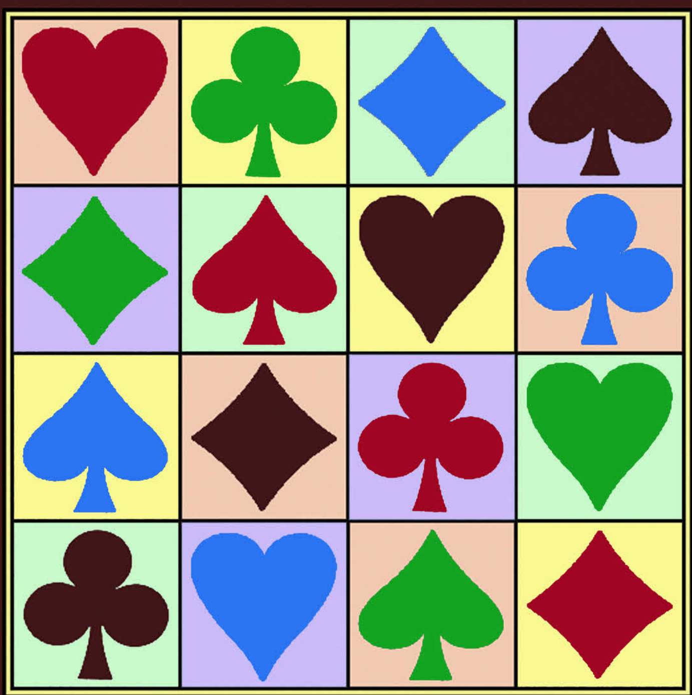
SLAVA BRODSKY

AN INTRODUCTION TO THE FACTORIAL DESIGN OF EXPERIMENTS

MATHEMATICAL FOUNDATIONS



Slava Brodsky (V.Z.Brodsky) graduated from Moscow University as a mathematician. He authored and co-authored several monographs in the field of applied mathematical statistics including "Multi-factorial Regular Designs" (The Moscow University Press), "An Introduction to the Factorial Design of Experiments" (Moscow, Nauka), "Mathematical Theory of Experimental Design" (Moscow, Nauka, FizMatGiz). In 1991, he came to the United States. Since then, he has worked in Manhattan at the largest financial companies in America. His website is www.slavabrodsky.com.

V.Z.Brodsky's book stands out for its high mathematical level and for presence of constructively new results obtained directly by the author.

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AN INTRODUCTION TO THE FACTORIAL DESIGN OF EXPERIMENTS

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Slava Brodsky (V. Z. Brodsky)
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This monograph is devoted to the theory of the design of optimal experiments. It introduces new ideas of the author that are an integral part of mathematical foundations of factorial experiments. The book presents a new concept of factorial models and addresses the issues of construction of effective plans for them. It contains numerous examples and a catalogue of factorial designs.

The monograph will be useful to practitioners involved in experiments in various fields of industry and science, and it will be useful to researchers. This book will also be a valuable addition to core curriculum for senior and graduate students studying the design of experiments.

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Preface to the First Edition

Mathematicians have long focused on the problem of efficient statistical analysis of experiments. This problem is studied as part of mathematical statistics, and practitioners involved in experiments in various areas of industry and science have found it be extremely useful in applications. The design of experiments is a much younger field of mathematical statistics. Applications of these two fields of statistics have shown that a reasonable allocation of resources for experiments, i.e., the efficient design of experiments, is no less important than efficient statistical analysis of the results of experiments. The skillful application of these two parts of mathematical statistics allows available resources to be more fully utilized and the effectiveness of experimental research to rise.

This book deals with the theory of factorial designs, which was where the theory of the design of experiments began its development. Factorial experiments were first considered by R. A. Fisher almost half a century ago. The problem of factorial designs first appeared in agricultural experiments, but since then factorial designs have been used in a variety of fields. There have been manifold successful applications in chemical, biological, and medical research, as well as in the manufacture of various products and materials, and also in metallurgy

The goal of this book is to consider from a single perspective all of the essential issues addressed by the theory of factorial designs. Achieving this goal required certain difficulties to be surmounted. This primarily refers to foundations of the theory.

Hundreds of publications contain the words "factorial designs" in their titles. Yet not all authors use the same definition of this concept. In this book, the concepts of "factorial designs" and "factorial models" are introduced in a way that, on the one hand, will not greatly surprise authors of papers on factorial designs, and on the other hand, will make these definitions productive.

In writing this book, the author has sought to make it both interesting from a theoretical standpoint and useful for applications.

To read this book, one does not need, apart from the basics of mathematical statistics, any knowledge beyond the ordinary mathematical university curriculum (necessary additional information is given in the first two chapters), but familiarity with elements of the mathematical theory of design and analysis of experiments is desirable. The texts by N. R. Draper and H. Smith (Applied Regression Analysis) and V. V. Nalimov and N. A. Chernova (Statistical methods for design of extremal experiments) are recommended for this. All chapters are accompanied by examples to assist readers without a thorough mathematical background to understand the materials in this book.

The author considers it his pleasurable duty to thank those who assisted him at various stages in the preparation of this book. V. V. Nalimov first prompted the author’s interest in this topic and has always given this work his sincere and critical attention. The author deeply appreciates the understanding and support of V. G. Gorsky, contact with whom was very fruitful. Many results, in particular those that form the basis of Chapter 3, were obtained after stimulating discussions with T. I. Golikova. The author is also grateful to E. P. Nikitina and V. S. Kuznetsov, who looked through several parts of the manuscript and made a number of valuable remarks.

Preface to the Second Edition

The first edition of my book came out in Soviet Russia in 1976, and this event involved various tragicomic circumstances.

In 1974, the book was submitted to the Publishing House “Nauka” (which means “Science” in Russian) by the Cybernetics Council of the USSR Academy of Sciences. Few people in Russia (even in scientific circles) knew what cybernetics was. Yet, at one point, you could pay with your life for belonging to this field of science, because in Russia, it was generally assumed that cybernetics were a central element in the development of plans by aggressors who wished to initiate a third world war. Later, the persecutors of cybernetics were, with the approval of the Soviet authorities, recognized as reactionaries. And at that point, you could have serious difficulties if you expressed any doubt in the usefulness of those who claimed to be doing any research in cybernetics.

So, right at the time that the word cybernetics became extremely popular in Russia, it turned out that the design of experiments was somehow related to cybernetics. This opened many doors for those working in it, including me. It was at this moment that the Publishing House “Nauka” made a decision to publish my book.

However, for the book to actually be accepted by the publisher, I needed to overcome difficulties that had little to do with science. The difficulties were related to the physical delivery of the manuscript to the publisher.

The first difficulty concerned the publishing requirements for manuscripts submitted to “Nauka”. Those responsible for accepting manuscripts, like all other Soviet bureaucrats, enjoyed making people run back and forth for the slightest deviation from the rules. Moreover, the rules themselves were unnecessarily complex and were kept in secret (as were all rules relating to anything whatsoever in Soviet Russia, incidentally). I spent a couple of months struggling for the right to acquaint myself with these rules. Only when I went too far in my battle and demanded a meeting with the director of “Nauka” were the rules finally provided to me.

As I discovered later, not only did authors not know the rules, but neither did those who accepted manuscripts. Each of them established his or her own rules, and then changed them from time to time. I was disappointed to learn from one of the published authors that no one had yet been able to submit a book on his first attempt. Nevertheless, I was optimistic: I possessed the requirements of the Publishing House “Nauka” and I made certain my manuscript was in full compliance with these requirements.

The second (but, as it happened, the most important) difficulty was that I needed to go through the Soviet censors. I needed a confirmation from them that my book contained no information restricted from publication. I prepared all the papers necessary and waited for the decision of the censors’ committee. I still had six months until the end of the year, which was the deadline for submission to “Nauka”. I assumed that I would get the required certificate in a few weeks. I thought so because it was obvious that my mathematical text contained no national secrets, and looking for political heresy in mathematical theorems, was, I thought, a pointless endeavor.

As it turned out, I really should not have assumed all this. The process took the Soviet censors eight months. I waited until the very end. On the last day before the submission deadline – December 30, 1974 – I brought my book to the publisher without the certificate of examination. I should have been kicked out immediately, of course. However, a miracle happened. The woman assigned to check my manuscript was, apparently, very shocked by the way her review went. She found one “serious” error after another, and each time, I immediately showed her the rules I had secured from “Nauka”, proving that everything had been done exactly as these rules demanded. All of this continued for hours. Several times she ran away in frustration, likely to consult with someone, but in the end, she gave up and just forgot to check for my certificate of examination. They first noticed its absence when they started editing my book – in March of 1975. By this point, the vigilant censors had ensured that my theorems contained neither national secrets nor anti-Soviet propaganda and had provided me with the approved certificate.

After this, everything went quite smoothly. My editor was a young pretty woman. She seemed fairly competent, although, before this, she had edited only fiction, which she honestly warned me about at the very beginning. Everything was running on rails. Her biggest issue with my text was the frequent use of the word “consider”: consider the design, consider the matrix, consider the model. Therefore, she tried, no matter how much I resisted, replacing this word with various synonyms. I reluctantly agreed. Later, I asked her to reserve a page of my book with all such synonyms, in memory of our work together, and for future reference. So now, I can recommend that all those who write mathematics books in Russian acquaint themselves with page 52 of the first edition of my book. On this page can be found all of the substitutes of the word “consider” suggested by my editor: use, take, apply, examine.

After the editing process had finished, we began to consider the cover of the book. I had prepared for it a sketch depicting playing cards, which you can see on the front cover of the current edition. I had expected to encounter serious difficulties with this suggestion. In Soviet Russia, for some reason, playing cards were banned. Not long before my book was submitted to the publisher, Soviet authorities issued a decree banning the card game bridge, along with athletic gymnastics, karate, women’s soccer, and Hatha yoga. That was probably the reason why my editor, when she looked at my sketch, told me, “I like it, but the head editor will not allow a cover like this.” I then suggested that we go to the head editor and talk to him.

The head editor praised the sketch but said it would not be suitable for a scientific book, placing a particular emphasis on the words “scientific book”. Then I asked him why the sketch would not be suitable for a scientific book. He said that he personally liked it and would leave it on the cover, but that the director would never allow something like this. He assured me that he was absolutely certain. I suggested we go to the director, and within a couple of days, the head editor and I were sitting in the director’s office.

We talked peacefully about something or other. Then the director looked at my sketch, said he really liked it, took a pen, and asked where he should sign to approve the cover. At which point my head editor asked the director how they should respond to the elderly retirees who would write furious letters about playing cards on the cover of a scientific book. The director put his pen back down on the table and said, “Ah! Somewhere over there...” – and he jerked with his thumb somewhere behind him – “... there, they would use strong colors, a glossy cover, and the book...” – he slashed the air with his hand – “... the book would sell! But we, you’re right...” – turning to the head editor – “... you’re right, we can’t. We can’t put playing cards on the cover of a scientific book. Think of something else.” This last was to me. Then, to both the head editor and me “Have a good day.” The director came out from behind the table and shook hands with us. Somewhere by the door, I managed to say that I would replace the cards with a stylized image of them, and the director said something approving about this.

There were sixteen thousand copies of my book printed, which was, in my opinion, clearly too much. At first, I doubted that more than fifty copies would sell. Nevertheless, the book sold out almost right away, which was hardly surprising if one thinks of the situation in Russia at the time. Hunger for books made people sweep anything (except Party publications) off the shelves in bookstores. It was considered practically indecent for a city resident not to have a large number of bookshelves. To fill them, people bought everything that was in bookstores. This ludicrousness, like all the others, was a consequence of the general atmosphere of absurdity that was characteristic of the socialist society built in Soviet Russia.

When they found out about the book at the place I then worked, I was advised to submit a proposal on the subject of the book to the State Committee for Science and Technology (GKNT in Russian) under the USSR Council of Ministers. I submitted such a proposal, and it was almost instantly accepted by the GKNT, even though no one on the committee had any idea what it was about. In a couple of months, a GKNT research program on my subject was created by special decree of the USSR government. In this way, Latin squares and all the rest of it became one of the leading fields of science and technology in the country. There was nothing unusual in this. That was how research was planned in a country with a command economy.

As the head of the program, I was allocated a great deal of money for research, even though both those who allocated the money and I, the person supposed to receive it, knew that I could not actually spend it. The money was only allocated on paper, by the decision of the GKNT. No one knew where to get it from. And even if, by some miracle, the money appeared out of nowhere, I would not be able to spend it. I could not hire anyone, and there was nothing anywhere that I could buy with this money.

The research on the subject took five years. The result only interested the bureaucrats of the GKNT and the executives of our institute in the sense of it being complete or not. If the work was not complete in time, the director and the executives of our institute would likely have lost their jobs for non-execution of the government resolution. However, the work was completed. It was concluded with a report, which I doubt anyone has ever read.

I had a chance to continue this research more than ten years later. I came to the US at the end of 1991 and found out that the National Institute of Standards and Technology had proposed a research program for 1992-1993 (the ASA/NSF/NIST Senior Research Fellow Program) that included the design of experiments. I submitted my proposal. Then I had several interviews and submitted additional materials. At some point, I was notified that my proposal had been conditionally approved, and that I needed to pass a concluding interview over the phone with a representative of the Institute.

The interviewer asked me a series of questions, which I answered. I did not, obviously, have any problems with the essence of the questions, or, more precisely, I should not have had any problems with the questions. But I had only been in the country for a couple of months and had trouble understanding American English, especially over the phone. At some point, the interviewer asked me whether I was familiar with the works of Addelman. I was, of course, familiar with all of his articles, and I even had a generalization of one of his results. However, the way my interviewer pronounced his name was not how I had assumed it should be pronounced, and the first-syllable stress utterly confused me. So I answered, “I don’t know him.” This probably sounded quite Biblical but apparently turned out to be the last straw in our already strained conversation (which was my fault entirely, of course). As a result, the National Institute of Standards and Technology rejected my proposal, and for the following twenty plus years, I applied my mathematical background and software development experience in a completely different area – the financial industry.

Was there any good that came of the first edition of my book in Russia? It is extremely difficult to answer this question. I do not know about all the theorems, which were the basis of the book. I do not know how many people read them, but practitioners did use it fairly extensively. Unfortunately, there is a simple explanation for this. Vasily Nalimov, the leader of the design of experiments in Soviet Russia, used to say that one of the three elephants supporting the design of experiments in Russia was the graduate student. And that was the truth. Graduate students from many fields of medicine, biology, pharmaceutics, chemical engineering, metallurgy, jumped on the design of experiments bandwagon in the 70’s. The buzzwords of the day – cybernetics, experimental design – created an illusion of scientific thought in their work. There is no particular scientific thought involved when you simply apply basic techniques of the design of experiments, and yet many graduate students wrote successful doctoral theses doing just that. As for why those who worked in industry and had nothing to do with academia needed to get a PhD, that was obvious to everyone: in accordance with the laws of a command economy, a PhD automatically doubled one’s salary. So my book was very useful for graduate students: it allowed them to get paid twice as much. Unfortunately, it follows that my book decreased the purchasing power of the money in the possession of the rest of the population, and therefore was harmful to them. I try not to think about my unwitting role in this deplorable state of affairs.

However, despite everything, I look back at the seventies (when I was writing this book) with great warmth. I remember working with many nice people bound by a common scientific idea that at the time seemed extraordinarily fruitful.

All of this, especially at first, took place at Moscow University, at the Inter-faculty Laboratory of Statistical Methods, headed by Andrey Kolmogorov, in the department of the design of experiments under Vasily Nalimov. I was always welcome in his department. I was an active participant in his seminar, was published alongside his colleagues by Moscow University's publishers, used the famous Kolmogorov library of statistical literature. I could even borrow the treasured statistics journals from the library. And, most importantly, it seemed to me that in this group, one did not feel bound by the Soviet spirit (though of course it penetrated everywhere).

Another such group of like-minded individuals was to be found in the mathematical section of the journal Industrial Laboratory where I worked (on a volunteer basis) for almost twenty-five years, until my departure from Soviet Russia in 1991. It was the only journal in the USSR that published theoretical and applied statistical work. The head of the section was Boris Gnedenko. However, he rarely came to our meetings, and Nalimov was the one who actually performed the duties of the head. There was something about the work of this section that distinguished it from other editorial boards. If an article contained a sound idea, then nothing – not a tangled explanation, not bad writing, not even certain repairable errors – could stop it from being published (albeit after revision), even if the author was completely unknown. An editorial style unachievable, as I now see, even for the leading statistical journals of the US.

These two oases were my salvation. They created the possibility of a meaningful existence in a country where it seemed there could not be a meaningful existence. They created an atmosphere that allowed us to wall ourselves off from the socialist bacchanalia that surrounded us (or at least allowed us to temporarily forget about it).

That, in short, is the story of the first edition of this book.

Now, regarding the second edition. It is not very different from the first, though I made some corrections and additions and augmented the bibliography of the factorial designs.

All of the additions made for the second edition are based on papers that were published by me, including collaborations with my colleagues, several years after the first edition came out (mostly at the end of the seventies). Nevertheless, I decided to publish the second edition now. The major reason for this is that despite the passing of time, I have not seen many developments in the field where I once worked. I am not talking about the methods for the construction of the designs, which does have a lot of new work. I am talking about foundations of the factorial design of experiments, which formed the main portion of my book. That is why I have decided to publish a second edition that will, I hope, be more accessible to potential readers than the first.

In the preface to the first edition, I said that the goal of this book was to establish foundations of the factorial design of experiments. I also said that hundreds of papers had no consensus about the definition of factorial designs. That was an understatement. Neither then, when I was first writing this book, nor now, when I am preparing its second edition, have I seen a meaningful definition of factorial designs in statistical publications.

D. Raghavarao, in his marvelous book "Construction and Combinatorial Problems in Design of Experiments" says that the factorial design of experiments occurs when different combinations of the factors at various levels influence a character under study. However, any multidimensional design includes different combinations of factors. How, then, are factorial designs different? It should be understood that D. Raghavarao excludes the one-dimensional case from his definition, though he does not state this outright.

In many books, the multidimensional condition is explicitly included in the definition of the factorial designs. For example, this is what R. Mukerjee and C. F. J. Wu do in their brilliant book "A Modern Theory of Factorial Designs". They define a factorial experiment as an experiment involving n ($\geqslant$2) factors that appear at $s_1, \ldots, s_n$ (≥ 2) levels. However, it is not clear from this definition how the factorial design of experiments is different from any other multidimensional design. Given this definition, any multidimensional experiment has to be considered as factorial. Therefore, such a definition is not very productive.

Unfortunately, that is not the only problem with this definition. Another problem is that the authors of numerous works in different fields of the design of experiments are unlikely to agree with such an approach to the definition of factorial designs. Will authors of articles on, say, polynomial designs (including in part rotatable designs) consider that they do research on factorial designs? I do not think so. In reality, none of them has ever used such a concept as "rotatable factorial designs". No one would consider, for example, the rotatable design of second order in two variables as a fractional factorial design 5^2 (even though it consists of treatment combinations of two five-level factors).

What can then be said of the designs constructed numerically and satisfying, say, criterion of *D*-optimality for different models and design spaces (as V. V. Fedorov did, developing the ideas of J. Kiefer and J. Wolfowitz)? Will researchers and the readers of their papers consider such designs "*D*-optimal factorial designs" only because they are multidimensional? Of course not.

What can we say about the authors of the book on the design of experiments? Do they use effectively the definition of factorial designs as multidimensional designs? Do they use such a definition, for example, when they think about a structure for their book? No, no one follows such a definition. On the contrary, authors of books on the general problem of the design of experiments (including the D. Raghavarao book quoted above) consider factorial designs separately from the sections devoted to other types of designs, for example, rotatable designs. On the other hand, books on factorial designs (including the R. Mukerjee and C. F. J. Wu book mentioned above) do not contain, say, a section devoted to rotatable designs. That means that authors of the book do not follow the definition of factorial designs as multidimensional ones. They structure their books based on an intuitive understanding of what factorial designs are. And this intuitive understanding has nothing to do with multidimensionality.

So one of the goals of my book was to introduce the concepts of "factorial designs" and "factorial models" in a way that would reflect this intuitive understanding. The most important part, however, was not simply to introduce definitions that would not frighten those who do research in the area of the design of experiments. The most important contribution of my book is that the definitions I introduced have turned out to be quite productive. These definitions support many important aspects of experimental design, including the effectiveness of statistical inferences and construction of the designs, thereby opening the way for advancements in the theory of experiments.

A few more words about terminology. A number of authors started using the term "regular" to refer to the designs generated from finite geometries. In the middle of the seventies, when the first edition of this book was published, I considered the concept of regular factorial designs to be connected only with the designs having certain statistical properties. So I called the designs generated from finite geometries, geometric. The second edition naturally retains the name of geometric designs for the designs generated from finite geometries.

This book does not only contain my results, it also includes the results of other authors (mostly related to the methods of construction of designs). In this regard, I would like to note that in the second edition, I have not sought to include all of the latest developments on construction of factorial designs for these reasons: firstly, I wished to consider the methods of construction only as an illustration of the more general ideas of the book, and secondly, I preferred to focus on those methods that are most important for applications.

The first two chapters of this book are meant as a reference. Chapter 1 contains the mathematical knowledge necessary for reading this book, and Chapter 2, the statistical. In the other chapters, I have attempted to lay out all the major results of the theory of factorial designs. A significant number of these results are mine, and in those cases I give the relevant theorems without citations. These results mostly date back to the middle of the seventies, when I was working on the first edition. If a theorem given here does not belong to me, I either give the corresponding citation directly after the word "Theorem" or give clarifications and the citation in the adjacent text. The theorems of the first two chapters are well known, and are given without citations.

A few words of gratitude as a conclusion. Vladimir Aleshin, Maria Tyutyunik, Igor Mandel, and Rebecca Gee gave me a great deal of help during the preparation of the second edition of the book, and I am very grateful to them for their assistance.

Chapter 1. Finite Fields and Finite Geometries

§ 1. Galois Fields

Definition 1.1.1. A finite commutative ring $\mathcal{R}$ of order s is a set of s elements $a_0, a_1, \dots, a_{s-1}$ with two operations called addition and multiplication and denoted by $+$ and $\cdot$ respectively (symbol $\cdot$ is usually omitted) such that the following axioms hold for all a_i, a_j, and a_n in $\mathcal{R}$:

1. Both $a_i + a_j$ and $a_i a_j$ are in $\mathcal{R}$ ($+$ and $\cdot$ are binary operations on $\mathcal{R}$).

2. Addition is commutative:
$a_i + a_j = a_j + a_i$.

3. Multiplication is commutative:
$a_i a_j = a_j a_i$.

4. Addition is associative:
$a_i + (a_j + a_n) = (a_i + a_j) + a_n$.

5. Multiplication is associative:
$a_i(a_j a_n) = (a_i a_j) a_n$.

6. Multiplication is distributive over addition:
$a_i(a_j + a_n) = a_i a_j + a_i a_n$.

7. There exists a reverse operation for addition – subtraction: for any two elements a_i and a_j, there is one and only one element a_n (called the difference of a_i and a_j and denoted by $a_n = a_i - a_j$) for which the following equality holds:
$a_i = a_j + a_n$.

Some basic properties follow from the definition of a finite commutative ring.

1. For any $a_i \in \mathcal{R}$, there is one and only one additive identity element a_0 such that
$a_i + a_0 = a_i$.

2. For any $a_i \in \mathcal{R}$, there is one and only one additive inverse element $(-a_i)$ such that
$a_i + (-a_i) = a_0$.

3. For any elements $a_i,\ a_j \in \mathcal{R}$,

$$a_i a_0 = a_0\ ,\ (-a_i)a_j = -a_i a_j\ ,\ (-a_i)(-a_j) = a_i a_j\ .$$

Definition 1.1.2. A finite field $\mathcal{F}$ of order s is a commutative ring of order s containing at least one nonzero element and such that there exists an inverse operation of multiplication (called division and denoted by /), i.e., for any a_i and nonzero a_j in $\mathcal{F}$, there is one and only one element (denoted by $a_n = a_i/a_j$) such that $a_i = a_j a_n$.

Some basic properties follow from the definition of a finite field.

1. For any $a_i \in \mathcal{F}$, there is one and only one multiplicative identity element a_1 such that

$$a_i a_1 = a_i\ .$$

2. For any $a_i \in \mathcal{F}$, there is one and only one multiplicative inverse element a_i^{-1} such that

$$a_i a_i^{-1} = a_1.$$

3. For any elements $a_i,\ a_j \in \mathcal{F}$,

$$a_i^{-1} = a_1/a_i\ ,\ \ a_i/a_j = a_i a_j^{-1},\ \ \left(a_i^{-1}\right)^n = (a_i^n)^{-1}\ .$$

Additive identity element a_0 and multiplicative identity element a_1 will be denoted also by 0 and 1 respectively.

Definition 1.1.3. Two integers a and b are congruent modulo p ($p > 1$, integer) if $a - b$ is divisible by p. This relation is denoted by $a \equiv b \pmod{p}$.

Definition 1.1.4. For a given p ($p > 1$, integer), a residue class (mod p) is a class of all integers congruent modulo p.

Every integer belongs to one and only one of p residue classes (mod p) $C_0, \dots, C_{p-1}$. A class C_i $(i = 0, 1,\ \dots, p-1)$ consists of integers with the same residue i when divided by p. We can define addition and multiplication of classes C_i and C_j by the following rules:

$$C_i + C_j = C_{i+j} \text{ for } \ i + j < p\ ,$$
$$C_i + C_j = C_{i+j-p} \text{ for } \ i + j \geq p\ ,$$
$$C_i C_j = C_r\ ,$$

where $ij = pq + r$ $\ (0 \leq r \leq p)$.

The set of residue classes (mod p) with the defined operations (addition and multiplication) is a commutative ring. This ring is a field if and only if p is prime. The field of residue classes (mod p) is called a prime field, or Galois field, of order p and denoted by $GF(p)$.

Let x be an algebraic number over the field $GF(p)$. Consider all polynomials in x with coefficients belonging to $GF(p)$. Let $P(x)$ be a given irreducible polynomial in x of degree h with coefficients belonging to $GF(p)$. For any polynomial $T(x)$ with integer coefficients, the polynomial

$$t(x) = a_0 + a_1x + a_2x^2 + \cdots + a_{h-1}x^{h-1}$$
$$(a_i \in GF(p),\ \ i = 0,1, \dots, h-1)$$

is called a residue of $T(x)$ modulus p and $P(x)$ if

$$T(x) = t(x) + pq(x) + P(x)Q(x),$$

where $q(x)$ and $Q(x)$ are polynomials in x with integer coefficients.

This relationship between $T(x)$ and t(x) may be written as

$$T(x) \equiv t(x) \bmod [p, P(x)].$$

The set of p^h residue classes (mod $[p, P(x)]$) is a finite field. It is called Galois field of order p^h and denoted by $GF(p^h)$.

A finite field of order s exists if and only if $s = p^h$ (p is prime, h is integer). All finite fields of the same order are isomorphic.

Definition 1.1.5. A nonzero element of $GF(s)$ is called a quadratic residue if it equals the square of an element of $GF(s)$. All other elements of $GF(s)$ are called quadratic nonresidues.

The Legendre symbol (a_i/s), where $a_i \in GF(s)$, is defined as

$$(a_i/s) = \begin{cases} +1, \text{if } a_i \text{ is a quadratic residue,} \\ -1, \text{if } a_i \text{ is a quadratic nonresidue.} \end{cases}$$

Well-known properties of the Legendre symbol are:

$$\sum_{n \neq i,j} \left(\frac{a_n - a_i}{s}\right)\left(\frac{a_n - a_j}{s}\right) = -1 \quad (i \neq j), \tag{1.1.1}$$

$$\sum_i \left(\frac{a_i}{s}\right) = 0, \tag{1.1.2}$$

$$\left(\frac{-1}{s}\right) = (-1)^{(s-1)/2} \quad (s > 2), \tag{1.1.3}$$

$$\left(\frac{a_i a_j}{s}\right) = \left(\frac{a_i}{s}\right)\left(\frac{a_j}{s}\right), \tag{1.1.4}$$

where $a_n,\ a_i,\ a_i \in GF(s)$.

Definition 1.1.6. An element $a_n \in GF(s)$ is called a primitive element if $a_n^{s-1} = 1$ and $a_n^v \neq 1$ for any $v < s - 1$.

There exists at least one primitive element $a_n \in GF(s)$. Any element a_i $(a_i \neq 0)$ of the field can be represented as $a_i = a_n^h$.

Example 1.1.1. For $GF(4)$ with the elements denoted by symbols 0, 1, 2, and 3, all axioms of a finite field are satisfied for the following addition and multiplication tables.

Addition Table

+	**0**	**1**	**2**	**3**
0	0	1	2	3
1	1	0	3	2
2	2	3	0	1
3	3	2	1	0

Multiplication Table

×	**0**	**1**	**2**	**3**
0	0	0	0	0
1	0	1	2	3
2	0	2	3	1
3	0	3	1	2

Definition 1.1.7. A finite additive group of order s is a set of s elements with one binary operation (addition) which is associative (but not necessarily commutative) and has a reverse operation – subtraction. The existence of subtraction means that for any two elements a_i, a_j, there exists one and only one element a_n such that $a_n + a_i = a_j$, and there exists one and only one element a_k such that $a_i + a_k = a_j$.

It is evident that any finite ring (in particular, any Galois field) is a finite additive group.

§ 2. Finite Projective Geometries

Definition 1.2.1. A finite projective plane is a finite set of elements (called points) and subset of the points (called lines) if the following axioms hold:

1. For every pair of points, there is one and only one line that contains both points.
2. For every pair of lines, there is one point, called intersection, that belongs to both lines.
3. There are four points such that no three of them belong to the same line.

It follows from axioms 1 and 2 that for every pair of lines, there is exactly one point that belongs to both lines. It follows from axiom 3 that any line contains at least three points and that any points belongs to at least three lines.

Theorem 1.2.1. Let $s \geq 2$ be integer. In projective plane π, any of the following properties implies all others:

1. Some line contains exactly $s + 1$ points.
2. Some point belongs to exactly $s + 1$ lines.
3. Any line contains exactly $s + 1$ points.
4. Any point belongs to exactly $s + 1$ lines.
5. There exist exactly $s^2 + s + 1$ points in π.
6. There exist exactly $s^2 + s + 1$ lines in π.

The proof of this theorem can be found, for example, in [1].

Definition 1.2.2. A finite projective plane is said to have order s if some of its line contains exactly $s + 1$ points.

Example 1.2.1. The simplest finite projective plane is the plane of order $s = 2$. By Theorem 1.2.1, the plane contains exactly 7 points and 7 lines. Any line contains exactly 3 points, and each point belongs to exactly 3 lines. Let the points of this plane are *A*, *B*, *C*, *D, E, F,* and *G* and the lines are *ADC*, *AGE*, *AFB*, *CGF, CEB, DGB,* and *DEF*. A geometric interpretation of this projective plane is presented in Figure 1.

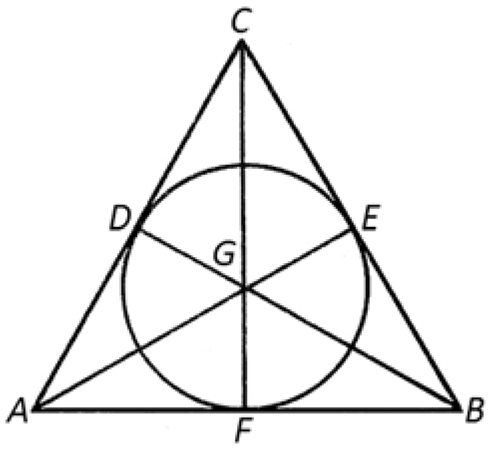

Figure 1. Projective plane of order 2

It is easy to check that for construction above, all axioms of finite projective plane are satisfied.

Now consider finite spaces of higher dimension [2].

Definition 1.2.3. A finite projective geometry is a finite set of elements (called points) and subset of the points (called lines) if the following axioms hold:

1. For every pair of points, there is one and only one line that contains both points.
2. Each line contains at least 3 points.
3. Let *A*, *B,* and *C* be points that do not belong to one line; D($\neq$ A) be a point belonging to the line that contains *A* and *B*; E($\neq$ A) be a point belonging to the line that contains *A* and *C*. Then there exists a point *F* belonging to both the line that contains *D* and *E* and the line that contains *B* and *C*.

A dimension of a finite projective geometry (or a finite projective space) is defined recurrently. A point is projective geometry of dimension 0, or 0-space. Let Z_{n-1} be a (n – 1)-space and A be a point that does not belong to Z_{n-1}. Then a set of all points belonging to all lines AB, where B is a point that belongs to Z_{n-1}, is a projective geometry of dimension n, or an n-space.

The existence of a projective geometry of dimension m $>$ 1 (or an m-space) is ensured by the following two axioms:

4. If $l < m$, not all points are in the same l-space.
5. There exists no $(m+1)$-space in the set.

A line is a 1-space. A finite projective 2-dimensional space is a finite projective plane (see definition 1.2.1). An l-space can be regarded as a subspace of a space of higher dimension. In this case it can be referred as an l-flat. An $(m-1)$-flat in m-dimensional space is called a hyperplane.

A method of construction of one type of a finite projective geometry is the following [2]. Define a point of an m-dimensional finite space (or an m-space) $PG(m,s)$ as an ordered set of m + 1 coordinates $(\chi_0, \chi_1, \ldots, \chi_m)$, where χ_i are elements of Galois field $GF(s)$ that are not simultaneously equal to zero. Coordinates χ_i will be regarded as homogeneous, i.e., the point $(\lambda\chi_0, \lambda\chi_1, \ldots, \lambda\chi_m)$ is considered the same as the point $(\chi_0, \chi_1, \ldots, \chi_m)$ for any $\lambda \neq 0$, $\lambda \in GF(s)$. Hence, the number of different points in $PG(m,s)$ equals

$$V(m,0,s) = \frac{s^{m+1}-1}{s-1}.$$

$PG(m,s)$ contains n-flats $(n = 0, 1, \ldots, m-1)$, or n-dimensional subspaces, defined as a set of all points with coordinates satisfying $m-n$ linearly independent homogeneous equations with coefficients from *GF(s)*:

$$\begin{aligned}
&a_{10}\chi_0 + a_{11}\chi_1 + \cdots + a_{1m}\chi_m = 0,\\
&a_{20}\chi_0 + a_{21}\chi_1 + \cdots + a_{2m}\chi_m = 0,\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
&a_{m-n,0}\chi_0 + a_{m-n,1}\chi_1 + \cdots + a_{m-n,m}\chi_m = 0.
\end{aligned} \tag{1.2.1}$$

We can define n-flats alternatively. Let $n + 1$ points

$$\boldsymbol{\chi}_0 = (\chi_{00}, \chi_{01}, \ldots, \chi_{0m}), \ldots, \boldsymbol{\chi}_n = (\chi_{n0}, \chi_{n1}, \ldots, \chi_{nm})$$

be linearly independent, i.e., the matrix

$$\begin{Vmatrix} \chi_{00} & \chi_{01} & \cdots & \chi_{0m} \\ \chi_{10} & \chi_{11} & \cdots & \chi_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_{n0} & \chi_{n1} & \cdots & \chi_{nm} \end{Vmatrix} = \begin{Vmatrix} \boldsymbol{\chi}_0 \\ \boldsymbol{\chi}_1 \\ \vdots \\ \boldsymbol{\chi}_n \end{Vmatrix}$$

has rank $n + 1$. Then an n-flat consists of all points

$$a_0\boldsymbol{\chi}_0 + a_1\boldsymbol{\chi}_1 + \ldots + a_n\boldsymbol{\chi}_n,$$

where $a_i \in GF(s)$ and all a_i are not simultaneously equal to zero; $\boldsymbol{\chi}_i$ are linearly independent points with coordinates satisfying (1.2.1). It can be proved [2] that $PG(m, s)$ satisfies all five axioms of a finite projective space.

It is useful to enumerate flats in $PG(m, s)$ [2]. The number of n-flats in $PG(m, s)$ equals the number of $(m - n - 1)$-flats and equals

$$V(m, n, s) = \frac{(s^{m+1} - 1)(s^m - 1) \ldots (s^{m-n+1} - 1)}{(s^{n+1} - 1)(s^n - 1) \ldots (s - 1)}.$$

The number of t-flats in $PG(m, s)$ that contain the given n-flat $(n \neq t)$ equals the number $(m - t - 1)$-flats in an $(m - n - 1)$-flat:

$$V(m - n - 1, m - t - 1, s) = V(m - n - 1, t - n - 1, s)$$

$$= \frac{(s^{m-n} - 1)(s^{m-n-1} - 1) \ldots (s^{t-n+1} - 1)}{(s^{m-t} - 1)(s^{m-t-1} - 1) \ldots (s - 1)}.$$

In particular, each n-flat contains

$$V(n, 0, s) = \frac{s^{n+1} - 1}{s - 1}$$

points. For example, 1-flat contains $s + 1$ points, 2-flat contains $s^2 + s + 1$ points.

Definition 1.2.4 [3]. Let $X_i \in PG(m, s)$ $(i = 1, \ldots, m;\ s = p^h)$, and for all X_i, coordinate $\chi_i = 1$, the rest of the coordinates, including χ_0, equal zero. The set of points $X_1, \ldots, X_m$ is called a fundamental simplex.

The points X_i are called vertices (or 0-cells) of the fundamental simplex. The lines X_iX_j $(i \neq j)$ are called its edges (or 1-cells). In general, the $(n-1)$-flat formed by any n of m vertices $X_1, \dots, X_m$ $(n < m)$ is called $(n-1)$-cells of the fundamental simplex.

§ 3. Finite Euclidean Spaces

Definition 1.3.1. A subset of points of $PG(m,s)$ with the first coordinate not equal to zero is called a finite m-dimensional Euclidean space and denoted by $EG(m,s)$.

Since coordinates of points of $PG(m,s)$ are homogeneous, we may set the first coordinate χ_0 to be 1. Therefore, $EG(m,s)$ are an ordered set of points $(\chi_1, \dots, \chi_m)$, where χ_i are elements of Galois field $GF(s)$. Hence, $EG(m,s)$ is formed from $PG(m,s)$ by excluding hyperplane $\chi_0 = 0$ together with all its flats. These flats are called flats at infinity. Those remaining flats, belonging to $EG(m,s)$, that intersect only at infinity are called parallel.

It is easy to show [2] that there are

$$V(m,n,s) - V(m-1,n,s) \tag{1.3.1}$$

n-flats in $EG(m,s)$. For example, there are $s(s^m-1)/(s-1)$ hyperplanes and s^m points in $EG(m,s)$. Using (1.3.1), we can find the number of n-flats in an m-flat in the space of higher dimension.

The number of t-flats passing through the given n-flat is the same as in $PG(m,s)$.

An n-flat in $EG(m,s)$ contains all s^n points satisfying $m-n$ linearly independent equations:

$$\begin{aligned} &a_{01} + a_{11}\chi_1 + \dots + a_{m1}\chi_m = 0, \\ &a_{02} + a_{12}\chi_1 + \dots + a_{m2}\chi_m = 0, \\ &\dots\dots\dots\dots\dots\dots\dots\dots \\ &a_{0,m-n} + a_{1,m-n}\chi_1 + \dots + a_{m,m-n}\chi_m = 0. \end{aligned}$$

In particular, hyperplane in $EG(m,s)$ is given by the following equation:

$$a_0 + a_1\chi_1 + \dots + a_m\chi_m = 0. \tag{1.3.2}$$

Any hyperplane (1.3.2) in $EG(m,s)$ can be extended to the flat

$$a_0\chi_0 + a_1\chi_1 + \dots + a_m\chi_m = 0 \tag{1.3.3}$$

in $PG(m,s)$. The points of (1.3.2) are the same as the finite points of (1.3.3), but the plane (1.3.3) has also points at infinity, which belong to an $(m-2)$-flat

$$a_1\chi_1 + a_2\chi_2 + \cdots + a_m\chi_m = 0,\ \ \chi_0 = 0. \tag{1.3.4}$$

If a_0 takes all s possible values of $GF(s)$ in (1.3.2), then for given a_1, ... , a_m, we get the pencil $P(a_1,\ \dots,\ a_m)$ of parallel $(m-1)$-flats in $EG(m,s)$. Any point of $EG(m,s)$ belongs to one (and only one) hyperplane of the pencil $P(a_1,\ \dots,\ a_m)$. No two of the parallel $(m-1)$-flats of the pencil $P(a_1,\ \dots,\ a_m)$ have any common point of $EG(m,s)$. But when extended to infinity, they intersect the flat (1.3.4). This intersection is called the vertex of the pencil $P(a_1,\ \dots,\ a_m)$. The numbers $a_1,\ \dots,\ a_m$ are called coordinates of the pencil.

It is evident that the pencil $P(a_1,\ \dots,\ a_m)$ of parallel hyperplanes in $EG(m,s)$ is the same as the pencil $P(\lambda a_1,\ \dots,\ \lambda a_m)$, where $\lambda \neq 0$. So we can set the first coordinate of the pencil to be 1. Hence, there are $(s^m-1)/(s-1)$ different pencils of parallel hyperplanes in $EG(m,s)$.

Let $\mathfrak{I}$ be any $(m-n-1)$-flat at infinity. Then there are exactly $(s^{n+1}-1)/(s-1)$ different $(m-n)$-flats of $PG(m,s)$ passing through $\mathfrak{I}$, and $(s^n-1)/(s-1)$ of them lie entirely at infinity while the remaining s^n belong to $EG(m,s)$. Therefore, there are exactly s^n $(m-n)$-flats in $EG(m,s)$ that when extended to infinity, pass through the $(m-n-1)$-flat $\mathfrak{I}$. These s^n $(m-n)$-flats may be said to form a parallel bundle with the vertex $\mathfrak{I}$.

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Chapter 2. Regression Analysis

§ 1. Model and General Assumptions

We will consider models that are linear in the parameters. That means the model has the following type:

$$\eta = \mathbf{f}^T(X_1, \dots, X_m)\mathbf{\Theta}, \tag{2.1.1}$$

where η is a response variable; $\mathbf{\Theta}^T = (\theta_1, \dots, \theta_k)$ is a vector of unknown parameters; $\mathbf{f}^T(X_1, \dots, X_m) = \{f_1(X_1, \dots, X_m), \ \dots, \ f_k(X_1, \dots, X_m)\}$ is a vector of given functions.

To estimate parameters of the model (2.1.1) we will use *N* observations $y_1, \dots, y_N$ assuming that

$$y_u = \eta_u + \varepsilon_u,$$

where ε_u $(u = 1, \dots, N)$ is the error of the u-th observation, $\eta_u = \eta(X_{1u}, \dots, X_{mu})$, $X_{1u}, \dots, X_{mu}$ are the values that the variables $X_1, \dots, X_m$ take respectively in the u-th observation. A part of the domain of the functions $f_1(X_1, \dots, X_m), \ \dots, \ f_k(X_1, \dots, X_m)$, where observations are conducted is called a design space.

For the errors $\varepsilon_1, \dots, \varepsilon_N$, we assume that

$$E\varepsilon_i = 0; \ \ E\varepsilon_i\varepsilon_j = 0; \ \ E\varepsilon_i^2 = \sigma^2 \ \ (i, j = 1, \dots, N),$$

or (in the matrix form)

$$E(\boldsymbol{\varepsilon}) = 0; \quad \mathbf{\Gamma}(\boldsymbol{\varepsilon}) = \mathbf{E}_N\sigma^2, \tag{2.1.2}$$

where $\boldsymbol{\varepsilon}^{\mathrm{T}} = (\varepsilon_1, \dots, \varepsilon_N)$; $\mathbf{\Gamma}(\boldsymbol{\varepsilon})$ is a covariance matrix of the vector $\boldsymbol{\varepsilon}$; $\mathbf{E}_{\mathrm{N}}$ is the unit matrix of order *N*.

Hence,

$$y_u = \mathbf{f}^T(X_{1u}, \dots, X_{mu})\mathbf{\Theta} + \boldsymbol{\varepsilon}_u. \tag{2.1.3}$$

The matrix

$$\mathbf{D}_X = \begin{Vmatrix} X_{11} & \dots & X_{m1} \\ \vdots & \ddots & \vdots \\ X_{1N} & \cdots & X_{mN} \end{Vmatrix} \tag{2.1.4}$$

is called a design matrix (or design, plan).

Equality (2.1.3) can be expressed in a matrix form:

$$\mathbf{y} = \mathbf{X\Theta} + \boldsymbol{\varepsilon}, \tag{2.1.5}$$

or, by (2.1.2),

$$E\mathbf{y} = \mathbf{X\Theta},$$

where $\mathbf{y}^T = (y_1, \dots, y_N)$ and

$$\mathbf{X} = \left\| \begin{matrix} f_1(X_{11}, \dots, X_{m1}) & \cdots & f_k(X_{11}, \dots, X_{m1}) \\ \vdots & \ddots & \vdots \\ f_1(X_{1N}, \dots, X_{mN}) & \cdots & f_k(X_{1N}, \dots, X_{mN}) \end{matrix} \right\|.$$

The matrix $\mathbf{X}$ is called a coefficient matrix of the design $\mathbf{D}_X$ for the model (2.1.5). The matrix $\mathbf{X}$ is often called a matrix of independent variables. However, further along with a case of a full rank matrix, we will consider a case when the matrix $\mathbf{X}$ is not full rank. Then the term coefficient matrix will be more appropriate.

§ 2. Estimation of Parameters and Parametric Functions

We will calculate estimates $\hat{\theta}_1, \dots, \hat{\theta}_k$ of unknown parameters $\theta_1, \dots, \theta_k$ using the least squares method, i.e., by minimizing the following expression:

$$\left(\mathbf{y} - \mathbf{X}\widehat{\mathbf{\Theta}}\right)^T \left(\mathbf{y} - \mathbf{X}\widehat{\mathbf{\Theta}}\right) = \boldsymbol{y}^T\mathbf{y} - 2\widehat{\mathbf{\Theta}}^T\mathbf{X}^T\mathbf{y} + \widehat{\mathbf{\Theta}}^T\mathbf{X}^T\mathbf{X}\widehat{\mathbf{\Theta}}\,. \tag{2.2.1}$$

The moment matrix, or the information matrix, $\mathbf{X}^T\mathbf{X}$ is positive semi-definite. If $\mathbf{X}$ is a full rank matrix, $\mathbf{X}^T\mathbf{X}$ is nonsingular and positive definite. In this case the only point $\widehat{\mathbf{\Theta}} = \left(\hat{\theta}_1, \dots, \hat{\theta}_k\right)$ that minimizes (2.2.1) can be found as unique solution of so-called normal equations of the method of least squares

$$(\mathbf{X}^T\mathbf{X})\widehat{\mathbf{\Theta}} = \mathbf{X}^T\mathbf{y}\,. \tag{2.2.2}$$

Then

$$\widehat{\mathbf{\Theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}\,. \tag{2.2.3}$$

The solution $\widehat{\mathbf{\Theta}} = \left(\hat{\theta}_1, \dots, \hat{\theta}_k\right)$ is called LS estimates of parameters $\theta_1, \dots, \theta_k$. These estimates have certain properties:

1. The vector $\widehat{\mathbf{\Theta}}$ is unbiased estimate of the vector $\mathbf{\Theta}$, i.e., $E\widehat{\mathbf{\Theta}} = \mathbf{\Theta}$.
2. The estimate $\hat{\theta}_i$ $(i = 1, \dots, k)$ is a linear function of the observations and has the minimum variance in the class of linear unbiased estimators.

We will consider the case of a full rank of the coefficient matrix unless otherwise stated.

The estimate $\mathbf{P}^T\widehat{\mathbf{\Theta}}$ of a parametric function $\mathbf{P}^T\mathbf{\Theta}$ (where $\widehat{\mathbf{\Theta}}$ is the LS estimate of the vector $\mathbf{\Theta}$) is called the LS estimate of the parametric function $\mathbf{P}^T\mathbf{\Theta}$.

The value of the function $\eta = \mathbf{f}^T(X_1, \dots, X_m)\mathbf{\Theta}$ at any point $(X_1, \dots, X_m)$ is a parametric function. The LS estimate of this function is the value of the regression function $\hat{y} = \mathbf{f}^T(X_1, \dots, X_m)\widehat{\mathbf{\Theta}}$ at the point $(X_1, \dots, X_m)$.

Properties of the LS estimate of a parametric function are similar to properties of the LS estimates of the vector of parameters $\widehat{\mathbf{\Theta}}$:

1. $\mathbf{P}^T\widehat{\mathbf{\Theta}}$ is an unbiased estimate of the parametric function $\mathbf{P}^T\mathbf{\Theta}$, i.e., $E(\mathbf{P}^T\widehat{\mathbf{\Theta}}) = \mathbf{P}^T\mathbf{\Theta}$.

2. The estimate $\mathbf{P}^T\widehat{\mathbf{\Theta}}$ is a linear function of the observations and has the minimum variance in the class of linear unbiased estimators.

The covariance matrix of the vector of LS estimate of $\widehat{\mathbf{\Theta}}$ is

$$\mathbf{\Gamma}(\widehat{\mathbf{\Theta}}) = (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2. \tag{2.2.4}$$

The variance of the LS estimate of the parametric function $\mathbf{P}^T\widehat{\mathbf{\Theta}}$ is

$$\sigma^2\{\mathbf{P}^T\widehat{\mathbf{\Theta}}\} = \mathbf{P}^T\mathbf{\Gamma}(\widehat{\mathbf{\Theta}})\mathbf{P}\,. \tag{2.2.5}$$

Consider the estimates of l parametric functions $\mathbf{P}_1^T\mathbf{\Theta}, \dots, \mathbf{P}_l^T\mathbf{\Theta}$ (or the estimate of the parametric vector $\mathbf{T\Theta}$). The covariance matrix of the vector of the LS estimate of $\mathbf{T}\widehat{\mathbf{\Theta}}$ is $\mathbf{T\Gamma}(\widehat{\mathbf{\Theta}})\mathbf{T}^T$.

For the given design $\mathbf{D}$ and for the model (2.1.3), consider a k-dimensional ellipsoid with a constant density inside and zero density outside, with the center that coincides with $\widehat{\mathbf{\Theta}}$ – the LS estimate of the vector of the parameters of the model (2.1.3) for the design $\mathbf{D}$, and with the moments of second order that form the covariance matrix (2.2.4) of the vector $\widehat{\mathbf{\Theta}}$ of LS estimates. This ellipsoid is called a dispersion ellipsoid of the vector $\widehat{\mathbf{\Theta}}$ of the parameter estimates.

More properties possessed by LS estimates are presented below.

3. For any unbiased linear estimate $\widetilde{\mathbf{\Theta}}$,

$$\mathbf{\Gamma}(\widehat{\mathbf{\Theta}}) = \mathbf{\Gamma}(\widetilde{\mathbf{\Theta}}) - \boldsymbol{\gamma}, \tag{2.2.6}$$

where $\boldsymbol{\gamma}$ is a positive semi-definite matrix.

Equality (2.2.6) implies the following three properties of LS estimates.

4. The LS estimates have a minimal generalized variance, i.e., a minimal determinant of the covariance matrix:

$$\det\{\mathbf{\Gamma}(\widehat{\mathbf{\Theta}})\} \le \det\{\mathbf{\Gamma}(\widetilde{\mathbf{\Theta}})\}\,.$$

5. The LS estimates correspond to a minimal volume of the dispersion ellipsoid of the parameter estimates.

6. For the LS estimates,

$$\mathrm{Tr}\{\boldsymbol{\Gamma}(\widehat{\boldsymbol{\Theta}})\} \le \mathrm{Tr}\{\boldsymbol{\Gamma}(\widetilde{\boldsymbol{\Theta}})\}.$$

§ 3. Variance Estimate and Model Adequacy Checking

It follows from (2.2.2) that the minimum of the sum of squares (2.2.1), or the residual sum of squares,

$$R_0^2 = \mathbf{y}^T\mathbf{y} - \widehat{\boldsymbol{\Theta}}^T\mathbf{X}^T\mathbf{y}.$$

It is well known that $E(R_0^2) = (N-k)\sigma^2$. Therefore,

$$\hat{\sigma}^2 = R_0^2/(N-k) \tag{2.3.1}$$

is an unbiased estimate of the variance σ^2.

Another method of calculation of the estimate of the variance uses a series of the following observations:

$$y_{11}, \dots, y_{1n_1},$$
$$\cdot\ \ \cdot\ \ \cdot\ \ \cdot\ \ \cdot\ \ \cdot$$
$$y_{r1}, \dots, y_{rn_r},$$

where $y_{ij} = \mathbf{f}^T(X_{1i}, \ \dots, \ X_{mi})\boldsymbol{\Theta} + \varepsilon_{ij}$.

Then an unbiased estimate of the variance is

$$s_e^2 = \frac{\sum_{i=1}^{r}\sum_{j=1}^{n_i}(y_{ij}-\bar{y}_i)^2}{\sum_{i=1}^{r} n_i - r} = \frac{R_e^2}{n_e}, \tag{2.3.2}$$

where

$$\bar{y}_i = \frac{\sum_{j=1}^{n_i} y_{ij}}{n_i}, \quad R_e^2 = \sum_{i=1}^{r}\sum_{j=1}^{n_i}(y_{ij} - \bar{y}_i)^2,$$
$$n_e = \sum_{i=1}^{r} n_i - r.$$

When the model (2.1.3) is valid, it is preferable to use the estimate (2.3.1). However, the estimate (2.3.2) can be used for adequacy checking of the model (2.1.3). To do this checking, we need to make additional assumptions about the distribution of the errors ε_i.

Assume that

$$\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \mathbf{E}_N\sigma^2). \tag{2.3.3}$$

Then the statistic

$$\frac{(R_0^2 - R_e^2)/(N-k-n_e)}{R_e^2/n_e} \tag{2.3.4}$$

has F-distribution with $N-k-n_e$ and n_e degrees of freedom. Therefore, the ratio (2.3.4) can be compared with the $100(1-\alpha)\%$-th point of $\mathrm{F}(N-k-n_e, n_e)$ distribution. If the ratio (2.3.4) exceeds the tabulated value, the hypothesis about the model (2.1.3) is rejected at the given level of significance. In this case the unbiased estimates of the variance of error will be only (2.3.2). If the ratio (2.3.4) does not exceed the tabulated value, there is no reason to reject the hypothesis.

§ 4. Test of Hypotheses and Interval Estimation

Suppose that the model (2.1.3) is correct with the assumption (2.3.3). The linear hypothesis to be tested is

$$\mathbf{T\Theta} = \mathbf{0}, \tag{2.4.1}$$

where $\mathrm{Rg}\,\mathbf{T} = q$.

Let a general solution of (2.4.1) be

$$\mathbf{\Theta} = \mathbf{Q\Theta}_n\,, \tag{2.4.2}$$

where $\mathbf{Q}$ is a $k \times (k-q)$ matrix; $\mathrm{Rg}\,\mathbf{Q} = k-q$ and $\mathbf{TQ} = \mathbf{0}$; $\mathbf{\Theta}_n$ is the vector of $(k-q)$ elements, which are, so to speak, new parameters.

If we substitute the solution (2.4.2) into the model (2.1.3), we get a reduced model

$$\mathrm{E}\mathbf{y} = \mathbf{X\Theta} = \mathbf{XQ\Theta}_n, \tag{2.4.3}$$

where $\mathbf{XQ}$ is a $N \times (k-q)$ matrix.

There will exist a unique solution for LS estimates of the parameters $\mathbf{\Theta}_n$ of the new model (2.4.3) if $\mathbf{XQ}$ is a full rank matrix. However,

$$\mathrm{Rg}(\mathbf{XQ}) = \mathrm{Rg}\left\|\begin{matrix}\mathbf{X}\\ \mathbf{T}\end{matrix}\right\| - \mathrm{Rg}\mathbf{T},$$

therefore, $\mathbf{XQ}$ is a full rank matrix if and only if

$$\left\|\begin{matrix}\mathbf{X}\\ \mathbf{T}\end{matrix}\right\|$$

is a full rank matrix.

The new residual sum of squares is

$$R_n^2 = \mathbf{y}^T\mathbf{y} - \widehat{\mathbf{\Theta}}_n^T\mathbf{Q}^T\mathbf{X}^T\mathbf{y},$$

where $\widehat{\mathbf{\Theta}}_n = \left(\mathbf{Q}^{\mathrm{T}}\mathbf{X}^T\mathbf{XQ}\right)^{-1}\mathbf{Q}^T\mathbf{X}^T\mathbf{y}$.

The ratio

$$\frac{(R_n^2 - R_0^2)/q}{R_0^2/(N-k)}$$

has F-distribution with q and $N = k$ degrees of freedom and can be compared with the $100(1-\alpha)$%-th point of the distribution.

All these calculations are presented in Table 1.

Table 1
Analysis of Variance

	Degrees of Freedom	Sum of Squares	Mean Square
Deviation from Hypothesis $\mathbf{T\Theta} = 0$	q	$R_n^2 - R_0^2$	$(R_n^2 - R_0^2)/q$
Residual Sum	$N-k$	$R_0^2 = \min\limits_{\hat{\Theta}} (\mathbf{y} - \mathbf{X}\hat{\mathbf{\Theta}})^T (\mathbf{y} - \mathbf{X}\hat{\mathbf{\Theta}})$	$R_0^2/(N-k)$
Residual Sum (with Hypothesis $\mathbf{T\Theta} = \mathbf{0}$)	$N-k+q$	$R_n^2 = \min\limits_{\mathbf{T}\hat{\mathbf{\Theta}} = 0} (\mathbf{y} - \mathbf{X}\hat{\mathbf{\Theta}})^T (\mathbf{y} - \mathbf{X}\hat{\mathbf{\Theta}})$	

The confidence intervals for the set of linearly independent parametric functions represented by the vector of parametric functions $\mathbf{T\Theta}$ can be found based on the following equality:

$$P\left\{\frac{\sigma^2(\mathbf{T}\hat{\mathbf{\Theta}}-\mathbf{T\Theta})^T[\mathbf{T}\Gamma(\hat{\mathbf{\Theta}})\mathbf{T}^T]^{-1}(\mathbf{T}\hat{\mathbf{\Theta}}-\mathbf{T\Theta})}{q\hat{\sigma}^2} \le F_\alpha\right\} = 1-\alpha,$$

where $\hat{\sigma}^2$ is calculated by (2.3.1).

§ 5. Bias of Regression Estimates

The LS estimate of $\hat{\mathbf{\Theta}}$ is an unbiased estimate of the parameter vector $\mathbf{\Theta}$ only if the postulated model (2.1.5) is valid. Otherwise, the estimates will be biased.

Suppose that the real model on the contrary to the postulated model (2.1.5) is

$$E\mathbf{y} = \mathbf{X\Theta} + \mathbf{X}_0\mathbf{\Theta}_0,$$

i.e., contains the terms $\mathbf{X}_0\mathbf{\Theta}_0$ that are not a part of the model (2.1.5).
Then

$$E\hat{\mathbf{\Theta}} = \mathbf{\Theta} + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_0\mathbf{\Theta}_0\,. \tag{2.5.1}$$

The matrix $\mathbf{A} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_0$ is called a bias matrix. The bias $\mathbf{A\Theta}_0$, as it is evident from (2.5.1), depends on the design. An optimal choice of the design helps to reduce and sometimes eliminate the bias.

§ 6. Estimation with Restrictions on Parameters

Suppose that for the parameters of the model (2.1.5), the following equality holds:

$$\mathbf{T\Theta} = \mathbf{0}. \tag{2.6.1}$$

We will estimate the parametric functions $\mathbf{P}^T\mathbf{\Theta}$ such that $\mathbf{P}^T$ is not represented by a linear combination of the rows of $\mathbf{T}$. This case can be resolved by the technique described in the §4 (which is called a reduction). Indeed, the original k-dimensional vector $\mathbf{\Theta}$ can be replaced with the $(k-q)$-dimensional vector $\mathbf{\Theta}_n$ using (2.4.2). That forms the reduced model (2.4.3).

Assume that $\mathrm{Rg}(\mathbf{XQ}) = k - q$. Then the unbiased estimate $\widehat{\mathbf{\Theta}}_n$ of the parameter vector $\mathbf{\Theta}_n$ can be calculated by the method of least squares.

Estimate $\widehat{\mathbf{\Theta}}$ is

$$\widehat{\mathbf{\Theta}} = \mathbf{Q}\widehat{\mathbf{\Theta}}_n.$$

This estimate can be also calculated by minimization of $(\mathbf{y} - \mathbf{X\Theta})^T(\mathbf{y} - \mathbf{X\Theta})$ with the restrictions (2.6.1) on the parameters. Therefore, $\widehat{\mathbf{\Theta}}$ is called the LS estimate of the parameter vector $\mathbf{\Theta}$ with the restrictions (2.6.1).

As in the previous paragraphs, we can (substituting k with $k - q$) calculate LS estimates of parametric functions (or the parametric vector $\mathbf{T\Theta}_n$), the covariance matrix of the vector of LS estimates $\mathbf{T}\widehat{\mathbf{\Theta}}_n$, estimate σ^2 and perform hypothesis testing.

Thus, theoretically, the restrictions (2.6.1) pose no additional problem.

All calculations can be also performed without new parameters. The technique of these calculations is presented in the book of C.R. Rao [1].

More information on this chapter issues can be found in the books [2, 3].

References

1. Rao, C.R. (1973). *Linear Statistical Inference and Its Applications*, 2^{nd} ed. New York: Wiley.

2. Scheffé, H. (1959). *The analysis of variance*. Oxford, England: Wiley.

3. Draper, N.R. and Smith, H. (1973). *Applied Regression Analysis*. New York, London, Sydney: Wiley.

Chapter 3. Factorial Models and Designs

§ 1. Factorial Design

Consider N observations $y_1, \dots, y_N$ and m variables $X_i (i = 1, \dots, m)$ with values X_{iu} corresponding to the u-th observation $(u = 1, \dots, N)$. Assume that a mathematical expectation of y_u is the following function of X_{iu} and parameters $\theta_1, \dots, \theta_k$:

$$Ey_u = \mathbf{\Theta}^T \mathbf{f}(X_{1u}, \dots, X_{mu}),$$

where $\mathbf{\Theta}^T = (\theta_1, \dots, \theta_k)$ is a vector of unknown parameters; $\mathbf{f} = (f_1, \dots, f_k)^T$ is a vector of given functions.

The variable X_i is said to be quantitative if all X_{iu} are numbers. The variable X_i is said to be qualitative if at least one of the values X_{iu} is a symbol (even if it is represented by number). This definition of quantitative and qualitative variables may not be regarded as strict. Rather it can be regarded as an explanation which model (for quantitative or qualitative factors) will be considered. In other words, quantitative variables are those for which the model for quantitative variables is considered; qualitative variables are those for which the model for qualitative variables is considered.

Each of different values of the variable X_i in the design matrix (or just design) $\mathbf{D}_X = \{X_{iu}\}$ $(i = 1, \dots, m;\ u = 1, \dots, N)$ is called a level. The number of different levels of the variable X_i is denoted by s_i. We will set up a correspondence between symbols $0, 1, \dots, s_i - 1$ and different levels of the variable X_i regardless of whether the variable X_i is a quantitative or qualitative. In this case we actually deal with the factor F_i (qualitative or quantitative) and its levels $0, 1, \dots, s_i - 1$. Then the design matrix can be rewritten as

$$\mathbf{D} = \begin{Vmatrix} F_{11} & \dots & F_{m1} \\ \cdots & \ddots & \cdots \\ F_{1N} & \dots & F_{mN} \end{Vmatrix},$$

where the columns correspond to the factors, and the rows correspond to the treatment combinations (or treatments, runs) of design $\mathbf{D}$; F_{iu} is the value of the factor F_i in the u-th treatment combination.

A design with N runs for factors $F_1, \dots, F_m$ with $s_1, \dots, s_m$ levels respectively will be denoted by $s_1 \times \dots \times s_m//N$ (or just $s_1 \times \dots \times s_m$).

It is clear that the maximum number of different rows in the design matrix is equal to $s_1 \dots s_m$.

Definition 3.1.1. A design $s_1 \times \dots \times s_m//N$ that consists of $N = s_1 \dots s_m$ different rows is called a full design. A design that does not contain at least one of $s_1 \dots s_m$ combinations of levels is called a fractional design.

We will not assume that a design does not contain identical treatment combinations.

Definition 3.1.2. A design is called symmetrical if all factors have the same number of levels. A design is called uniform if for any given factor, its levels appear equally in the design.

A design will be called factorial only with respect to a specific type of a model for which the design is considered [1]. The types of factorial models will be listed below.

§ 2. Factorial Model for Quantitative Factors

Assume that in the design **D**, all m factors $F_1, \dots, F_m$ (with $s_1, \dots, s_m$ levels respectively) are quantitative. Then consider the following model:

$$\begin{aligned} &Ey(X_1, \dots, X_m) \\ &= b_0 + b_1^{(1)} f_1^{(1)}(X_1) + \ \dots \ + b_1^{(s_i-1)} f_1^{(s_i-1)}(X_1) \\ &+ b_m^{(1)} f_m^{(1)}(X_m) + \ \dots \ + b_m^{(s_m-1)} f_m^{(s_m-1)}(X_m) + \Pi. \end{aligned} \tag{3.2.1}$$

In the model (3.2.1), the following notations and assumptions are used. $y(X_1, \dots, X_m)$ is an observation that depends on $X_1, \dots, X_m$. Π contains terms with products $k_{i_1 \ \dots \ i_r}^{(q_1 \ \dots \ q_r)} f_{i_1}^{(q_1)}(X_{i_1}) \ \dots \ f_{i_r}^{(q_r)}(X_{i_r})$ ($k_{i_1 \ \dots \ i_r}^{(q_1 \ \dots \ q_r)}$ are constants, $i_1 \neq \dots \neq i_r$). The functions $1, f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ are linearly independent at points $X_{i1}, \dots, X_{iN}$, i.e., $\mathrm{Rg}\, \mathbf{G}_i = s_i$ for any $i = 1, \dots, m,$ where

$$\mathbf{G}_i = \left\| \begin{matrix} 1 & f_i^{(1)}(X_{i1}) & \dots & f_i^{(s_i-1)}(X_{i1}) \\ 1 & f_i^{(1)}(X_{i2}) & \dots & f_i^{(s_i-1)}(X_{i2}) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & f_i^{(1)}(X_{iN}) & \dots & f_i^{(s_i-1)}(X_{iN}) \end{matrix} \right\|. \tag{3.2.2}$$

The functions $f_i^{(q)}(X_i)$ can be polynomials in X_i of degree q. In particular, for any $i = 1, \dots, m$, the functions $f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ can be the Chebyshev orthogonal polynomials at points $X_{i1}, \dots, X_{iN}$. In this case, the columns of the matrix $\mathbf{G}_i$ are pairwise orthogonal. The corresponding model is called the Chebyshev model.

Definition 3.2.1. The model (3.2.1) is called a full factorial model for quantitative factors (or an A^f-model) for the factorial design **D** if Π contains all possible terms with the products $k_{i_1 \dots i_r}^{(q_1 \dots q_r)} f_{i_1}^{(q_1)}(X_{i1}) \dots f_{i_r}^{(q_r)}(X_{i_r})$ $(i_1 \neq \dots \neq i_r)$.

The coefficient matrix for the A^f-model (3.2.1) is

$$\mathbf{X} = \begin{Vmatrix} 1 & f_1^{(1)}(X_{11}) & \dots & f_m^{(s_m-1)}(X_{m1}) & \dots \\ 1 & f_1^{(1)}(X_{12}) & \dots & f_m^{(s_m-1)}(X_{m2}) & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots \\ 1 & f_1^{(1)}(X_{1N}) & \dots & f_m^{(s_m-1)}(X_{mN}) & \dots \end{Vmatrix}. \tag{3.2.3}$$

Definition 3.2.2. A set of factors $F_1, \dots, F_m$, pairs of factors $F_{i_1}F_{i_2}$ $(i_1 \neq i_2)$, triples of factors $F_{j_1}F_{j_2}F_{j_3}$ $(j_1 \neq j_2 \neq j_3)$, etc., is called a factorial set Ω if the following requirements are satisfied: if $F_{n_1} \dots F_{n_r} \in \Omega$, then $F_{l_1} \dots F_{l_v} \in \Omega$ for all $v = 1, \dots, r-1$ and $l_1, \dots, l_v = n_1, \dots, n_r$, $l_1 \neq \dots \neq l_v$.

Example 3.2.1. For $m = 4$, elements $F_1, F_2, F_3, F_4, F_1F_2, F_1F_4, F_1F_2F_4$ do not form a factorial set Ω. Indeed, since $F_1F_2F_4 \in \Omega$, it requires that $F_1F_2 \in \Omega$, $F_1F_4 \in \Omega$, and $F_2F_4 \in \Omega$. However, the last relation does not hold. We will get a factorial set Ω if we add element F_2F_4 to the set.

Definition 3.2.3. The model for the factorial design **D**

$$\begin{aligned} &Ey(X_1, \dots, X_m) = \\ &b_0 + \textstyle\sum_{i=1}^m \left[b_i^{(1)} f_i^{(1)}(X_i) + \dots + b_i^{(s_i-1)} f_i^{(s_i-1)}(X_i)\right] \\ &+ \textstyle\sum_{i_1 i_2} \Big[b_{i_1 i_2}^{1,1} k_{i_1 i_2}^{1,1} f_{i_1}^{(1)}(X_{i_1}) f_{i_2}^{(1)}(X_{i_2}) + \cdots \\ &+ b_{i_1 i_2}^{s_{i_1}-1, s_{i_2}-1} k_{i_1 i_2}^{s_{i_1}-1, s_{i_2}-1} f_{i_1}^{(s_{i_1}-1)}(X_{i_1}) f_{i_2}^{(s_{i_2}-1)}(X_{i_2})\Big] + \cdots \end{aligned} \tag{3.2.4}$$

is called a factorial model for quantitative factors for the factorial set Ω (or an A^Ω-model) if the following requirements are satisfied: if the model (3.2.4) includes the term $k_{i_1 \dots i_r}^{q_1 \dots q_r} f_{i_1}^{(q_1)}(X_{i_1}) \dots f_{i_r}^{(q_r)}(X_{i_r})$ for some set of $q_1, \dots, q_r$, then the model includes all terms for all $q_1 = 0, \dots, s_1 - 1, \dots, q_r = 0, \dots, s_r - 1$ (by definition, $f_i^{(0)}(X_i) = 1$).

It is evident that Definition 3.2.3 is consistent with Definition 3.2.2.

An A^{Ω}-model (3.2.4) is a general model for quantitative factors. An A^{f}-model, for example, is a special case of an A^{Ω}-model.

§ 3. Main Effects and Interaction Effects

In an N-dimensional Euclidean space E_N, we set up a correspondence between the u-th coordinate of each vectors and the u-th treatment combination of the design **D.**

Definition 3.3.1. A nonzero vector $\mathbf{z}^{\mathrm{T}} = (z_1, \dots, z_N) \in E_N$ is defined to be a contrast if

$$\sum_{u=1}^{N} z_u = 0. \qquad (3.3.1)$$

Definition 3.3.2. The vector of the main effect of the factor F_i of the design **D** is a contrast with equal coordinates for the same levels of the factor F_i in the design **D.** The vector of the main effect is also called the vector of the interaction effect of order 0.

The definition of the vector of the interaction effect of $(r-1)$-th order $(r \geq 2)$ is based on the definition of the vector of the interaction effect of $(r-2)$-th order.

Definition 3.3.3. The vector of the interaction effect of $(r-1)$-th order (or the vector of the r-factorial interaction effect) of the factors $F_1, \dots, F_r$ of the design **D** is a contrast with equal coordinates for the same combinations of levels of the factors $F_1, \dots, F_r$ in the design **D**, orthogonal to all vectors of interaction effects up to $(r-2)$-th order of the factors $F_1, \dots, F_r$.

We may omit word “vector” in the above two definitions.

A linear combination of several interaction effects of $(r-1)$-th order $(r \geq 1)$ of r factors is, obviously, an interaction effect of $(r-1)$-th order of the same factors or zero-vector. Therefore, a set of all interaction effects of $(r-1)$-th order of r factors, together with the zero-vector, is a linear subspace of the space E_N.

Definition 3.3.4. The number of degrees of freedom carried by interaction effects of $(r-1)$-th order for the design **D** is the dimension of the corresponding linear subspace.

It is evident that the number of degrees of freedom carried by main effects of the factor F_i for any design is equal to $s_i - 1$.

The requirement of orthogonality of the $(r-1)$-th order interaction effects to all interaction effects up to $(r-2)$-th order of the same factor is obviously equivalent to the requirement of orthogonality to maximal linearly independent subset of the corresponding interaction effects.

Definition 3.3.5. The matrix $\mathbf{F}_i$ composed of the maximum subset of $s_i - 1$ independent vectors of main effects of the factor F_i is called a matrix of main effects of the factor F_i. The matrix $\mathbf{F}_{ij}$, composed of the maximum subset of independent vectors of interaction effects of the factors F_i and F_j is called a matrix of interaction effects of the factors F_i and F_j, etc.

Introduce the following notation:

$$\boldsymbol{\Phi}_{1\ldots r} = \| \ \mathbf{I}, \mathbf{F}_1, \ldots, \mathbf{F}_r, \mathbf{F}_{12}, \ldots, \mathbf{F}_{1\ldots r} \ \|,$$

where $\mathbf{I}$ is a unit vector (with the elements equal to 1).

We will assume that any matrix in $\boldsymbol{\Phi}_{1\ldots r}$ is normalized in such a way that sum of squares of elements of any its column is equal to N. In the matrix $\mathbf{F}_i$, for each subset of identical rows, we delete all but one row and add a left column consisting of 1. Denote the resulting matrix by $\bar{\boldsymbol{\Phi}}_i$.

Matrices $\mathbf{F}_i$ can be used as matrices $\mathbf{G}_i$ (3.2.2) for the A^f -model (3.2.1), since

$$\text{Rg} \ \| \ \mathbf{I}, \mathbf{F}_i \ \| = \text{Rg} \ \bar{\boldsymbol{\Phi}}_i = s_i.$$

Example 3.3.1. Consider a matrix of the full design 3×2 for factors F_1 and F_2:

$$\begin{array}{cc} & \begin{array}{cc} F_1 & F_2 \end{array} \\ \mathbf{D} = & \left\| \begin{array}{cc} 0 & 0 \\ 1 & 0 \\ 2 & 0 \\ 0 & 1 \\ 1 & 1 \\ 2 & 1 \end{array} \right\|. \end{array}$$

The number of degrees of freedom carried by main effects of the factor F_2 is equal to 1, Any main effect is, apart from proportionality factor, $(-1, -1, -1, +1, +1, +1)^T$. The number of degrees of freedom carried by main effects of the factor F_1 equals 2. Therefore, there exist two linearly independent vectors of main effects of the factor F_1, forming a matrix $\mathbf{F}_1$ of main effects. This matrix may be as follows (hereinafter we present matrices in integers and put multipliers under the corresponding columns):

$$\mathbf{F}_1 = \left\| \begin{array}{cc} -1 & +1 \\ 0 & -2 \\ +1 & +1 \\ -1 & +1 \\ 0 & -2 \\ +1 & +1 \end{array} \right\|$$

$$\times \left\| \sqrt{3/2} \quad \sqrt{1/2} \right\|^T.$$

Any nontrivial combination of columns of $\mathbf{F}_1$ produces a vector of a main effect of the factor F_1. An example of such a main effect is linear combination with parameters (1/2, 1/2): $(0, -1, +1, 0, -1, +1)^{\mathrm{T}}$.

It is easy to verify that

$$\mathbf{F}_{12} = \begin{Vmatrix} +1 & -1 \\ 0 & +2 \\ -1 & -1 \\ -1 & +1 \\ 0 & -2 \\ +1 & +1 \end{Vmatrix} \times \begin{Vmatrix} \sqrt{3/2} & \sqrt{1/2} \end{Vmatrix}^T.$$

is the matrix of interaction effects of the factors F_1 and F_2. Indeed, two vectors of the matrix $\mathbf{F}_{12}$ are orthogonal to vector $\mathbf{I}$ and to vectors of matrices $\mathbf{F}_1$ and $\mathbf{F}_2$. Since vector $\mathbf{I}$ and vectors of matrices $\mathbf{F}_1$ and $\mathbf{F}_2$ are orthogonal, $\mathbf{F}_{12}$ contains as much as possible number of vectors. Hence, the matrix $\mathbf{\Phi}_{12}$ is

$$\mathbf{\Phi}_{12} = \begin{Vmatrix} +1 & -1 & +1 & -1 & +1 & -1 \\ +1 & 0 & -2 & -1 & 0 & +2 \\ +1 & +1 & +1 & -1 & -1 & -1 \\ +1 & -1 & +1 & +1 & -1 & +1 \\ +1 & 0 & -2 & +1 & 0 & -2 \\ +1 & +1 & +1 & +1 & +1 & +1 \end{Vmatrix} \times \begin{Vmatrix} 1 & \sqrt{3/2} & \sqrt{1/2} & 1 & \sqrt{3/2} & \sqrt{1/2} \end{Vmatrix}^T.$$

§ 4. The Main Theorem for Full Design

Definition 3.4.1. For two vectors $\mathbf{a} = (a_1, \dots, a_N)^T$ and $\mathbf{c} = (c_1, \dots, c_N)^T$, introduce operation $\otimes$ called multiplication, such that product

$$\mathbf{a} \otimes \mathbf{c} = (a_1 c_1, \dots, a_N c_N)^T.$$

Let columns of the (N x n)-matrix $\mathbf{A}$ be $\mathbf{a}_1, \dots, \mathbf{a}_n$, and columns of the ($N$ x l)-matrix $\mathbf{C}$ be $\mathbf{c}_1, \dots, \mathbf{c}_l$. Then, by definition,

$$\mathbf{A} \otimes \mathbf{C} = \|(\mathbf{a}_1 \otimes \mathbf{c}_1), (\mathbf{a}_1 \otimes \mathbf{c}_2), \dots, (\mathbf{a}_n \otimes \mathbf{c}_l)\|.$$

Theorem 3.4.1. For a full factorial design, any interaction effect of a set of factors is orthogonal to any interaction effect of other set of factors and the number of columns of the matrix $\mathbf{F}_{i_1 \dots i_r}$ is equal to $(s_{i_1} - 1) \dots (s_{i_r} - 1)$.

P r o o f. Consider any two rows of the matrix of the full design $\mathbf{D}^f$. It can be shown that for these two rows, there exists a column corresponding to some factor, such that for selected two rows, the factor has different levels. Without loss of generality, it can be assumed that the first two rows and the last column are considered. Select the columns in the matrices $\mathbf{F}_i = \{F_i^{pq}\}$ to make them pairwise orthogonal. It is evident that in the full design, all levels of the given factor occur equally. Therefore, the columns of the matrix $\overline{\boldsymbol{\Phi}}_i = \{\overline{\Phi}_i^{jl}\}$ will be pairwise orthogonal. Besides, for any j and l,

$$\sum_j \left(\overline{\Phi}_i^{jl}\right)^2 = \sum_l \left(\overline{\Phi}_i^{jl}\right)^2. \tag{3.4.1}$$

It follows from (3.4.1) that for any p

$$\sum_q F_i^{pq} = const. \tag{3.4.2}$$

Define $\mathbf{R}_1 = \|\mathbf{I},\ \mathbf{F}_1\|$. The number of columns of the matrix $\mathbf{R}_1$ equals

$$\lambda_{R_1} = s_1. \tag{3.4.3}$$

Define $\mathbf{R}_i (i = 2, \dots, m)$ by the following recurrence relation:

$$\mathbf{R}_i = \|\mathbf{R}_{i-1}, (\mathbf{R}_{i-1} \otimes \mathbf{F}_i)\|.$$

The number of the columns λ_{R_i} of the matrix $\mathbf{R}_i$ and the number of the columns $\lambda_{R_{i-1}}$ of the matrix $\mathbf{R}_{i-1}$ are connected by the following obvious relation:

$$\lambda_{R_i} = \lambda_{R_{i-1}} s_i. \tag{3.4.4}$$

Consider the matrix $\mathbf{R}_m = \|\mathbf{R}_{m-1}, (\mathbf{R}_{m-1} \otimes \mathbf{F}_m)\|$. The number of the columns λ_{R_m} of the matrix $\mathbf{R}_m$, by (3.4.3) and (3.4.4), equals $\lambda_{R_m} = s_1 \dots s_m = N$. Hence, $\mathbf{R}_m$ is a square matrix.

We will prove that the selected two first rows of the matrix $\mathbf{R}_m$ are orthogonal. Let the first two rows of the matrix $\mathbf{R}_{m-1}$ be $\mathbf{a}^T$ and $\mathbf{c}^T$. Then the first two rows of the matrix $\mathbf{R}_m$ are

$$(\mathbf{a}\overline{\Phi}_m^{11})^T \dots \left(\mathbf{a}\overline{\Phi}_m^{1s_m}\right)^T \text{ and } (\mathbf{c}\overline{\Phi}_m^{21})^T \dots \left(\mathbf{c}\overline{\Phi}_m^{2s_m}\right)^T.$$

Their scalar product

$$(\mathbf{a}, \mathbf{c}) \sum_{j=1}^{s_m} \overline{\Phi}_m^{1j} \overline{\Phi}_m^{2j} = 0.$$

Hence, any two rows of the matrix $\mathbf{R}_m$ are orthogonal.

To prove that any two columns of the matrix $\mathbf{R}_m$ are orthogonal we need to show that sum of squares of elements of any row of the matrix $\mathbf{R}_m$ is constant:

$$\sum_{l=1}^{s_1 \ldots s_m} r_m^{jl} = \text{const}, \tag{3.4.5}$$

where r_i^{jl} is element of the j-th row and the l-th column of the matrix $\mathbf{R}_i$.

By definition $\mathbf{R}_i$,

$$\sum_{l=1}^{s_1 \ldots s_i} \left(r_i^{jl}\right)^2 = \sum_{l=1}^{s_1 \ldots s_i} \left(r_{i-1}^{jl}\right)^2 \sum_{n=1}^{s_i} \left(F_i^{jn}\right)^2,$$
$$\sum_{l=1}^{s_1} \left(r_i^{jl}\right)^2 = 1 + \sum_{n=1}^{s_1-1} \left(F_1^{jn}\right)^2.$$

Therefore,

$$\sum_{l=1}^{s_1 \ldots s_m} \left(r_m^{jl}\right)^2 = \prod_{i=1}^{m} \sum_{n=1}^{s_i} \left(F_i^{jn}\right)^2 + \prod_{i=2}^{m} \sum_{n=1}^{s_i} \left(F_i^{jn}\right)^2.$$

Hence, by (3.4.2), we get (3.4.5).

Matrices of the form $\mathbf{F}_{i_1} \otimes \ \ldots \ \otimes \mathbf{F}_{i_r}$, included in the matrix $\mathbf{R}_m$, contain $\left(s_{i_1} - 1\right) \ \ldots \ \left(s_{i_r} - 1\right)$ columns. For each of these columns, its elements are equal for all treatments of the design $\mathbf{D}^f$ with the same combinations of levels of the factors $F_{i_1}, \ldots, F_{i_r}$. By what we have already proved, each of these columns is orthogonal to all other columns. Hence, it can be proved by induction that these columns are interaction effects of the factors $F_{i_1}, \ldots, F_{i_r}$.

The number of different combinations of levels of the factors $F_{i_1}, \ldots, F_{i_m}$ equals $s_{i_1} \ldots s_{i_m}$. All vectors of main effects and interaction effects of these factors belong to an l-dimensional subspace E_l ($l = s_1 \ldots s_m - 1$) of an N-dimensional space E_N, because elements of each of the vector of main effects or interaction effects are equal for all treatments with the same combinations of levels of the factors and all vectors of these effects are orthogonal to the unit vector.

Since

$$\sum_{i=1}^{m} (s_i - 1) + \sum_{i \neq j} (s_i - 1)\left(s_j - 1\right)$$
$$+ \cdots + (s_1 - 1) \ldots (s_m - 1) = s_1 \ldots s_m - 1,$$

the number of linearly independent r-factorial interaction effects of the factors $F_{i_1}, \ldots, F_{i_r}$ may not exceed

$$\left(s_{i_1} - 1\right) \ldots \left(s_{i_r} - 1\right) \tag{3.4.6}$$

and, therefore, is equal to (3.4.6).

By using matrices $\mathbf{F}_i$ with pairwise orthogonal columns, we get sets of orthogonal interaction effects. It can be shown that by using linearly independent (not necessarily pairwise orthogonal) main effects of the matrix $\mathbf{F}'_r$, we get linearly independent interaction effects. To prove that, consider the following lemma.

Lemma 3.4.1. Let $\mathbf{A}$, $\mathbf{A}'$, and $\mathbf{C}$ be matrices of size $N \times p$, $N \times p$, and $N \times q$ respectively and

$$\mathbf{A} = \mathbf{A}'\boldsymbol{\Lambda}, \tag{3.4.7}$$

where $\boldsymbol{\Lambda}$ is a nonsingular square matrix of order *p*. Then the matrices $\mathbf{A} \otimes \mathbf{C}$ and $\mathbf{A}' \otimes \mathbf{C}$ are related by a nonsingular linear transformation.

P r o o f. Let $\boldsymbol{c}_i$ be the *i*-th column of the matrix $\mathbf{C}$. Then, by (3.4.7),

$$\mathbf{A} \otimes \mathbf{c}_i = (\mathbf{A}'\boldsymbol{\Lambda}) \otimes \mathbf{c}_i = (\mathbf{A}' \otimes \mathbf{c}_i)\boldsymbol{\Lambda}.$$

Therefore, for any i $(i = 1, \dots, q)$, the matrices $\mathbf{A} \otimes \mathbf{c}_i$ and $\mathbf{A}' \otimes \mathbf{c}_i$ are related by a nonsingular linear transformation. This proves the lemma.

Matrices $\mathbf{F}_i$ and $\mathbf{F}'_i$ for any i are related by a nonsingular linear transformation. Therefore, using Lemma 3.4.1 repeatedly, we get that $\mathbf{F}_{i_1} \otimes \dots \otimes \mathbf{F}_{i_r}$ is related by a nonsingular linear transformation with $\mathbf{F}'_{i_1} \otimes \dots \otimes \mathbf{F}'_{i_r}$. Hence, $\mathbf{F}'_{i_1} \otimes \dots \otimes \mathbf{F}'_{i_r}$ consists of linearly independent interaction effects of the factors $F_{i_1}, \dots, F_{i_r}$.

This completes the proof of Theorem 3.4.1.

Definition 3.4.2. A set of linearly independent interaction effects of the factors $F_{i_1}, \dots, F_{i_r}$ is called full if the number of those effects of the set is given by (3.4.6).

Note 1 to Theorem 3.4.1. The proof of Theorem 3.4.1 gives us a method of construction of interaction effects for the design $\mathbf{D}^f$ as a product of main effects of the factors. By using a full set of orthogonal main effects of the factors, we get a full set of orthogonal interaction effects. By using a full set of linearly independent main effects of the factors, we get a full set of linearly independent interaction effects.

Note 2 to Theorem 3.4.1. If for any $i = 1, \dots, m$, the functions $f_i^{(q)}(X_i)$ of the A^f-model (3.2.1) are chosen in such a way that

$$\textstyle\sum_{u=1}^{N} f_i^{(q)}(X_{iu}) = 0,$$

all columns of the matrix (3.2.2) except the first are vectors of main effects of the factor F_i. If, in addition,

$$\textstyle\sum_{u=1}^{N} \left\{f_i^{(q)}\left(X_{i_u}\right)\right\}^2 = N,$$

then, by the proof of Theorem 3.4.1, a scalar square of any column $\mathbf{F}_{i_1} \otimes \dots \otimes \mathbf{F}_{i_r}$ equals *N*. Therefore, by Theorem 3.4.1 and Note 1 to the Theorem 3.4.1, the coefficient matrix (3.2.3) for a full factorial model is the matrix $\mathbf{\Phi}_{1\,\dots\,m}$ of main effects and interaction effects of the factors $F_1, \dots, F_m$ for the design $\mathbf{D}^f$.

Example 3.4.1. Consider the matrix $\mathbf{D}^f$ of the full design 3^2 and the corresponding matrix $\mathbf{\Phi}_{12}$:

$$
\begin{array}{c}
\begin{array}{cc} F_1 & F_2 \end{array} \\
\mathbf{D}^f = \left\|\begin{array}{cc}
0 & 0 \\
1 & 0 \\
2 & 0 \\
0 & 1 \\
1 & 1 \\
2 & 1 \\
0 & 2 \\
1 & 2 \\
2 & 2
\end{array}\right\|
\end{array},
\quad
\begin{array}{c}
\begin{array}{c|cc|cc|cccc} \mathbf{I} & \mathbf{F}_1 & & \mathbf{F}_2 & & \mathbf{F}_{12} = \mathbf{F}_1 \otimes \mathbf{F}_2 & & & \end{array} \\
\mathbf{\Phi}_{12} = \left\|\begin{array}{c|cc|cc|cccc}
1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 0 & -2 & -1 & 1 & 0 & 0 & 2 & -2 \\
1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
1 & -1 & 1 & 0 & -2 & 0 & 2 & 0 & -2 \\
1 & 0 & -2 & 0 & -2 & 0 & 0 & 0 & 4 \\
1 & 1 & 1 & 0 & -2 & 0 & -2 & 0 & -2 \\
1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 \\
1 & 0 & -2 & 1 & 1 & 0 & 0 & -2 & -2 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{array}\right\| \\
\times \left\| \begin{array}{ccccccccc} 1 & \sqrt{3/2} & \sqrt{1/2} & \sqrt{3/2} & \sqrt{1/2} & 3/2 & \sqrt{3}/2 & \sqrt{3}/2 & 1/2 \end{array} \right\|^T
\end{array}
$$

Since each of the factors F_1 and F_2 is three-level, there are exactly two linearly independent main effects for each of them. Each of the columns of the submatrix $\mathbf{F}_1$ is orthogonal to $\mathbf{I}$ and has equal elements for the same levels of the factor F_1. Each of the columns of the submatrix $\mathbf{F}_2$ is orthogonal to $\mathbf{I}$ and has equal elements for the same levels of the factor F_2. Hence, two columns of the matrix $\mathbf{F}_1$ and two columns of the matrix $\mathbf{F}_2$ are main effects of the factors F_1 and F_2 respectively. The columns of the matrix $\mathbf{F}_1$ are orthogonal. The same is true for the columns of the matrix $\mathbf{F}_2$. Therefore, matrix product $\mathbf{F}_1 \otimes \mathbf{F}_2$, by Note 1 to Theorem 3.4.1, has four pairwise orthogonal vectors of interaction effects of the factors F_1 and F_2. We can verify that all requirements of the definition of interaction effects are satisfied. Besides, by Theorem 3.4.1, all columns of the matrix $\mathbf{\Phi}_{12}$ are pairwise orthogonal.

§ 5. A Model of True Effects for Quantitative Factors

Hereafter, we will consider the Chebyshev model only if the structure of the design $\mathbf{D}$ leads to orthogonality of all effects. Otherwise, we will consider so-called model of true effects for quantitative factors.

Consider a full design $\mathbf{D}^f$ with N^f runs for all factors of the design $\mathbf{D}$. Define a vector of true values $\boldsymbol{\eta}^f$ for the design $\mathbf{D}^f$ as follows:

$$\boldsymbol{\eta}^f = E\mathbf{y}^f = E\left(y_1, \dots, y_{N^f}\right)^T.$$

To define a vector of true effects $\mathbf{B}$ for quantitative factors, form the following matrix for the design $\mathbf{D}^f$:

$$\mathbf{\Phi}^f_{1\dots m} = \left\|\mathbf{I}, \mathbf{F}^f_1, \dots, \mathbf{F}^f_m, \ \mathbf{F}^f_{12}, \dots, \mathbf{F}^f_{1\dots m}\right\|, \tag{3.5.1}$$

where all matrices $\mathbf{F}^f$ have pairwise orthogonal columns (scalar squares of the columns of the matrix $\mathbf{\Phi}^f_{1\ldots m}$ equal N^f). Then define

$$\mathbf{B} = \frac{1}{N^f}\mathbf{\Phi}^{f^T}_{1\ \ldots\ m}\boldsymbol{\eta}^f. \tag{3.5.2}$$

It is evident that

$$\boldsymbol{\eta}^f = \mathbf{\Phi}^f_{1\ldots m}\mathbf{B}, \tag{3.5.3}$$

because, by (3.5.2) and Theorem 3.4.1,

$$\mathbf{\Phi}^f_{1\ldots m}\mathbf{B} = \frac{1}{N^f}\mathbf{\Phi}^f_{1\ldots m}\mathbf{\Phi}^{f^T}_{1\ldots m}\boldsymbol{\eta}^f = \boldsymbol{\eta}^f.$$

Therefore, the following theorem has been proved.

Theorem 3.5.1. For the vector of observations $\mathbf{y}^f = (y_1, \ldots, y_{N^f})$,

$$E\mathbf{y}^f = \mathbf{\Phi}^f_{1\ldots m}\mathbf{B} \tag{3.5.4}$$

at the points of the design $\mathbf{D}^f$ with the factors $F_1, \ldots, F_m$, where $\mathbf{B}$ is the vector of true effects (3.5.2).

By the definition of the matrix of main effects and Note 2 to Theorem 3.4.1, the model (3.5.3) – (3.5.4) is a special case of the A^f-model and, therefore, a special case of the general factorial A^Ω-model for quantitative factors. We will call (3.5.3) – (3.5.4) the A^f-model of true effects.

Denote the parts of the matrix $\mathbf{\Phi}^f_{1\ \ldots\ m}$ and the vector $\mathbf{B}$ for the factorial set Ω by $\mathbf{\Phi}^\Omega$ and $\mathbf{B}^\Omega$ respectively. If elements of the vector $\mathbf{B}$ that do not correspond to the factorial set Ω equal zero, (3.5.4) will be as follows:

$$E\mathbf{y}^f = \mathbf{\Phi}^\Omega\mathbf{B}^\Omega. \tag{3.5.5}$$

It is evident that the model (3.5.5) is also a special case of the factorial A^Ω-model. We will call (3.5.5) the A^Ω-model of true effects. If it does not matter or if it is clear which type of a model for quantitative factors we consider, we will omit the words "true effects".

The A^Ω-model (3.5.5) can be extended to a wider domain:

$$Ey(X_1, \ldots, X_m) = \mathbf{f}^T(X_1, \ldots, X_m)\mathbf{B}^\Omega, \tag{3.5.6}$$

where $f^T(X_{1u}, \ldots, X_{mu})$ is the u-th row of the matrix $\mathbf{\Phi}^\Omega$.

We will discuss an interpretation of the coefficients of the model (3.5.6) after the following example:

Example 3.5.1. Consider the design $\mathbf{D}$ and the corresponding vector of mathematical expectation of observations $\boldsymbol{\eta}$:

$$\begin{array}{cc} & \begin{array}{ccc} F_1 & F_2 & F_3 \end{array} \\ \mathbf{D} = & \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{Vmatrix} \end{array}; \quad \mathbf{D}_X = \begin{Vmatrix} X_1^{(1)} & X_2^{(0)} & X_3^{(0)} \\ X_1^{(0)} & X_2^{(1)} & X_3^{(0)} \\ X_1^{(0)} & X_2^{(0)} & X_3^{(1)} \\ X_1^{(0)} & X_2^{(0)} & X_3^{(0)} \\ X_1^{(1)} & X_2^{(1)} & X_3^{(1)} \end{Vmatrix};$$

$$E\mathbf{y} = \boldsymbol{\eta} = \begin{Vmatrix} \eta_2 \\ \eta_3 \\ \eta_5 \\ \eta_1 \\ \eta_8 \end{Vmatrix}.$$

Then the full design $\mathbf{D}^f$ and the corresponding vector $\boldsymbol{\eta}^f$ of mathematical expectations of observations will be as follows:

$$\mathbf{D}^f = \begin{Vmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{Vmatrix}; \quad E\mathbf{y}^f = \boldsymbol{\eta}^f = (\eta_1, \dots, \eta_8)^T.$$

For the design $\mathbf{D}^f$ the matrix $\boldsymbol{\Phi}_{123}^f$ can be, for example, as follows:

$$\boldsymbol{\Phi}_{123}^f = \begin{Vmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{Vmatrix}.$$

Then the vector of true effects

$$\mathbf{B} = (b_0, b_1, b_2, b_3, b_{12}, b_{13}, b_{23}, b_{123})^T = \frac{1}{8} \boldsymbol{\Phi}_{123}^{f^T} \boldsymbol{\eta}^f, \tag{3.5.7}$$

and the A^f-model of true effects (3.5.4) becomes an identity at the points of $\mathbf{D}^f$. To define the model in a wider domain, consider the following functions:

$$f_i^{(1)}(X_i) = x_i = \frac{X_i - \bar{X}_i}{\Delta X_i} \quad (i = 1,2,3),$$

where

$$\bar{X}_i = \frac{X_i^{(1)} + X_i^{(0)}}{2} \text{ and } \Delta X_i = \frac{X_i^{(1)} - X_i^{(0)}}{2}.$$

It is evident that x_i at points of $\mathbf{D}^f$ forms the vectors $\mathbf{F}_i$. Also, x_1x_2, x_1x_3, x_2x_3, $x_1x_2x_3$ at points of $\mathbf{D}^f$ form the vectors $\mathbf{F}_{12}, \mathbf{F}_{13}, \mathbf{F}_{23}, \mathbf{F}_{123}$ respectively. Then we get an extended A^f-model of true effects:

$$Ey = b_0 + b_1x_1 + b_2x_2 + b_3x_3$$
$$+b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + b_{123}x_1x_2x_3. \tag{3.5.8}$$

Suppose, for example, that $b_{13} = b_{23} = b_{123} = 0$. Then we get the following A^Ω-model of true effects:

$$Ey = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2. \tag{3.5.9}$$

The coefficient matrix $\mathbf{X}^\Omega$ of the design $\mathbf{D}$ for the model (3.5.9) is

$$\mathbf{X}^\Omega = \begin{Vmatrix} 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{Vmatrix}.$$

The coefficients of the model (3.5.8), i.e., elements of the vector of true effects (or just true effects), can have a clear interpretation. For example, it follows from (3.5.7) that

$$b_0 = \frac{1}{8}\sum_{u=1}^{8} \eta_u$$

is the average of all $\eta_u = Ey_u$. The number

$$2b_3 = \frac{1}{4}\sum_{u=5}^{8} \eta_u - \frac{1}{4}\sum_{u=1}^{4} \eta_u$$

shows what is an "influence" of the factor F_3, i.e., what is the difference between the average of all mathematical expectations with one level of the factor F_3 and the average of all mathematical expectations with other level of the factor F_3.

The number

$$4b_{12} = \left\{\frac{\eta_1 + \eta_5}{2} - \frac{\eta_2 + \eta_6}{2}\right\} - \left\{\frac{\eta_3 + \eta_7}{2} - \frac{\eta_4 + \eta_8}{2}\right\}$$

shows what is the difference between the "influence" of the factor F_1 for one level of the factor F_2 and the "influence" of the factor F_1 for other level of the factor F_2.

§ 6. Full Rank Theorem

The following three paragraphs are devoted to finding a condition under which it is possible to construct an orthogonal design [2].

Let in the design **D**, the number of different combinations of levels of factors $F_1, \dots, F_r$

$$C^{1\dots r} = s_1 \dots s_r. \tag{3.6.1}$$

Theorem 3.6.1. I. The condition (3.6.1) is necessary and sufficient for the number of degrees of freedom carried by any n-factor interaction effects $(n \le r)$ of n factors $F_{i_1}, \dots, F_{i_n}$ of $F_1, \dots, F_r$ is determined by (3.4.6). II. If (3.6.1) holds, $\mathbf{\Phi}_{1\dots r}$ is a matrix of full rank.

P r o o f. Necessity of the condition (3.6.1) is evident. Show sufficiency of the condition (3.6.1) and that statement II of the theorem is true.

By the hypothesis of the theorem, the design **D** contains a subset $\mathbf{D}^f$ forming a full design for the factors $F_1, \dots, F_r$. For the design $\mathbf{D}^f$, we generate matrices of effects up to order $(r-1)$ of the factors $F_1, \dots, F_r$ and the matrix

$$\mathbf{\Phi}_{1\dots r}^f = \left\| \mathbf{I}, \mathbf{F}_1^f, \dots, \mathbf{F}_r^f, \mathbf{F}_{12}^f, \dots, \mathbf{F}_{1\dots r}^f \right\|.$$

Theorem 3.4.1 implies that for $\mathbf{D}^f$ any interaction effect of a given subset of factors orthogonal to any interaction effect of a different subset of factors. Hence, the columns of the matrix $\mathbf{\Phi}_{1\dots r}^f$ taken one from each matrix of effects are pairwise orthogonal. Therefore, $\mathbf{\Phi}_{1\dots r}^f$ is a matrix of full rank.

For each combination of levels of the factors $F_1, \dots, F_r$ in the design **D,** select the row that corresponds to this combination in the matrix $\mathbf{\Phi}_{1\dots r}^f$. Denote the resulting matrix by

$$\mathbf{\Phi}_{1\dots r}^{\mathbf{D}} = \left\| \mathbf{I}, \mathbf{F}_1^{\mathbf{D}}, \dots, \mathbf{F}_r^{\mathbf{D}}, \mathbf{F}_{12}^{\mathbf{D}}, \dots, \mathbf{F}_{1\dots r}^{\mathbf{D}} \right\|,$$

where the number of columns of the matrix $\mathbf{F}_{i_1\dots i_n}^{\mathbf{D}}$ equals the number of columns of the matrix $\mathbf{F}_{i_1\dots i_n}^f$. It is evident that $\mathbf{\Phi}_{1\dots r}^{\mathbf{D}}$ is also a matrix of full rank.

Now we will construct the matrix

$$\mathbf{\Phi}_{1\dots r} = \|\mathbf{I}, \mathbf{F}_1, \dots, \mathbf{F}_r, \mathbf{F}_{12}, \dots, \mathbf{F}_{1\dots r}\|$$

that contains vectors main effects, interaction effects of the factors F_1, $\dots, F_r$ of the design $\mathbf{D}$, and the vector $\mathbf{I}$. The number of columns of the matrix $\mathbf{F}_{i_1\dots i_n}$ is equal to the number of columns of the matrix $\mathbf{F}^{\mathbf{D}}_{i_1\dots i_n}$. Denote the j-th columns of the matrices $\mathbf{F}_{i_1\dots i_n}$ and $\mathbf{F}^{\mathbf{D}}_{i_1\dots i_n}$ by $\mathbf{F}^{j}_{i_1\dots i_n}$ and $\mathbf{F}^{\mathbf{D}j}_{i_1\dots i_n}$ respectively. The first column of the matrix $\mathbf{\Phi}_{1\dots r}$ is the first column of the matrix $\mathbf{\Phi}^{\mathbf{D}}_{1\dots r}$. We will construct the next columns recurrently. Assume that we have constructed first p independent columns of the matrix $\mathbf{\Phi}_{1\dots r}$ in such a way that the l-th column of the matrix $\mathbf{\Phi}_{1\dots r}$ is a linear combination of the first l columns of the matrix $\mathbf{\Phi}^{\mathbf{D}}_{1\dots r}$ $(l = 1, \dots, p)$. Also assume that any of the columns that belong to the matrix $\mathbf{F}_{j_1\dots j_l}$ are linearly independent interaction effects of the factors $F_{j_1}, \dots, F_{j_l}$. Then the method of construction of the $(p+1)$-th column is the following.

Let the $(p+1)$-th column of the matrix $\mathbf{\Phi}_{1\dots r}$ is $\mathbf{F}^{j}_{i_1\dots i_n}$. Then make the following assignment:

$$\mathbf{F}^{j}_{i_1\dots i_n} = \mathbf{A}^{j}_{i_1\dots i_n}\left(\mathbf{A}^{jT}_{i_1\dots i_n}\mathbf{A}^{j}_{i_1\dots i_n}\right)^{-1}\mathbf{A}^{jT}_{i_1\dots i_n}\mathbf{F}^{\mathbf{D}j}_{i_1\dots i_n} - \mathbf{F}^{\mathbf{D}j}_{i_1\dots i_n},$$

where

$$\mathbf{A}^{j}_{i_1\dots i_n} = \left\|\mathbf{I}, \mathbf{F}_{i_1}, \dots, \mathbf{F}_{i_n}, \mathbf{F}_{i_1 i_2}, \dots, \mathbf{F}_{i_1\dots i_n}, \mathbf{F}^{1}_{i_1\dots i_n}, \dots, \mathbf{F}^{j-1}_{i_1\dots i_n}\right\|.$$

The first p columns of the matrix $\mathbf{\Phi}_{1\dots r}$ are independent, therefore $\mathbf{A}^{jT}_{i_1\dots i_n}\mathbf{A}^{j}_{i_1\dots i_n}$ is nonsingular, its inverse exists, and

$$\mathbf{A}^{j}_{i_1\dots i_n}\left(\mathbf{A}^{jT}_{i_1\dots i_n}\mathbf{A}^{j}_{i_1\dots i_n}\right)^{-1}\mathbf{A}^{jT}_{i_1\dots i_n}\mathbf{F}^{\mathbf{D}j}_{i_1\dots i_n} \neq \mathbf{F}^{\mathbf{D}j}_{i_1\dots i_n},$$

$\mathbf{F}^{j}_{i_1\dots i_n}$ is nonzero column. $\mathbf{F}^{j}_{i_1\dots i_n}$ is a linear combination of columns of $\mathbf{A}^{j}_{i_1\dots i_n}$ and $\mathbf{F}^{\mathbf{D}j}_{i_1\dots i_n}$, therefore, we get $p+1$ independent columns. The elements of $\mathbf{F}^{j}_{i_1\dots i_n}$ for the same combinations of level of the factors $F_{i_1}, \dots, F_{i_n}$ are equal. It is evident that

$$\mathbf{A}^{jT}_{i_1\dots i_n}\mathbf{F}^{j}_{i_1\dots i_n} = 0.$$

Hence, $\mathbf{F}^{j}_{i_1\dots i_n}$ is an interaction effect of the factors $F_{i_1}, \dots, F_{i_n}$.

Therefore, the matrix $\mathbf{\Phi}_{1\dots r}$ contains linearly independent columns of main effects, interaction effects of the factors $F_1, \dots, F_r$, and **I.**

By Theorem 3.4.1, for the design $\mathbf{D}^f$, the number of degrees of freedom carried by main effects of the factor F_i and interaction effects of the factors $F_{i_1}, \dots, F_{i_n}$ are equal $(s_i - 1)$ and $(s_{i_1} - 1) \dots (s_{i_n} - 1)$ respectively. Therefore, each of the matrices $\mathbf{F}_i^f$ and $\mathbf{F}_i$ contains $s_i - 1$ independent columns; each of the matrix $\mathbf{F}_{i_1 \dots i_n}^f$ and $\mathbf{F}_{i_1 \dots i_n}$ contains $(s_{i_1} - 1) \dots (s_{i_n} - 1)$ independent columns. The number of linearly independent columns in $\mathbf{F}_i$ equals $s_i - 1$, therefore $\mathbf{F}_i$ contains a maximum set of linearly independent main effects of the factor F_i for the design $\mathbf{D}$.

Suppose that $\mathbf{I}$ and columns of the matrices $\mathbf{F}_1, \dots, \mathbf{F}_r$ constitute a set of linearly independent vectors. Since a nontrivial linear combination of independent main effects of the factors F_i is a main effect of the factor F_i, there exists a nontrivial linear combination of the vectors $\mathbf{I}, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_r$ that equals zero (where $\boldsymbol{\xi}_i$ are vectors of main effects). On the other hand, $\boldsymbol{\xi}_i$ can be expressed as nontrivial linear combinations of the columns of the matrix $\mathbf{F}_i$. It follows that there exists a nontrivial linear combination of $\mathbf{I}$ and columns of matrices $\mathbf{F}_1, \dots, \mathbf{F}_r$ that equals zero, which is a contradiction. Therefore, $\mathbf{I}$ and all columns of matrices $\mathbf{F}_1, \dots, \mathbf{F}_r$ are linearly independent. By using simple algebraic operations, we can get that the number of degrees of freedom carried by interaction effects of the factors F_i and F_j equals $(s_i - 1)(s_j - 1)$. Therefore, any matrix of interaction effects of first order in $\boldsymbol{\Phi}_{1 \dots r}$ contains a maximum set of linear independent interaction effects of first order.

By using the same type of argument, we can get the following. If any of matrices of linearly independent interaction effects of order $(n - 1)$ in $\boldsymbol{\Phi}_{1 \dots r}$ contains a maximum set of vectors, then any of matrices of linearly independent interaction effects of order n in $\boldsymbol{\Phi}_{1 \dots r}$ contains a maximum set of vectors.

This completes the proof of Theorem 3.6.1.

Consider the matrix $\boldsymbol{\Phi}_i^{f\mathbf{D}} = \|\mathbf{I},\ \mathbf{F}_i^{f\mathbf{D}}\|$ and the matrix $\mathbf{G}_i$ (3.2.2). It is evident that these matrices are related by a linear nonsingular transformation. It follows that the matrices $\boldsymbol{\Phi}_{1 \dots r}^{f\mathbf{D}} = \|\mathbf{I},\ \mathbf{F}_1^{f\mathbf{D}}\| \otimes \dots \otimes \|\mathbf{I},\ \mathbf{F}_r^{f\mathbf{D}}\|$ and $\mathbf{G}_{1 \dots r} = \mathbf{G}_1 \otimes \dots \otimes \mathbf{G}_r$ are related by a linear nonsingular transformation as well. Therefore, we get a simple corollary.

Corollary to Theorem 3.6.1. If the condition (3.6.1) is satisfied, then $\mathbf{G}_{1 \dots r}$ is a matrix of full rank; coefficient matrices $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ of the design $\mathbf{D}$ for any two A^{Ω}-models are related by nonsingular linear transformation.

When considering r-factorial interaction effects, we will assume that the condition (3.6.1) is satisfied.

When considering a factorial set Ω as a set of factors and their subsets in accordance with Definition 3.2.2, we will also consider a factorial set Ω as a set of main effects and interaction effects in accordance with the following definition.

Definition 3.6.1. A set of main effects and interaction effects of the factors $F_1, \dots, F_m$ is called a factorial set Ω if the following condition holds. If interaction effect of the factors $F_{n_1}, \dots, F_{n_r}$ belongs to the set Ω, full set of interaction effects of factors $F_{l_1}, \dots, F_{l_v}$ belong to the set Ω for all $v = 1, \dots, r$ and $l_1, \dots, l_v = n_1, \dots, n_r, \quad l_1 \neq \ \dots \ \neq l_v$.

Definition 3.2.2 is consistent with Definition 3.6.1, because of obvious one-to-one correspondence between subsets of factors and subsets of main effects and interaction effects of these factors.

§ 7. The Condition of Proportional Frequencies

This paragraph is devoted to the fundamental concept introduced by R.L. Plackett [3] – the condition of proportional frequency.

Let the l-th level of the factor F_i occurs ω_i^l times and the n-th level of the factor F_j occurs ω_j^n times in the design **D**. Let the l-th level of the factor F_i occurs ω_{ij}^{ln} times with the n-th level of the factor F_j. Consider the $(s_i \times s_j)$-matrix $\mathbf{W} = \{\omega_{ij}^{ln}\}$. It is evident that

$$\mathbf{W}_i = \left\| \begin{array}{c} w_i^0 \\ w_i^1 \\ \vdots \\ w_i^{s_i-1} \end{array} \right\| = \mathbf{WI}, \quad \mathbf{W}_j = \left\| \begin{array}{c} w_j^0 \\ w_j^1 \\ \vdots \\ w_j^{s_j-1} \end{array} \right\| = \mathbf{W}^T\mathbf{I}.$$

Consider the N-dimensional vector **S** and the $(N \text{ x } s_1 \dots s_r)$-matrix $\mathbf{\Phi}_{1\dots r}$. Matrix $\mathbf{\Phi}_{1\dots r}$ has N rows including $s_1 \dots s_r$ different rows (corresponding different combinations of levels of the factors $F_1, \dots, F_r$) and $s_1 \dots s_r$ columns that are linearly independent.

For each subset of the identical rows of $\mathbf{\Phi}_{1\dots r}$, select only one. For the corresponding elements of vector **S**, calculate their average. Denote the resulting matrix and the column by $\overline{\mathbf{\Phi}}_{1\dots r}$ and $\overline{\mathbf{S}}$ respectively.

Any column of main effect is orthogonal to the unit vector. Hence,

$$\overline{\mathbf{\Phi}}_i^T \mathbf{W}_i = \left\| \begin{array}{c} N \\ 0 \\ \vdots \\ 0 \end{array} \right\| = \mathbf{\Delta}_i,$$

or

$$\mathbf{W}_i = \bar{\mathbf{\Phi}}_i^{T-1}\mathbf{\Delta}_i. \tag{3.7.1}$$

Analogically,

$$\mathbf{W}_j = \bar{\mathbf{\Phi}}_j^{T-1}\mathbf{\Delta}_j. \tag{3.7.2}$$

Theorem 3.7.1 [3]. If

$$\mathbf{F}_i^T\mathbf{F}_j = 0, \tag{3.7.3}$$

then

$$N\mathbf{W} = \mathbf{W}_i\mathbf{W}_j^T.$$

P r o o f. Rewrite (3.7.3) as follows:

$$\bar{\mathbf{\Phi}}_i^T\mathbf{W}\bar{\mathbf{\Phi}}_j = \begin{Vmatrix} N & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{Vmatrix} = \frac{1}{N}\mathbf{\Delta}_i\mathbf{\Delta}_j^T.$$

Then, by (3.7.1) and (3.7.2),

$$N\mathbf{W} = \bar{\mathbf{\Phi}}_i^{T-1}\mathbf{\Delta}_i\mathbf{\Delta}_j\bar{\mathbf{\Phi}}_j^{-1} = \mathbf{W}_i\mathbf{W}_j^T.$$

This proves the theorem.

Therefore, Theorem 3.7.1 presents a necessary condition of pairwise orthogonality of vectors of main effects (one from each factor). This condition – the condition of proportional frequencies – states that the levels of one factor occur with each of the levels of other factor with proportional frequencies.

Definition 3.7.1. Let $w_{i_1 \dots i_t}^{j_1 \dots j_t}$ be the number of the appearances of the combination of levels $j_1, \dots, j_t$ of the factors $F_{i_1}, \dots, F_{i_t}$ respectively in the design **D**. Then the set of requirements

$$N^{t-1}w_{i_1 \dots i_t}^{j_1 \dots j_t} = w_{i_1}^{j_1} \dots w_{i_t}^{j_t} \quad (\text{for any } j_1, \dots, j_t) \tag{3.7.4}$$

is called the condition of proportional frequencies for the factors $F_{i_1}, \dots, F_{i_t}$.

Definition 3.7.2. The condition of proportional frequencies (3.7.4) is said to be satisfied for a factorial set Ω if (3.7.4) is satisfied for each group of factors of any two elements of the set Ω.

Let the design includes all level combinations of the factors F_i and F_j. Then the number of independent first-order interaction effects of these factors will be determined by (3.4.6). In this and only this case, the matrix $\bar{\bar{\mathbf{\Phi}}}_{ij}$ will be square. Assume that the condition

$$\mathbf{\Phi}_{ij}^T \mathbf{F}_n = 0$$

is satisfied for the factor F_n. As in the proof of Theorem 3.7.1, we get that the levels of the factor F_n occur with each combination of the levels of the factors F_i and F_j with proportional frequencies:

$$N w_{nij}^{k_n k_i k_j} = w_n^{k_n} w_{ij}^{k_i k_j}.$$

If the condition (3.7.3) is satisfied for the factors F_i and F_j, then, by Theorem 3.7.1,

$$N w_{ij}^{k_i k_j} = w_i^{k_i} w_j^{k_j}.$$

Therefore

$$N^2 w_{nij}^{k_n k_i k_j} = w_n^{k_n} w_i^{k_i} w_j^{k_j}.$$

A similar conclusion can be made for any number of factors. For this purpose, we will consider the following partitioning of a set of the factors $F_1, \dots, F_r$. The first partition splits the factors $F_1, \dots, F_r$ into two sets. The second partition splits each of the sets of the first partition (if it contains more than one factor) into two subsets. And so on. The resulting partition of the factors is called a full partition if each subset of the last partition contains only one factor.

Theorem 3.7.2. Suppose that for t factors $F_1, \dots, F_t$, there exists a full partition such that the following condition holds. Any subset of the l-th partition is split by the $(l+1)$-th partition into two subsets $F_{i_1}, \dots, F_{i_p}$ and $F_{i_{p+1}}, \dots, F_{i_q}$ such that

$$\mathbf{\Phi}_{i_1 \dots i_p}^T \mathbf{\Phi}_{i_{p+1} \dots i_q} = \begin{Vmatrix} N^2 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{Vmatrix}.$$

Then

a) the combinations of the levels of the factors $F_{i_1}, \dots, F_{i_p}$ occur with each combination of the levels of the factors $F_{i_{p+1}}, \dots, F_{i_q}$ with proportional frequencies;

b) the condition of proportional frequencies is satisfied for the factors $F_1, \dots, F_t$.

Now we are going to prove a sufficiency of the condition (3.7.4) for pairwise orthogonality of main effects and interaction effects (one from each matrix of effects). The proof will follow from the following lemma.

Lemma 3.7.1. Suppose that for the factors $F_1, \dots, F_t$ and the column **S**,

$$\mathbf{S}^T \boldsymbol{\Phi}_{1\dots r} = \mathbf{0}.$$

Then the sum of the elements of **S** corresponding to any combination of the levels of the factors $F_1, \dots, F_t$ equals zero.

P r o o f. $\mathrm{Rg}(\overline{\boldsymbol{\Phi}}_{1\dots r}) = \mathrm{Rg}(\boldsymbol{\Phi}_{1\dots r})$, and, by Theorem 3.6.1, $\overline{\boldsymbol{\Phi}}_{1\dots r}$ is a square nonsingular matrix. $\overline{\mathbf{S}}$ is orthogonal to all columns of the matrix $\overline{\boldsymbol{\Phi}}_{1\dots r}$. Hence, all elements of **S** equal zero, which was to be proved.

It follows from Lemma 3.7.1 that orthogonality of the interaction effect $\boldsymbol{\xi}_{1\dots r+1}$ r-th order of the factors $F_1, \dots, F_{r+1}$ to all interaction effects n-th $(n < r)$ order of these factors implies that the sum of elements of $\boldsymbol{\xi}_{1\dots r+1}$ corresponding to any combination of the levels of any n factors of the factors $F_1, \dots, F_{r+1}$ are equal to zero.

Theorem 3.7.3. If the condition of proportional frequencies (3.7.4) is satisfied for t factors, all main effects and interaction effects of these factors (one from each set of effects) are pairwise orthogonal.

P r o o f. Let P and R are two arbitrary subsets (of p and r factors respectively) of the set of t factors such that the condition of proportional frequencies (3.7.4) is satisfied. Summing up both parts of (3.7.4) for all levels of certain factors, we get that the condition of proportional frequencies (3.7.4) is satisfied for any subset of the factors of the given set of t factors. In particular, the condition of proportional frequencies is satisfied for the set of factors belonging to the union $T = P \cup R$. Denote by $\boldsymbol{\xi}_P$ and $\boldsymbol{\xi}_R$ arbitrary interaction effects (p –1)-th and (r – 1)-th order respectively of the factors belonging to P and R. Consider two cases:

1) the set $Q = P \cap R$ is empty;

2) the set Q is not empty.

C a s e 1 . $\boldsymbol{\xi}_P$ is a contrast, therefore, the sum of its elements equals zero. The condition of proportional frequencies is satisfied for the factors of the set T. Therefore, the combinations of the levels of the factors from the set R occur with each combination of the levels of the factors from the set P with proportional frequencies. The elements of $\boldsymbol{\xi}_P$ are equal for the same combinations of the factors from the set P. Hence, the sum of elements of $\boldsymbol{\xi}_P$ corresponding to any combination of the levels of the factors from R equals zero. Therefore, $\boldsymbol{\xi}_P$ and $\boldsymbol{\xi}_R$ are orthogonal.

C a s e 2 . Any effect $\boldsymbol{\xi}_P$, by the definition of interaction effects, orthogonal to any effects of the factors from the set Q. By Lemma 3.7.1, for the part $\boldsymbol{D}_Q$ of the design corresponding to any combination of the levels of the factors from Q, the sum of elements of $\boldsymbol{\xi}_P$ equals zero. The combinations of the levels of the factors from the set P occur with each combination of the levels of the factors from the set $R \setminus Q$ with proportional frequencies. In particular, the same is true for the combinations of the levels of the factors from P for the part $\mathbf{D}_Q$ of the design. Hence, the sum of elements of $\boldsymbol{\xi}_P$ equals zero for any combination of the levels of the factors from R. Therefore, $\boldsymbol{\xi}_P$ is orthogonal to $\boldsymbol{\xi}_R$.

This completes the proof of the theorem.

It is evident that for any matrix of effects, all effects can be selected pairwise orthogonal. In this case if the condition of proportional frequencies is satisfied for any t factors of the design, all main effects and interaction effects up to order $t-1$ are pairwise orthogonal.

§ 8. Construction of Interaction Effects

Theorem 3.8.1. For any t factors $F_1, \dots, F_t$ for which the condition of proportional frequencies is satisfied, the product $\mathbf{S}_1 \otimes \dots \otimes \mathbf{S}_t$ of the vectors $\mathbf{S}_1, \dots, \mathbf{S}_t$ of main effects of the factors $F_1, \dots, F_t$ respectively is a vector $\mathbf{S}_{1\dots t}$ of interaction effects of the factors $F_1, \dots, F_t$.

Proof. It is evident that elements of $\mathbf{S}_{1\dots t}$ depend only on the combinations of the levels of the factors $F_1, \dots, F_t$. Hence, we need only to prove that $\mathbf{S}_{1\dots t}$ is orthogonal to $\mathbf{I}$ and any main effects and interaction effects up to order $t-2$ of the factors $F_1, \dots, F_t$.

For two factors F_1 and F_2, orthogonality of $\mathbf{S}_1 \otimes \mathbf{S}_2$ and $\mathbf{S}'_1$ ($\mathbf{S}'_1$ is any vector of main effects of the factor F_1, perhaps, identical to $\mathbf{S}_1$) is equivalent to orthogonality $\mathbf{S}_1 \otimes \mathbf{S}'_1$ and $\mathbf{S}_2$. By the term of the theorem, $\mathbf{S}_2$ is orthogonal to all vectors of main effects of the factor F_1. Therefore, by Lemma 3.7.1, the sum of the elements of $\mathbf{S}_2$ corresponding to any level of the factor F_1 equals zero. Since $\mathbf{S}_1 \otimes \mathbf{S}'_1$ has equal elements for the same levels of the factors F_1, $\mathbf{S}_1 \otimes \mathbf{S}'_1$ is orthogonal to $\mathbf{S}_2$.

Continue the proof by induction. On the $(n-1)$-th step $(n \le t)$, we get the column $\mathbf{S}_1 \otimes \mathbf{S}_2 \otimes \dots \otimes \mathbf{S}_n$. Its orthogonality to any columns $\mathbf{S}_{1\dots l}$ $(i \le n-1)$ of main effects and interaction effects up to order $(l-1)$ is equivalent to orthogonality of two columns $\mathbf{S}_1 \otimes \dots \otimes \mathbf{S}_l \otimes \mathbf{S}_{1\dots l}$ and $\mathbf{S}_{l+1} \otimes \dots \otimes \mathbf{S}_n$. By the induction hypothesis, $\mathbf{S}_{l+1} \otimes \dots \otimes \mathbf{S}_n$ is interaction effect $(n-l-1)$-th order and, therefore, orthogonal to all main effects and interaction effects of the factors $F_1, \dots, F_l$. Hence, by

Lemma 3.7.1, the sum of elements of $\mathbf{S}_{l+1} \otimes \ldots \otimes \mathbf{S}_n$ corresponding to any combination of the levels of the factors $F_1, \ldots, F_l$ equals zero.

Thus, the proof is complete.

Theorem 3.8.2. Suppose that the condition of proportional frequencies (3.7.4) is satisfied for given set of the factors $F_1, \ldots, F_t$. Let all matrices of main effects contain pairwise orthogonal columns. Then all possible products of the columns $\mathbf{S}_1, \ldots, \mathbf{S}_t$ (one for each factor) produce the full set of $(s_1 - 1) \times \ldots \times (s_t - 1)$ pairwise orthogonal interaction effects of the factors $F_1, \ldots, F_t$.

P r o o f. Consider two different products of the columns (one for each factor): $\mathbf{S}_1 \otimes \ldots \otimes \mathbf{S}_t$ and $\mathbf{S'}_1 \otimes \ldots \otimes \mathbf{S'}_t$. For these two sets of columns, at least one pair (let it be $\mathbf{S}_1$ and $\mathbf{S'}_1$) contains different columns. The elements of the column $\mathbf{S}_2 \otimes \ldots \otimes \mathbf{S}_t \otimes \mathbf{S'}_2 \otimes \ldots \otimes \mathbf{S'}_t$ depend only on the levels of the factors $F_2, \ldots, F_t$. Now we have to prove that the sum of the elements $\mathbf{S}_1 \otimes \mathbf{S'}_1$ for any combination of the levels of the factors $F_2, \ldots, F_t$ equals zero. Indeed, by Theorem 3.7.2, for any combination of the levels of the factors $F_2, \ldots, F_t$, the levels of F_1 occur with proportional frequencies. Hence, for all combinations of the levels of the factors $F_2, \ldots, F_t$, the sums of the elements of $\mathbf{S}_1 \otimes \mathbf{S'}_1$ have the same sign. By the term of the theorem, $\mathbf{S}_1$ and $\mathbf{S'}_1$ are orthogonal. Hence, these sums equal zero.

Thus, the proof is complete.

Theorem 3.8.2 can be generalized for the case of matrices of main effects that not necessarily contain orthogonal columns.

Theorem 3.8.3. Suppose that the condition of proportional frequencies (3.7.4) is satisfied for given set of the factors $F_1, \ldots, F_t$. Then all possible products of the columns $\mathbf{S}_1, \ldots, \mathbf{S}_t$ (one for each factor) produce the full set of $(s_1 - 1) \times \ldots \times (s_t - 1)$ linearly independent interaction effects of the factors $F_1, \ldots, F_t$.

The proof of the theorem is similar to the proof of the corresponding part of Theorem 3.4.1.

§ 9. Effects of Levels and Interaction Effects of Levels

For the sake of simplicity, without loss of generality, consider a design with three factors.

Let $\eta_{ijn} = Ey_{ijn}$, where y_{ijn} is an observation that corresponds to the point of a full design $\mathbf{D}^f$ with the i-th level of the factor F_1, the j-th level of the factor F_2, and the n-th level of the factor F_3. An asterisk instead of an index means that we take the average over all levels of the corresponding factor. For example,

$$\eta_{*jn} = \frac{1}{s_1}\sum_{i=0}^{s_1-1} \eta_{ijn}.$$

Definition 3.9.1. The number $\beta_0 = \eta_{***}$ is called a true average; the number $\beta_1^i = \eta_{i**} - \eta_{***}$ is called an effect of the i-th level of the factor F_1.

Definition 3.9.2. The difference between the effect of the i-th level of the factor F_1 for a subset with the j-th level of the factor F_2 and the effect of the i-th level of the factor F_1 is called an interaction effect of the i-th level of the factor F_1 and the j-th level of the factor F_2 and denoted by β_{12}^{ij}.

Definition 3.9.3. The difference between the interaction effect of the i-th level of the factor F_1 and the j-th level of the factor F_2 for a subset with the n-th level of the factor F_3 and the interaction effect of the i-th level of the factor F_1 and the j-th level of the factor F_2 is called an interaction effect of the i-th level of the factor F_1, the j-th level of the factor F_2 , and the n-th level of the factor F_3 and denoted by β_{123}^{ijn}.

It is evident that definitions 3.9.2 and 3.9.3 are correct, since they are symmetrical for the factors F_1, F_2, and F_3. For example, for the design with three factors,

$$\begin{aligned}\beta_{123}^{ijn} &= (\eta_{ijn} - \eta_{*jn} - \eta_{i*n} + \eta_{**n}) \\ &-(\eta_{ij*} - \eta_{*j*} - \eta_{i**} + \eta_{***}) \\ &= \eta_{ijn} - \eta_{ij*} - \eta_{i*n} - \eta_{*jn} + \eta_{i**} + \eta_{*j*} + \eta_{**n} - \eta_{***}.\end{aligned} \tag{3.9.1}$$

Other effects of levels and interaction effects of levels are defined analogously.

Any effect of the level or any interaction effect of the levels is a linear combination of the mathematical expectations of observations for $\mathbf{D}^f$. The coefficients of such linear combinations form the vectors that we will call vectors of effects of levels and vectors of interaction effects of levels. Denote by $\boldsymbol{\psi}_1^{(i)}$ the vector of the effect of the i-th level of the factor F_1 and denote by $\boldsymbol{\psi}_{12}^{ij}$ the vector of the interaction effect of the i-th level of the factor F_1 and the j-th level of the factor F_2, etc.

In (3.9.1), coefficient for the treatment combination with the levels i, j, and n of the factors F_1, F_2, and F_3 respectively is $1/N\,(s_1s_2s_3 - s_1s_2 - s_1s_3 - s_2s_3 + s_1 + s_2 + s_3 - 1) = 1/N\,(s_1 - 1)(s_2 - 1)(s_3 - 1)$.

Coefficient for the treatment combination in which the factors F_1 and F_2 appear at the levels i and j respectively and the factor F_3 appears at the level other than *n,* equals $1/N\,(-s_1s_2+s_1+s_2-1)=-(1/N)(s_1-1)(s_2-1)$.

Coefficient for the treatment combination in which the factor F_1 appears at the level i and the factors F_2 and F_3 appear at the levels other than j and n respectively, equals $1/N\,(s_1-1)$.

Coefficient for the treatment combination in which the factors F_1, F_2, and F_3 appear at the levels other than *i, j,* and *n* respectively equals -1.

The summary for all elements of the vector of the interaction effects of the levels *i*, *j*, and *n* is given in Table 2.

Table 2
Vector of Interaction Effect of Levels *i*, *j*, and *n*

F_1	F_2	F_3	Elements of Vector of Interaction Effect of Levels *i*, *j*, and *n* of Factors F_1, F_2, and F_3 Respectively
i	j	n	$1/N\,(s_1-1)(s_2-1)(s_3-1)$
i	j		$-1/N\,(s_1-1)(s_2-1)$
i		n	$-1/N\,(s_1-1)(s_3-1)$
	j	n	$-1/N\,(s_2-1)(s_3-1)$
i			$1/N\,(s_1-1)$
	j		$1/N\,(s_2-1)$
		n	$1/N\,(s_3-1)$
			$-1/N$

Each of rows of Table 2 corresponds to a set of treatments. If, for example, the factor F_1 appears at the level i in the set, the corresponding cell of the table has index *i*. If the factor F_1 appears at the level other than *i*, the corresponding cell is left empty. The table cells for the factors F_2 and F_3 are filled analogously.

Let

$$\Delta_{i\,j\,*}^{+-}=\begin{cases}1 & \text{if for the } u\text{-th obsevation, the factor } F_1 \text{ appears} \\ & \text{at the level } i \text{ and the factor } F_2 \text{ appears at the level} \\ & \text{other than } j, \\ 0 & \text{otherwise.}\end{cases}$$

We will also use the similar notations in the similar cases.

The element of the vector of the interaction effect of the levels i, j, and n for the u-th obsevation is

$$\psi_{123}^{ijn}(u) = \frac{1}{N}\{\Delta_{i\,j\,n}^{+++}(s_1-1)(s_2-1)(s_3-1)$$
$$-\Delta_{i\,j\,n}^{++-}(s_1-1)(s_2-1)$$
$$-\Delta_{i\,j\,n}^{+-+}(s_1-1)(s_3-1)$$
$$-\Delta_{i\,j\,n}^{-++}(s_2-1)(s_3-1)$$
$$+\Delta_{i\,j\,n}^{+--}(s_1-1)+\Delta_{i\,j\,n}^{-+-}(s_2-1)+\Delta_{i\,j\,n}^{--+}(s_3-1)-\Delta_{i\,j\,n}^{---}\} =$$
$$= \frac{1}{N}\{\Delta_{i**}^{+}(s_1-1)-\Delta_{i**}^{-}\}\{\Delta_{*j*}^{+}(s_2-1)-\Delta_{*j*}^{-}\}\{\Delta_{**n}^{+}(s_3-1)-\Delta_{**n}^{-}\}.$$

We can easily prove it if we take into account the following equalities:

$$\Delta_{i**}^{+}\Delta_{*j*}^{+}\Delta_{**n}^{+} = \Delta_{i\,j\,n}^{+++}; \quad \Delta_{i**}^{+}\Delta_{*j*}^{+}\Delta_{**n}^{-} = \Delta_{i\,j\,n}^{++-};$$
$$\Delta_{i**}^{+}\Delta_{*j*}^{-}\Delta_{**n}^{-} = \Delta_{i\,j\,n}^{+--}; \quad \Delta_{i**}^{-}\Delta_{*j*}^{-}\Delta_{**n}^{-} = \Delta_{i\,j\,n}^{---}.$$

Analogously, in the general case, the element of the vector $\boldsymbol{\psi}_{1\dots r}^{i_1\dots i_r}$ of the interaction effect of the levels i_j $(j = 1, \dots, r)$ of the factors $F_1, \dots, F_r$ is

$$\psi_{1\dots r}^{i_1\dots i_r}(u) = \frac{1}{N}\left\{\Delta_{i_1*\dots*}^{+}(s_1-1)-\Delta_{i_1*\dots*}^{-}\right\} \times \dots$$
$$\times \left\{\Delta_{*\dots*i_r*\dots*}^{+}(s_r-1)-\Delta_{*\dots*i_r*\dots*}^{-}\right\}.$$

In particular, the element of the vector of the effect of the level i of the factor F_1 is

$$\psi_1^{i_1}(u) = \frac{1}{N}\left\{\Delta_{i_1*\dots*}^{+}(s_1-1)-\Delta_{i_1*\dots*}^{-}\right\}. \tag{3.9.2}$$

Hence,

$$N\psi_{1\dots r}^{i_1\dots i_r}(u) = N\psi_1^{i_1}(u)\dots N\psi_r^{i_r}(u),$$

or

$$N\boldsymbol{\psi}_{1\dots r}^{i_1\dots i_r} = N\boldsymbol{\psi}_1^{i_1} \otimes \dots \otimes N\boldsymbol{\psi}_r^{i_r}. \tag{3.9.3}$$

Therefore, the following theorem has been proved.

Theorem 3.9.1. The vector of the interaction effect of the levels $i_1, \dots, i_r$ of the factors $F_1, \dots, F_r$ respectively is, apart from a proportionality factor, the product of the vectors of the effects of the levels $i_1, \dots, i_r$ of the factors $F_1, \dots, F_r$ respectively.

It is evident that $\boldsymbol{\psi}_1^{i_1}, \dots, \boldsymbol{\psi}_r^{i_r}$ are the vectors of main effects of the factors $F_1, \dots, F_r$ respectively. Hence, the vector of the interaction effect of levels $\boldsymbol{\psi}_{1\dots r}^{i_1\dots i_r}$, by Note 1 to Theorem 3.4.1, is the vector of the interaction effect of the factors $F_1, \dots, F_r$ for the design $\mathbf{D}^f$.

It is easy to verify that any $i-1$ vectors of all vectors of main effects of the factor F_1, with the elements $\Delta^{+}_{i_{*\dots *}}(s_1-1)-\Delta^{-}_{i_{*\dots *}}$ $(i=0,1,\dots,s_1-1)$, form the set of linearly independent vectors. A similar statement holds for the factors $F_2,\dots,F_r$. All possible products of the selected independent main effects (one from each factor) form $(s_1-1)\dots(s_r-1)$ interaction effects of levels of the factors $F_1,\dots,F_r$. By Note 1 to Theorem 3.4.1, these $(s_1-1)\dots(s_r-1)$ interaction effects of levels form a set of linearly independent vectors. Therefore, the following theorem has been proved.

Theorem 3.9.2. Any vector of the interaction effect of levels of the factors $F_1,\dots,F_r$ is a vector of an interaction effect of the factors $F_1,\dots,F_r$. Maximum linearly independent subset of vectors of interaction effects of levels of the factors $F_1,\dots,F_r$ contains exactly $(s_1-1)\dots(s_r-1)$ vectors.

§ 10. A Model of True Effects for Qualitative Factors

Denote the matrix of all vectors of effects of levels of the factor F_i by $\boldsymbol{\psi}_i=\left\|\boldsymbol{\psi}_i^0,\boldsymbol{\psi}_i^1,\ \dots,\ \boldsymbol{\psi}_i^{s_i-1}\right\|$, denote the matrix of all interaction effects of levels of the factors F_i and F_j by $\boldsymbol{\psi}_{ij}$, etc.

Then, by (3.9.3), the following equality holds:

$$N\boldsymbol{\psi}_{i_1\dots i_r}=N\boldsymbol{\psi}_{i_1}\otimes\dots\otimes N\boldsymbol{\psi}_{i_r}.$$

Denote

$$\boldsymbol{\Psi}_{1\dots m}=\left\|\frac{1}{N}\mathbf{I},\boldsymbol{\psi}_1,\dots,\boldsymbol{\psi}_m,\boldsymbol{\psi}_{12},\dots,\boldsymbol{\psi}_{1\dots m}\right\|.$$

Let

$$x_i^{(j)}(u)=\begin{cases}1 & \text{if the factor } F_i \text{ appears at the level } j \\ & \text{ in the } u\text{-th observation,}\\ 0 & \text{otherwise.}\end{cases}\qquad(3.10.1)$$

We will use also the following notations:

$$\begin{aligned}&\mathbf{x}_i^{jT}=\left(x_i^{(j)}(1),\dots,x_i^{(j)}(N)\right),\mathbf{x}_i=\left\|\mathbf{x}_i^0,\dots,\mathbf{x}_i^{s_i-1}\right\|,\\&\mathbf{x}_{i_1\dots i_r}=\mathbf{x}_{i_1}\otimes\dots\otimes\mathbf{x}_{i_r},\\&\mathbf{X}_{1\dots m}=\|\mathbf{I},\mathbf{x}_1,\dots,\mathbf{x}_m,\mathbf{x}_{12},\dots,\mathbf{x}_{1\dots m}\|.\end{aligned}\qquad(3.10.2)$$

Theorem 3.10.1.

$$\mathbf{X}_{1\dots m}\boldsymbol{\Psi}^T_{1\dots m}=\mathbf{E}_N.\qquad(3.10.3)$$

P r o o f. For the sake of simplicity, without loss of generality, consider a design with three factors.

In the matrix $\mathbf{X}_{123}$, consider the row corresponding to the i-, j-, and n-th levels of the factors F_1, F_2, and F_3 respectively. In the matrix $\mathbf{\Psi}_{123}$, consider the row corresponding to some combination of levels of the factors F_1, F_2, and F_3. Then a scalar square of these two rows of the matrices $\mathbf{X}_{123}$ and $\mathbf{\Psi}_{123}$ equals

$$\begin{aligned}
&\tfrac{1}{N}\{1 + [\Delta^{+}_{i**}(s_1 - 1) - \Delta^{-}_{i**}] + [\Delta^{+}_{*j*}(s_2 - 1) - \Delta^{-}_{*j*}] \\
&+[\Delta^{+}_{**n}(s_3 - 1) - \Delta^{-}_{**n}] \\
&+[\Delta^{+}_{i**}(s_1 - 1) - \Delta^{-}_{i**}]\,[\Delta^{+}_{*j*}(s_2 - 1) - \Delta^{-}_{*j*}] \\
&+[\Delta^{+}_{i**}(s_1 - 1) - \Delta^{-}_{i**}]\,[\Delta^{+}_{**n}(s_3 - 1) - \Delta^{-}_{**n}] \\
&+[\Delta^{+}_{*j*}(s_2 - 1) - \Delta^{-}_{*j*}]\,[\Delta^{+}_{**n}(s_3 - 1) - \Delta^{-}_{**n}] \\
&+[\Delta^{+}_{i**}(s_1 - 1) - \Delta^{-}_{i**}]\,[\Delta^{+}_{*j*}(s_2 - 1) - \Delta^{-}_{*j*}][\Delta^{+}_{**n}(s_3 - 1) - \Delta^{-}_{**n}]\}.
\end{aligned} \tag{3.10.4}$$

If the given row of $\mathbf{\Psi}_{123}$ corresponds to the levels i, j, and n of the factor F_1, F_2, and F_3 respectively, then

$$\Delta^{+}_{i**} = \Delta^{+}_{*j*} = \Delta^{+}_{**n} = 1, \quad \Delta^{-}_{i**} = \Delta^{-}_{*j*} = \Delta^{-}_{**n} = 0,$$

Therefore, (3.10.4) becomes

$$\begin{aligned}
&\tfrac{1}{N}\{1 + (s_1 - 1) + (s_2 - 1) + (s_3 - 1) + \\
&+(s_1 - 1)(s_2 - 1) + (s_1 - 1)(s_3 - 1) + (s_2 - 1)(s_3 - 1) + \\
&+(s_1 - 1)(s_2 - 1)(s_3 - 1)\} = \tfrac{1}{N} = s_1 s_2 s_3 = 1.
\end{aligned}$$

Hence, it has been proved that the diagonal elements of $\mathbf{X}_{123}\mathbf{\Psi}^{T}_{123}$ are equal to 1.

Assume that in the given row of $\mathbf{\Psi}_{123}$, at least one of the factors F_1, F_2, and F_3 appears at the level other than i, j, and n respectively. Without loss of generality, assume that the factor F_3 appears at the level other than n. Then (3.10.4) becomes

$$A + A[\Delta^{+}_{**n}(s_3 - 1) - \Delta^{-}_{**n}] = 0,$$

where

$$\begin{aligned}
A = {} & 1 + [\Delta^{+}_{i**}(s_1 - 1) - \Delta^{-}_{i**}] + [\Delta^{+}_{*j*}(s_2 - 1) - \Delta^{-}_{*j*}] \\
&+[\Delta^{+}_{i**}(s_1 - 1) - \Delta^{-}_{i**}]\,[\Delta^{+}_{*j*}(s_2 - 1) - \Delta^{-}_{*j*}].
\end{aligned}$$

This proves the theorem.

Now we will define the vector $\mathfrak{B}$ of true effects for qualitative factors:

$$\mathfrak{B} = \boldsymbol{\Psi}_{1\ldots m}^{T} \boldsymbol{\eta}^{f}, \tag{3.10.5}$$

where $\boldsymbol{\eta}^{f}$, as before, is the vector of mathematical expectations at the points of full design. By (3.10.3) and (3.10.5), the following equality holds:

$$\boldsymbol{\eta}^{f} = \mathbf{X}_{1\ldots m} \mathfrak{B}. \tag{3.10.6}$$

We can consider (3.10.6) as a model, that is true for all points of $\mathbf{D}^{f}$.

Denote by $\mathbf{X}^{\Omega}$ and $\mathfrak{B}^{\Omega}$ the parts of the matrix $\mathbf{X}_{1\ldots m}$ and the vector $\mathfrak{B}$ respectively corresponding to the factorial set Ω. Assume that the elements of the vector $\mathfrak{B}$ that do not correspond to the factorial set Ω are equal to zero. Then (3.10.6) becomes

$$\boldsymbol{\eta}^{f} = \mathbf{X}^{\Omega} \mathfrak{B}^{\Omega}. \tag{3.10.7}$$

The coefficients of the model (3.10.6) and, therefore, the model (3.10.7) are easy to interpret. This interpretation becomes evident if we recall the definition of the effects of levels and interaction effects of levels.

Example 3.10.1. Let

$$\mathbf{D} = \begin{array}{c} \begin{array}{cc} F_1 & F_2 \end{array} \\ \left\| \begin{array}{cc} 0 & 0 \\ 1 & 0 \\ 1 & 1 \\ 2 & 1 \\ 0 & 2 \\ 2 & 2 \end{array} \right\| \end{array}; \quad \mathbf{Ey} = \boldsymbol{\eta} = \left\| \begin{array}{c} \eta_1 \\ \eta_2 \\ \eta_5 \\ \eta_6 \\ \eta_7 \\ \eta_9 \end{array} \right\|.$$

In this case, the full design and the corresponding vector of mathematical expectations of the observations will be as follows:

$$\mathbf{D}^{f} = \left\| \begin{array}{cc} 0 & 0 \\ 1 & 0 \\ 2 & 0 \\ 0 & 1 \\ 1 & 1 \\ 2 & 1 \\ 0 & 2 \\ 1 & 2 \\ 2 & 2 \end{array} \right\|; \quad \mathbf{Ey}^{f} = \boldsymbol{\eta}^{f} = \left\| \begin{array}{c} \eta_1 \\ \vdots \\ \eta_9 \end{array} \right\|.$$

The matrix $\boldsymbol{\Psi}_{12}$ for $\mathbf{D}^{f}$ is

$$9\boldsymbol{\Psi}_{12} = \begin{array}{c} \begin{array}{cccc} \mathbf{I} & 9\boldsymbol{\psi}_1 & 9\boldsymbol{\psi}_2 & 9\boldsymbol{\psi}_{12} = 9\boldsymbol{\psi}_1 \otimes 9\boldsymbol{\psi}_2 \end{array} \\ \left\| \begin{array}{c|ccc|ccc|ccccccccc} 1 & 2 & -1 & -1 & 2 & -1 & -1 & 4 & -2 & -2 & -2 & 1 & 1 & -2 & 1 & 1 \\ 1 & -1 & 2 & -1 & 2 & -1 & -1 & -2 & 1 & 1 & 4 & -2 & -2 & -2 & 1 & 1 \\ 1 & -1 & -1 & 2 & 2 & -1 & -1 & -2 & 1 & 1 & -2 & 1 & 1 & 4 & -2 & -2 \\ 1 & 2 & -1 & -1 & -1 & 2 & -1 & -2 & 4 & -2 & 1 & -2 & 1 & 1 & -2 & 1 \\ 1 & -1 & 2 & -1 & -1 & 2 & -1 & 1 & -2 & 1 & -2 & 4 & -2 & 1 & -2 & 1 \\ 1 & -1 & -1 & 2 & -1 & 2 & -1 & 1 & -2 & 1 & 1 & -2 & 1 & -2 & 4 & -2 \\ 1 & 2 & -1 & -1 & -1 & -1 & 2 & -2 & -2 & 4 & 1 & 1 & -2 & 1 & 1 & -2 \\ 1 & -1 & 2 & -1 & -1 & -1 & 2 & 1 & 1 & -2 & -2 & -2 & 4 & 1 & 1 & -2 \\ 1 & -1 & -1 & 2 & -1 & -1 & 2 & 1 & 1 & -2 & 1 & 1 & -2 & -2 & -2 & 4 \end{array} \right\| \end{array}.$$

The vector of true effects is

$$\mathfrak{B} = \left(\beta_0, \beta_1^{(0)}, \beta_1^{(1)}, \beta_1^{(2)}, \beta_2^{(0)}, \beta_2^{(1)}, \beta_2^{(2)}, \beta_{12}^{(00)}, \beta_{12}^{(01)}, \beta_{12}^{(02)},\right.$$
$$\left.\beta_{12}^{(10)}, \beta_{12}^{(11)}, \beta_{12}^{(12)}, \beta_{12}^{(20)}, \beta_{12}^{(21)}, \beta_{12}^{(22)}\right) = \boldsymbol{\Psi}_{12}^T \boldsymbol{\eta}^f.$$

Then, by (3.10.6), the following model will be true at the points of $\mathbf{D}^f$:

$$\eta = \mathbf{X}_{12}\mathfrak{B},$$

where, by (3.10.2),

$$\mathbf{D}^f = \begin{array}{c} \begin{array}{cc} F_1 & F_2 \end{array} \\ \left\| \begin{array}{cc} 0 & 0 \\ 1 & 0 \\ 2 & 0 \\ 0 & 1 \\ 1 & 1 \\ 2 & 1 \\ 0 & 2 \\ 1 & 2 \\ 2 & 2 \end{array} \right\| \end{array};$$

$$\mathbf{X}_{12} = \begin{array}{c} \begin{array}{cccc} \mathbf{I} & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_{12} = \mathbf{x}_1 \otimes \mathbf{x}_2 \end{array} \\ \left\| \begin{array}{c|ccc|ccc|ccccccccc} 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right\| \end{array}.$$

Assuming that all interaction effects of levels are equal to zero, we get the following model:

$$\boldsymbol{\eta}^f = \beta_0 + \beta_1^{(0)}\mathbf{x}_1^0 + \beta_1^{(1)}\mathbf{x}_1^1 + \beta_1^{(2)}\mathbf{x}_1^2$$

$$+\beta_2^{(0)}\mathbf{x}_2^0 + \beta_2^{(0)}\mathbf{x}_2^1 + \beta_2^{(2)}\mathbf{x}_2^2, \qquad (3.10.8)$$

where the value of $\mathbf{x}_i^j$ at the u-th point of $\mathbf{D}^f$ is $x_i^{(j)}(u)$ calculated by (3.10.1).

The coefficient matrix $\mathbf{X}$ of the design $\mathbf{D}$ for the model (3.10.8) is

$$\mathbf{X} = \begin{array}{c} \begin{array}{ccccccc} \mathbf{I} & \mathbf{x}_1^0 & \mathbf{x}_1^1 & \mathbf{x}_1^2 & \mathbf{x}_2^0 & \mathbf{x}_2^1 & \mathbf{x}_2^2 \end{array} \\ \left\| \begin{array}{ccccccc} 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{array} \right\| \end{array}.$$

The coefficient matrix $\mathbf{X}_{1\dots m}$ for the model (3.10.6) for the full design is not full rank matrix. For example, the sum of the columns belonging to $\mathbf{x}_1$ is $\mathbf{I}$. Therefore, the solution of the normal equations of the method of least squares for the parameters $\mathfrak{B}$ of the model is not unique. However, there exists a system of linear equalities for these parameters

$$\mathbf{H}\mathfrak{B} = 0 \qquad (3.10.9)$$

such that the matrix

$$\left\| \begin{matrix} \mathbf{X}_{1\dots m} \\ \mathbf{H} \end{matrix} \right\| \qquad (3.10.10)$$

has full rank and no row of $\mathbf{H}$ is represented by a linear combination of rows of the matrix $\mathbf{X}_{1\dots m}$. In this case, for the matrix design $\mathbf{X}_{1\dots m}$, i.e., for the full design with the restriction (3.10.9) on the parameters $\mathfrak{B}$, there exists a unique solution for LS estimates of the parameters [4].

Consider the u-th row $\left[\psi_1^{(0)}(u),\ \psi_1^{(1)}(u),\ \dots,\ \psi_1^{(s_1-1)}(u)\right]$ of the matrix $\boldsymbol{\psi}_1$ of the vector of effects of levels of the factor F_1.

$$\textstyle\sum_{n=0}^{s_1-1} \Delta^+_{n*\dots*} = 1, \quad \sum_{n=0}^{s_1-1} \Delta^-_{n*\dots*} = s_1 - 1\,,$$

we get, by (3.9.2), that

$$\textstyle\sum_{n=0}^{s_1-1} \psi_1^{(n)}(u) = \sum_{n=0}^{s_1-1}\{\Delta^+_{n*\dots*}(s_1-1) - \Delta^-_{n*\dots*}\} = 0.$$

Hence, for any factor F_i

$$\boldsymbol{\psi}_i \mathbf{I}_{s_i} = \mathbf{0} \quad (i = 1, \dots, m). \qquad (3.10.11)$$

It follows that

$$\boldsymbol{\psi}_i \otimes \boldsymbol{\psi}_j^{n_j} \mathbf{I}_{s_j} = \mathbf{0},$$

. . . .

$$\boldsymbol{\psi}_1 \otimes \boldsymbol{\psi}_2^{n_2} \otimes \dots \otimes \boldsymbol{\psi}_m^{n_m} \mathbf{I}_{s_1} = \mathbf{0},$$

. . . .

$$\boldsymbol{\psi}_1^{n_1} \otimes \boldsymbol{\psi}_2^{n_2} \otimes \dots \otimes \boldsymbol{\psi}_m \mathbf{I}_{s_m} = \mathbf{0}$$

$$(i, j = 1, \dots, m;\ i \neq j;\ n_l = 0, \dots, s_l - 1).$$

Therefore, by (3.10.11), we get

$$\begin{aligned} &\textstyle\sum_{n_i=0}^{s_i-1} \beta_i^{(n_i)} = 0,\ \sum_{n_i=0}^{s_i-1} \beta_{ij}^{(n_i n_j)} = 0, \dots , \\ &\textstyle\sum_{n_1=0}^{s_1-1} \beta_{12\dots m}^{(n_1 n_2 \dots n_m)} = 0, \dots , \sum_{n_m=0}^{s_m-1} \beta_{12\dots m}^{(n_1 n_2 \dots n_m)} = 0, \\ &i, j = 1,\ \dots, m;\ i \neq j;\ n_l = 0, \dots, s_l - 1. \end{aligned} \tag{3.10.12}$$

Then (3.10.12) becomes

$$\mathbf{H}\mathfrak{B} = \mathbf{0}, \tag{3.10.13}$$

where **H** is the coefficient matrix of (3.10.12).

Split the matrix **H** into submatrices to correspond to the partitions of $\mathbf{X}_{1\dots m}$ and $\boldsymbol{\Psi}_{1\dots m}$:

$$\mathbf{H} = \|\mathbf{H}_0, \mathbf{H}_1, \dots, \mathbf{H}_m, \mathbf{H}_{12}, \dots, \mathbf{H}_{1\dots m}\|.$$

Then for the full design 3^2, for example, the matrix **H** is

$$\mathbf{H} = \begin{array}{c} \begin{array}{cccc} \mathbf{H}_0 & \mathbf{H}_1 & \mathbf{H}_2 & \mathbf{H}_{12} \end{array} \\ \left\| \begin{array}{c|ccc|ccc|ccccccccc} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{array} \right\| \end{array}.$$

Denote the columns of the matrices **H** and $\mathbf{X}_{1\dots m}$ by **h** and **x** respectively, adding the indices corresponding to the indices of $\boldsymbol{\psi}$. The columns of the matrix **H** is $\mathbf{h}_0$, $\mathbf{h}_1^0$, $\mathbf{h}_1^1$, $\mathbf{h}_1^2$, $\mathbf{h}_2^0$, $\mathbf{h}_2^1$, $\mathbf{h}_2^2$, $\mathbf{h}_{12}^{00}$, $\mathbf{h}_{12}^{01}$, $\mathbf{h}_{12}^{02}$, $\mathbf{h}_{12}^{10}$, $\mathbf{h}_{12}^{11}$, $\mathbf{h}_{12}^{12}$, $\mathbf{h}_{12}^{20}$, $\mathbf{h}_{12}^{21}$, $\mathbf{h}_{12}^{22}$.

Lemma 3.10.1. If for the vector $\boldsymbol{\gamma}$

$$\mathbf{H}_{1\dots r}\boldsymbol{\gamma} = \mathbf{0}, \quad \boldsymbol{\gamma}^T\boldsymbol{\gamma} \neq 0, \tag{3.10.14}$$

then $\mathbf{x}_{1\dots r}\boldsymbol{\gamma}$ is the vector of the interaction effect of the factors $F_1, \dots, F_r$ and for any vector of the interaction effect $\boldsymbol{\psi}$ of these factors there exists the vector $\boldsymbol{\gamma}$, such that (3.10.14) holds and $\boldsymbol{\psi} = \mathbf{x}_{1\dots r}\boldsymbol{\gamma}$.

Proof. It is evident that any column of the matrix $\boldsymbol{\psi}_{1\ldots r}$, as any other vector of the interaction effect of the factors $F_1, \ldots, F_r$, can be represented by a linear combination of columns of the matrix $\mathbf{x}_{1\ldots r}$, namely $\mathbf{x}_{1\ldots r}\boldsymbol{\gamma}$.

Let

$$\mathbf{x}_{1\ldots r}\boldsymbol{\gamma} = \sum_{i_1=0}^{s_1-1} \sum_{i_r=0}^{s_r-1} \mathbf{x}_{1\ldots r}^{i_1\ldots i_r} \gamma_{1\ldots r}^{(i_1\ldots i_r)}.$$

By the definition of a vector of an interaction effect, $\mathbf{x}_{1\ldots r}\boldsymbol{\gamma}$ is orthogonal to all columns of the matrix

$$\boldsymbol{\Phi}_{i_1\ldots i_{r-1}} = \| \ \mathbf{I}, \mathbf{F}_{i_1}, \ldots, \mathbf{F}_{i_{r-1}}, \ \mathbf{F}_{i_1 i_2}, \ldots, \mathbf{F}_{i_1\ldots i_{r-1}} \ \|$$

for any factors $F_{i_1}, \ldots, F_{i_{r-1}}$ of $F_1, \ldots, F_r$. Therefore, by Lemma 3.7.1, the sum of the elements of $\mathbf{x}_{1\ldots r}\boldsymbol{\gamma}$ corresponding to any combination of levels of the factors $F_{i_1}, \ldots, F_{i_{r-1}}$ is equal to zero, i.e.,

$$\sum_{i_1=0}^{s_1-1} \gamma_{1\ldots r}^{(i_1\ldots i_r)} = 0, \ldots, \sum_{i_r=0}^{s_r-1} \gamma_{1\ldots r}^{(i_1\ldots i_r)} = 0. \tag{3.10.15}$$

Hence,

$$\mathbf{H}_{1\ldots r}\gamma = \left\| \begin{matrix} \left\{\sum_{i_1=0}^{s_1-1} \gamma_{1\ldots r}^{(i_1\ldots i_r)}\right\} \\ \vdots \\ \left\{\sum_{i_r=0}^{s_r-1} \gamma_{1\ldots r}^{(i_1\ldots i_r)}\right\} \end{matrix} \right\| = 0\,. \tag{3.10.16}$$

Therefore, the condition (3.10.14) holds.

Now we have to prove that if the condition (3.10.14) holds, $\mathbf{x}_{1\ldots r}\boldsymbol{\gamma}$ is the vector of the interaction effect of the factors $F_1, \ldots, F_r$.

Summing up, for example, the first equality of (3.10.15), we get

$$\sum_{i_1=0}^{s_1-1} \cdots \sum_{i_r=0}^{s_r-1} \gamma_{1\ldots r}^{(i_1\ldots i_r)} = 0.$$

That means that $\mathbf{x}_{1\ldots r}\boldsymbol{\gamma}$ is a contrast. It follows, by (3.10.14), that (3.10.16) holds, and, therefore, (3.10.15) holds as well. Hence, the sum of elements of $\mathbf{x}_{1\ldots r}\boldsymbol{\gamma}$ corresponding to any combination of level of the factors $F_{i_1}, \ldots, F_{i_{r-1}}$ of the factors $F_1, \ldots, F_r$ is equal to zero.

This completes the proof of the lemma.

Theorem 3.10.1. The matrix (3.10.10) is a full rank matrix and no row of **H** can be represented by a linear combination of the rows of the matrix $\mathbf{X}_{1\ldots m}$.

Proof. The fact that no row of **H** can be represented by a linear combination of the rows of the matrix $\mathbf{X}_{1\ldots m}$ is obvious. Now we have to prove that there is no nonzero vector $\boldsymbol{\gamma}$ such that

$$\left\| \begin{matrix} \mathbf{X_{1\ldots m}} \\ \mathbf{H} \end{matrix} \right\| \boldsymbol{\gamma} = \mathbf{0}. \tag{3.10.17}$$

Indeed, (3.10.17) implies that

$$\mathbf{H}\boldsymbol{\gamma} = \mathbf{0}. \tag{3.10.18}$$

By Lemma 3.10.1 and (3.10.18), it follows that

$$\boldsymbol{\gamma}^T = (\gamma_0, \boldsymbol{\gamma}_1^T, \ldots, \boldsymbol{\gamma}_m^T, \boldsymbol{\gamma}_{12}^T, \ldots, \boldsymbol{\gamma}_{1\ldots m}^T),$$

where $\mathbf{x}_i\boldsymbol{\gamma}_i$ is the vector of the main effect of the factor F_i; $\mathbf{x}_{i_1\ldots i_r}\boldsymbol{\gamma}_{i_1\ldots i_r}$ is the vector of the interaction effect of the factors $F_{i_1}, \ldots, F_{i_r}$. Hence,

$$\mathbf{X}_{1\ldots m}\boldsymbol{\gamma} = \\ \mathbf{I}\gamma_0 + \mathbf{x}_1\boldsymbol{\gamma}_1 + \cdots + \mathbf{x}_m\boldsymbol{\gamma}_m + \mathbf{x}_{12}\boldsymbol{\gamma}_{12} + \cdots + \mathbf{x}_{1\ldots m}\boldsymbol{\gamma}_{1\ldots m}. \tag{3.10.19}$$

By Theorem 3.4.1, all vectors in the right-hand side of (3.10.19) are orthogonal. Therefore,

$$\mathbf{X}_{1\ldots m}\boldsymbol{\gamma} \neq 0,$$

which contradicts (3.10.17).

This completes the proof of Theorem 3.10.1.

The model (3.10.6) with the restrictions (3.10.13) is called a full factorial model of true effects for qualitative factors (or a C^f-model of true effects).

Let $\mathbf{H}^{\Omega}$ be a submatrix of the matrix $\mathbf{H}$ corresponding to the factorial set Ω. Then the model (3.10.7) with the restrictions $\mathbf{H}^{\Omega}\mathfrak{B}^{\Omega} = \mathbf{0}$ is called a factorial model of true effects for the factorial set Ω for quantitative factors (or a C^{Ω}-model of true effects) . Hereafter, we will not necessarily keep the words "true effects" in the notation of these models.

For the C^{Ω}-model, obviously, the following two conditions are satisfied:

1. The C^{Ω}-model (3.10.7) of true effects contains an absolute term and terms with all effects of levels for any factor.
2. If the model contains at least one term with an interaction effect of levels of the factors $F_{i_1}, \ldots, F_{i_r}$, then the model contains all terms with interaction effects of levels of any n $(n \leq r)$ factors of the factors $F_{i_1}, \ldots, F_{i_r}$.

§ 11. A Mixed Model

Consider the full design $\mathbf{D}^f$ together with the design $\mathbf{D}$ for the case when the factors $F_1, \ldots, F_n$ are qualitative and the factors $F_{n+1}, \ldots, F_m$ are quantitative.

For the qualitative factors, as in §10, we will use the matrices $\boldsymbol{\rho}_i = \boldsymbol{\psi}_i = \left\|\boldsymbol{\psi}_i^0, \dots, \boldsymbol{\psi}_i^{s_i-1}\right\|$ of all vectors of effects of levels of the factors F_i $(i = 1, \dots, n)$. For quantitative factors, as in §5, we will use the matrices $\boldsymbol{\rho}_j = \left(1/N^f\right)\mathbf{F}_j^f$ of vectors of main effects of the factors F_j $(j = n+1, \dots, m)$ for the design $\mathbf{D}^f$. For vectors of interaction effects of qualitative factors $F_{i_1}, \dots, F_{i_r}$ $(i_1, \dots, i_r \le n)$, we will apply the matrix $\boldsymbol{\rho}_{i_1 \dots i_r}$ of all vectors of interaction effects of levels of the factors $F_{i_1}, \dots,$ F_{i_r}:

$$N^f \boldsymbol{\rho}_{i_1 \dots i_r} = N^f \boldsymbol{\psi}_{i_1 \dots i_r} = N^f \boldsymbol{\psi}_{i_1} \otimes \dots \otimes N^f \boldsymbol{\psi}_{i_r}.$$

For quantitative factors $F_{j_1}, \dots, F_{j_l}$ $(j_1, \dots, j_l \ge n+1)$, we will apply the matrix $\boldsymbol{\rho}_{j_1 \dots j_l}$ of interaction effects of the factors $F_{j_1}, \dots, F_{j_l}$:

$$N^f \boldsymbol{\rho}_{j_1 \dots j_l} = \mathbf{F}_{j_1 \dots j_l}^f.$$

For the qualitative factors $F_{i_1}, \dots, F_{i_r}$ $(i_1, \dots, i_r \le n)$ and the quantitative factors $F_{j_1}, \dots, F_{j_l}$ $(j_1, \dots, j_l \ge n+1)$ we will use the matrix $\boldsymbol{\rho}_{i_1, \dots, i_r, j_1, \dots, j_l}$:

$$N^f \boldsymbol{\rho}_{i_1 \dots i_r j_1 \dots j_l} = N^f \boldsymbol{\psi}_{i_1 \dots i_r} \otimes \mathbf{F}_{j_1 \dots j_l}^f. \tag{3.11.1}$$

By using the line of proof of Theorem 3.9.2, we get the following theorem.

Theorem 3.11.1. Any vector of the matrix (3.11.1) is a vector of an interaction effect of the factors $F_{i_1}, \dots, F_{i_r}, F_{j_1}, \dots, F_{j_l}$. A maximum linearly independent subset of vectors of interaction effects of the matrix (3.11.1) contains exactly $\left(s_{i_1} - 1\right) \dots \left(s_{i_r} - 1\right)\left(s_{j_1} - 1\right) \dots \left(s_{j_l} - 1\right)$ vectors.

Denote

$$\begin{aligned}
&\mathbf{P}_{1 \dots m} = \left\| \tfrac{1}{N^f}\mathbf{I}, \boldsymbol{\rho}_1, \dots, \boldsymbol{\rho}_m, \boldsymbol{\rho}_{12}, \dots, \boldsymbol{\rho}_{1 \dots m} \right\|, \\
&\mathbf{z}_i = \mathbf{x}_i \ \ (i = 1, \dots, n), \\
&\mathbf{z}_i = \mathbf{F}_j^f \ \ (j = n+1, \dots, m), \\
&\mathbf{z}_{i_1 \dots i_r j_1 \dots j_l} = \mathbf{x}_{i_1 \dots i_r} \otimes \mathbf{F}_{j_1 \dots j_l}^f \\
&\ (i_1, \dots, i_r \le n; j_1, \dots, j_l \ge n+1), \\
&\mathbf{Z}_{1 \dots m} = \| \ \mathbf{I}, \mathbf{z}_1, \dots, \mathbf{z}_m, \mathbf{z}_{12}, \dots, \mathbf{z}_{1 \dots m} \ \|.
\end{aligned} \tag{3.11.2}$$

Theorem 3.11.2.

$$\mathbf{Z}_{1 \dots m}\mathbf{P}_{1 \dots m}^T = \mathbf{E}_{N^F}. \tag{3.11.3}$$

P r o o f. Consider the full design $\mathbf{D}'$ with s_i runs for the only factor F_i. By Theorems 3.4.1 and 3.10.1, we can easily see that

$$\mathbf{X'}_i\mathbf{\Psi'}_i^T = \frac{1}{s_i}\mathbf{\Phi'}_i\mathbf{\Phi'}_i^T = \mathbf{E}_{s_i}.$$

Besides,

$$\left\| \begin{matrix} \mathbf{X'}_i \\ \vdots \\ \mathbf{X'}_i \end{matrix} \right\| = \| \ \mathbf{I}, \mathbf{x}_i \ \|; \quad \left\| \begin{matrix} \mathbf{\Psi'}_i \\ \vdots \\ \mathbf{\Psi'}_i \end{matrix} \right\| = \frac{N^f}{s_i} \left\| \ \frac{1}{N^f}\mathbf{I}, \boldsymbol{\psi}_i \ \right\|;$$

$$\left\| \begin{matrix} \mathbf{\Phi'}_i \\ \vdots \\ \mathbf{\Phi'}_i \end{matrix} \right\| = \| \ \mathbf{I}, \mathbf{F}_i^f \ \|.$$

Therefore,

$$\frac{N^f}{s_i}\| \ \mathbf{I}, \mathbf{x}_i \ \| \cdot \left\| \ \frac{1}{N^f}\mathbf{I}, \boldsymbol{\psi}_i \ \right\|^T = \frac{1}{s_i}\| \ \mathbf{I}, \mathbf{F}_i^f \ \| \cdot \| \ \mathbf{I}, \mathbf{F}_i^f \ \|^T,$$

and

$$\mathbf{x}_i\boldsymbol{\psi}_i^T = \tfrac{1}{N^f}\mathbf{F}_i^f\mathbf{F}_i^{f\mathrm{T}} = \mathbf{z}_i\boldsymbol{\rho}_i^T. \tag{3.11.4}$$

Then, by (3.11.2) and (3.11.4), we get for $i_1, \dots, i_r \le n$ and $j_1, \dots, j_l \ge n+1$ that

$$\mathbf{z}_{i_1\dots i_r j_1\dots j_l}\boldsymbol{\rho}_{i_1\dots i_r j_1\dots j_l}^T = \left(\mathbf{x}_{i_1\dots i_r} \otimes \mathbf{F}_{j_1\dots j_l}^f\right)\left(\boldsymbol{\psi}_{i_1\dots i_r} \otimes \mathbf{F}_{j_1\dots j_l}^f\right)^T$$
$$= \left(N^f\right)^{r+l-1}\left(\mathbf{x}_{i_1} \otimes \dots \otimes \mathbf{x}_{i_r} \otimes \mathbf{F}_{j_1}^f \otimes \dots \otimes \mathbf{F}_{j_l}^f\right)$$
$$\times\left(\boldsymbol{\psi}_{i_1} \otimes \dots \otimes \boldsymbol{\psi}_{i_r} \otimes \frac{1}{N^f}\mathbf{F}_{j_1}^f \otimes \dots \otimes \mathbf{F}_{j_l}^f\right)^T$$
$$= \left(N^f\right)^{r+l-1}\left(\mathbf{x}_{i_1}\boldsymbol{\psi}_{i_1}^T\right) * \dots * \left(\mathbf{x}_{i_r}\boldsymbol{\psi}_{i_r}^T\right) * \left(\frac{1}{N^f}\mathbf{F}_{j_1}^f\mathbf{F}_{j_1}^{fT}\right) * \dots * \left(\frac{1}{N^f}\mathbf{F}_{j_l}^f\mathbf{F}_{j_l}^{fT}\right)$$
$$= \left(N^f\right)^{r+l-1}\left(\mathbf{x}_{i_1}\boldsymbol{\psi}_{i_1}^T\right) * \dots * \left(\mathbf{x}_{j_l}\boldsymbol{\psi}_{j_l}^T\right) = \mathbf{x}_{i_1\dots i_r j_1\dots j_l}\boldsymbol{\psi}_{i_1\dots i_r j_1\dots j_l}^T,$$

where $*$ denotes term by term multiplication of matrices.

Then (3.10.3) implies (3.11.3).

Denote by

$$\mathbf{\Theta} = \mathbf{P}_{1\dots m}^T\boldsymbol{\eta}^f \tag{3.11.5}$$

a vector of true effects of the mixed model. Theorem 3.11.2 implies that

$$\boldsymbol{\eta}^f = \mathbf{Z}_{1\dots m}\mathbf{\Theta}. \tag{3.11.6}$$

There exist equalities similar to equalities (3.10.12), for the parameters (3.11.5) of the mixed model (3.11.6) with the summation indices $i,\ j \le n$. Let **V** denote the matrix of coefficient of the corresponding system. Then

$$\mathbf{V\Theta} = \mathbf{0}. \tag{3.11.7}$$

Using methods similar to the methods of §10, we can show that the following theorem holds.

Theorem 3.11.3.

$$\left\| \begin{array}{c} \mathbf{Z}_{1\ldots m} \\ \mathbf{V} \end{array} \right\|$$

is a full rank matrix, and no row of **V** is represented by a linear combination of the rows of $\mathbf{Z}_{1\ldots m}$.

The model (3.11.6) with the restriction (3.11.7) will be called the mixed full factorial model of true effects (or the G^f-model of true effects).

Example 3.11.1. For the full design 3^2, consider a factorial model with the qualitative factor F_1 and the quantitative factor F_2. Then

$$\mathbf{Z}_{1\ldots m} = \begin{array}{c} \mathbf{I} \qquad \mathbf{z}_1 \qquad\qquad \mathbf{z}_2 \qquad\qquad\qquad \mathbf{z}_{12} = \mathbf{z}_1 \otimes \mathbf{z}_2 \\ \left\| \begin{array}{c|ccc|cc|cccccc} 1 & 1 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & -1 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 1 \\ 1 & 1 & 0 & 0 & 0 & -2 & 0 & -2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & -2 & 0 & 0 & 0 & -2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & -2 \\ 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \end{array} \right\| \end{array}$$

$$\times \left\| \begin{array}{cccccccccccc} 1 & 1 & 1 & 1 & \sqrt{3/2} & \sqrt{1/2} & \sqrt{3/2} & \sqrt{1/2} & \sqrt{3/2} & \sqrt{1/2} & \sqrt{3/2} & \sqrt{1/2} \end{array} \right\|^T,$$

$$\mathbf{P}_{1\ldots m} = \begin{array}{c} \frac{1}{9}\mathbf{I} \qquad \boldsymbol{\rho}_1 \qquad\qquad \boldsymbol{\rho}_2 \qquad\qquad\qquad \boldsymbol{\rho}_{12} = \boldsymbol{\rho}_1 \otimes \boldsymbol{\rho}_2 \\ \left\| \begin{array}{c|ccc|cc|cccccc} 1 & 2 & -1 & -1 & -1 & 1 & -2 & 2 & 1 & -1 & 1 & -1 \\ 1 & -1 & 2 & -1 & -1 & 1 & 1 & -1 & -2 & 2 & 1 & -1 \\ 1 & -1 & -1 & 2 & -1 & 1 & 0 & -1 & 1 & -1 & -2 & 2 \\ 1 & 2 & -1 & -1 & 0 & -2 & 0 & -4 & 0 & 2 & 0 & 2 \\ 1 & -1 & 2 & -1 & 0 & -2 & 0 & 2 & 0 & -4 & 0 & 2 \\ 1 & -1 & -1 & 2 & 0 & -2 & 0 & 2 & 0 & 2 & 0 & -4 \\ 1 & 2 & -1 & -1 & 1 & 1 & 2 & 2 & -1 & -1 & -1 & -1 \\ 1 & -1 & 2 & -1 & 1 & 1 & -1 & -1 & 2 & 2 & -1 & -1 \\ 1 & -1 & -1 & 2 & 1 & 1 & -1 & -1 & -1 & -1 & 2 & 2 \end{array} \right\| \end{array}$$

$$\times \left\| \begin{array}{cccccccccccc} 1/9 & 1/9 & 1/9 & 1/9 & \frac{1}{9}\sqrt{3/2} & \frac{1}{9}\sqrt{1/2} & \frac{1}{9}\sqrt{3/2} & \frac{1}{9}\sqrt{1/2} & \frac{1}{9}\sqrt{3/2} & \frac{1}{9}\sqrt{1/2} & \frac{1}{9}\sqrt{3/2} & \frac{1}{9}\sqrt{1/2} \end{array} \right\|^T,$$

$$\begin{array}{cc} & \begin{array}{cccccccccccc} \mathbf{V}_0 & \mathbf{V}_1 & & & \mathbf{V}_2 & & \mathbf{V}_{12} & & & & & \end{array} \\ \mathbf{V} = & \left\| \begin{array}{c|ccc|cc|cccccc} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \end{array} \right\|. \end{array}$$

Denote by $\mathbf{Z}^{\Omega}, \mathbf{V}^{\Omega}$, and $\mathbf{\Theta}^{\Omega}$ the parts of the matrices $\mathbf{Z}_{1\dots m}, \mathbf{V},$ and the vector $\mathbf{\Theta}$ respectively corresponding to the factorial set Ω. Assume that elements of the vector $\mathbf{\Theta}$ that do not correspond to the set Ω are equal to zero. Then the following model (which will be called the mixed factorial model of true effects for the factorial set Ω, or the G^{Ω}-model of true effects) holds:

$$\boldsymbol{\eta}^{f} = \mathbf{Z}^{\Omega}\mathbf{\Theta}^{\Omega} \quad \left(\mathbf{V}^{\Omega}\mathbf{\Theta}^{\Omega} = \mathbf{0}\right). \tag{3.11.8}$$

We may omit the words “true effects” in the notation of the model.

The model (3.11.8) can be extended to a wider domain. In this case, we get the following model:

$$Ey(X_1, \dots, X_m) = \mathbf{f}_g^T(X_1, \dots, X_m)\mathbf{\Theta}^{\Omega} \quad \left(\mathbf{V}^{\Omega}\mathbf{\Theta}^{\Omega} = \mathbf{0}\right),$$

where $\mathbf{f}_g^T(X_{1u}, \dots, X_{mu})$ is the u-th row of the matrix $\mathbf{Z}^{\Omega}$.

§ 12. Equivalence of Factorial Models

We now focus on equivalence of factorial models in the sense of properties of related regression. The A^{Ω}-model and the C^{Ω}-model of true effects are special cases of the G^{Ω}-model of true effects. Hence, the only model (of considered factorial models) that is not a special case of the G^{Ω}-model of true effects is the general A^{Ω}-model. Therefore, to prove equivalence of all types of factorial models for factorial set Ω we have to prove equivalence of any two G^{Ω}-models (i.e., any G^{Ω}-model of true effects and any A^{Ω}-model of true effects) and equivalence of A^{Ω}-models of true effects and the general A^{Ω}-model.

Consider a set $S^{\Omega f}$ that consists of vector **I** and a full set of linearly independent effects for the factorial set Ω for the full design $\mathbf{D}^f$. For the fractional design **D** (i.e., for the design that does not include some combinations of the levels), consider a set $S^{\Omega D}$ of vectors with the following property. Its coordinates corresponding to some combination of levels of the factors are equal to the elements of vectors of the set $S^{\Omega f}$ corresponding to the same combination of levels for the design $\mathbf{D}^f$. We will call the vectors of effects of the set $S^{\Omega D}$, the vectors of effects generated by the design **D** and the factorial set Ω, and denote them by upper index **D**. Let $\mathbf{Z}^{\Omega D}$ be the coefficient matrix of the design **D** for the G^{Ω}-model (3.11.8).

We now focus on the problem of estimability of the parameters of the model (3.11.8) for the fractional design **D** that includes some treatment combinations (not necessarily different) of the full design $\mathbf{D}^f$.

Lemma 3.12.1. The matrix

$$\left\| \begin{matrix} \mathbf{Z}^{\Omega D} \\ \mathbf{V}^{\Omega} \end{matrix} \right\| \qquad (3.12.1)$$

is a matrix of full rank if and only if vectors of effects generated by the design **D** and the factorial set Ω are linearly independent.

Proof. Let $\boldsymbol{\gamma}$ be a nonzero vector such that

$$\left\| \begin{matrix} \mathbf{Z}^{\Omega D} \\ \mathbf{V}^{\Omega} \end{matrix} \right\| \boldsymbol{\gamma} = \mathbf{0}. \qquad (3.12.2)$$

Then $\mathbf{V}^{\Omega}\boldsymbol{\gamma} = \mathbf{0}$, and, by Lemma 3.10.1,

$$\boldsymbol{\gamma}^T = \left(\gamma_0, \boldsymbol{\gamma}_1^T, \dots, \boldsymbol{\gamma}_m^T, \boldsymbol{\gamma}_{i_1 i_2}^T, \dots\right),$$

where $\mathbf{z}_i\boldsymbol{\gamma}_i$ is the vector of the main effects of the factor F_i; $\mathbf{x}_{i_1 \dots i_r}\boldsymbol{\gamma}_{i_1 \dots i_r}$ is the vector of the interaction effect of the factors $F_{i_1}, \dots, F_{i_r}$.

Therefore,

$$\mathbf{Z}^{\Omega D}\boldsymbol{\gamma} = \gamma_0 \mathbf{I} + \textstyle\sum_{i=1}^m \mathbf{z}_i^D \boldsymbol{\gamma}_i^T + \sum_{i_1 i_2} \mathbf{z}_{i_1 i_2}^D \boldsymbol{\gamma}_{i_1 i_2} + \cdots = 0, \qquad (3.12.3)$$

where $\mathbf{z}^D$ includes those and only those rows of $\mathbf{z}$ that correspond to treatments combinations of the fractional design **D**, i.e., **I**, $\mathbf{z}_i^D \boldsymbol{\gamma}_i^T$, $\mathbf{z}_{i_1 i_2}^D \boldsymbol{\gamma}_{i_1 i_2}^T, \dots$ (the vectors of effects generated by the design **D** and the factorial set Ω). It follows from (3.12.3) that these vectors effects generated by the design **D** and the factorial set Ω are linearly independent. By Lemma 3.10.1, any vector of the interaction effect of the factors $F_{i_1}, \dots, F_{i_r}$ can be represented as $\mathbf{z}_{i_1 \dots i_r}\boldsymbol{\gamma}_{i_1 \dots i_r}$ $\left(\mathbf{V}_{i_1 \dots i_r}\boldsymbol{\gamma}_{i_1 \dots i_r} = \mathbf{0}\right)$. Then the corresponding vector of the effect generated by the design **D** is

$$\mathbf{z}_{i_1 \dots i_r}^D \boldsymbol{\gamma}_{i_1 \dots i_r} \quad \left(\mathbf{V}_{i_1 \dots i_r}\boldsymbol{\gamma}_{i_1 \dots i_r} = \mathbf{0}\right).$$

By virtue of the assumption, there exist $\lambda_0, \lambda_1, \dots, \lambda_m, \lambda_{i_1 i_2}, \dots$ (not equal simultaneously zero) such that

$$\lambda_0 \mathbf{I} + \textstyle\sum_{i=1}^m \lambda_i \mathbf{z}_i^D \boldsymbol{\gamma}_i + \sum_{i_1, i_2} \lambda_{i_1 i_2} \mathbf{z}_{i_1 i_2}^D \boldsymbol{\gamma}_{i_1 i_2} + \cdots = 0.$$

Then for the vector $\boldsymbol{\gamma}^T = \left(\lambda_0,\ \lambda_1\boldsymbol{\gamma}_1^T, \dots, \lambda_m\boldsymbol{\gamma}_m^T, \lambda_{i_1i_2}\boldsymbol{\gamma}_{i_1i_2}^T, \dots\right)$,

$$\mathbf{Z}^{\Omega D}\boldsymbol{\gamma} = \mathbf{0} \text{ and } \mathbf{V}^{\Omega}\boldsymbol{\gamma} = \mathbf{0},$$

i.e., (3.12.2) is satisfied.

Thus, the proof is complete.

Consider three set of factors corresponding to the fractional design **D**: $F_1, \dots, F_m$; $F_1', \dots, F_m'$ and the quantitative factors $F_1'', \dots, F_m''$ such that $s_i = s_i' = s_i''$. For the factors $F_1, \dots, F_m$, consider the G^{Ω}-model of true effects

$$\boldsymbol{\eta}^f = \mathbf{Z}^{\Omega}\boldsymbol{\Theta}^{\Omega} \tag{3.12.4}$$

with the restrictions on the parameters

$$\mathbf{V}^{\Omega}\boldsymbol{\Theta}^{\Omega} = \mathbf{0}\ . \tag{3.12.5}$$

For the factors $F_1', \dots, F_m'$, consider the G^{Ω}-model of true effects

$$\boldsymbol{\eta}^f = \mathbf{Z}'^{\Omega}\boldsymbol{\Theta}'^{\Omega}$$

with the restrictions on parameters

$$\mathbf{V}'^{\Omega}\boldsymbol{\Theta}'^{\Omega} = \mathbf{0}.$$

For the factors $F'_1, \dots, F'_m$, consider the general A^{Ω}-model (3.2.4) with the coefficient matrix **X**.

Theorem 3.12.1. If for the design **D**, one of the matrices

$$\left\| \begin{matrix} \mathbf{Z}^{\Omega D} \\ \mathbf{V}^{\Omega} \end{matrix} \right\|, \quad \left\| \begin{matrix} \mathbf{Z}'^{\Omega D} \\ \mathbf{V}'^{\Omega} \end{matrix} \right\|, \text{and } \mathbf{X}$$

is a full rank matrix, then any of them is a full rank matrix.

The proof of the theorem follows from Lemma 3.12.1 and the Corollary to Theorem 3.6.1.

Theorem 3.12.1 and Lemma 3.12.1 imply that the existence of unique solution of the normal equations of the method of least squares does not depend on whether the factors are qualitative or quantitative. It depends only on whether the vectors of effects generated by the design **D** and the factorial set Ω are linearly independent or not. The design **D** is called nonsingular if these vectors of effects (generated by the design **D** and the factorial set Ω) are linearly independent.

Theorem 3.12.2. For nonsingular factorial design **D**, all factorial models for the same factorial set Ω are equivalent in the sense of properties of related regression (for any point, estimates of the regression function are equal and variances of these estimates are equal).

P r o o f. First, we will prove that the general A^{Ω}-model and any A^{Ω}-model of true effects are equivalent. Second, we will prove that any G^{Ω}-model of true effects and any A^{Ω}-model of true effects are equivalent.

Consider the A^{Ω}-model of true effects

$$\begin{aligned} &Ey_t(X_1, \dots, X_m) = \mathbf{f}_t^T(X_1, \dots, X_m)\mathbf{B}_t^{\Omega} \\ &= B_{t0} + \textstyle\sum_i \mathbf{f}_{ti}^T(X_i)\,\mathbf{B}_{ti} \\ &+ \textstyle\sum_{i_1,i_2}[\mathbf{f}_{ti_1}(X_{i_1}) \otimes \mathbf{f}_{ti_2}(X_{i_2})]^T\mathbf{B}_{ti_1i_2} + \cdots, \end{aligned} \tag{3.12.6}$$

with the domain Z_t that not necessarily coincides with $\mathbf{D}^f$ such that

$$\mathbf{F}_i^f = \begin{Vmatrix} \mathbf{f}_{ti}^T(X_{i1}) \\ \vdots \\ \mathbf{f}_{ti}^T(X_{iN^f}) \end{Vmatrix}.$$

Then it is evident that

$$\mathbf{\Phi}^{\Omega} = \begin{Vmatrix} \mathbf{f}_t^T(X_{11}, \dots, X_{m1}) \\ \vdots \\ \mathbf{f}_t^T(X_{1N^f}, \dots, X_{mN^f}) \end{Vmatrix}.$$

The coefficient matrix of the design $\mathbf{D}$ for the model (3.12.6) $\mathbf{X}_t = \mathbf{\Phi}^{\Omega D}$.

Consider the general A^{Ω}-model with the domain Z_g:

$$\begin{aligned} &Ey(X_1, \dots, X_m) \\ &= \mathbf{f}^T(X_1, \dots, X_m)\mathbf{B}^{\Omega} = B_0 + \textstyle\sum_i \mathbf{f}_i^T(X_i)\,\mathbf{B}_i \\ &+ \textstyle\sum_{i_1,i_2}\left[\mathbf{f}_{i_1}(X_{i_1}) \otimes \mathbf{f}_{i_2}(X_{i_2})\right]^T \mathbf{B}_{i_1i_2} + \cdots \end{aligned} \tag{3.12.7}$$

Denote the coefficient matrix of the design $\mathbf{D}$ for the model (3.12.7) by $\mathbf{X}$. The submatrix $\mathbf{\Phi}_i^{fD} = \| \ \mathbf{I},\ \mathbf{F}_i^{fD} \ \|$ of the matrix $\mathbf{X}_t = \mathbf{\Phi}^{\Omega D}$ has the size $N \times s_i$ and the rank s_i. The submatrix

$$\mathbf{G}_i = \begin{Vmatrix} 1 & \mathbf{f}_i^T(X_{i1}) \\ & \vdots \\ 1 & \mathbf{f}_i^T(X_{iN}) \end{Vmatrix}$$

of the matrix $\mathbf{X}$ has the same size $N \times s_i$ and rank s_i. By the Corollary to Theorem 3.6.1, these submatrices are related by the nonsingular linear transformation $\mathbf{A}_i$:

$$\mathbf{\Phi}_i^{fD} = \mathbf{G}_i\mathbf{A}_i. \tag{3.12.8}$$

The matrices $\mathbf{X}_t$ and $\mathbf{X}$ are also related by the nonsingular linear transformation:

$$\mathbf{X}_t = \mathbf{XA}. \tag{3.12.9}$$

Besides, for the treatment combinations of $\mathbf{D}^f$, the following equality holds:

$$\mathbf{f}_t^T(X_1, \ldots, X_m) = \mathbf{f}^T(X_1, \ldots, X_m)\mathbf{A}. \tag{3.12.10}$$

Then for the point $(X_1, \ldots, X_m) \in \mathbf{D}^f$, LS estimate for the model (3.12.6), by (3.12.9) and (3.12.10), coincides with LS estimate for the model (3.12.7):

$$\begin{aligned} &\hat{y}_t(X_1, \ldots, X_m) = \mathbf{f}_t^T(X_1, \ldots, X_m)\widehat{\mathbf{B}}_t \\ &= \mathbf{f}_t^T(X_1, \ldots, X_m)(\mathbf{X}_t^T\mathbf{X}_t)^{-1}\mathbf{X}_t\mathbf{y} \\ &= \mathbf{f}^T(X_1, \ldots, X_m)\mathbf{A}(\mathbf{A}^T\mathbf{X}^T\mathbf{XA})^{-1}\mathbf{A}^T\mathbf{X}^T\mathbf{y} \\ &= \mathbf{f}^T(X_1, \ldots, X_m)(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \hat{y}(X_1, \ldots, X_m). \end{aligned} \tag{3.12.11}$$

The variance of the estimate $\hat{y}_t(X_1, \ldots, X_m)$ at the point $(X_1, \ldots, X_m) \in \mathbf{D}^f$, by (3.12.9) and (3.12.10), coincides with the variance of the estimate $\hat{y}(X_1, \ldots, X_m)$:

$$\begin{aligned} &\frac{\sigma^2(\hat{y}_t)}{\sigma^2} = \mathbf{f}_t^T(X_1, \ldots, X_m)(\mathbf{X}_t^T\mathbf{X}_t)^{-1}\mathbf{f}_t(X_1, \ldots, X_m) \\ &= \mathbf{f}^T(X_1, \ldots, X_m)\mathbf{A}(\mathbf{A}^T\mathbf{X}^T\mathbf{XA})^{-1}\mathbf{A}^T\mathbf{f}(X_1, \ldots, X_m) \\ &\mathbf{f}^T(X_1, \ldots, X_m)(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{f}(X_1, \ldots, X_m) = \frac{\sigma^2(\hat{y})}{\sigma^2}. \end{aligned} \tag{3.12.12}$$

Assume that the model (3.12.6) is defined on Z_t such that the equality similar to (3.12.8) holds over the domain $Z = Z_t \cap Z_g$, i.e., that

$$\mathbf{f}_{ti}^T(X_i) = \mathbf{f}_i^T(X_i)\mathbf{A}_i.$$

Then (3.12.10) and, therefore, (3.12.11) and (3.12.12) are satisfied for all points $(X_1, \ldots, X_m) \in Z$.

To prove equivalence of the G^Ω-model and A^Ω-model, we will show the following: a reduction of the model (3.12.4) – (3.12.5) to the model without restrictions on parameters, with a coefficient matrix of a full rank, leads to the A^Ω-model of true effects

$$\boldsymbol{\eta}^f = \boldsymbol{\Phi}^\Omega\mathbf{B}^\Omega, \tag{3.12.13}$$

where $\boldsymbol{\Phi}^\Omega$ contains the vectors of effects of the factorial set Ω for the design $\mathbf{D}$.

Consider the model (3.12.4) with the restrictions on the parameters (3.12.5). These restrictions are split into the following partial restrictions:

$$\mathbf{V}_{1\ldots r}\boldsymbol{\Theta}_{1\ldots r} = \mathbf{0}, \tag{3.12.14}$$

where $\mathbf{\Theta}_{1\dots r}$ is the corresponding part of the vector $\mathbf{\Theta}^{\Omega}$, i.e., $\mathbf{\Theta}_{1\dots r} = \boldsymbol{\rho}_{1\dots r}^{T}\boldsymbol{\eta}^{f}$. Let $\boldsymbol{\gamma}_i$ be one of the solution of (3.12.14). Then, by Lemma 3.10.1, the vector $\boldsymbol{\gamma}_i$ corresponds to the vector $\mathbf{z}_{1\dots r}\boldsymbol{\gamma}_i$ of the interaction effect of the factors $F_1, \dots, F_r$.

Lemma 3.12.2. A set of linearly independent vectors $\boldsymbol{\gamma}_i$ such that $\mathbf{V}_{1\dots r}\boldsymbol{\gamma}_i = \mathbf{0}$ corresponds to a set of the linearly independent vectors $\mathbf{z}_{1\dots r}\boldsymbol{\gamma}_i$ $(i = 1, \dots, l)$ of the interaction effects of the factors $F_1, \dots, F_r$.

Proof. The equality

$$\sum_{i=1}^{l} \lambda_i \mathbf{z}_{1\dots r}\boldsymbol{\gamma}_i = 0 \qquad (3.12.15)$$

implies that

$$\mathbf{z}_{1\dots r}^{T}\mathbf{z}_{1\dots r} \sum_{i=1}^{l} \lambda_i \boldsymbol{\gamma}_i = \mathbf{0}.$$

Since $\mathbf{z}_{1\dots r}^{T}\mathbf{z}_{1\dots r} = n\mathbf{E}$,

$$\sum_{i=1}^{l} \lambda_i \boldsymbol{\gamma}_i = \mathbf{0}. \qquad (3.12.16)$$

It is easy to see that (3.12.16) implies (3.12.15). This proves the lemma.

Since $\operatorname{Rg} \mathbf{V}_{1\dots r} = s_1 \dots s_r - (s_1 - 1) \dots (s_r - 1)$, the general solution of (3.12.14) is

$$\mathbf{\Theta}_{1\dots r} = \mathbf{\Gamma}_{1\dots r}\mathbf{B}_{1\dots r}, \qquad (3.12.17)$$

where $\mathbf{\Gamma}_{1\dots r}$ is the $(s_1 \dots s_r) \times [(s_1 - 1) \dots (s_r - 1)]$ matrix such that

$$\mathbf{V}_{1\dots r}\mathbf{\Gamma}_{1\dots r} = \mathbf{0}, \quad \operatorname{Rg} \mathbf{\Gamma}_{1\dots r} = (s_1 - 1) \dots (s_r - 1), \qquad (3.12.18)$$

and $\mathbf{B}_{1\dots r}$ is an arbitrary $[(s_1 - 1) \dots (s_r - 1)]$-dimensional vector. Now transform (3.12.4) to

$$\boldsymbol{\eta}^{f} = \Theta_0 + \sum_{i=1}^{m} \mathbf{z}_i \mathbf{\Theta}_i + \sum_{i_1, i_2} \mathbf{z}_{i_1 i_2} \mathbf{\Theta}_{i_1 i_2} + \cdots \qquad (3.12.19)$$

With the substitute (3.12.17), we get the following relationship:

$$\mathbf{z}_{1\dots r}\mathbf{\Theta}_{1\dots r} = \mathbf{z}_{1\dots r}\mathbf{\Gamma}_{1\dots r}\mathbf{B}_{1\dots r} = \mathbf{X}_{1\dots r}\mathbf{B}_{1\dots r}, \qquad (3.12.20)$$

where $\mathbf{X}_{1\dots r}$, by (3.12.18) and Lemma 3.12.2, contains the vectors of the interaction effects of the factors $F_1, \dots, F_r$.

The similar substitutes can be done for all terms of (3.12.3). With the notations

$$\mathbf{X} = \| \ \mathbf{I}, \mathbf{X}_1, \dots, \mathbf{X}_m, \mathbf{X}_{12}, \dots \ \|,$$

$$\mathbf{B}^{\Omega T} = \left\| \ \frac{1}{N}\mathbf{I}, \mathbf{B}_1^{T}, \dots, \mathbf{B}_m^{T}, \mathbf{B}_{12}^{T}, \dots \ \right\|,$$

we get the required model (3.12.13).

§ 13. Generalized Inverse of Information Matrix

We will follow the article [5] regarding one method of a generalized inverse of information matrix for a factorial model.

Consider the factorial design **D** and the model for the qualitative factors $F_1, \dots, F_n$ with $s_1, \dots, s_n$ levels respectively and the quantitative factors $F_{n+1}, \dots, F_m$ with $s_{n+1}, \dots, s_m$ levels respectively. For the sake of simplicity, without loss of generality, consider the model of main effects:

$$Ey = b_0 + \sum_{i=1}^{n}[b_{i0}x_{i0} + \cdots + b_{i\,(s_i-1)}x_{i\,(s_i-1)}]$$

$$+\sum_{i=\mathrm{n}+1}^{m}[b_{i1}x_{i1} + \cdots + b_{i\,(s_i-1)}x_{i\,(s_i-1)}]. \tag{3.13.1}$$

For the parameters $b_{i0}, \dots, b_{i\,(s_i-1)}$, the following restrictions exist:

$$b_{i0} + \dots + b_{i\,(s_i-1)} = 0 \ \ (i = 1, \dots, n), \tag{3.13.2}$$

or

$$b_{i\,(s_i-1)} = -b_{i0} - \dots - b_{i\,(s_i-2)}. \tag{3.13.3}$$

Let $\mathbf{X}^{(1)}$ be the coefficient matrix of the design **D** for the model (3.13.1). Denote the LS estimates of the parameters $b_{i0}, \dots, b_{i\,(s_i-1)}$ by $\hat{b}_{i0}, \dots, \hat{b}_{i\,(s_i-1)}$. Then the LS estimate $\widehat{\mathbf{B}}^{(1)}$ of the vector $\mathbf{B}^{(1)}$ of the parameters of the model (3.13.1) with the restrictions

$$\hat{b}_{i0} + \dots + \hat{b}_{i\,(s_i-1)} = 0 \ \ (i = 1, \dots, n) \tag{3.13.4}$$

can be found as one of the solutions of the normal equations

$$\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{B} = \mathbf{X}^{(1)T}\mathbf{Y} \tag{3.13.5}$$

that satisfies (3.13.4).

Any solution $\widehat{\widehat{\mathbf{B}}}^{(1)}$ of the normal equations (3.13.5) is given by the matrix $(\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{-}$, which is the generalized inverse (G-inverse) of the matrix $\mathbf{X}^{(1)T}\mathbf{X}^{(1)}$:

$$\widehat{\widehat{\mathbf{B}}}^{(1)} = (\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{-}\mathbf{X}^{(1)T}\boldsymbol{Y}.$$

The vector $\widehat{\widehat{\mathbf{B}}}^{(1)}$ is one of the LS estimates of the parameters of the model without restrictions.

Theorem 3.11.3 implies that for any factorial model, we can find a nonsingular design (for example, a full design) such that there exist the unique LS estimates of parameters of the model, satisfying the factorial restrictions (kind of equalities (3.13.4)).

For the nonsingular design $\mathbf{D}$, among all possible matrices $(\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{-}$, we will find the matrix (denote it by $(\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{+}$) such that for any corresponding solution $\hat{\hat{\mathbf{B}}}^{(1)}$, the following equality holds:

$$\hat{\hat{\mathbf{B}}}^{(1)} = \hat{\mathbf{B}}^{(1)}.$$

Substituting $b_{i\,(s_i-1)}$ from (3.13.3) into (3.13.1), we get the following expression for the sum with qualitative factors:

$$\sum_{i=1}^{n}[b_{i0}(x_{i0} - x_{i\,(s_i-1)}) + \cdots + b_{i\,(s_i-2)}(x_{i\,(s_i-2)} - x_{i\,(s_i-1)})]. \quad (3.13.6)$$

The coefficients in (3.13.6) are the new parameters. The vector of new parameters $\boldsymbol{B}_i^{(2)} = (b_{i0}, \dots, b_{\boldsymbol{i}(s_i-2)})$ and the vector of old parameters $\boldsymbol{B}_i^{(1)} = \left(b_{i0}, \dots, b_{\boldsymbol{i}\,(s_i-1)}\right)$ are connected by the following relationship:

$$\mathbf{B}_i^{(1)} = \mathbf{A}_i\mathbf{B}_i^{(2)}, \quad (3.13.7)$$

where

$$\mathbf{A}_i = \begin{Vmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ -1 & -1 & \cdots & -1 \end{Vmatrix} \ (i = 1, \dots, n).$$

For quantitative factors, the transformation to new parameters is as follows:

$$\mathbf{B}_i^{(1)} = \mathbf{A}_i\mathbf{B}_i^{(2)} \quad (i = n+1, \dots, m),$$

where $\mathbf{A}_i$ $(i = 1, \dots n+1)$ is the identity matrix.

As a result, we get the following reduced model, which can be also considered as a factorial model:

$$\begin{aligned} Ey = b_0 + \sum\nolimits_{i=1}^{n} &[b_{i0}(x_{i0} - x_{i\,(s_i-1)}) + \cdots \\ &+ b_{i\,(s_i-2)}(x_{i\,(s_i-2)} - x_{i\,(s_i-1)})] \\ &+ \sum\nolimits_{i=n+1}^{m}\left[b_{i1}x_{i1} + \cdots + b_{i\,(s_i-1)}x_{i\,(s_i-1)}\right]. \end{aligned} \quad (3.13.8)$$

Therefore, the vector of parameters of the model (3.13.8)

$$\begin{aligned}\mathbf{B}^{(2)} = (&b_0, b_{10}, \dots, b_{1\,(s_1-2)}, \dots, b_{n0}, \dots, b_{n\,(s_n-2)}, \\ &b_{(n+1)1}, \dots, b_{(n+1)\,(s_{n+1}-1)}, \dots, b_{m1}, \dots, b_{m\,(s_m-1)})\end{aligned}$$

connected with the vector of parameters of the model (3.13.1)

$$\mathbf{B}^{(1)} = (b_0, b_{10}, \dots, b_{1\,(s_1-1)}, \dots, b_{n1}, \dots, b_{n\,(s_n-1)}, \\ b_{(n+1)1}, \dots, b_{(n+1)\,(s_n-1)}, \dots, b_{m1}, \dots, b_{m\,(s_m-1)})$$

by the relationship

$$\mathbf{B}^{(1)} = \mathbf{A}\mathbf{B}^{(2)}, \tag{3.13.9}$$

where

$$\mathbf{A} = \begin{Vmatrix} 1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_1 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{A}_m \end{Vmatrix}.$$

Assume that the design **D** is nonsingular for the model (3.13.1) with the restrictions (3.13.2). Then, by Theorem 3.12.1, this design will be nonsingular for the model (3.13.8) as well. The coefficient matrix $\mathbf{X}^{(2)}$ of the design **D** for the model (3.13.8) is, evidently,

$$\mathbf{X}^{(2)} = \mathbf{X}^{1}\mathbf{A}. \tag{3.13.10}$$

Hence, the LS estimate $\widehat{\mathbf{B}}^{(2)}$ of the vector $\mathbf{B}^{(2)}$ of parameters is

$$\widehat{\mathbf{B}}^{(2)} = (\mathbf{X}^{(2)T}\mathbf{X}^{(2)})^{-1}\mathbf{X}^{(2)T}\boldsymbol{Y},$$

which, by (3.13.10), becomes

$$\widehat{\mathbf{B}}^{(2)} = (\mathbf{A}^T\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{A})^{-1}\mathbf{A}^T\mathbf{X}^{(1)T}\boldsymbol{Y},$$

where **Y** is the vector of observations corresponding to the design **D** with the covariance matrix (2.1.2).

The covariance matrix of the vector $\widehat{\mathbf{B}}^{(2)}$ is

$$\boldsymbol{\Gamma}^{(2)} = (\mathbf{X}^{(2)T}\mathbf{X}^{(2)})^{-1}\sigma^2 = (\mathbf{A}^T\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{A})^{-1}\sigma^2.$$

Then, by (3.13.9), the LS estimate $\widehat{\mathbf{B}}^{(1)}$ (satisfying (3.13.4)) of the vector $\mathbf{B}^{(1)}$ and the covariance matrix $\boldsymbol{\Gamma}^{(1)}$ of the vector of estimates $\widehat{\mathbf{B}}^{(1)}$ are

$$\widehat{\mathbf{B}}^{(1)} = \mathbf{A}(\mathbf{A}^T\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{A})^{-1}\mathbf{A}^T\mathbf{X}^{(1)T}\boldsymbol{Y}, \tag{3.13.11}$$

$$\boldsymbol{\Gamma}^{(1)} = \mathbf{A}(\mathbf{A}^T\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{A})^{-1}\mathbf{A}^T\sigma^2. \tag{3.13.12}$$

Therefore, *G*-inverse matrix is:

$$(\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{+} = \mathbf{A}(\mathbf{A}^T\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{A})^{-1}\mathbf{A}^T,$$

and (3.13.11) and (3.13.12) can be transformed to

$$\widehat{\mathbf{B}}^{(1)} = (\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{+}\mathbf{X}^{(1)\mathrm{T}}\mathbf{Y},$$
$$\boldsymbol{\Gamma}^{(1)} = (\mathbf{X}^{(1)T}\mathbf{X}^{(1)})^{+}\sigma^{2}.$$

Consider one more way to get the LS estimate of $\mathbf{B}^{(1)}$. Denote the k-dimensional unit vector by $\mathbf{I}_k$ and denote a zero-vector by $\mathbf{0}$. Now add m rows of the matrix

$$\mathbf{X}_0 = \begin{Vmatrix} 0 & \mathbf{I}_{s_1}^T & \mathbf{0}^T & \cdots & \mathbf{0}^T & \mathbf{0}^T \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \mathbf{0}^T & \mathbf{0}^T & \cdots & \mathbf{0}^T & \mathbf{I}_{s_m}^T \end{Vmatrix}$$

to the matrix $\mathbf{X}^{(1)}$.

Then consider the third regression with the coefficient matrix

$$\mathbf{X}^3 = \begin{Vmatrix} \mathbf{X}^{(1)} \\ \mathbf{X}_0 \end{Vmatrix}$$

and with the vector of observations

$$\mathbf{Y}^3 = \begin{Vmatrix} \mathbf{Y} \\ \mathbf{0} \end{Vmatrix}.$$

Denote by *SS* the sum of squares of deviations between observations and the values predicted by the regression. The low index *LS* will indicate the sum of squares belonging to the method of least squares. The upper indices (2) and (3) for SS, **B**, and **X** will indicate corresponding regression. Accent $\widehat{\ }$ will correspond to the LS estimate, accent $\widehat{\widehat{\ }}$ will correspond to any estimate.

Theorem 3.13.1.

$$SS_{LS}^{(2)} = SS_{LS}^{(3)}, \tag{3.13.13}$$
$$\widehat{\mathbf{B}}^{\mathbf{3}} = \mathbf{A}\widehat{\mathbf{B}}^{(2)}. \tag{3.13.14}$$

P r o o f. There exist such estimates of parameters of the third regression that

$$SS^{(3)} = SS_{LS}^{(2)}. \tag{3.13.15}$$

Indeed, let

$$\widehat{\widehat{\mathbf{B}}}^{\mathbf{3}} = \mathbf{A}\widehat{\mathbf{B}}^{(2)}. \tag{3.13.16}$$

Then it is easy to check that for the estimates (3.13.16), equality (3.13.15) holds. It follows from (3.13.15) that

$$SS_{LS}^{(3)} \le SS_{LS}^{(2)}. \tag{3.13.17}$$

On the other hand, there exist such estimates of parameters of the model (3.13.8) that

$$SS^{(2)} = SS_{LS}^{(3)}. \tag{3.13.18}$$

Indeed, let

$$\hat{\hat{b}}_0^{(2)} = \hat{b}_0^{(3)} + \sum_{i=1}^{n} \frac{\hat{b}_{i0}^{(3)} + \cdots + \hat{b}_{i\,(s_{i-1})}^{(3)}}{s_i},$$

$$\hat{\hat{b}}_{i0}^{(2)} = \frac{\left[(s_i - 1)\hat{b}_{i0}^{(3)} - \hat{b}_{i1}^{(3)} - \cdots - \hat{b}_{i\,(s_i-1)}^{(3)}\right]}{s_i}, \tag{3.13.19}$$

. . . .

$$\hat{\hat{b}}_{i\,(s_i-2)}^{(2)} = \frac{\left[-\hat{b}_{i0}^{(3)} - \cdots + (s_i - 1)\hat{b}_{i\,(s_i-2)}^{(3)} - \hat{b}_{i\,(s_i-1)}^{(3)}\right]}{s_i}$$

$(i = 1, \ldots, n)$,

and for the rest of estimates $\hat{\hat{b}}^{(2)}$, let

$$\hat{\hat{b}}^{(2)} = \hat{b}^{(3)}. \tag{3.13.20}$$

It is also easy to check that for the estimates (3.13.19) and (3.13.20), equality (3.13.18) holds. Hence,

$$SS_{LS}^{(2)} \le SS_{LS}^{(3)}. \tag{3.13.21}$$

Comparing (3.13.17) and (3.13.21), we get (3.13.13).

Thus, the proof is complete.

Note to Theorem 3.13.1. The LS estimates of parameters of the third regression can be found based on Theorem 3.13.1 if one uses the matrix $M\mathbf{X_0}$ (M is any positive number) instead of the matrix $\mathbf{X_0}$. Then each element of the matrix

$$(\mathbf{X}^{(3)T}\mathbf{X}^{(3)})^{-1}\sigma^2$$

will converge to the corresponding element of the covariance matrix of LS estimates of parameters (for $M \to \infty$).

Example 3.13.1. Consider the design

$$\mathbf{D} = \begin{array}{c} \mathrm{F} \\ \begin{Vmatrix} 0 \\ 1 \end{Vmatrix} \end{array}$$

for the only qualitative factor F and the model of main effects

$$Ey = b_0 + b_{10}x_{10} + b_{11}x_{11}, \tag{3.13.22}$$

where

$$x_{10} = \begin{cases} 0 & \text{if the value of the factor } F \text{ is } 0, \\ 1 & \text{if the value of the factor } F \text{ is } 1. \end{cases}$$

$$x_{11} = \begin{cases} 1 & \text{if the value of the factor } F \text{ is } 0, \\ 0 & \text{if the value of the factor } F \text{ is } 1. \end{cases}$$

The factorial restriction on the parameters is

$$b_{10} + b_{11} = 0.$$

Than the coefficient matrix of the design **D** for the model (3.13.22) is

$$\mathbf{X}^{(1)} = \begin{Vmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \end{Vmatrix}.$$

Using the first method, we get the following matrix **A**:

$$\mathbf{A} = \begin{Vmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{Vmatrix}.$$

Then the covariance matrix of LS estimates is

$$\mathbf{A}(\mathbf{A}^T\mathbf{X}^{(1)T}\mathbf{X}^{(1)}\mathbf{A})^{-1}\sigma^2 = \begin{Vmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & -1/2 \\ 0 & -1/2 & 1/2 \end{Vmatrix} \sigma^2 . \tag{3.13.23}$$

Using the second method, we get

$M\mathbf{X}_0 = M\|0 \quad 1 \quad 1\|.$

Then

$$(\mathbf{X}^{(3)T}\mathbf{X}^{(3)})^{-1}\sigma^2 = \begin{Vmatrix} \frac{1+2M^2}{4M^2} & -\frac{1}{4M^2} & -\frac{1}{4M^2} \\ -\frac{1}{4M^2} & \frac{1+2M^2}{4M^2} & \frac{1-2M^2}{4M^2} \\ -\frac{1}{4M^2} & \frac{1-2M^2}{4M^2} & \frac{1+2M^2}{4M^2} \end{Vmatrix} \sigma^2. \tag{3.13.24}$$

As $M \to \infty$, each element of the matrix (3.13.24) converges to corresponding element of (3.13.23).

§ 14. Blocking

We need to divide a factorial design into homogeneous blocks in the following situation. Let the design **D** for the factorial model

$$E\mathbf{y} = \mathbf{\Theta}^T\mathbf{f}(X_1, \dots, X_m)$$

with possible restrictions on parameters $\mathbf{T\Theta} = \mathbf{0}$ contains N runs. Sometimes all these N experiments cannot be performed in homogeneous environments. For example, if homogeneous parts of experimental materials (in a chemical experiment) are only enough for n experiments ($n < N$), if the uniform plots of land are small (in an agricultural experiment), etc. In such cases, we actually have one more factor, which is called a block factor or nuisance factor and which may affect the measured result but is not of primary interest. The number of levels of this factor is equal to the number of heterogeneous parts, plots, etc. This situation can be described with the following model:

$$E\mathbf{y} = \mathbf{\Theta}^T \mathbf{f}(X_1, \dots, X_m) + \sum_{i=1}^{r} \beta^{(i)} x^{(i)} \tag{3.14.1}$$

with the restrictions on parameters

$$\mathbf{T\Theta} = \mathbf{0},\ \sum_{i=1}^{r} \beta^{(i)} = 0,$$

where $\beta^{(i)}$ is the effect of the level i of the block factor F and

$$x^{(i)} = \begin{cases} 1 & \text{if the block factor } F \text{ appears at the level } i, \\ 0 & \text{if the block factor } F \text{ appears at the level other than } i. \end{cases}$$

It is obvious that this model is also a factorial model for the design $\mathbf{D}'$ that contains all factors of the design $\mathbf{D}$ and the block factor F (all factors of the design $\mathbf{D}'$ except F have the same number of levels as in the design $\mathbf{D}$).

Let $\mathbf{X}'$ be the coefficient matrix of the design $\mathbf{D}'$ for the model (3.14.1). Delete from $\mathbf{X}'$ the columns corresponding to the block factor F and denote the resulting matrix by $\mathbf{X}$. We will consider an orthogonal blocking if any main effect of the factor F is orthogonal to any column of the matrix $\mathbf{X}$.

We will consider a blocking problem (in particular, an orthogonal blocking) in parallel with the task of construction of optimal factorial designs.

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Chapter 4. The Effectiveness of Designs

For the given design, the LS estimates possess some optimal properties. Hereafter, we will fix a method of statistical estimation (the LS method) and will solve the task of finding effective designs for factorial models. We will distinguish between two shades of meaning of the concept of an effective design: the criteria of optimality and the desirable properties of the design. There is no clear distinction between these two concepts. However, they can be described as follows.

The criteria of optimality are mathematically clear requirements for the design. These requirements in the majority of cases may be seen as an expansion of the concept of the best linear estimates. The desirable properties are those properties that are not very clear from the point of view of a mathematician but natural for the practitioners involved in experiment.

Hereafter we assume that all designs are nonsingular. By Theorem 3.12.1, whether the design is singular or nonsingular does not depend on the type of the factorial model for the factorial set Ω. Therefore, we introduce the types of nonsingular designs in accordance with the following definition.

Definition 4.0.1. A nonsingular design for the factorial model for the factorial set Ω containing all possible elements of n factors $(n \leq r-1)$ is called the design of resolution $2r-1$. A nonsingular design for the factorial model for the set Ω containing all possible elements of n factors $(n \leq r-1)$ is called the design of resolution $2r$ if all effects of the set Ω are estimated with no bias in the model for the set Ω' containing all possible elements of l factors $(l \leq r)$. The design of resolution 3 is also called the design of main effects and the corresponding model is called the model of main effects.

§ 1. Optimality Criteria of Designs

If for the model (2.1.3) and the design (2.1.4), the information matrix $\mathbf{M}$ is a full rank matrix, the covariance matrix of the vector $\widehat{\mathbf{\Theta}}$ of estimates is

$$\mathbf{\Gamma}(\widehat{\mathbf{\Theta}}) = \mathbf{M}^{-1}\sigma^2.$$

The matrix $\bar{\mathbf{M}} = \frac{1}{N}\mathbf{M}$ is called a normalized information matrix and the matrix $\bar{\mathbf{\Gamma}} = \bar{\mathbf{M}}^{-1}\sigma^2$ is called a normalized covariance matrix.

The first three criteria of optimality will be introduced for the model without restrictions on parameters. They allow an interpretation that is associated with the size of the dispersion ellipsoid of the parameter estimates.

Definition 4.1.1. The design $\mathbf{D}^*$ is called *D*-optimal on the set of designs $\mathcal{D}$ if

$$\det \bar{\mathbf{M}}(\mathbf{D}^*) = \max_{\mathbf{D}\in\mathcal{D}} \det \bar{\mathbf{M}}(\mathbf{D}). \tag{4.1.1}$$

The dispersion ellipsoid of the parameter estimates of the *D*-optimal design has minimal volume.

The criterion of *D*-optimality (also called the Mood's criterion) is the most popular one. It will be used also for the model (2.1.5) with the restrictions (2.6.1) on parameters. In this case, the matrix $\bar{\boldsymbol{M}}$ in (4.1.1) will correspond to the information matrix $\mathbf{M} = \mathbf{Q}^T\mathbf{X}^T\mathbf{X}\mathbf{Q}$ for the reduced model (2.4.3). A property of *D*-optimality of a design is invariant to any nonsingular linear transformation of the parameter vector. Based on that it is easy to prove that a property of *D*-optimality of a design is invariant to a selection of the vector of new parameters $\mathbf{Q}_n$ of the reduced model.

Definition 4.1.2. The design $\mathbf{D}^*$ is called *A*-optimal on the set of designs $\mathcal{D}$ if

$$\mathrm{Tr}\, \mathbf{\Gamma}(\mathbf{D}^*) = \min_{\mathbf{D}\in\mathcal{D}} \mathrm{Tr}\, \mathbf{\Gamma}(\mathbf{D}). \tag{4.1.2}$$

The dispersion ellipsoid of the parameter estimates of the *A*-optimal design has minimal length of a diagonal of the circumscribed parallelepiped.

The criterion of *A*-optimality is also called the Kishen's criterion.

Definition 4.1.3. The design $\mathbf{D}^*$ is called *E*-optimal on the set of the designs $\mathcal{D}$ if

$$\max_q q\{\mathbf{\Gamma}(\mathbf{D}^*)\} = \min_{\mathbf{D}\in\mathcal{D}} \max_q q\{\mathbf{\Gamma}(\mathbf{D})\}, \tag{4.1.3}$$

where $q\{\mathbf{\Gamma}\}$ is an eigenvalue of the matrix $\mathbf{\Gamma}$.

The maximum axe of the dispersion ellipsoid of the parameters of estimates of an *E*-optimal design has minimal length.

The criterion of *E*-optimality is also called the Ehrenfeld's criterion.

The following two criteria are related to the properties of the regression function in the domain.

Definition 4.1.4. The design $\mathbf{D}^*$ is called *G*-optimal in the domain *Z* on the set of the designs $\mathcal{D}$ if

$$\max_{Z} N^* d(\mathbf{D}^*, X_1, \dots, X_m) = \min_{\mathbf{D}\in\mathcal{D}} \max_{Z} N d(\mathbf{D}, X_1, \dots, X_m), \qquad (4.1.4)$$

where $d(\mathbf{D}, X_1, \dots, X_m)$ is the variance of the estimate of the regression function at the point $(X_1, \dots, X_m) \in Z$.

The value

$$\bar{d}(\mathbf{D}, X_1, \dots, X_m) = \int \underset{Z}{\cdots} \int d(\mathbf{D}, X_1, \dots, X_m) dX_1 \dots dX_m$$

is called an average variance over the domain Z.[1]

Definition 4.1.5. The design $\mathbf{D}^*$ is called Q-optimal in the domain Z on the set of the designs $\mathcal{D}$ if

$$\bar{d}(\mathbf{D}^*, X_1, \dots, X_m) = \min_{\mathbf{D}\in\mathcal{D}} \bar{d}(\mathbf{D}, X_1, \dots, X_m). \qquad (4.1.5)$$

The following two criteria (orthogonality and regularity) will be often used in the book, although, at first glance, they have no such statistical justification as the previous criteria of this paragraph. However, at the end of this chapter, we will show why these criteria are important for applications.

Definition 4.1.6. A design is called orthogonal for the given model if the covariance matrix of the parameter vector of estimates for this model and for the design is diagonal.

Definition 4.1.7. A factorial design is called regular of strength t if the condition of proportional frequencies is satisfied for any t factors.

The following theorem is a corollary to Theorem 3.7.3.

Theorem 4.1.1. A regular factorial design of strength $t = 2n$ allows obtaining a set of pairwise orthogonal main effects and interaction effects up to the order $n - 1$. A regular factorial design of strength $t = 2n + 1$ allows obtaining a set of pairwise orthogonal main effects and interaction effects up to the order $n - 1$ such that each of them is orthogonal to all interaction effects of the order n.

Theorem 4.1.1 implies that a regular factorial design of strength t is a special case of the design of resolution $t + 1$.

Definition 4.1.8. A factorial design is called regular for the factorial set Ω if there exists a factorial model for the factorial set Ω for which this design is orthogonal.

By the definition 4.1.8, a regular factorial design of strength $t = 2n$ is a special case of the regular factorial design for the factorial set Ω, containing all possible elements of l factors ($l \le n$).

---

[1] For a discrete domain Z of N points

$$\bar{d}(\mathbf{D}, X_1, \dots, X_m) = 1/N \textstyle\sum_Z d(\mathbf{D}, X_1, \dots, X_m).$$

Note that regularity of the design for the factorial set Ω does not imply orthogonality of the design for any model for the set Ω.

Theorem 4.1.2. The following three statements are equivalent:

1) the design **D** is regular for the factorial set Ω;

2) for the design **D**, all main effects and interaction effects corresponding to the factorial set Ω (one from each set of effects) are pairwise orthogonal;

3) in the design **D**, the condition of proportional frequencies is satisfied for the factorial set Ω.

Proof. Equivalence of the statements 2 and 3 follows from Theorems 3.7.2 and 3.7.3. Now we will show that the statement 1 of the theorem implies the statement 2. Indeed, it follows from the statement 1 that the coefficient matrix **X** has pairwise orthogonal columns. Hence, the columns corresponding functions

$$f_1^{(1)}(X_1), \dots, f_1^{(s_1-1)}(X_1), \dots, f_m^{(1)}(X_m), \dots, f_m^{(s_m-1)}(X_m)$$

are orthogonal to the unit vector and, therefore, are main effects of the factors $F_1, \dots, F_m$.

The column $\mathbf{f}_{i_1 \dots i_n}$ corresponding to the product $f_{i_1}^{(j_1)}(X_{i_1}) \times \dots \times f_{i_n}^{(j_n)}(X_{i_n})$ has equal elements for the given combination of levels of the factors $F_{i_1}, \dots, F_{i_n}$. Hence, it follows from the statement 1 that this column is orthogonal to all main effects of the factors $F_{i_1}, \dots, F_{i_n}$ and all interaction effects of these factors of the order $l < n - 1$. Therefore, the column $\mathbf{f}_{i_1 \dots i_n}$ is an interaction effect of the factors $F_{i_1}, \dots, F_{i_n}$. Hence, the statement 2 holds.

It is easy to see from Theorem 3.8.2 that the statement 2 implies the statement 1.

This completes the proof of the theorem.

Very often, it is not easy to construct the design that satisfies all or even some of optimality criteria. So the designs that satisfy only one of the criteria are also important and useful.

§ 2. Desirable Properties of Designs

We start considering the desirable properties of designs with the property related to the number of treatments of the design, which is very important for practitioners involved in experiment.

Definition 4.2.1. A design is called saturated for the factorial A^{Ω}-model if the number of runs of the design is equal to the number of parameters of the model A^{Ω}.

We also apply the definition 4.2.1 to models that include qualitative factors (with the restrictions on parameters). In this case we reduce the number of parameters in the definition 4.2.1 by the number of linearly independent restrictions.

Among of other desirable properties of designs we note the following two:

- simplicity of calculations and interpretation of the results of observations;
- possibility to split the design into blocks when all experiments cannot be carry out in homogeneous conditions.

In the next chapters, we will address issues of construction of optimal designs with desirable properties.

§ 3. Equivalence of *D*- and *G*-optimal Designs

Let **D** be a set of all designs with the domain Z that is closed and bounded. Then the following theorem of Kiefer-Wolfowitz holds:

Theorem 4.3.1 [1]. The following statements are equivalent:

1) the design $\mathbf{D}^*$ is D-optimal on **D**;
2) the design $\mathbf{D}^*$ is G-optimal on **D**;
3) $\max_Z N^* d(\mathbf{D}^*, X_1, \dots, X_m) = k$.

Theorem 4.3.2 [1]. The information matrix of *D-(G-)*optimal design is unique on **D**. The maximum of the variance of the estimate of the regression function on Z is reached at points of the design.

Theorem 4.3.1, generally speaking, does not hold if **D** is a subset of the set of all designs. For example, for the subset of designs with the fixed number of treatments, D- and G-optimal designs are not equivalent. In this case the statement 3 of Theorem 4.3.1 holds neither for D- nor for G-optimal design.

§ 4. Criterion of Average Variance

Let **D** be a factorial design for the A^{Ω}-model (3.2.4). By (2.2.5), the variance of the estimate of the regression function at point

$$\mathbf{x}^T = \Big[1, f_1^{(1)}(X_1), \dots, f_1^{(s_1-1)}(X_1), \dots, k_{i_1 i_2}^{1,1} f_{i_1}^{(1)}\big(X_{i_1}\big) f_{i_2}^{(1)}\big(X_{i_2}\big),$$
$$\dots, k_{i_1 i_2}^{s_{i_1}-1, s_{i_2}-1} f_{i_1}^{(s_{i_1}-1)}\big(X_{i_1}\big) f_{i_2}^{(s_{i_2}-1)}\big(X_{i_2}\big), \dots\Big] = \{\mathbf{x}^T(X_1, \dots, X_m)\}$$

is equal to

$$\sigma_{\mathbf{x}}^2 = \sigma^2 \mathbf{x}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}.$$

By Theorem 3.4.1 and Note 2 to Theorem 3.4.1, functions in the A^{Ω}-model (3.2.4) can be selected in such a way that

$$\sum_{u=1}^{N^f} x_u^{(j)} x_u^{(l)} = N^f \delta_{jl} \tag{4.4.1}$$

where $\{x_u^{(n)}\} = \mathbf{x}^T(X_{1u}, \dots, X_{mu})$; $\quad n = j, l$.

Then the average variance over $\mathbf{D}^f$ is

$$\sigma_a^2 = \sigma^2/N^f \sum_{x\in\mathbf{D}^f} \mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}$$
$$= \sigma^2/N^f \sum_{u=1}^{N^f} \sum_{j=1}^{k} \sum_{l=1}^{k} x_u^{(j)} x_u^{(l)} c_{jl}$$
$$= \sigma^2/N^f \sum_{j=1}^{k} \sum_{l=1}^{k} c_{jl} \sum_{u=1}^{N^f} x_u^{(j)} x_u^{(l)}$$
$$= \sigma^2 \sum_{j=1}^{k} \sum_{l=1}^{k} c_{jl}\delta_{jl} = \sigma^2 \sum_{j=1}^{k} c_{jj} = \sigma^2 \mathrm{Tr}\{(\mathbf{X}^T\boldsymbol{X})^{-1}\},$$

where k is the number of parameters in the model and $(\mathbf{X}^T\mathbf{X})^{-1} = \{c_{jl}\}$. By the results of §12 of chapter 3, it follows that the variance of the estimate of the regression function depends neither on the type of the model for the factorial set Ω nor on the choice of the functions in the model. Therefore, the following theorem holds.

Theorem 4.4.1. The factorial design is Q-optimal on $\mathbf{D}^f$ for any factorial model for the factorial set Ω if and only if it is A-optimal for the A^{Ω}-model satisfied the condition (4.4.1).

Theorem 4.4.1 can also be obtained as a consequence of Theorem 2.12.1 of the book [2] by V.V. Fedorov.

Let the levels $0,1,\dots,(s_i-1)$ of the factor F_i occur $n_i^{(0)}, n_i^{(1)}, \dots, n_i^{(s_i-1)}$ times respectively in the design $\mathbf{D}$. In this case, obviously,

$$\sum_{j=0}^{s_i-1} n_i^{(j)} = N.$$

Definition 4.4.1. The number

$$U_i^{j_i} = \frac{N - n_i^{(j_i)}}{n_i^{(j_i)}(s_i-1)} \tag{4.4.2}$$

is called the coefficient of uniformity of the j_i-th level of the factor F_i.

It is evident that if the j_i-th level of the factor F_i occurs in the design $\mathbf{D}$ more than N/s_i times, $U_i^{j_i} < 1$; if the j_i-th level of the factor F_i occurs in the design $\mathbf{D}$ less than N/s_i times, $U_i^{j_i} > 1$; if the j_i-th level of the factor F_i occurs in the design $\mathbf{D}$ exactly N/s_i times, $U_i^{j_i} = 1$.

The last equality holds, in particular, for uniform designs for any level of any factor.

Definition 4.4.2. The average of the coefficients $U_i^{j_i}$ over all levels of the factor F_i

$$U_i = \sum_{j_i=0}^{s_i-1} \frac{U_i^{j_i}}{s_i} = \frac{N\sum_{j=0}^{s_i-1}\left(1/n_i^{(j_i)} - s_i\right)}{s_i(s_i-1)} \tag{4.4.3}$$

is called a coefficient uniformity of the factor F_i.

Definition 4.4.3. A factor is called uniform if all its levels occur in the design with equal frequency. Otherwise, a factor is called nonuniform.

It is evident that for uniform factors $U_i = 1$, for nonuniform factors $U_i > 1$.

Consider the regular design **D** of main effects for the factors $F_1, \dots, F_m$, i.e., the regular design for the factorial set Ω that consists of only the factors $F_1, \dots, F_m$. Then all functions in the model

$$\begin{aligned} Ey = b_0 + b_1^{(1)} f_1^{(1)}(X_1) + \dots + b_1^{(s_1-1)} f_1^{(s_1-1)}(X_1) + \\ \dots + b_m^{(1)} f_m^{(1)}(X_m) + \dots + b_m^{(s_m-1)} f_m^{(s_m-1)}(X_m) \end{aligned} \tag{4.4.4}$$

can be selected in such a way that the design **D** will be orthogonal for the model.

Let the values of the functions $f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ at the points of the design **D** form the matrix $\mathbf{F}_i$ of main effects of the factor F_i (§3 of chapter 3). Hence, the coefficient matrix **X** of the design **D** for the model (4.4.4) is

$$\mathbf{X} = \| \ \mathbf{I}, \mathbf{F}_1, \dots, \mathbf{F}_m \ \|.$$

All columns of **X** are pairwise orthogonal and scalar square of any of them equals N.

The covariance matrix of the vector of parameter estimates of the model (4.4.4) is

$$(\mathbf{X}^T\mathbf{X})^{-1}\sigma^2 = \frac{\sigma^2}{N}\mathbf{E}_k \quad \left(k = \sum_{i=1}^{m}(s_i - 1) + 1\right). \tag{4.4.5}$$

Let $\mathbf{x}(j_1, \dots, j_m) = \left[1, f_1^{(1)}\left(X_1^{j_1}\right), \dots, f_1^{(s_1-1)}\left(X_1^{(j_1)}\right), \dots, f_m^{(1)}\left(X_m^{j_m}\right), \dots, \ f_m^{(s_m-1)}\left(X_m^{(j_m)}\right)\right]$ be the vector of functions corresponding to the levels $j_1, \dots, j_m$ of the factors $F_1, \dots, F_m$ respectively. The variance at this point is

$$\sigma_{\mathbf{x}}^2 = \mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}\sigma^2 = \frac{\sigma^2}{N}\mathbf{x}^T\mathbf{x}.$$

The normalized (per one treatment combination) variance at this point is $\bar{\sigma}_{\mathbf{x}}^2 = \sigma^2\mathbf{x}^T\mathbf{x}$.

Consider the matrix

$$\boldsymbol{\Phi}_i = \| \ \mathbf{I}, \mathbf{F}_i \ \| = \left\| \begin{array}{c} \mathbf{a}_i^{0^T} \\ \vdots \\ \mathbf{a}_i^{0^T} \\ \vdots \\ \mathbf{a}_i^{s_i-1^T} \\ \vdots \\ \mathbf{a}_i^{s_i-1^T} \end{array} \right\| = \left\| \begin{array}{cc} 1 & \mathbf{c}_i^{0^T} \\ \vdots & \vdots \\ 1 & \mathbf{c}_i^{0^T} \\ \vdots & \vdots \\ 1 & \mathbf{c}_i^{s_i-1^T} \\ \vdots & \vdots \\ 1 & \mathbf{c}_i^{s_i-1^T} \end{array} \right\| \begin{array}{l} \left.\vphantom{\begin{array}{c}1\\ \vdots\\ 1\end{array}}\right\} n_i^{(0)} \\ \vdots \\ \left.\vphantom{\begin{array}{c}1\\ \vdots\\ 1\end{array}}\right\} n_i^{(s_i-1)} \end{array}.$$

Then

$$\boldsymbol{\Phi}_i^T \boldsymbol{\Phi}_i = N\mathbf{E}_{s_i}. \tag{4.4.6}$$

Now introduce the following matrix:

$$\widetilde{\boldsymbol{\Phi}}_i = \left\| \begin{array}{c} \sqrt{n_i^{(0)}}\mathbf{a}_i^{0^T} \\ \vdots \\ \sqrt{n_i^{(s_i-1)}}\mathbf{a}_i^{s_i-1^T} \end{array} \right\|.$$

$\widetilde{\boldsymbol{\Phi}}_i$ is a square matrix of order s_i. It follows from (4.4.6) that

$$\widetilde{\boldsymbol{\Phi}}_i^T \widetilde{\boldsymbol{\Phi}}_i = N\mathbf{E}_{s_i}.$$

Therefore,

$$\mathbf{a}_i^{j_iT}\mathbf{a}_i^{j_i} = \frac{N}{n_i^{(j_i)}}, \quad \mathbf{c}_i^{j_iT}\mathbf{c}_i^{j_i} = \frac{N}{n_i^{(j_i)}} - 1. \tag{4.4.7}$$

By (4.4.2) and (4.4.7),

$$\begin{aligned} \frac{\overline{\sigma}_{\mathbf{x}}^2}{\sigma^2} &= \mathbf{x}^T\mathbf{x} = 1 + \mathbf{c}_1^{j_1\mathrm{T}}\mathbf{c}_1^{j_1} + \cdots + \mathbf{c}_m^{j_m\mathrm{T}}\mathbf{c}_m^{j_m} \\ &= 1 + \left(\frac{N}{n_1^{(j_1)}} - 1\right) + \cdots + \left(\frac{N}{n_m^{(j_m)}} - 1\right) \\ &= 1 + \textstyle\sum_{i=1}^m (s_i - 1)\ U_i^{j_i}. \end{aligned} \tag{4.4.8}$$

Therefore, the normalized variance at any point $\mathbf{x}(j_1, \dots, j_m)$ of $\mathbf{D}^f$ can be expressed via the coefficient of uniformity of the levels $j_1, \dots, j_m$ of the factors $F_1, \dots, F_m$ respectively.

Calculate the sum of the normalized variances over all points of $\mathbf{D}^f$:

$$\sigma^2 \left\{ \textstyle\sum_{\mathbf{D}^f} \left(\frac{N}{n_1^{(j_1)}} - 1\right) + \cdots + \sum_{\mathbf{D}^f} \left(\frac{N}{n_m^{(j_m)}} - 1\right) + s_1 \dots s_m \right\}$$

$$= \sigma^2 \left\{ s_2 \dots s_m \sum_{j_1=0}^{s_1-1} \left(\frac{N}{n_1^{(j_1)}} - 1 \right) + \dots \right.$$
$$\left. + s_1 \dots s_{m-1} \sum_{j_m=0}^{s_m-1} \left(\frac{N}{n_m^{(j_m)}} - 1 \right) + s_1 \dots s_m \right\}.$$

The average normalized variance over $\mathbf{D}^f$

$$\bar{\sigma}_a^2 = \sigma^2 \sum_{\mathbf{D}^f} \frac{\mathbf{x}^T \mathbf{x}}{s_1 \dots s_m} = \sigma^2 \left\{ \frac{1}{s_1} \sum_{j_1=0}^{s_1-1} \left(\frac{N}{n_1^{(j_1)}} - 1 \right) + \cdots \right.$$
$$\left. + \frac{1}{s_m} \sum_{j_m=0}^{s_m-1} \left(\frac{N}{n_m^{(j_m)}} - 1 \right) + 1 \right\}. \tag{4.4.9}$$

Denote

$$A_i = \frac{\sigma^2}{s_i} N \left(\sum_{j_i=0}^{s_i-1} \frac{1}{n_i^{(j_i)}} - s_i \right)$$

and call it an average (over $\mathbf{D}^f$) normalized (per one treatment combination) variance for the factor F_i. Then (4.4.9) implies that

$$\bar{\sigma}_a^2 = \sigma^2 \sum_{\mathbf{D}^f} \mathbf{x}^T \mathbf{x} / (s_1 \dots s_m) = 1 + \sum_{i=1}^m A_i.$$

It is evident that

$$A_i = (s_i - 1) U_i \sigma^2.$$

Hence,

$$\bar{\sigma}_a^2 = \sigma^2 \{ 1 + \sum_{i=1}^m (s_i - 1) U_i \}, \tag{4.4.10}$$

Therefore, the average normalized variance is expressed via the coefficients of uniformity of factors.

In uniform regular designs, $U_i = 1 \quad (i = 1, \dots, m)$, therefore, for such designs

$$\bar{\sigma}_a^2 = \sigma^2 \{ 1 + \sum_{i=1}^m (s_i - 1) \} = k\sigma^2.$$

In nonuniform regular designs, $U_i > 1$ for some of i, therefore, for such designs $\bar{\sigma}_a^2 > k\sigma^2$.

Consider a regular design $\mathbf{D}$ for a factorial model for a factorial set Ω.

Let

$$\mathbf{x}(j_1, \dots, j_m) = \left[1, f_1^{(1)}\left(X_1^{(j_1)}\right), \dots, f_1^{(s_1-1)}\left(X_1^{(j_1)}\right), \dots, f_m^{(1)}\left(X_m^{(j_m)}\right), \dots, \right.$$
$$f_m^{(s_m-1)}\left(X_m^{(j_m)}\right), f_{i_1}^{(1)}\left(X_{i_1}^{(j_{i_1})}\right) f_{i_2}^{(1)}\left(X_{i_2}^{(j_{i_2})}\right), \dots,$$
$$\left. f_{i_1}^{(s_{i_1}-1)}\left(X_{i_1}^{(j_{i_1})}\right) f_{i_2}^{(s_{i_2}-1)}\left(X_{i_2}^{(j_{i_2})}\right), \dots \right]^T.$$

Then

$$\sigma_{\mathbf{x}}^2 = \frac{\sigma^2}{N}\mathbf{x}^T\mathbf{x}. \tag{4.4.11}$$

Similar to (4.4.8), we can get the following:

$$\begin{aligned}\bar{\sigma}_{\mathbf{x}}^2 &= \sigma^2\left\{1 + \sum_{i=1}^m \mathbf{c}_i^{j_i T}\mathbf{c}_i^{j_i} + \sum_{i_1,i_2}\left(\mathbf{c}_{i_1}^{j_{i_1}} \otimes \mathbf{c}_{i_2}^{j_{i_2}}\right)^T\left(\mathbf{c}_{i_1}^{j_{i_1}} \otimes \mathbf{c}_{i_2}^{j_{i_2}}\right) + \cdots\right\} \\ &= \sigma^2\left\{1 + \sum_{i=1}^m \mathbf{c}_i^{j_i T}\mathbf{c}_i^{j_i} + \sum_{i_1,i_2}\left(\mathbf{c}_{i_1}^{j_{i_1} T}\mathbf{c}_{i_2}^{j_{i_2}}\right)\left(\mathbf{c}_{i_2}^{j_{i_2} T}\mathbf{c}_{i_2}^{j_{i_2}}\right) + \cdots\right\} \\ &= \sigma^2\left\{1 + \sum_{i=1}^m (s_i - 1)U_i^{j_i} + \sum_{i_1,i_2}(s_{i_1} - 1)(s_{i_2} - 1)U_{i_1}^{j_{i_1}}U_{i_2}^{j_{i_2}} + \cdots\right\}.\end{aligned} \tag{4.4.12}$$

Similar to (4.4.9), for the design under consideration, we can calculate the average (over $\mathbf{D}^f$) normalized variance:

$$\bar{\sigma}_a^2 = \sigma^2\{1 + \frac{1}{s_1}\sum_{j_1=0}^{s_1-1}\left(\frac{N}{n_1^{(j_1)}} - 1\right) + \cdots + \frac{1}{s_m}\sum_{j_m=0}^{s_m-1}\left(\frac{N}{n_m^{(j_m)}} - 1\right)$$
$$\left. + \sum_{i_1,i_2}\frac{1}{s_{i_1}s_{i_2}}\sum_{j_{i_1}=0}^{s_{i_1}-1}\left(\frac{N}{n_{i_1}^{(j_{i_1})}} - 1\right)\sum_{j_{i_2}=0}^{s_{i_2}-1}\left(\frac{N}{n_{i_2}^{(j_{i_2})}} - 1\right) + \cdots\right\}.$$

Taking into account (4.4.3), we get

$$\bar{\sigma}_a^2 = \sigma^2\{1 + \sum_{i=1}^m (s_i - 1)U_i + \sum_{i_1,i_2}(s_{i_1} - 1)(s_{i_2} - 1)U_{i_1}U_{i_2} + \cdots\}$$

It is evident that in uniform regular designs, $\bar{\sigma}_a^2 = \sigma^2 k,$ where k is the number of parameters of the model; in nonuniform regular designs, $\bar{\sigma}_a^2 > \sigma^2 k.$

Consider the following efficiency function related to the criterion of the average variance:

$$\varphi = \frac{k\sigma^2}{\bar{\sigma}_a^2}.$$

Then for uniform regular designs, $\varphi = 1$. For nonuniform regular designs, $\varphi < 1$. Hence,

$$\varphi \leq 1\,. \tag{4.4.13}$$

Therefore, it makes sense to express the efficiency function related to the criterion of the average variance as $\varphi 100\%$.

Emphasize that (4.4.13) holds only for factorial models and designs. In connection with the last comment, consider the following example.

Example 4.4.1. In the domain

$$0 \leq X_i \leq 1 \quad (i = 1, 2, 3),$$

consider the design

$$\begin{array}{ccc} X_1 & X_2 & X_3 \\ \end{array}$$
$$\begin{Vmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{Vmatrix}$$

for the model

$$Ey = b_1X_1 + b_2X_2 + b_3X_3. \tag{4.4.14}$$

It can be verified that this design is *D*-optimal. The lack of an absolute term makes the model "nonfactorial". And, therefore, we should not expect that (4.4.13) still holds. Calculate now the variances of estimates of the regression function (divided by σ^2) at 8 points of $\mathbf{D}^f$. They are 1, 1, 1, 3/4, 3/4, 3/4, 3/4, 0. The average variance is $6\sigma^2/8$. Hence, an efficiency of the design equals 133%.

§ 5. *D*-optimality of Regular Factorial Designs

In this paragraph we will obtain conditions under which regular factorial designs are D-optimal [3] and establish the relationship with other criteria of optimality.

First, consider the regular design of main effects for the model (4.4.4). It follows from (4.4.8) that for a uniform design, a normalized variance at any point $\mathbf{x}$ (in particular, at any point of the design $\mathbf{D}$) is equal to the number of parameters to be estimate:

$$k = 1 + \textstyle\sum_{i=1}^{m}(s_i - 1),$$

i.e., maximum of a normalized variance over $\mathbf{D}^f$ is reached at points of the design $\mathbf{D}$. Hence, the design $\mathbf{D}$ is *D*-optimal on $\mathbf{D}^f$.

Assume that in the design $\mathbf{D}$, at least one factor, say F_1, is nonuniform. For each factor, select the level with the maximum value of coefficient of uniformity. Let these levels be $j_1, \dots, j_m$. Since

$$U_1^{j_1} > 1, \quad U_i^{j_i} \geq 1 \quad (i = 2, \dots, m),$$

it follows from (4.4.8) that $\bar{\sigma}^2_{\mathbf{x}(j_1,\dots,j_m)} > k\sigma^2$. Therefore, a nonuniform regular design cannot be *D*-optimal for the model (4.4.4.) even on $\mathbf{D}^f$. Hence, the following theorem has been proved.

Theorem 4.5.1. A regular factorial design of main effects is *D*-optimal for the model (4.4.4) on $\mathbf{D}^f$ if and only if it is uniform.

Suppose that the functions $f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ in the model (4.4.4) form a set of orthogonal polynomials in X_i at the points of the design $\mathbf{D}$ such that (4.4.5) holds. Denote by a_i and b_i minimal and maximum values of the variable X_i respectively. The property of D-optimality of the design on $\mathbf{D}^f$, by Theorem 4.5.1, holds for any choice of values of X_i for each of levels of the factor F_i.We will now try to answer the question how to select the values of X_i to ensure that the resulting design is optimal on the cube $a_i \leq X_i \leq b_i$. Hereafter, without loss of generality, we will consider a design on the cube $-1 \leq X_i \leq 1$.

Let **D** be the regular uniform design for the quantitative factors $F_1, \dots, F_m$ for the model of main effects. Let s_i values $X_i^{(0)}, \dots, X_i^{(s_i-1)}$ of the variable X_i that appear in the design **D** be the following: endpoints of the interval $[-1, 1]$ and roots of the first derivative of the $(s_i - 1)$-th Legendre polynomial. Well known [4, 5] that the one-dimension design on interval $[-1, 1]$ that consists of these s_i points is a *D*-optimal for the model

$$Ey = b_0 + b_i^{(1)} f_i^{(1)}(X_i) + \cdots + b_i^{(s_i-1)} f_i^{(s_i-1)}(X_i).$$

That implies the following:

$$\max_{X_i \in [-1,+1]} \sum_{j=1}^{s_i-1} \left[f_i^{(j)}(X_i) \right]^2 = s_i - 1, \tag{4.5.1}$$

The maximum in (4.5.1) is reached on interval $[-1, 1]$ at the points $X_i^{(0)}, \dots, X_i^{(s_i-1)}$. For the design **D** the normalized variance at the point

$$\mathbf{x}^T = \left[1, f_1^{(1)}(X_1), \dots, f_1^{(s_1-1)}(X_1), \dots, f_m^{(1)}(X_m), \dots, f_m^{(s_m-1)}(X_m) \right],$$

by (4.4.5), is equal to

$$\bar{\sigma}_{\mathbf{x}}^2 = \left\{ 1 + \sum_{j=1}^{s_1-1} \left[f_1^{(j)}(X_1) \right]^2 + \cdots + \sum_{j=1}^{s_m-1} \left[f_m^{(j)}(X_m) \right]^2 \right\} \sigma^2.$$

Taking into account (4.5.1), we get that

$$\max_{X_i \in [-1,+1]} \bar{\sigma}_{\mathbf{x}}^2 = \sigma^2 \{ 1 + \sum_{i=1}^{m} (s_i - 1) \} = \sigma^2 k.$$

Therefore, the design **D** is *D*-optimal. The design **D** is also *D*-optimal for the model, obtained from the model (4.4.4) by a linear transformation of its functions. Hence, the following theorem has been proved.

Theorem 4.5.2. Consider a regular design **D** of main effects for the factors $F_1, \dots, F_m$ with the $s_1, \dots, s_m$ levels respectively for the model (4.4.4), where $f_i^{(j)}(X_i)$ is polynomial in X_i of degree *j*. Suppose that the variables X_i take s_i values at the endpoints of the interval $[-1, +1]$ and at roots of the first derivative of the $(s_i - 1)$-th Legendre polynomial. Then the design **D** is *D*-optimal for the model (4.4.4) on the cube $-1 \leq X_i \leq +1$ if and only if it is uniform.

Example 4.5.1. Consider the model

$$Ey = \theta_0 + \theta_1 x_1 + \theta_{11} x_1^2 + \theta_{111} x_1^3$$
$$+\theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4 + \theta_5 x_5. \quad (4.5.2)$$

Using the condition of proportional frequencies, it is easy to show that the design

$$\mathbf{D} = \begin{Vmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 2 & 1 & 0 & 1 & 0 \\ 3 & 0 & 0 & 1 & 1 \\ 3 & 1 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{Vmatrix}$$

is a regular uniform factorial design of main effects for one four-level and four two-level factors. Hence, the *D*-optimal design on the $[-1, +1]$-cube for the model (4.5.2) is

$$\mathbf{D}' = \begin{Vmatrix} -1 & -1 & -1 & -1 & -1 \\ -1/\sqrt{5} & 1 & -1 & -1 & 1 \\ +1/\sqrt{5} & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ +1/\sqrt{5} & -1 & 1 & -1 & 1 \\ -1/\sqrt{5} & -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 \end{Vmatrix}.$$

This design is presented in Figure 2.

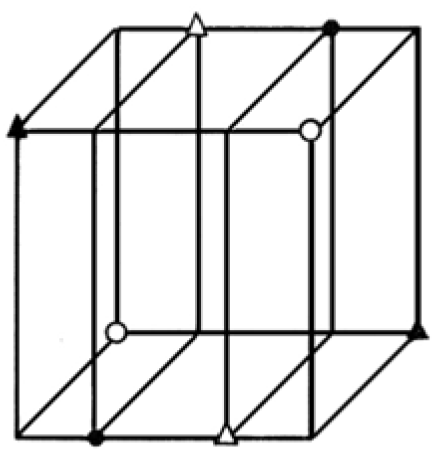

Figure 2. *D*-optimal design for the model (4.5.2)

Figure 2 plots x_1 on the abscissa axis, x_2 on the ordinate axis, x_3 on the applicate axis; circles and triangles indicate that x_4 takes the values -1 and +1 respectively; light and dark shapes indicate that x_5 takes the values -1 and +1 respectively.

Consider now the regular design **D** for the factorial set Ω for the A^{Ω}-model:

$$\begin{aligned}
Ey &= b_0 + b_1^{(1)} f_1^{(1)}(X_1) + \cdots + b_1^{(s_1-1)} f_1^{(s_1-1)}(X_1) + \cdots \\
&+ b_m^{(1)} f_m^{(1)}(X_m) + \cdots + b_m^{(s_m-1)} f_m^{(s_m-1)}(X_m) \\
&+ \sum\nolimits_{i_1,i_2} \Big[b_{i_1 i_2}^{(1,1)} f_{i_1}^{(1)}(X_{i_1}) f_{i_2}^{(1)}(X_{i_2}) + \cdots \\
&+ b_{i_1 i_2}^{(s_{i_1}-1,\ s_{i_2}-1)} f_{i_1}^{(s_{i_1}-1)}(X_{i_1}) f_{i_2}^{(s_{i_2}-1)}(X_{i_2}) \Big] + \cdots
\end{aligned} \tag{4.5.3}$$

It follows from (4.4.12) that for the uniform design, normalized variance at any point $\mathbf{x} \in \mathbf{D}^f$ (in particular, at any point of the design **D**) is equal to the number of parameters to be estimated. Therefore, the design **D** is *D*-optimal in the domain $\mathbf{D}^f$. On the other hand, by (4.4.12), if at least one factor of the design **D** is nonuniform, there exists the point $\mathbf{x} \in \mathbf{D}^f$ for which the normalized variance exceeds the number of parameters. Hence, a nonuniform design cannot be *D*-optimal for the model (4.5.3) even on the $\mathbf{D}^f$. Therefore, the following theorem has been proved.

Theorem 4.5.3. A regular factorial design for the factorial set Ω is *D*-optimal for the factorial A^{Ω}-model on $\mathbf{D}^f$ if and only if it is uniform.

Let the function $f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ be the set of orthogonal polynomials in X_i at points of the design **D**. X_i is defined on the interval $[-1, +1]$. A property of *D*-optimality of a regular design for the factorial set Ω on $\mathbf{D}^f$ does not depend on the values X_i for each of s_i levels of the factor. We will find the set of the values X_i that makes the design *D*-optimal on the cube $-1 \le X_i \le +1$.

Consider a regular uniform design for the factorial set Ω. Assume that s_i different values $X_i^{(0)}, \dots, X_i^{(s_i-1)}$ of variable X_i in the design **D** are the endpoints of the interval $[-1, +1]$ and the roots of the first derivative of the $(s_i - 1)$-th Legendre polynomial on this interval.

For the design **D** for A^{Ω}-model (4.5.3), the normalized variance at the point

$$\mathbf{x}^T = [1, f_1^{(1)}(X_1), \dots, f_1^{(s_1-1)}(X_1), \dots, f_m^{(1)}(X_m), \dots, f_m^{(s_m-1)}(X_m),$$
$$f_{i_1}^{(1)}(X_{i_1}) f_{i_2}^{(1)}(X_{i_2}), \dots, f_{i_1}^{(s_{i_1}-1)}(X_{i_1}) f_{i_2}^{(s_{i_2}-1)}(X_{i_2})\Big]$$

equals, by (4.4.11),

$$\bar{\sigma}_{\mathbf{x}}^2 = \sigma^2 \Big\{ 1 + \textstyle\sum_{j=1}^{s_1-1} \Big[f_1^{(j)}(X_1)\Big]^2 + \dots + \sum_{j=1}^{s_m-1} \Big[f_m^{(j)}(X_m)\Big]^2$$
$$+ \textstyle\sum_{i_1,i_2} \Big\{ \sum_{j=1}^{s_{i_1}-1} \Big[f_{i_1}^{(j)}(X_{i_1})\Big]^2 \sum_{j=1}^{s_{i_2}-1} \Big[f_{i_2}^{(j)}(X_{i_2})\Big]^2 \Big\} + \cdots \Big\}.$$

Taking into account (4.5.1), we get

$$\max_{X_i \in [-1,+1]} \bar{\sigma}_{\mathbf{x}}^2$$
$$= \sigma^2 \{ 1 + \textstyle\sum_{i=1}^m (s_i - 1) + \sum_{i_1,i_2} (s_{i_1} - 1)(s_{i_2} - 1) + \cdots \} = k\sigma^2.$$

Therefore, the design **D** is *D*-optimal. The design **D** is also *D*-optimal for the model obtained from the model (4.5.3) by linear nonsingular transformation of the set its functions. Hence, the following theorem has been proved.

Theorem 4.5.4. Let $f_i^{(j)}(X_i)$ in the A^Ω-model (4.5.3) be a polynomial in X_i of degree *j*. Then the regular factorial design **D** for the factorial set Ω with the variables X_i that have s_i different values at the endpoints of the interval $[-1, +1]$ and at the roots of the first derivative of the $(s_i - 1)$-th Legendre polynomial is *D*-optimal for the A^Ω-model (4.5.3) on the cube $-1 \le X_i \le +1$ if and only if the design **D** is uniform.

Let $\mathbf{D}_i$ be a *D*-optimal uniform design with s_i runs on the interval $[-1, +1]$ for the model

$$Ey = b_0 + b_i^{(1)} f_i^{(1)}(X_i) + \cdots + b_i^{(s_i-1)} f_i^{(s_i-1)}(X_i).$$

The following theorem is a generalization of Theorem 4.5.4 and can be proved analogously.

Theorem 4.5.5. A regular factorial design **D** for the factorial set Ω where for each i $(i = 1, \dots, m)$ s_i levels of the variables X_i match with s_i levels of the variables of the design $\mathbf{D}_i$, is a *D*-optimal for the A^Ω-model (4.5.3) on the cube $-1 \le X_i \le +1$ if and only if the design **D** is uniform.

Theorem 4.5.6. The *D*-optimal regular uniform design **D** from Theorem 4.5.5 is *Q*-optimal and *A*-optimal if the set of the functions $f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ satisfies the condition (4.4.1).

P r o o f. The theorem is a corollary to Theorem 2.11.1 of the book [2] and the results of this chapter.

Now consider the mixed factorial G^{Ω}-model for the factorial set Ω for the qualitative factors $F_1, \dots, F_n$ and the quantitative factors $F_{n+1}, \dots, F_m$:

$$\mathrm{E}y = \mathbf{f}^T(X_1, \dots, X_m)\mathbf{\Theta}. \tag{4.5.4}$$

The domain is defined as follows:

$$F_j = 0, 1, \dots, s_j - 1 \quad (j = 1, \dots, n),$$
$$-1 \le X_i \le 1 \quad (i = n + 1, \dots, m). \tag{4.5.5}$$

It follows from §11 of chapter 3 that for a k-dimensional vector $\mathbf{\Theta}$ of parameters of the G^{Ω}-model, the following equality holds:

$$\mathbf{T\Theta} = \mathbf{0} \;\; (Rg\mathbf{T} = q). \tag{4.5.6}$$

Let the general solution of (4.5.6) be

$$\mathbf{\Theta} = \mathbf{Q}\boldsymbol{\theta}_m,$$

where $\mathbf{Q}$ is a k x $(k - q)$matrix; $Rg\mathbf{Q} = k - q, \mathbf{TQ} = \mathbf{0}$; $\boldsymbol{\theta}_n$ is the vector of $k - q$ elements, which are the new parameters. The value $k - q$ can be calculated based on Theorem 3.9.2. After the reparametrization we will have the following model:

$$\mathrm{E}y = \mathbf{f}^T(X_1, \dots, X_m)\mathbf{Q}\boldsymbol{\theta}_m. \tag{4.5.7}$$

For different new parameters $\boldsymbol{\theta}_n$, we will have different matrices $\mathbf{Q}$, related to each other by linear nonsingular transformations. This is equivalent to linear nonsingular transformations of the set of functions of the model (4.5.7). Property of *D*-optimality is invariant to such transformations. In view of the last remark, we give the following definition.

Definition 4.5.1. The design **D** is called *D*-optimal for the G^{Ω}-model with the restrictions (4.5.6) on (4.5.5) if it *D*-optimal for any model (4.5.7) that is the result of reparametrization of the model (4.5.4).

Let **D** be a regular uniform design for the factorial set Ω for the qualitative factors $F_1, \dots, F_n$ and quantitative factors $F_{n+1}, \dots, F_m$. Assume that the functions $f_i^{(1)}(X_i), \dots, f_i^{(s_i-1)}(X_i)$ (which are included to the G^{Ω}-model for quantitative factors) are pairwise orthogonal so that condition (4.4.1) holds. Then, by using methods similar to those in §4 and §5 of chapter 4, we can show that the normalized (per one treatment combination) variance of the estimate of the regression function at the point $(j_1, \dots, j_n, \mathrm{X}_{n+1}, \dots, X_m)$ is equal to

$$\sigma_a^2(j_1, \dots, j_n, X_{n+1}, \dots, X_m) = \sigma^2 \Big\{1 + \textstyle\sum_{j=1}^{s_1-1}[f_{n+1}^{(j)}(X_{n+1})]^2 + \cdots$$
$$+ \textstyle\sum_{j=1}^{s_{m}-1}[f_{m}^{(j)}(X_{m})]^2 + (s_1 - 1) + \cdots + (s_n - 1) + \qquad (4.5.8)$$
$$\textstyle\sum_{i_1,i_2}(s_{i_1} - 1)\sum_{j=1}^{s_{i_2}-1}[f_{i_2}^{(j)}(X_{i_2})] + \cdots \Big\}.$$

If the variables X_i take s_i values at the points of the design $\mathbf{D}_i$, then, by (4.5.8) and Theorem 3.9.2,

$$\sigma_a^2(j_1, \dots, j_n, X_{n+1}, \dots, X_m,)$$
$$= \sigma^2[1 + \textstyle\sum_{i=1}^{m}(s_i - 1) + \sum_{i_1,i_2}(s_{i_1} - 1)(s_{i_2} - 1) + \dots] \qquad (4.5.9)$$
$$= \sigma^2(k - q).$$

The multiplier $k - q$ in (4.5.9) matches with the number of parameters of the model (4.5.7). Now it is evident that by using the line of the proof of Theorem 4.5.4, we can prove the following generalization of Theorem 4.5.5.

Theorem 4.5.7. Let the design **D** be a regular factorial design for the factorial set Ω for the quantitative variables $X_1, \dots, X_m$ and the qualitative factors $F_{m+1}, \dots, F_n$. Let for each i $(i = 1, \dots, m)$, s_i levels of the variables X_i match with s_i levels of the variables of the design $\mathbf{D}_i$. Then the design **D** is *D*-optimal for the G^{Ω}-model (4.5.4) with the restrictions (4.5.6) on (4.5.5) if and only if it is uniform.

Note to Theorem 4.5.7. It is easy to prove that for the design **D** from Theorem 4.5.7, a statement similar to Theorem 4.5.6 holds.

The results of this chapter provide a justification for the applicability of the criterion of regularity in the design of experiments.

§ 6. *BG*-Criterion

A geometric interpretation of *D*-optimal (and close to *D*-optimal) designs is based on the volume of a multi-dimensional ellipsoid. This interpretation does not give a clear understanding on a relative effectiveness of designs when we want to compare them. In this paragraph we will consider a transformation that reduces the multi-dimensional characteristic of +*D*-optimality to the linear one. The transformation was introduced by V.Z. Brodsky and T.I. Golikova [6]. It is applicable not only to factorial models but also to other polynomial model.

Consider one preliminary example (from the original paper [6]) for the design of second order. Let $\mathbf{D}^*$ be the *D*-optimal design on the cube

$$-1 \le X_i \le 1 \ \ (i = 1, \dots, 7)$$

for the polynomial model of second order. Let $\mathbf{M}^*$ be the information matrix of the design $\mathbf{D}^*$.

For the same model, consider another design $\mathbf{D_1}$ obtained by multiplication of all coordinates of any point of $\mathbf{D}^*$ by 0.99. Practically, these two designs can be regarded as "almost the same".

It is easy to calculate that

$$detM_1 = 0.28 \cdot det\mathbf{M}^*,$$

where M_1 is an information matrix for the design D_1.

Hence, the design $\mathbf{D_1}$ is "three times worse" than the design $\mathbf{D}^*$ (based on determinant of information matrix). Therefore, it is obvious that it does not make much sense to compare designs based on the determinant of the information matrix. This is not surprising: the clarity of the comparison is lost in moving to multidimensional characteristics. Therefore, all criteria are usually reduced to linear characteristics.

It is for this reason that a number of authors performs certain transformations on this criterion (the determinant of the information matrix). The most popular transformation is a root of degree q. Some authors assume that $q = k$, where k is the number of parameters of the model. However, more often, they assume $q = 2k$. Now we will see what this yields for the example above.

It is easy to calculate that

$$\frac{(det\mathbf{M_1})^{1/k}}{(det\mathbf{M}^*)^{1/k}} 100\% = 96.5\%\,,$$

$$\frac{(det\mathbf{M_1})^{1/2k}}{(det\mathbf{M}^*)^{1/2k}} 100\% = 98.3\%\,.$$

I.e., the design that has to have an 99%-efficiency is interpreted as 96.5%-optimal (for $q = k$) or 98.3%-optimal (for $q = 2k$). The difference is not so big, especially for $q = 2k$. So it may seem that the transformation meets the goal. However, one more example will show that it does not.

In our example, replace the design $\mathbf{D_1}$ with the design $\mathbf{D_2}$ obtained by multiplication of all coordinates of any point of $\mathbf{D}^*$ by 0.90. It is easy to calculate that for $q = 2k$ it will be interpreted as 83%-optimal (instead of 90%-optimal) and for $q = k$, as 69%-optimal. It is possible to give even stronger examples.

It turns out that the use of these transformations only aggravates the situation. Indeed, since determinants of information matrices usually differ by several orders of magnitude, nobody wants to compare them. It is simply stated, instead, which is the greater. The transformations give the impression of comparability of criteria. The researcher might choose a not quite appropriate design (e.g., one with a large number of experiments) just because it has a "significantly" better characteristic than others, while in reality, the characteristics of all designs might be very close to each other.

Is it possible to find a transformation that never distort (in the sense mentioned above) characteristic of *D*-optimality? Such a transformation for polynomial models is a root of degree

$$q = 2n_1 + 4n_2 + \cdots + 2ln_l, \tag{4.6.1}$$

where n_i is the number of terms of order i in the model $(i = 1, \dots, l)$.

We will call a corresponding criterion the *BG*-criterion.

Denote the number of variables by m and the number of parameters of the model, by k. Then for the designs of the first order (for example, two-level factorial design of main effects), (4.6.1) will be as follows:

$$q = 2k - 2.$$

For designs of second order,

$$q = 4k - 2n - 4.$$

For the example under consideration, $q = 126$ (instead of usually used 36 and 72).

Therefore, *BG*-criterion of optimality of the design **D** (related to the criterion of *D*-optimality and expressed by determinant of the information matrix **M** of the design **D**) is:

$$\frac{(det\mathbf{M})^{1/q}}{(det\mathbf{M}^*)^{1/q}}\, 100\% \,, \tag{4.6.2}$$

where q is defined by (4.6.1).

Using (4.6.2), we get that the value of *BG*-criterion equals 99% for the design $\boldsymbol{D}_1$ and equals 90% for the design $\boldsymbol{D}_2$.

A geometric interpretation of the *BG*-criterion is obvious. If for the given design **D**, the value of *BG*-criterion equals, say, 95%, then a *D*-optimal design with coordinates of any points multiplied by 0.95 has the same determinant of information matrix as the design **D**.

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Chapter 5. Regular Designs

§ 1. Classification

In this paragraph we will consider various special cases of regular factorial designs and compare them with known combinatorial constructions.

Definition 5.1.1. A symmetrical design $s^m//N$ is called an orthogonal array of strength t and index λ and denoted by $(N,\ m,\ s,\ t)$ if for any t factors, the design contains all s^t different combinations of levels with the same frequency λ.

In combinatorial mathematics, the orthogonal arrays are usually considered in a transposed form.

It is evident that if a symmetrical regular factorial design of strength t is uniform, then for any t factors all s^t different combinations of levels occur with the same frequency.

Assume now that in a symmetrical design for any t factors, all s^t different combinations of levels occur with the same frequency. Consider all levels of the given factor. Then all s^{t-1} different combinations of the rest $t-1$ factors occur exactly λs times. Similarly, all s different levels of any factor occur exactly λs^{t-1} times. Therefore, the design is uniform and the condition of proportional frequencies (3.7.4) is satisfied. Indeed,

$$(\lambda s^t)^{t-1}\lambda = (\lambda s^{t-1})^t.$$

Therefore, the following theorem has been proved.

Theorem 5.1.1. A symmetrical regular uniform s-level factorial design with m factors and N runs of strength t is equivalent to an orthogonal array $(N,\ m,\ s,\ t)$ of strength t.

Definition 5.1.2. If for the orthogonal array $(N,\ m,\ s,\ t)$, the condition $\lambda = s^l$ (l integer) holds, the design is called a hypercube of strength t.

Definition 5.1.3. An $(s \times s)$-array filled with s integers $0,1,\dots,s-1$ is called a square of order s. A square is called a Latin square if each integer occurs exactly once in each row and exactly once in each column.

Definition 5.1.4. If in two squares of the same order, when superimposed on one another, every ordered pair of integers occurs exactly once, the two squares are called orthogonal.

There exists a pair of orthogonal squares (called standard) such that any of them is orthogonal to any Latin squares the same order. The first of standard squares has the first row of 0, the second row of 1, etc. The second standard square is the first standard square transposed.

Theorem 5.1.2. The total number of pairwise orthogonal Latin squares of order s is at most $s-1$.

A direct proof of Theorem 5.1.2 can be found in the book [1] by Raghavarao. However, we will give it here since it will become obvious after the proof of Theorem 5.1.3 and inequality (5.2.5).

Definition 5.1.5. A set of $s-1$ pairwise orthogonal Latin squares of order s is called a full set of orthogonal Latin squares.

The full set of orthogonal Latin squares and two standard squares form the set of $s+1$ pairwise orthogonal squares.

For $s=3$, an example of the set of four pairwise orthogonal squares is:

$$\begin{matrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 2 & 2 & 2 \end{matrix}, \quad \begin{matrix} 0 & 1 & 2 \\ 0 & 1 & 2 \\ 0 & 1 & 2 \end{matrix}, \quad \begin{matrix} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \end{matrix}, \quad \begin{matrix} 0 & 2 & 1 \\ 1 & 0 & 2 \\ 2 & 1 & 0 \end{matrix}. \tag{5.1.1}$$

Definition 5.1.6. A pair of orthogonal Latin squares is called a Graeco-Latin square if the integers of the first of the Latin squares are replaced with Latin letters and the integers of the second, by Greek letters. Similarly, a set of more than two pairwise orthogonal Latin squares is called a hyper-Graeco-Latin square.

Two orthogonal Latin squares in (5.1.1) can be represented by the following Graeco-Latin square:

$$\begin{matrix} a\alpha & b\gamma & c\beta \\ b\beta & c\alpha & a\gamma \\ c\gamma & a\beta & b\alpha \end{matrix}. \tag{5.1.2}$$

Transform every square of (5.1.1) to a vector-column, putting the second column of the square under the first one, and the third column of the square under the second one. As a result, we get four vector-columns forming, obviously, an orthogonal array (9, 4, 3, 2) of index 1, or a hypercube of strength 2:

$$\left\| \begin{matrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 2 & 0 & 2 & 2 \\ 0 & 1 & 1 & 2 \\ 1 & 1 & 2 & 0 \\ 2 & 1 & 0 & 1 \\ 0 & 2 & 2 & 1 \\ 1 & 2 & 0 & 2 \\ 2 & 2 & 1 & 0 \end{matrix} \right\|. \tag{5.1.3}$$

It is evident that rows any orthogonal array (9, 4, 3, *2)* can be arranged so that the first two columns match with the first two columns of (5.1.3). This gives us a method of construction the squares (5.1.1). Using similar constructions with n orthogonal Latin squares of order s, we get the following theorem.

Theorem 5.1.3 [2]. The existence of a set of n orthogonal Latin squares of order s is equivalent to the existence of an orthogonal array $(s^2,\ n+2,\ s,\ 2)$.

Latin squares, orthogonal Latin (Graeco-Latin and hyper-Graeco-Latin) squares have been generalized by Kishen [3, 4]. He introduced the concept of Latin cubes and hypercubes, orthogonal Latin (Graeco-Latin and hyper-Graeco-Latin) cubes and hypercubes.

Definition 5.1.7. Three-dimensional $(s \times s \times s)$-matrix consisting of s layers (squares) each having s row and s columns and filled with s integers $0,1,\dots,s-1$, is called a cube of side s. A cube is called a first order Latin cube of side s if each integer occurs exactly s times in each layer (square), in the i-th row of all squares $(i = 1,\dots,s)$, and in the j-th column of all squares $(j = 1,\dots,s)$. Two cubes of the same side are called orthogonal if when superimposed on one another, every ordered pair of integers occurs exactly s times.

There exist three pairwise orthogonal cubes (called standard) such that any of them is orthogonal to any of first order Latin cube of the same side. The standard cubes for $s = 2$ are presented in Figure 3. Their construction is similar for any s.

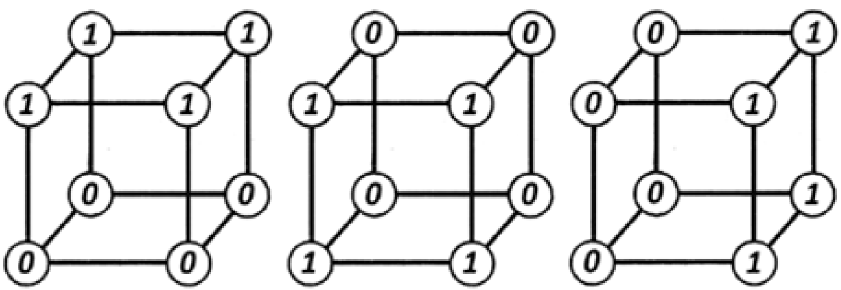


Figure. 3. Three standard pairwise orthogonal cubes of side 2

Definition 5.1.8. A pair of orthogonal Latin cubes is called a Graeco-Latin cube if the integers of the first of the Latin cubes are replaced with Latin letters and the integers of the second, with Greek letters. Similarly, a set of more than two pairwise orthogonal Latin cubes is called a hyper-Graeco-Latin cube.

An example of a first order Graeco-Latin cube of side 3 is presented in Figure 4.

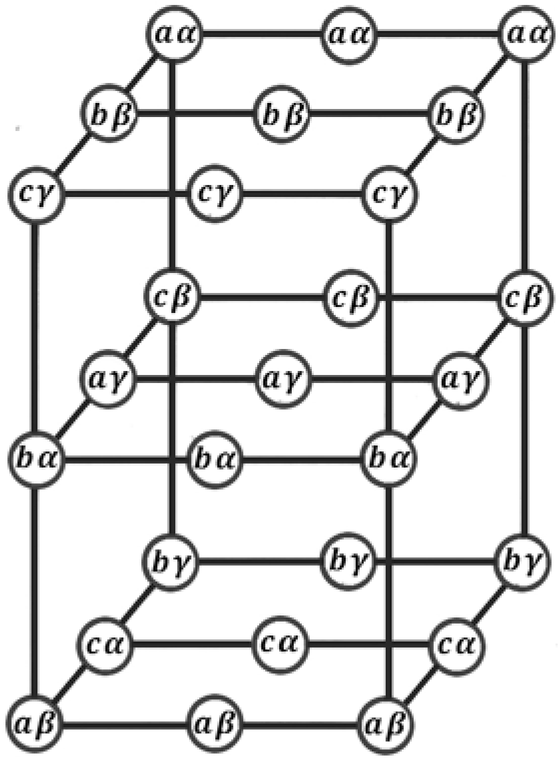


Figure 4. A first order Graeco-Latin cube of side 3

Consider a system of orthogonal Latin cubes together with three standard cubes. The same way as in the proof of Theorem 5.1.3, we can prove equivalence between the set of orthogonal cubes and some orthogonal array of strength 2. Hence, the following theorem holds.

Theorem 5.1.4. The existence of a set of n pairwise orthogonal first order Latin cubes of side s is equivalent to the existence of the orthogonal array $(s^3,\ n+3,\ s,\ 2)$.

Kishen proved [4] that the maximum number of pairwise orthogonal first order Latin cubes of side s equals (s^2+s-2). Together with the standard cubes, they form a set of (s^2+s+1) pairwise orthogonal cubes. A direct proof of this statement is omitted here because it will be evident after we establish inequality (5.2.5).

Theorems 5.1.3 and 5.1.4 are related to orthogonal arrays of strength 2 and index 1 and 5 respectively. Similar to definition of the first order cubes and standard cubes, it is possible to define the first order Latin hypercubes and standard hypercubes and establish equivalence of the existence of a set of n pairwise orthogonal first order l-dimensional hypercubes of side s and the existence of an orthogonal array $(s^l,\ n+1,\ s,\ 2)$ of strength 2 and index s^{l-2} $(l > 3)$.

Therefore, the concept of orthogonal first order Latin hypercubes, introduced by Kishen, fully covers the case of hypercubes of strength 2.

Consider an orthogonal array $(s^3,\ n+3,\ s,\ 3)$ of strength 3 and index 1, a set of n pairwise orthogonal first order Latin cubes (corresponding to the array $(s^3,\ n+3,\ s,\ 3)$ by Theorem 5.1.4), and three standard cubes. Since strength of the array equals 3, the following condition should be satisfied. In any three of $n+3$ cubes under consideration when superimposed on each other, every ordered combination of three integers occurs once. Now consider all cases when two of these three cubes are the standard ones. For any row (column) of any square of any of the superimposed cubes, there exist two standard cubes containing the same combinations in the given row (column). Hence, any row (column) of any of the superimposed cubes contains different integers. Therefore, any square of any of n Latin cubes is a Latin square.

Now consider all cases when one of three cubes is the standard one. For any square of any of the superimposed cubes, there exists a standard cube with the same integer for the given square. Therefore, all combinations of any of the squares of the rest two of the superimposed cubes are different. Hence, any pair of these superimposed cubes contains corresponding pairs of orthogonal Latin squares.

It is evident that we can construct an orthogonal array $(s^3,\ n+3,\ s,$ $3)$ based on the given set of n orthogonal first order Latin cubes of side s if the following three conditions hold:

a) in three Latin cubes (if any) when superimposed on each other, any ordered combination of integers occurs exactly once;

b) any square of any Latin cube is a Latin square;

c) any pair of Latin cubes contains corresponding pairs of orthogonal Latin squares.

Therefore, we have the following theorem.

Theorem 5.1.5. The existence of a set of n first order Latin cubes of side s satisfied the conditions a, b, and c is equivalent to the existence of the orthogonal array $(s^3, n+3, s, 3)$ of strength 3 and index 1.

An example of the set of three orthogonal first order Latin cubes (or hyper-Graeco-Latin cube) of side 4 satisfied the conditions a, b, and c and, therefore, equivalent to the orthogonal array (64, 6, 4, 3) is presented in Figure 5.

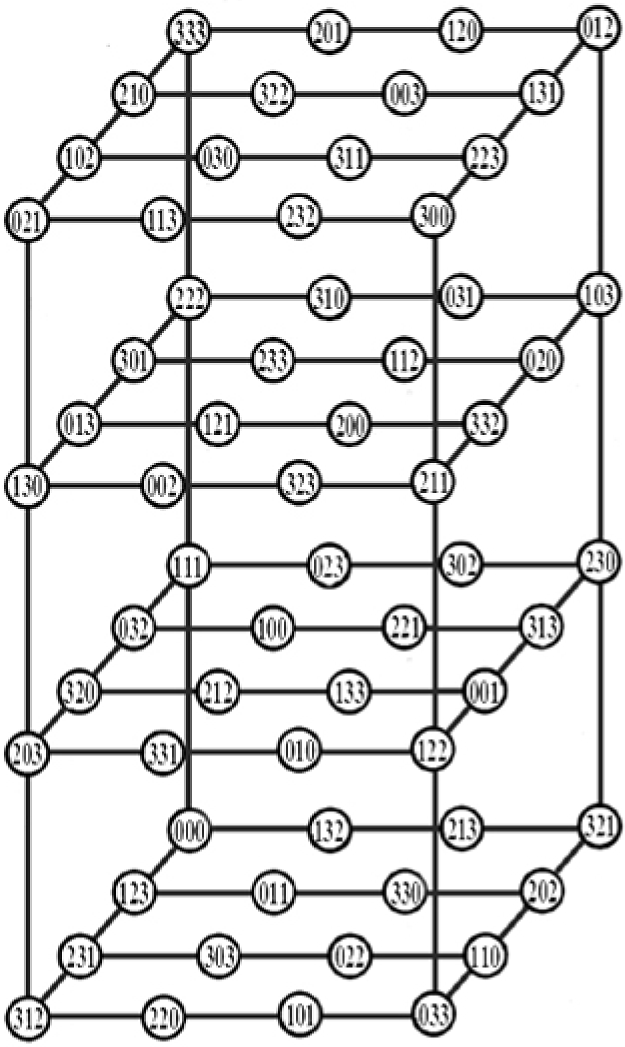


Figure 5. Hyper-Graeco-Latin first order cube of side 4 equivalent to orthogonal array (64, 6, 4, 3)

Definition 5.1.9. Three-dimensional $(s \times s \times s)$-matrix consisting of s layers (squares) each having s row and s columns and filled with $s^2 - 1$ integers $0,1,\ldots,s^2 - 1$ is called a Latin second order cube of side s if each integer occurs exactly once in each layer (square), in the i-th row of all squares ($i = 1, \dots, s$), and in the j-th column of all squares ($j = 1, \dots, s$).

It is evident that a pair of orthogonal second order Latin cube of side s does not exist, because the number of ordered pair of integers $0,1, \dots, s^2 - 1$ equals s^4 but the number of the positions in the cube equals s^3. However, the existence of a set of n first order Latin cubes and one second order Latin cube that are pairwise orthogonal is possible. Their existence is equivalent to the existence of the regular factorial design of strength 2 for $n + 3$ factors with s levels and one factor with s^2 levels.

An example of two orthogonal Latin cubes – a second order Latin cube of side 2 and a first order Latin cube of side 2 – is presented in Figure 6 (as a Graeco-Latin cube of side 2).

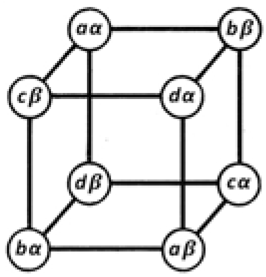


Figure 6. Orthogonal second order Latin cube of side 2 and first order Latin cube of side 2

This Graeco-Latin cube corresponds to regular factorial design $2^4 \times 4$ of strength 2:

$$\begin{Vmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 2 \\ 1 & 1 & 0 & 0 & 3 \\ 0 & 0 & 1 & 1 & 3 \\ 1 & 0 & 1 & 0 & 2 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{Vmatrix}.$$

Consider a regular factorial design **D** of strength 2 with N runs. We will not assume that the design is symmetrical or uniform. Let the design **D** contains m factors $F_1, \dots, F_m$ with the levels $s_1, \dots, s_m$ respectively; $N = s^2$; $s = s_1 = s_2 = \max_i\{s_i\}$. Assume that each level of the factors F_1 and F_2 occurs in the design s times. Fill a square matrix of size s with the levels of the factor F_3. We set the element of the i-th row and the j-th column ($i, j = 0,1, \dots, s - 1$) to be equal the level of F_3 that occurs with the j-th level of the factor F_2 and the i-th level of the factor F_1 in the design

D. Since the design **D** is regular (i.e., the proportional frequency condition is satisfied for any two factors) a given level of the factor F_3 occurs with each level of the factor F_1 the same number of times. A given level of the factor F_3 occurs with each level of the factor F_2 the same number of times. Therefore, in the square matrix, the n-th level of the factor F_3 occurs λ_n times in each row and in each column.

Definition 5.1.10. Let $C = (c_1, \dots, c_l)$ be an ordered set of l different elements and $\mathbf{A} = \{a_{ij}\}$ be a square matrix of order s $(a_{ij} \in C)$. Assume that c_n occurs exactly λ_n times ($\lambda_n > 0$) in each row and in each column of the matrix **A** for any $n = 1, \dots, l$. Then the matrix **A** is called a frequency square (or an F-square) on C of size s and with the frequency vector $(\lambda_1, \dots, \lambda_l)$.

An F-square of size s with the frequency vector $(\lambda_1, \dots, \lambda_l)$ is denoted by $F(s; \lambda_1, \dots, \lambda_l)$. The notation $F(s; \lambda^l)$ means frequency square $F(s; \lambda, \dots, \lambda)$.

A special case of an F-square is $F(s; 1^s)$, which, obviously, is a Latin square of order s.

An example of the frequency square $F(6; 2^3)$ on $C = (1, 2, 3)$:

$$\begin{matrix} 1 & 2 & 3 & 3 & 2 & 1 \\ 2 & 3 & 1 & 1 & 3 & 2 \\ 3 & 1 & 2 & 2 & 1 & 3 \\ 3 & 1 & 2 & 2 & 1 & 3 \\ 2 & 3 & 1 & 1 & 3 & 2 \\ 1 & 2 & 3 & 3 & 2 & 1 \end{matrix}.$$

Theorem 5.1.6 [5]. $F(s; \lambda_1, \dots, \lambda_l)$ square exists if and only if

$$s = \sum_{i=1}^{l} \lambda_i. \qquad (5.1.4)$$

P r o o f. Necessity of the condition (5.1.4) for the existence of the square $F(s; \lambda_1, \dots, \lambda_l)$ follows from the definition of an F-square. Now we will prove sufficiency of the condition (5.1.4). Construct a Latin square of order s, or a square $F(s; 1^s)$, on an ordered set $B = (b_1, \dots, b_s)$. Divide B into l different subsets $S_1, \dots, S_l$ such that S_i contains λ_i elements. Define the function f from B to C as follows:

$$f(x) = a_i \text{ if } x \in S_i \quad (i = 1, \dots, l).$$

Applying the function f to the elements of $F(s; 1^s)$, we get $F(s; \lambda_1, \dots, \lambda_l)$ on C.

The definition of orthogonal Latin squares can be generalized to F-squares.

Definition 5.1.11. Two F-squares $F(s; \lambda_1, \dots, \lambda_l)$ on $C = (c_1, \dots, c_l)$ and $F(s; \lambda'_1, \dots, \lambda'_l)$ on $C = (c'_1, \dots, c'_l)$ is called orthogonal if when superimposed on one another, every ordered pair c_i and c'_j occurs exactly $\lambda_i\lambda'_j$ times.

An example of the set of five pairwise orthogonal F-squares of order 4:

$$F(4;1^4) = \begin{matrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 3 & 2 \\ 2 & 3 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{matrix}; \quad F(4;2,1^2) = \begin{matrix} 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 2 & 0 & 1 & 0 \\ 0 & 1 & 0 & 2 \end{matrix};$$

$$F(4;2^2) = \begin{matrix} 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{matrix}; \quad F(4;2^2) = \begin{matrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{matrix};$$

$$F(4;2^2) = \begin{matrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{matrix}.$$

Consider again a regular factorial design **D** of strength 2. Fill a square matrix of size s with the levels of the factor F_4 similar to the factor F_3. The n-th level of the factor F_4 occurs in each row and in each column of the square matrix λ'_n times. The resulting matrix is the F-square on $C' = (c'_1, \dots, c'_l)$ with the frequency vector $(\lambda'_1, \dots, \lambda'_l)$. Superimpose $F(s;\lambda_1, \dots, \lambda_l)$ on $F(s;\lambda'_1, \dots, \lambda'_l)$. Based on the condition of proportional frequencies, the level c_i of the factor F_3 occurs with the level c'_j of the factor F_4 $\lambda_i\lambda'_j$ times. Therefore, these F-squares are orthogonal. With similar constructions for the rest factors of the design **D**, we get a set of $m-2$ pairwise orthogonal F-squares of order s.

It is evident that all constructions above with the regular design **D** are reversible. Therefore, the following theorem holds.

Theorem 5.1.7. The following two statements are equivalent:

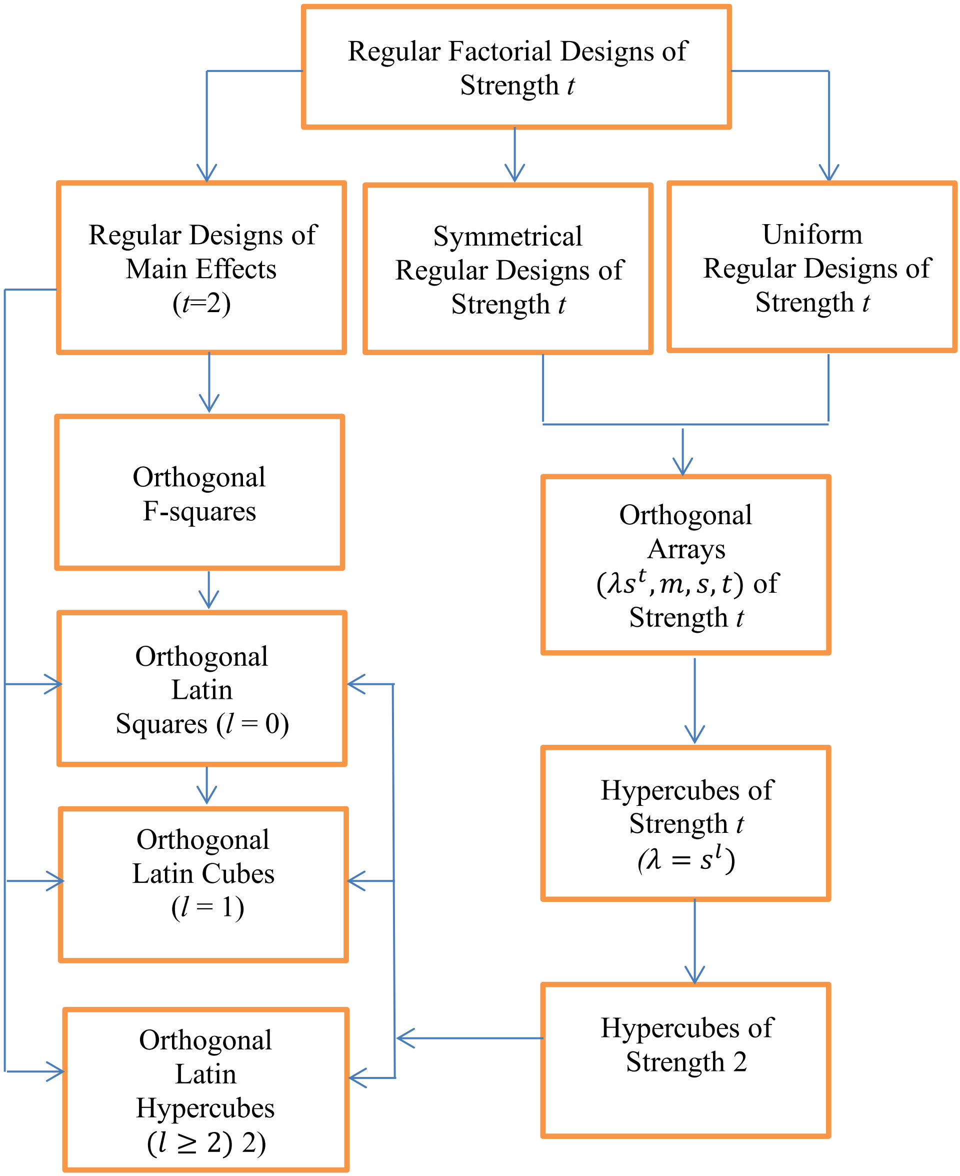
1) there exists a set of $m-2$ pairwise orthogonal frequency squares $F\left(s;\lambda_1^{(j)}, \dots, \lambda_{i_j}^{(j)}\right)$ $(j = 1, \dots, m-2)$;

2) there exists a regular factorial design $s^2 \times l_1 \times \dots \times l_{m-2}$ of strength 2 in s^2 runs.

One important special case of the set of orthogonal F-squares is introduced by the following definition.

Definition 5.1.12. Let $\mathbf{A}_1$ and $\mathbf{A}_2$ be orthogonal F-squares, and let $\mathbf{A}_1$ be a Latin square. Then $\mathbf{A}_2$ is called an orthogonal partition of the Latin square $\mathbf{A}_1$. Several pairwise orthogonal F-squares that are orthogonal partitions of a given Latin squares is called mutually orthogonal partitions of this F-squares.

Scheme below presents a relationship between various regular factorial designs.



§ 2. Bounds for Number of Factors and Number of Runs

Consider a regular factorial design of strength t with orthogonal matrices of effects. Let $n = [t/2]$, ($[t/2]$ is the integer part of $t/2$). By Theorem 4.1.1, if t is even, then **I** and all main effects and interaction effects up to order $n-1$ are orthogonal. Total number of these orthogonal vectors equals

$$1 + \sum_{i=1}^{m}(s_i - 1) + \sum_{i>j}(s_i - 1)(s_j - 1) + \cdots$$
$$+ \sum_{i_1 > \cdots > i_n}(s_{i_1} - 1) \dots (s_{i_n} - 1).$$

Hence, we get the inequality for the number of runs N:

$$N - 1 \geq \sum_{i=1}^{m}(s_i - 1) + \cdots + \sum_{i_1 > \cdots > i_n}(s_{i_1} - 1) \dots (s_{i_n} - 1). \qquad (5.2.1)$$

If t is odd, then, by Theorem 3.7.2, **I**, main effects and interaction effects up to order $n-1$, and all interaction effects of order n including one factor F (for example, with maximum number of levels $s_{\max}$) are orthogonal. Then, obviously, the following inequality holds:

$$\begin{aligned} N - 1 \geq &\sum_{i=1}^{m}(s_i - 1) + \cdots + \sum_{i_1 > \cdots > i_n}(s_{i_1} - 1) \dots (s_{i_n} - 1) \\ &+ \sum_{i_1 > \cdots > i_n}(s_{\max} - 1)(s_{i_1} - 1) \dots (s_{i_n} - 1). \end{aligned} \qquad (5.2.2)$$

For a special case of a symmetrical design, (5.2.1) and (5.2.2) become the inequalities obtained by Rao [6] for orthogonal arrays of strength t:

$$N - 1 \geq \sum_{i=1}^{n}\binom{m}{i}(s-1)^i, \qquad (5.2.3)$$

if t is even, and

$$N - 1 \geq \sum_{i=1}^{n}\binom{m}{i}(s-1)^i + \binom{m-1}{n}(s-1)^{n+1}, \qquad (5.2.4)$$

if t is odd.

It is evident that the following trivial inequality holds for regular factorial designs of strength t:

$$N \geq s_{i_1} \dots s_{i_t}$$

for any $i_1, \dots, i_t$.

A special case of (5.2.3) for $t = 2$ is inequality of Plackett and Burman [7]:

$$m \leq \left[\frac{\lambda s^2 - 1}{s - 1}\right], \qquad (5.2.5)$$

where λ is index of orthogonal array.

A special case of (5.2.4) for $t = 3$ is the following inequality:

$$m \leq \left[\frac{\lambda s^2-1}{s-1}\right] + 1. \qquad (5.2.6)$$

In the following four theorems we give some bounds for the number of factors of orthogonal arrays, omitting the proofs (they can be found in cited works).

The inequalities (5.2.5) and (5.2.6) can be extended for orthogonal arrays of strength 2 and 3 when $\lambda - 1$ is not divisible by $s - 1$.

Theorem 5.2.1 [8]. The inequality

$$m \leq \left[\frac{\lambda s^2-1}{\lambda-1}\right] - [\nu] - 1 \qquad (5.2.7)$$

holds for orthogonal arrays $(\lambda s^2,\ m,\ s,\ 2)$, and the inequality

$$m \leq \left[\frac{\lambda s^2-1}{\lambda-1}\right] - [\nu] \qquad (5.2.8)$$

holds for orthogonal arrays $(\lambda s^3,\ m,\ s,\ 3)$, where ν is a positive number given by the equality

$$\nu = {}^1\!/_2 \left\{\sqrt{1 + 4s(s-1-b)} - (2s - 2b - 1)\right\};$$

a and b are integers in the decomposition of $\lambda - 1$:

$$\lambda - 1 = a(s-1) + b, 0 \leq b \leq s-1, \quad a \geq 0.$$

When $\lambda - 1$ is divisible by $s - 1$, (5.2.6) can also be extended.

Theorem 5.2.2 [8]. For orthogonal arrays $(\lambda s^3,\ m,\ s,\ 3)$

$$m \leq \left[\frac{\lambda s^2-1}{\lambda-1}\right] - 1, \qquad (5.2.9)$$

if $\lambda - 1 = a(s-1)$ (a integer) and $(s-1)^2(s-2)$ is not divisible by $as + 2$.

The inequalities (5.2.3) and (5.2.4) can be extended for orthogonal arrays of index 1.

Theorem 5.2.3 [9]. For orthogonal arrays $(s^t,\ m,\ s,\ t)$ for $t \leq s$

$$m \leq s + t - 1 \text{ if } s \text{ is even,} \qquad (5.2.10)$$

and

$$m \leq s + t - 2 \text{ if } s \text{ is odd and } t > 3. \qquad (5.2.11)$$

When $s \leq t$, the following theorem holds.

Theorem 5.2.4 [9]. For orthogonal arrays $(s^t,\ m,\ s,\ t)$

$$m \leq t + 1 \text{ if } s \leq t. \qquad (5.2.12)$$

The next theorem compares the maximum number of factors that can be included into orthogonal arrays of strength t and $t - 1$.

Theorem 5.2.5 [10]. Let m' and m be the maximum number of factors for orthogonal arrays $(\lambda s^{t-1},\ m',\ s,\ t-1)$ and $(\lambda s^{t},\ m,\ s,\ t)$ respectively. Then

$$m \le m' + 1. \tag{5.2.13}$$

Proof. Without loss of generality, it can be assumed that the first λs^{t-1} elements of the last column of the orthogonal array $(\lambda s^{t},\ m,\ s,\ t)$ are the same. Then it is obvious that submatrix consisted of the first λs^{t-1} rows and the first $m-1$ columns forms the orthogonal array $(\lambda s^{t-1},\ m-1,\ s,\ t-1)$. That implies (5.2.13).

In the following theorem we give some other bounds for the maximum number of factors, omitting the proofs.

Theorem 5.2.6 [11]. Let $\lambda > 1$ be odd and $\lambda \le t-1$. Then the maximum number of factors in the design $(\lambda s^{t},\ m,\ s,\ t)$ equals $t+1$.

§ 3. Parameter Estimation

Let **D** be a nonsingular factorial design for the factorial set Ω (i.e., the vector of effects generated by the design **D** and the set Ω are linearly independent). If **D** is the design for quantitative factors and $\mathbf{X} = \mathbf{\Phi}_{1\ldots m}^{\Omega D}$ is the coefficient matrix of the design for the factorial A^{Ω}-model, then $\mathbf{X}^{T}\mathbf{X}$ is nonsingular. In this case the vector $\widehat{\mathbf{B}}^{\Omega}$ of LS estimates of the vector $\mathbf{B}^{\Omega}$ of parameters of the A^{Ω}-model, by (2.2.3), is calculated from the following equality:

$$\widehat{\mathbf{B}}^{\Omega} = (\mathbf{X}^{T}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{y},$$

where upper index Ω indicates the factorial model for the factorial set Ω.

If the design **D** is regular for the factorial set Ω, there exists the model for the set Ω such that $\mathbf{X}^{T}\mathbf{X}$ is diagonal. If, in addition, the design **D** is uniform, this model is the model of true effects (3.5.6). Then

$$\widehat{\mathbf{B}}^{\Omega} = \frac{1}{N}\mathbf{X}^{T}\mathbf{y}. \tag{5.3.1}$$

Introduce the following notations:

$$\mathbf{B}_{i_1\ldots i_n} = \frac{1}{N^f}\mathbf{F}_{i_1\ldots i_n}^{f\mathrm{T}}\boldsymbol{\eta}^f; \quad \mathbf{\Theta}_{i_1\ldots i_n} = \boldsymbol{\rho}_{i_1\ldots i_n}^{T}\boldsymbol{\eta}^f.$$

It follows from (5.3.1) that LS estimate of the vector $\mathbf{B}_{i_1\ldots i_n}$

$$\widehat{\mathbf{B}}_{i_1\ldots i_n} = \frac{1}{N}\mathbf{F}_{i_1\ldots i_n}^{fD^T}\mathbf{y}. \tag{5.3.2}$$

Assume that in the design **D** for the mixed G^{Ω}-model, the factors $F_{i_1},\ldots,F_{i_r}$ are qualitative and the factors $F_{j_1},\ldots,F_{j_r}$ are quantitative.

Theorem 5.3.1. For regular uniform design $\mathbf{D}$,

$$\widehat{\boldsymbol{\Theta}}_{i_1 \dots i_r j_1 \dots j_l} = \boldsymbol{\rho}^{DT}_{i_1 \dots i_r j_1 \dots j_l} \mathbf{y} \tag{5.3.3}$$

is the LS estimate of the vector $\boldsymbol{\Theta}_{i_1 \dots i_r j_1 \dots j_l}$ with the restrictions

$$\mathbf{V}_{i_1 \dots i_r j_1 \dots j_l} \widehat{\boldsymbol{\Theta}}_{i_1 \dots i_r j_1 \dots j_l} = \mathbf{0}.$$

P r o o f. If (5.3.3) holds, then

$$\mathbf{z}_{i_1 \dots i_r j_1 \dots j_l} \widehat{\boldsymbol{\Theta}}_{i_1 \dots i_r j_1 \dots j_l} = \mathbf{F}^{f}_{i_1 \dots i_r j_1 \dots j_l} \widehat{\mathbf{B}}_{i_1 \dots i_r j_1 \dots j_l}. \tag{5.3.4}$$

Indeed, by (3.11.1), (3.11.2), (3.11.4), and (5.3.2),

$$\mathbf{z}_{i_1 \dots i_r j_1 \dots j_l} \widehat{\boldsymbol{\Theta}}_{i_1 \dots i_r j_1 \dots j_l} = \mathbf{z}_{i_1 \dots i_r j_1 \dots j_l} \boldsymbol{\rho}^{\mathbf{D}T}_{i_1 \dots i_r j_1 \dots j_l} \mathbf{y}$$
$$= \left(\mathbf{x}_{i_1 \dots i_r} \otimes \mathbf{F}^{f}_{j_1 \dots j_l}\right) \left(\boldsymbol{\psi}^{\mathbf{D}}_{i_1 \dots i_r} \otimes \mathbf{F}^{f\mathbf{D}}_{j_1 \dots j_l}\right)^T \mathbf{y}$$
$$= \left(\mathbf{x}_{i_1} \otimes \dots \otimes \mathbf{x}_{i_r} \otimes \mathbf{F}^{f}_{j_1} \otimes \dots \otimes \mathbf{F}^{f}_{j_l}\right)$$
$$\times \left(N\boldsymbol{\psi}^{\mathbf{D}}_{i_1} \otimes \dots \otimes N\boldsymbol{\psi}^{\mathbf{D}}_{i_r} \otimes \mathbf{F}^{f\mathbf{D}}_{j_1} \otimes \dots \otimes \mathbf{F}^{f\mathbf{D}}_{j_l}\right)^T \mathbf{y}\frac{1}{N}$$
$$= N\left(\mathbf{x}_{i_1} \boldsymbol{\psi}^{\mathbf{D}T}_{i_1}\right) * \dots * N\left(\mathbf{x}_{i_r} \boldsymbol{\psi}^{\mathbf{D}T}_{i_r}\right) * \left(\mathbf{F}^{f}_{j_1} \mathbf{F}^{f\mathbf{D}T}_{j_1}\right) * \dots * \left(\mathbf{F}^{f}_{j_l} \mathbf{F}^{f\mathbf{D}T}_{j_l}\right) \mathbf{y}\frac{1}{N}$$
$$= \left(\mathbf{F}^{f}_{i_1} \mathbf{F}^{f\mathbf{D}T}_{i_1}\right) * \dots * \left(\mathbf{F}^{f}_{j_l} \mathbf{F}^{f\mathbf{D}T}_{j_l}\right) \mathbf{y}\frac{1}{N}$$
$$= \left(\mathbf{F}^{f}_{i_1} \otimes \dots \otimes \mathbf{F}^{f}_{j_l}\right) \left(\mathbf{F}^{f\mathbf{D}}_{i_1} \otimes \dots \otimes \mathbf{F}^{f\mathbf{D}}_{j_l}\right)^T \mathbf{y}\frac{1}{N}$$
$$= \mathbf{F}^{f}_{i_1 \dots i_r j_1 \dots j_l} \mathbf{F}^{f\mathbf{D}T}_{i_1 \dots i_r j_1 \dots j_l} \mathbf{y}\frac{1}{N} = \mathbf{F}^{f}_{i_1 \dots i_r j_1 \dots j_l} \widehat{\mathbf{B}}_{i_1 \dots i_r j_1 \dots j_l}.$$

Besides,

$$\mathbf{V}_{i_1 \dots i_r j_1 \dots j_l} \widehat{\boldsymbol{\Theta}}_{i_1 \dots i_r j_1 \dots j_l} = \mathbf{V}_{i_1 \dots i_r j_1 \dots j_l} \boldsymbol{\rho}^{\mathbf{D}T}_{i_1 \dots i_r j_1 \dots j_l} \mathbf{y} = \mathbf{0}\,. \tag{5.3.5}$$

Now the theorem statement follows from (5.3.4) and (5.3.5).

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Chapter 6. Geometric Designs

§ 1. Splitting of Degrees of Freedom

This and the next paragraphs are devoted to the fundamental concept introduced by R.C. Bose [1] – the nature of degrees of freedoms split in a full symmetrical design s^m, where $s = p^h$, p is prime.

Definition 6.1.1. Let $y_1, \dots, y_l$ and $y_{l+1}, \dots, y_{2l}$ be two sets of observations. Then a vector of coefficients of the linear function of observations

$$y_1 + \cdots + y_l - y_{l+1} - \cdots - y_{2l} \tag{6.1.1}$$

is called a contrast between these two sets of observations.

It is evident that (3.3.1) is satisfied for the vector of coefficients of the linear function (6.1.1).

Assume that all N observations are divided into q sets of $N_1 = N/q$ observations in each in such a way that no one observation belongs to two sets. Then there exist $\binom{q}{2} = q\,(q-1)/2$ different contrast between these sets. It is evident that maximum number of linearly independent contrasts equals $q - 1$. An example of $q - 1$ linearly independent contrasts could be the contrasts between any fixed set and all other sets. The contrasts between these sets are said to carry $q - 1$ degrees of freedom.

The following lemma is evident.

Lemma 6.1.1 [1]. Suppose that all N observations are divided into q_1 subsets of $N_1 = N/q_1$ observations each in one way, and into q_2 sets of $N_2 = N/q_2$ observations each in another way so that for every split, each of N observations belong to one and only one of subset. Then if for any subset of the first split, N_1/q_2 observations belong to any subset of the second split, a contrast between any two subsets of the first split is orthogonal to a contrast between any two subsets of the second split.

Consider the full symmetrical design s^m, where $s = p^h$, p is prime, h is integer. In the design s^m, every level of a factor corresponds to an element of Galois field $GF(s)$. Then any treatment combination of the design with the factors $F_1, \dots, F_m$ at levels $\chi_1, \dots, \chi_m$ can be represented by the point of an m-dimensional finite Euclidean space $EG(m, s)$.

Let $P(a_1, \dots, a_m)$ be the pencil of parallel flats in $EG(m, s)$. By this pencil, all s^m treatments are divided into s subsets of s^{m-1} treatments (each subset corresponds to one flat of the pencil). Different flats of the pencil have no points in common, and there exists one flat that passes thorough each point of $EG(m, s)$. Hence, each treatment belongs to one and only one subset. Therefore, the maximal number of linearly independent contrasts between these subsets is $s - 1$. In this case the pencil $P(a_1, \dots, a_m)$ of parallel flats is said to carry $s - 1$ degrees of freedom.

Consider two different pencils P_1 and P_2 of parallel flats.

Theorem 6.1.1 [1]. A contrasts between any two subsets generated by the pencil P_1 is orthogonal to a contrast between any two subset generated by the pencil P_2.

Proof. Any given flat of the pencil P_1 intersects s different flats of the pencil P_2 in s different $(m-2)$-flats. No two of $(m-2)$-flats have any point in common (otherwise two different flats of the pencil P_2 would have a point in common). Any $(m-2)$-flat contains exactly s^{m-2} points. Therefore, each $(m-1)$-flats of the pencil P_2 contains exactly s^{m-2} points of s^{m-1} points belonging to the given $(m-1)$-flat of the pencil P_1. Now the theorem statement follows from Lemma 6.1.1.

In accordance with chapter 1, the number of different pencils of parallel flats is equal to $(s^m - 1)/(s - 1)$. Each pencil carries $s - 1$ degrees of freedom. Hence, all $s^m - 1$ degrees of freedom carried by all contrasts can be split up to $(s^m - 1)/(s - 1)$ sets (generated by pencils of parallel flats) of $s - 1$ degrees of freedom each so that any contrast corresponding to one set is orthogonal to any contrast corresponding to another set.

§ 2. Nature of Degrees of Freedom Carried by Parallel Pencils

Following R.C. Bose [1], consider the nature of $s - 1$ degrees of freedom carried by the pencil

$$P(a_1, \dots, a_m). \tag{6.2.1}$$

Suppose that of m coordinates $a_1, \dots, a_m$ of the pencil (6.2.1), n coordinates are nonzero (without loss of generality, $a_1, \dots, a_n$) and the rest of them $(a_{n+1}, \dots, a_n)$ are equal to zero. Any $(m-1)$-flat of the pencil (6.2.1) is

$$a_0 + a_1\chi_1 + \cdots + a_n\chi_n = 0, \tag{6.2.2}$$

where a_0 is one of the s elements of $GF(s)$. Consider two points such that the i-th coordinate of one of them equals the i-th coordinate of other point for all $i = 1, \dots, n$. It is evident that these two points either simultaneously satisfy (6.2.2) or do not. Therefore, coordinates of a contrast between any two flats of the pencil (6.2.1) are the same for the same combinations of $\chi_1, \dots, \chi_n$.

When $n = 1$, coordinates of a contrast between any two flats of the pencil

$$P(a, 0, \dots, 0) \tag{6.2.3}$$

depend only on levels of the factor F_1 and, by the definition, form a main effect of the factor. Since the pencil of parallel flats carries $s - 1$ degrees of freedom, the pencil (6.2.3) generates a full set of linearly independent main effects.

When $n = 2$, coordinates of a contrast between any two flats of the pencil

$$P(a_1, a_2, 0, \dots, 0) \tag{6.2.4}$$

depend only on levels of the factors F_1 and F_2. By Theorem 6.1.1, this contrast is orthogonal to all main effects of the factors F_1 and F_2. Therefore, it is an interaction effect of the factors F_1 and F_2. The number of different pencils of type (6.2.4) equals $s - 1$. Each of them carries $s - 1$ degrees of freedom, and these degrees of freedom for one pencil of type (6.2.4), by Theorem 6.1.1, are orthogonal to degrees of freedom of other pencil of type (6.2.4). Therefore, all pencils of type (6.2.4) produce the full set of $(s-1)^2$ linearly independent interaction effects of the factors F_1 and F_2.

Increasing n, we get the following theorem.

Theorem 6.2.1 [1]. If n coordinates $a_{i_1}, \dots, a_{i_n}$ of the pencil (6.2.1) are nonzero and the rest of them are zero, a contrast between any flats of the pencil (6.2.1) is an interaction effect of the factors $F_{i_1}, \dots, F_{i_n}$. The pencil (6.2.1) carries $s - 1$ degrees of freedom. The number of different pencils generating interaction effects of the factors $F_{i_1}, \dots, F_{i_n}$ equals $(s-1)^{n-1}$.

Example 6.2.1. Consider the full symmetrical design 3^2 (the design $\mathbf{D}^f$) including all combinations of levels of two three-level factors F_1 and F_2. Set up a one-to-one correspondence between the levels of the factors F_1

and F_2 and elements of Galois field $GF(3)\colon 0, 1, 2$. This design in 9 runs presented in the first two columns of Table 3.

Table 3
Full Design 3^2

F_1	F_2	$F_1 + F_2$	$F_1 + 2F_2$
0	0	0	0
1	0	1	1
2	0	2	2
0	1	1	2
1	1	2	0
2	1	0	1
0	2	2	1
1	2	0	2
2	2	1	0

The flats of the pencil corresponding to main effects of the factor F_1 are defined naturally. Each of three flats consists of three treatments where the factor F_1 appears at the levels 0, 1 and 2 respectively. Hence, two linearly independent main effects of the factor F_1 can be represented, for example, as contrasts between the first and the second and between the first and the third flats. The coordinates of these contrasts are presented in Table 4 (the first two columns).

Table 4
Main Effects and Interaction Effects of Design 3^2

Main Effects				Interaction Effects			
Factor F_1		Factor F_2		Factors F_1 and F_2			
–1	–1	–1	–1	–1	–1	–1	–1
1	0	–1	–1	1	0	1	0
0	1	–1	–1	0	1	0	1
–1	–1	1	0	1	0	0	1
1	0	1	0	0	1	–1	–1
0	1	1	0	–1	–1	1	0
–1	–1	0	1	0	1	1	0
1	0	0	1	–1	–1	0	1
0	1	0	1	1	0	–1	–1

To find the parallel flats of the first pencils corresponding to the interaction effects of the factors F_1 and F_2, we need to calculate the sum of elements of the first two columns of Table 3 (see third column of Table 3). To find the parallel flats of the second pencil, we need to multiply the elements of the second column of Table 3 by 2 and sum up the result with the elements of the first columns (see forth column of Table 3). The flats of pencils corresponding to the interaction effects of the factors F_1 and F_2 can be found as follows. The first pencil contains three flats. Each flat consists of three treatments, where $F_1 + F_2$ equals 0, 1, and 2 respectively. Coordinates of contrasts between the first and the second flats and between the first and the third flats are presented in the 5-th and the 6-th columns of Table 4 respectively. The contrasts of the second pencil corresponding to the interaction effects of the factors F_1 and F_2 are calculated analogously.

Let $X_i \in PG(m, s)$ be the vertex of the fundamental simplex. Consider the bundle of the parallel flats $P(a_1, \dots, a_m)$ in $PG(m, s)$. Assume that the coordinates $a_{i_1}, \dots, a_{i_n}$ of this bundle are nonzero, and the rest coordinates are equal to zero. Then the vertex of the bundle is

$$\chi_0 = 0, \quad a_{i_1}\chi_{i_1} + \dots + a_{i_n}\chi_{i_n} = 0. \tag{6.2.5}$$

The vertex (6.2.5) passes thorough all vertices of the fundamental simplex, except the vertices $\mathrm{X}_{i_1}, \dots, \mathrm{X}_{i_n}$. Then the following theorem follows from Theorem 6.2.1.

Theorem 6.2.2 [1]. The pencil $P(a_1, \dots, a_m)$ of parallel flats corresponds to interaction effects of order $(n-1)$ of the factors $F_{i_1}, \dots, F_{i_n}$ if and only if the vertex of the corresponding bundle passes through all the vertices of the fundamental simplex other than $\mathrm{X}_{i_1}, \dots, \mathrm{X}_{i_n}$.

§ 3. Hypercubes of Strength *t*

Consider a full symmetrical design with each factor at *s* levels.

Set up a one-to-one correspondence between the levels of the factors F_i $(i = 1, \dots, m)$ and the elements of Galois field $GF(s)$ denoted by $0, 1, \dots, s-1$. The full design corresponds to the points of a finite Euclidean space $EG(m, s)$. Denote coordinates of points of this space as $(\chi_1, \dots, \chi_m)$. Then the system of l independent equations

$$\begin{aligned} &a_{11}\chi_1 + \dots + a_{m1}\chi_{\mathrm{m}} = 0, \\ &\dots\dots\dots\dots\dots\dots \\ &a_{1l}\chi_1 + \dots + a_{ml}\chi_m = 0 \end{aligned} \tag{6.3.1}$$

with coefficients $a_{ij} \in GF(s)$ in accordance with §3 of chapter 1 defines the subset of s^{m-l} points of $EG(m,s)$, or the subset of the full design s^m.

Definition 6.3.1. The design consisting of s^{m-l} points satisfying the system of l linearly independent equations (6.3.1) is called a geometric design.

We will also use Definition 6.3.1 of geometric designs when right-hand sides of (6.3.1) have any elements (not necessarily zero). However, hereafter, except §9 of chapter 6, we will assume that right-hand sides of (6.3.1) are zero.

Theorem 6.3.1 [2]. s^{m-l} points satisfying the system (6.3.1) form a hypercube of strength t if and only if there is no nontrivial linear combination of (6.3.1) that contains less than $t+1$ nonzero coefficients.

Proof. Assume that any nontrivial linear combination of (6.3.1) contains at least $(t+1)$ nonzero coefficients. Then any combination of any set of t factors satisfies the system (6.3.1). Indeed, without loss of generality, we can select the factors $F_1, \dots, F_t$ as a set of t factors. Fix them at certain levels. Then (6.3.1) is transformed into the following system:

$$\begin{aligned} a_1 &= a_{t+1,1}\chi_{t+1} + \dots + a_{m1}\chi_1, \\ &\dots\dots\dots\dots\dots\dots \\ a_l &= a_{t+1,l}\chi_{t+1} + \dots + a_{ml}\chi_m. \end{aligned} \qquad (6.3.2)$$

Each equation of (6.3.2) contains at least one nonzero coefficient. Without loss of generality, assume that $a_{ml} \neq 0$. Sum up the $(l-1)$-th equation and the l-th equation with appropriate multiplier. Then we get the equation with $a_{m,l-1} = 0$. This equation also have at least one nonzero coefficient. We can assume that $a_{m-1,l-1} \neq 0$. Going further with this process of diagonalization, transform the system (6.3.2) to a semi-diagonal type. Then we get that the system (6.3.2) always has at least one solution, and the number of different solutions is constant and equals s^{m-l-t}. Hence, any combination of levels of any t factors occurs exactly s^{m-l-t} times. Therefore, the design is a hypercube of strength t.

Now suppose that there exists a linear combination of (6.3.1) that forms the equation

$$a_1\chi_{i_1} + \dots + a_n\chi_{i_n} = 0, \qquad (6.3.3)$$

where $n < t+1$. Then, it is evident that all combinations of levels of n factors $F_{i_1}, \dots, F_{i_n}$ will not satisfy (6.3.1). This proves the theorem.

Theorem 6.3.2 [3]. Suppose that there exists the matrix $\mathbf{C} = \{c_{ij}\}$ of size $m \times n$ ($c_{ij} \in GF(s)$, $s = p^h$, p is prime) such that any of its submatrix of size $t \times n$ has rang t. Then there exists an orthogonal array (s^n, m, s, t).

P r o o f. Consider the matrix $Q = \{q_{ij}\}$ of the full design s^n of size $s^n \times n$ $\left(q_{ij} \in GF(s)\right)$. We will show that the matrix $\mathbf{A} = \mathbf{QC}^T$ of size $s^n \times m$ is the orthogonal array (s^n, m, s, t).

Let $\mathbf{A}'$ be a submatrix of size $s^n \times t$ of the matrix $\mathbf{A}$, and $\mathbf{C}'$ is a submatrix of size $t \times n$ of the matrix $\mathbf{C}$ corresponding to $\mathbf{A}'$. Since Rg $\mathbf{C}' = t$, each row of $\mathbf{A}'$ is a combination of s^{n-t} different rows of the matrix $\mathbf{Q}$. Hence, each row in $\mathbf{A}'$ occurs s^{n-t} times. Therefore, $\mathbf{A}$ is an orthogonal array of strength t and index $\lambda = s^{n-t}$.

Elements of rows of the matrix $\mathbf{C}$ can be interpreted as coordinates of points in a finite projective space $PG\left(n-1, p^h\right)$ such that no t of them belong to a subspace of dimension $t-2$ or less. Therefore, this condition is equivalent to the condition of Theorem 6.3.2.

We will show that two conditions of Theorem 6.3.2 are equivalent to the condition of Theorem 6.3.1.

Theorem 6.3.3. The following three statements are equivalent:

1. There exists the matrix $\mathbf{C} = \{c_{ij}\}$ of size $m \times n$ ($c_{ij} \in GF\left(p^h\right)$, p is prime) such that any its submatrix of size $t \times n$ has rank t.
2. There exist m points in projective space $PG\left(n-1, p^h\right)$ such that no t of them belong to a subspace of dimension $\mathrm{t}-2$ or less.
3. There exists a system of $l = m - n$ equations (6.3.1) such that there is no nontrivial linear combination of the equations that contains less than $\mathrm{t}+1$ nonzero coefficients.

P r o o f. Suppose that the statement 3 of the theorem holds. We will use the following transformation of the matrix: addition a multiple of one row to another and permutation of rows or columns, and call them elementary transformations. It is evident that the matrix $\mathbf{V} = \{v_{ij}\}$ $(i = 1, \dots, m;\quad j = 1, \dots, l)$ of coefficient of the system (6.3.1) by elementary transformations can be converted to the following matrix:

$$\left\| \begin{matrix} g_{11} & g_{21} & \dots & g_{n1} & 0 & 0 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ g_{1l} & g_{2l} & \dots & g_{nl} & 1 & 0 & \dots & 0 \end{matrix} \right\|. \tag{6.3.4}$$

Each row of the matrix (6.3.4) is a nontrivial linear combination of rows of the matrix $\mathbf{V}$. Hence, each row of the matrix (6.3.4) contains at least $t+1$ nonzero elements. I.e., for any j, there is at least t nonzero elements among numbers $g_{1j}, \dots, g_{nj}$. A similar statement can be made for any nontrivial combination of rows of the matrix (6.3.4). Namely, a nontrivial linear combination with $a(>0)$ nonzero coefficients of rows of the matrix (6.3.4) contains at least $t+1$ nonzero elements, and at least $t+1-a$ of them occur in the first n columns.

Consider the matrix

$$\left\|\begin{matrix} g_{11} & g_{21} & \cdots & g_{n1} & 0 & 0 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ g_{1l} & g_{2l} & \cdots & g_{nl} & 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{matrix}\right\| \tag{6.3.5}$$

and some nontrivial linear combination of its t rows with a rows selected from the first l rows and $(t-a)$ rows selected from the rest rows. It is evident that the first n elements of this linear combination contain at least $(t+1-a)-(t-a)=1$ nonzero elements. That means that any submatrix of size $t\times n$ $(t\leq n)$ of the matrix

$$\left\|\begin{matrix} g_{11} & g_{21} & \cdots & g_{n1} \\ \vdots & \vdots & \ddots & \vdots \\ g_{1l} & g_{2l} & \cdots & g_{nl} \\ 0 & 0 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \end{matrix}\right\| \tag{6.3.6}$$

of size $m\times n$ has rang t.

Suppose that the statement 1 of the theorem holds and rank of the matrix $\mathbf{C}=\{c_{ij}\}$ equals n' $(t\leq n'\leq n)$. Select n' independent rows in the matrix $\mathbf{C}$ (without loss of generality, assume that these rows are the last n' rows of $\mathbf{C}$). Then each row $\mathbf{c}_i$ $(i=1,\ldots,m-n')$ of the matrix $\mathbf{C}$ can be represented by a linear combination of rows $\mathbf{c}_u$ $(u=m-n'+1,\ldots,m)$ of the matrix:

$$\begin{aligned} &\mathbf{c}_1=\lambda_{11}\mathbf{c}_{m-n'+1}+\cdots+\lambda_{1n'}\mathbf{c}_m, \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &\mathbf{c}_{m-n'}=\lambda_{(m-n')1}\mathbf{c}_{m-n'+1}+\cdots+\lambda_{(m-n')\,n'}\mathbf{c}_m. \end{aligned} \tag{6.3.7}$$

Consider the matrix $\mathbf{\Lambda}=\{\lambda_{ij}\}$ $(i=1,\ldots,m-n';\ j=1,\ldots,n')$. The number of nonzero elements in the i-th row of the matrix $\mathbf{\Lambda}$ cannot be less than t. Otherwise, by (6.3.7), $\mathbf{c}_i$ could be represented by a linear combination of these nonzero elements and therefore, there would exist t

linearly independent rows of the matrix **C**. Thus, we have arrived at a contradiction.

For the same reason, a nontrivial linear combination r $(r \leq m - n')$ rows of the matrix $\mathbf{\Lambda}$ cannot contain less than $t - r + 1$ nonzero elements.

Form the following matrix of size $(m - n') \times m$:

$$\left\| \begin{matrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n'} & 1 & 0 & \cdots & 0 \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n'} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_{(m-n')\,1} & \lambda_{(m-n')\,2} & \cdots & \lambda_{(m-n')\,n'} & 0 & 0 & \cdots & 1 \end{matrix} \right\|. \tag{6.3.8}$$

Using the properties of the matrix $\mathbf{\Lambda}$, we can get that any nontrivial linear combination of any rows of the matrix (6.3.8) contains at least $t + 1$ nonzero elements. Since $n' \leq n$, the matrix of required size can be generated from the matrix (6.3.8) by deleting any $n - n'$ rows.

This completes the proof of the theorem.

We will say that we are using geometric method of construction of hypercubes of strength t when we construct them based on Theorem 6.3.1 or Theorem 6.3.2. In this case s^{m-l} points of the hypercube satisfy the system of type (6.3.1).

Example 6.3.1 of construction a system of two equations with 6 variables. Consider the matrix

$$\left\| \begin{matrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{matrix} \right\| \tag{6.3.9}$$

with elements of $GF(2)$. It is easy to check that any submatrix of size (3×4) of the matrix (6.3.9) has rank 3. It is evident that rank of the matrix (6.3.9) equals 4 and the last 4 rows are linearly independent. The first row of the matrix (6.3.9) is the sum of the 4-th, 5-th, and 6-th rows, the second row is the sum of the 3-rd, 4-th, and 5-th rows. Using notations of Theorem 6.3.3, we get the following equalities:

$$\mathbf{c}_1 = \mathbf{c}_4 + \mathbf{c}_5 + \mathbf{c}_6; \quad \mathbf{c}_2 = \mathbf{c}_3 + \mathbf{c}_4 + \mathbf{c}_5.$$

Hence, the matrix (6.3.8) is as follows:

$$\left\| \begin{matrix} 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{matrix} \right\|,$$

and the system (6.3.1) is:

$$\chi_2 + \chi_3 + \chi_4 + \chi_5 = 0,$$
$$\chi_1 + \chi_2 + \chi_3 + \chi_6 = 0.$$

Any nontrivial linear combination of equalities of this system contains at least 4 nonzero coefficients.

§ 4. Alias sets of pencils of parallel flats

In this paragraph, we will concentrate on the nature of pencils of parallel flats in fractional geometric designs [4].

Consider the full symmetrical design s^m (the design $\mathbf{D}^f$) and all pencils $P(a_1, \dots, a_m)$ of parallel flats

$$a_0 + a_1\chi_1 + \cdots + a_m\chi_m = 0. \qquad (6.4.1)$$

The nature of the contrasts generated by these pencils is defined by Theorem 6.2.1. Let $\mathbf{D}$ be the subset of s^{m-l} points of the design $\mathbf{D}^f$ generated by l independent equations (6.3.1).

The equations (6.3.1) is called generating relations of the design $\mathbf{D}$. The pencil $P(a_{11}, \dots, a_{m1})$, …, $P(a_{1l}, \dots, a_{ml})$ is called generators of the design $\mathbf{D}$. Note that for the given design $\mathbf{D}$, a selection of the generators is not unique. The pencils

$$P(\lambda_1 a_{11} + \cdots + \lambda_l a_{1l}, \dots, \lambda_l a_{m1} + \cdots + \lambda_l a_{ml}) \qquad (6.4.2)$$

(λ_i are not equal simultaneously to zero) is called defining pencils of the design $\mathbf{D}$. It is evident that we can get a unique representation of the defining pencils (6.4.2) if we set to 1 the first of nonzero coordinates. Therefore, the total number of different defining pencils of the design $\mathbf{D}$ generated by (6.3.1) equals $(s^l - 1)/(s - 1)$.

For the design $\mathbf{D}$ consider vector $\boldsymbol{\xi}$ with coordinates equal coordinates of the contrast $\boldsymbol{\xi}^f$ generated by the pencil $P(a_1, \dots, a_m)$ in $\mathbf{D}^f$. In this case we will say that the contrast $\boldsymbol{\xi}^f$ in $\mathbf{D}^f$ generates $\boldsymbol{\xi}$ in $\mathbf{D}$. If $P(a_1, \dots, a_m)$ is a defining pencil of the design $\mathbf{D}$, then all points of $\mathbf{D}$ belong to one of the flats of (6.4.1) (for $a_0 = 0$) and no points of $\mathbf{D}$ belong to other flats of (6.4.1) (for $a_0 \neq 0$). In this case $\boldsymbol{\xi}^f$ generates zero vector $\mathbf{0}$ in $\mathbf{D}$. It is evident that the vector $\mathbf{0}$ is generated by those and only those contrasts $\boldsymbol{\xi}^f$ that correspond to defining pencils of the design $\mathbf{D}$. In this case we shall say that the vector $\mathbf{0}$ and vectors generated by defining pencils of the design $\mathbf{D}$ belong to the same alias set (for the design $\mathbf{D}$). We also shall say that defining pencils of the design $\mathbf{D}$ belong to the same alias set.

If $P(a_1, \dots, a_m)$ is not a defining pencil of the design $\mathbf{D}$, each flat of the pencil (6.4.1) intersect $\mathbf{D}$ in s^{m-l-1} points of $(m - l - 1)$-flat, which we denote by $P(a_0, a_1, \ldots, a_m)$. In this case each point of the design **D** belong to one and only one flat of the pencil (6.4.1) and, therefore, one and only one flat $P(a_0, a_1, \ldots, a_m)$. Hence, a pencil of parallel flats in $\mathbf{D}^f$ generates a pencil of parallel $(m-l-1)$-flats $P(a_0, a_1, \ldots, a_m)$ in the design **D**, which we denote by $P'(a_1, \ldots, a_m)$.

Consider the flat

$$\begin{aligned} &a_0 + (\lambda_0 a_1 + \lambda_1 a_{11} + \cdots + \lambda_l a_{1l})\chi_1 + \cdots \\ &+(\lambda_0 a_m + \lambda_1 a_{m1} + \cdots + \lambda_l a_{ml})\chi_m = 0 \\ &(\lambda_0 \neq 0) \end{aligned} \tag{6.4.3}$$

of the pencil

$$\begin{aligned} &P(\lambda_0 a_1 + \lambda_1 a_{11} + \cdots + \lambda_l a_{1l}, \ldots, \\ &\lambda_0 a_m + \lambda_1 a_{m1} + \cdots + \lambda_l a_{ml}). \end{aligned} \tag{6.4.4}$$

It is evident that the flat (6.4.3) intersects (6.3.1) in the same points as (6.4.1). Besides, all flats intersecting (6.3.1) in the same points as (6.4.1) are represented by (6.4.3).

Since the pencils $P(a_1, \ldots, a_m), P(a_{11}, \ldots, a_{m1}), \ldots, P(a_{1l}, \ldots, a_{ml})$ are linearly independent, different sets (6.4.4) correspond to different pencils. Therefore, the total number of different pencils of type (6.4.4) equals s^l. Hence, for any pencil $P(a_1, \ldots, a_m)$ that is not defining pencil of the design **D** there exists s^l pencils, including $P(a_1, \ldots, a_m)$, that generate the same pencil $P'(a_1, \ldots, a_m)$ in the design **D**. We shall say about such s^l pencils that they belong to the same alias set of the design **D**. We shall also say that contrasts generated by these pencils belong to one alias set.

The total number of the pencils in $\mathbf{D}^f$ equal $(s^m - 1)/(s-1)$. An alias set of defining pencils of the design **D** consists of $(s^l - 1)/(s-1)$ pencils. Therefore, the number of different alias sets of nondefining pencils equals

$$\frac{(s^m - 1)/(s-1) - (s^l - 1)/(s-1)}{s^l} = \frac{s^{m-l} - 1}{s-1}.$$

Consider two different pencils $P'(a_1, \ldots, a_m)$ and $P'(g_1, \ldots, g_m)$ that are generated by pencils of two different alias sets for the design **D**. The rows of the matrix

$$\begin{Vmatrix} a_1 & \cdots & a_m \\ g_1 & \cdots & g_\mathrm{m} \\ a_{11} & \cdots & a_{m1} \\ \vdots & \ddots & \vdots \\ a_{1l} & \cdots & a_{ml} \end{Vmatrix}$$

are linearly independent. Hence, any given $(m-l-1)$-flat of the pencil $P'(a_1, \dots, a_m)$ intersects s different $(m-l-1)$-flats of the pencil $P'(g_1, \dots, g_m)$ in s different $(m-l-2)$-flats. Any two of these $(m-l-2)$-flats have no point in common, because two different $(m-l-1)$-flats of the pencil $P'(g_1, \dots, g_m)$ have no point in common. Any $(m-l-2)$-flat contains exactly s^{m-l-2} points. Therefore, each $(m-l-1)$-flat of the pencil $P'(g_1, \dots, g_m)$ contains exactly s^{m-l-2} points of s^{m-l-1} points belonging to the given $(m-l-1)$-flat of the pencil $P'(a_1, \dots, a_m)$. Therefore, by Lemma 6.1.1, degrees of freedom carried by the pencil $P(a_1, \dots, a_m)$ are orthogonal to degrees of freedom carried by the pencil $P'(g_1, \dots, g_m)$. Therefore, the following theorem has been proved.

Theorem 6.4.1. All $(s^m-1)/(s-1)$ pencils of parallel flats in $\mathbf{D}^f$ are split into $\left(s^{m-l}-1\right)/(s-1)$ alias sets with s^l pencils in each and one alias set with $\left(s^l-1\right)/(s-1)$ defining pencils. The pencils belonging to the same alias set generate identical pencils of parallel flats in the design **D**. The pencils from different alias sets generate pencils of parallel flats in the design **D** with orthogonal degrees of freedom.

It follows from the proof of Theorem 6.3.1 that if the design contains all combinations of levels of t factors $F_{i_1}, \dots, F_{i_t}$, no defining pencil has all coordinates other than $a_{i_1}, \dots, a_{i_t}$ simultaneously equal to zero. The pencil that have part of coordinates $a_{i_1}, \dots, a_{i_t}$ (namely, $a_{j_1}, \dots, a_{j_t}$) not equal to zero and the rest of coordinates equal to zero, cannot be a defining pencil and cannot be in the same alias set with the pencil that has all coordinates other than $a_{i_1}, \dots, a_{i_t}$ simultaneously equal to zero.

Therefore, if the design **D** contains all levels of the factor F_i, the pencil P_i corresponding to main effects of this factor in $\mathbf{D}^f$ cannot be a defining pencil of the design **D**. Hence, the pencil P_i' in **D** generated by the pencil P_i forms $s-1$ contrasts orthogonal to the vector **I**, with coordinates that depend only on levels of the factor F_i. Therefore, the pencil P_i' also forms a full set of main effects of the factor F_i in the design **D**.

If the design **D** contains all combinations of levels of two factors F_i and F_j, any pencil P_{ij} corresponding to interaction effects of these factors in $\mathbf{D}^f$ cannot be a defining pencil of the design **D**. Hence, the pencil P_{ij}' in **D** generated by the pencil P_{ij} forms $s-1$ contrasts orthogonal to the vector **I** and all main effects of the factors F_1 and F_2 (because the pencils corresponding to main effects of factors F_1 and F_2 cannot be in the alias set together with the pencil P_{ij}). Since the pencil P_{ij}' forms contrasts with coordinates that depend only on levels of the factors F_i and F_j, these contrasts are interaction effects of the factors F_i and F_j. Contrasts corresponding to all pencils P_{ij} form a full set of $(s-1)^2$ interaction effects of the factors F_i and F_j.

Continuing this reasoning by induction, we get the following theorem.

Theorem 6.4.2. If the design contains all combinations of levels of the factors $F_{i_1}, \dots, F_{i_t}$, or (which is the same) no defining pencil has all coordinates other than $a_{i_1}, \dots, a_{i_t}$ simultaneously equal to zero, all pencils corresponding to interaction effects of the factors $F_{i_1}, \dots, F_{i_t}$ in $\mathbf{D}^f$ generate pencils of parallel flats in the design **D** corresponding to a full set of interaction effects of these factors in the design **D**.

We will get independent effects if we select not more than one pencil from each alias set.

Example 6.4.1. Consider the full symmetrical design 3^4 (the design $\mathbf{D}^f$) and the design **D** with 9 treatment combinations generated by two independent equations

$$\chi_1 + \chi_2 + 2\chi_3 = 0, \quad \chi_1 + 2\chi_2 + 2\chi_4 = 0.$$

The pencils $P(1,1,2,0)$ and $P(1,2,0,2)$ are generators of the design **D**. Pencils $P(1,1,2,0)$, $P(1,2,0,2)$, $P(1,0,1,1)$, and $P(0,1,1,2)$ are four defining pencils. They form the alias set of defining pencils. It is evident that in the design **D** no three factors have all combinations of their levels. I.e., for any i $(i = 1, \dots, 4)$, there exists a defining pencil with the i-th coordinate equal to zero.

There are four alias sets of nondefining pencils, with 9 pencils each.

Alias Sets

1-st	**2-nd**	**3-rd**	**4-th**
$P(1,0,0,0)$	$P(0,1,0,0)$	$P(0,0,1,0)$	$P(0,0,0,1)$
$P(1,2,1,0)$	$P(1,2,2,0)$	$P(1,1,0,0)$	$P(1,1,2,1)$
$P(1,1,0,1)$	$P(1,0,0,2)$	$P(1,2,1,2)$	$P(1,2,0,0)$
$P(1,0,2,2)$	$P(1,1,1,1)$	$P(1,0,2,1)$	$P(1,0,1,2)$
$P(1,1,1,2)$	$P(0,1,2,1)$	$P(0,1,2,2)$	$P(0,1,1,0)$
$P(0,1,2,0)$	$P(1,0,2,0)$	$P(1,1,1,0)$	$P(1,1,2,2)$
$P(0,1,0,1)$	$P(1,1,0,2)$	$P(1,2,2,2)$	$P(1,2,0,1)$
$P(0,0,1,1)$	$P(1,2,1,1)$	$P(1,0,0,1)$	$P(1,0,1,0)$
$P(1,2,2,1)$	$P(0,0,1,2)$	$P(0,1,0,2)$	$P(0,1,1,1)$

We will get independent effects if we select not more than one pencil from each alias set, for example, pencils $P(1,0,0,0)$, $P(0,1,0,0)$,

$P(0,0,1,0)$, and $P(0,0,0,1)$. Each of these pencils carries two degrees of freedom that correspond to main effects of the factors F_1, F_2, F_3, and F_4.

Another example of independent effects: pencils $P(0,1,0,0)$ and $P(0,0,1,0)$ from the 2-nd and the 3-rd alias sets respectively and pencils $P(0,1,2,0)$ and $P(0,1,1,0)$ from the 1-st and the 4-th sets respectively. The first two pencils generate main effects of the factors F_2 and F_3, the second two pencils generate all their interaction effects.

§ 5. Defining Relation

Consider a geometric design **D** generated by l independent equations (6.3.1). We will call the following relationship a defining relation of the design **D**:

$$\begin{aligned}
&0 = a_{11}\chi_1 + \cdots + a_{m1}\chi_m = a_{12}\chi_1 + \cdots + a_{m2}\chi_m = \cdots \\
&= a_{1l}\chi_1 + \cdots + a_{ml}\chi_m = (a_{11} + a_{12})\chi_1 + \cdots \\
&+(a_{m1} + a_{m2})\chi_m = \cdots = [a_{11} + (s-1)a_{12}]\chi_1 + \cdots \\
&+[a_{m1} + (s-1)a_{m2}]\chi_m = \cdots \\
&= [a_{11} + \cdots + a_{1l}]\chi_1 + \cdots + [a_{m1} + \cdots + a_{ml}]\chi_m = \cdots \\
&= [a_{11} + (s-1)a_{12} + \cdots + (s-1)a_{1l}]\chi_1 + \cdots \\
&+[a_{m1} + (s-1)a_{m2} + \cdots + (s-1)a_{ml}]\chi_m.
\end{aligned} \tag{6.5.1}$$

The coefficients in (6.5.1) match with the coordinates of the defining pencils. A so-called standard defining relation is derived from the defining relation (6.5.1) by multiplying of each of its side by the element $\lambda \in GF(s)$ such that the first nonzero coefficient of the side equals 1. In Example 6.4.1, the standard defining relation is:

$$\begin{aligned}
&0 = \chi_1 + \chi_2 + 2\chi_3 = \chi_1 + 2\chi_2 + 2\chi_4 \\
&= \chi_1 + \chi_3 + \chi_4 = \chi_2 + \chi_3 + 2\chi_4.
\end{aligned}$$

By Theorem 6.3.1, the geometric design **D** is a hypercube of strength t if and only if no side of the defining relation (6.5.1) contains less than $t + 1$ nonzero coefficients.

§ 6. Packing Problem

Definition 6.6.1. The set of m points of the projective geometry $PG(n-1, s)$ is called an (m, t)-set if no t of them belong to a subspace of dimension $t - 2$ or less.

According to §3 of chapter 6, the existence of an (m, t)-set in $PG(n-1, s)$ implies the existence of an orthogonal array (s^n, m, s, t).

The existence of a geometric method of the construction of an orthogonal array (s^n, m, s, t) implies the existence of an (m, t)-set in $PG(n-1, s)$.

Hereafter, for some specific case, we will use this fact for the construction of orthogonal arrays and try to construct (m, t)-sets with the maximal value of m.

Definition 6.6.2. An (m, t)-set is said to be complete if an (m', t)-set with $m' > m$ does not exist. The number m corresponding to the complete (m, t)-set in $PG(n-1, s)$ is denoted by $m_t(n, s)$.

The construction of (m, t)-sets and, in particular, the complete (m, t)-sets is also useful for blocking (see §7 of chapter 8).

The problem of finding complete (m, t)-sets and the numbers $m_t(n, s)$ is called the packing problem. When the value $m_t(n, s)$ is unknown, it is useful to have the upper bounds for $m_t(n, s)$.

Theorem 6.6.1 [5,6].

$$m_2(n, s) = (s^n - 1)/(s - 1).$$

This case will be considered in detail in §7 of the chapter.

Theorem 6.6.2 [1].

$$m_3(n, s) = 2^{n-1}.$$

The proof of the theorem is given in §4 of chapter 7.

Theorem 6.6.3 [1].

$$m_3(3, s) = \begin{cases} s+1 & \text{if } s \text{ is odd,} \\ s+2 & \text{if } s \text{ is even.} \end{cases}$$

The proof is given in §3 of chapter 7.

Theorem 6.6.4 [7].

$$m_4(4, 2) = 5; \quad m_4(6, 2) = 8;$$
$$m_4(5, 2) = 6; \quad m_4(7, 2) = 11.$$

The proof of the theorem is given in §4 of chapter 7.

For the next two theorem, we will omit the proof but will give the corresponding complete (m, t)-sets.

Theorem 6.6.5 [8].

$$m_4(4, s) = \max(5, s + 1).$$

For $s = 2, 3,$ and 4, the set of 5 points (vector-columns) such that no 4 of them are linearly dependent, form the matrix

$$\begin{Vmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{Vmatrix}.$$

For $s > 4$ such a set is generated by columns of the following matrix:

$$\begin{Vmatrix} 1 & 0 & 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 1 & a & a^2 & a^3 & \cdots & a^{s-2} \\ 0 & 0 & 1 & a^2 & a^4 & a^6 & \cdots & a^{2s-4} \\ 0 & 1 & 1 & a^3 & a^6 & a^9 & \cdots & a^{3s-6} \end{Vmatrix},$$

where a is a primitive element of $GF(s)$**.** Indeed, consider the submatrix $\mathbf{C}'$ of the matrix $\mathbf{C}$:

$$\mathbf{C}' = \begin{Vmatrix} 1 & 1 & 1 & 1 \\ a^{i_1} & a^{i_2} & a^{i_3} & a^{i_4} \\ (a^2)^{i_1} & (a^2)^{i_2} & (a^2)^{i_3} & (a^2)^{i_4} \\ (a^3)^{i_1} & (a^3)^{i_2} & (a^3)^{i_3} & (a^3)^{i_4} \end{Vmatrix}.$$

A determinant of $\mathbf{C}'$ is the Vandermonde determinant and, therefore,

$$\det \mathbf{C}' = \prod_{j<l}\left(a^{i_j} - a^{i_l}\right) \ (j, l = 0, 1, 2, 3, 4).$$

The elements a^i of the second row of the matrix $\mathbf{C}$ are different. Hence, $a^{i_j} \neq a^{i_l}$ and, therefore, $\det \mathbf{C}' \neq 0$.

Similarly, it can be shown that a determinant of any submatrix 4×4 of the matrix $\mathbf{C}$ is not equal to zero.

Theorem 6.6.6 [8].

$m_4(5, 3) = 11.$

The set of 11 points (vector-columns) such that no 4 of them are linearly dependent forms the following matrix:

$$\begin{Vmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 2 & 2 \\ 0 & 0 & 1 & 0 & 0 & 1 & 2 & 2 & 0 & 2 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 2 & 1 & 2 & 0 & 2 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 1 & 0 \end{Vmatrix}.$$

Here are a few more theorems without proof.

Theorem 6.6.7 [1, 9].

$$m_3(4, s) = s^2 + 1.$$

Theorem 6.6.8 [10].

$$m_3(n, s) < s^{n-2} + 1 \quad (s > 2,\ n \geq 4).$$

Theorem 6.6.9 [11].

$$m_3(n,s) \le s^{n-2} - (s-5)\sum_{i=0}^{n-5} s^i + 1 \;\; (n \ge 5, s \ge 7 \text{ is odd}),$$
$$m_3(5,5) \le 124,$$
$$m_3(n,5) \le s^{n-2} - 10\sum_{i=0}^{n-6}(5^i - 1) \;\; (n \ge 6),$$
$$m_3(5,s) \le s^3 \;\; (s \text{ is even}),$$
$$m_3(n,s) \le s^{n-2} - s\sum_{i=0}^{n-6} s^i \;\; (s \text{ is even}, n \ge 6).$$

Theorem 6.6.10 [12]. The $m_3(n,s)$ does not exceed a positive root of the equation

$$x^2(s^2 - s - 1) - x\{(s^2 - 2s - 1) + (n + x)(s - 2)\} - 2(n + x) = 0$$

if $s > 2$ and $n \ge 4$.

Theorem 6.6.11 [8].

$$m_4(5,s) \le s(s-1) \quad (s \ge 4),$$
$$m_4(n,s) \le s^{n-3} - (s+1)\sum_{j=0}^{n-5} s^j + 1 \quad (n \ge 6, \; s \ge 4).$$

§ 7. Construction of Designs of Strength 2

We will consider a problem of the construction of symmetrical factorial designs from projective geometries starting with the construction of the regular symmetrical factorial design of strength 2 in $N = s^2$ runs for $s + 1$ factors with s levels each from the finite projective plane of order s.

Consider any given line in $PG(2,s)$. By Theorem 1.2.1, this line contains $s + 1$ points. Denote them by $F_0, \dots, F_s$. Set up a correspondence between each of these points and the factor, which we denote the same way as the point. Set up a correspondence between each point that does not belong to line $F_0, \dots, F_s$ and a treatment combination of the design. Hence, the number of factor equals $s + 1$, the number of treatment combinations equals $(s^2 + s + 1) - (s + 1) = s^2$.

By Theorem 1.2.1, a given point F_i belongs to s lines in addition to the line $F_0, \dots, F_s$. Set up a correspondence between each of these lines and one of s levels of the factor F_i (all points of any of these lines correspond to the same level). Denote the resulting design by $\mathbf{D}(2,s)$.

Theorem 6.7.1. The design $\mathbf{D}(2,s)$ is a regular factorial design of strength 2.

P r o o f. Since any pair of points belong only one line, there exists exactly one line passing through points F_i and point that does not belong to line $F_0, \ldots, F_s$. That means that each treatment combination corresponds exactly to one level of each factor.

Since any two lines have only one point in common, any combination of any two factors occurs exactly one time.

Therefore, the design $\mathbf{D}(2, s)$ is an orthogonal array of strength 2 and index 1.

Example 6.7.1. Consider the projective plane $PG(2,2)$ of order 2 illustrated by Figure 1 (§2 of chapter 1). Select any line in $PG(2,2)$, for example, those which represented by the circle in Figure 1. Set up a correspondence between the points of this line and the factors F_1, F_2, F_3. Then set up a correspondence between the rest points and treatments combinations 1, 2, 3, and 4 (Figure 7).

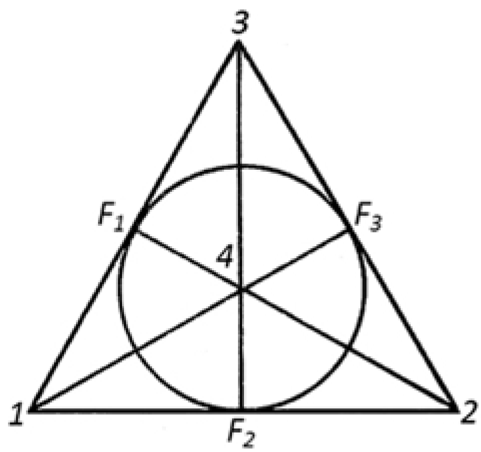

Figure 7. Projective geometry $PG(2, 2)$ and construction of orthogonal array (4, 3, 2, 2)

Now we have to determine the level of the given factor that occurs in the given treatment of the design. I.e., we have to fill in the cells of Table 5. Two lines pass through point F_1 (in addition to the line F_1, F_2, F_3): line $(F_1, 4, 2)$ and line $(1, F_1, 3)$. Therefore, in the treatments 1 and 3, the factor F_1 occurs at one of two possible levels (denote it by 0); in the treatments 2 and 4, the factor F_1 occurs at other level (denote it by 1). Two lines pass through point F_2 (in addition to the line F_1, F_2, F_3): line $(1, F_2, 2)$ and line $(3, 4, F_2)$. Therefore, in the treatments 1 and 2, the factor F_2 occurs at the level 0; in the treatments 3 and 4, the factor F_2 occurs at the level 1. Two lines pass through point F_3 (in addition to the line F_1, F_2, F_3): line $(1, 4, F_3)$ and line $(2, F_3, 3)$. Therefore, in the treatments 1 and 4, the factor F_3 occurs at the level 0; in the treatments 2 and 3, the factor F_3 occurs at the level 1. This design is presented in Table 5 and, obviously, is the orthogonal arrays (4, 3, 2, 2), i.e., the regular three-level design of strength 2.

Table 5
Construction of Orthogonal Array (4, 3, 2, 2)

# of Treatment Combination	Factor		
	F_1	F_2	F_3
1	0	0	0
2	1	0	1
3	0	1	1
4	1	1	0

Following C.R. Rao [13], consider the method of construction of orthogonal arrays from projective geometries $PG(n, s)$. There are $(s^n - 1)/(s - 1)$ $(n - 2)$-flats at infinity in $PG(n, s)$:

$$\chi_0 = 0, \quad a_1\chi_1 + \cdots + a_n\chi_n = 0 \quad \left(a_i \in GF(s)\right). \tag{6.7.1}$$

The bundle of s $(n - 1)$-flats

$$a_{0i}\chi_0 + a_1\chi_1 + \cdots + a_n\chi_n = 0 \quad \left(a_{0i} \in GF(s)\right) \tag{6.7.2}$$

passes through the $(n - 2)$-flat (6.7.1).

Set up a correspondence between the vertex (6.7.1) of the bundle (6.7.2) of flats and the factor, which we denote by $(a_1, \dots, a_n)$. The number of different bundles of flats and, therefore, the number of factors $(a_1, \dots, a_n)$ equals $(s^n - 1)/(s - 1)$. Obviously, we will not distinguish between factors $(a_1, \dots, a_n)$ and $(\rho a_1, \dots, \rho a_n)$ $(\rho \neq 0)$. Hence, we will represent coordinates $(a_1, \dots, a_n)$ of factors (and pencils of bundles of flats as well) in such a way that the first nonzero coordinate equals 1.

There are s^n finite points $(1, \chi_1, \dots, \chi_n)$ in $PG(n, s)$. Exactly one $(n - 1)$-flat of each of $(s^n - 1)/(s - 1)$ bundles of $(n - 1)$-flats passes through each of the these finite points. Set up a correspondence between the finite point and a treatment. We will assume that the factor $(a_1, \dots, a_n)$ occurs at the i-th level in the treatment $(1, \chi_1, \dots, \chi_n)$ if the point $(1, \chi_1, \dots, \chi_n)$ belongs to the i-th flat (6.7.2) of the bundle with the vertex at the flat (6.7.1).

Therefore, we get the design in s^n runs for $(s^n - 1)/(s - 1)$ factors at s levels each. It is easy to check that the design is an orthogonal array

$(s^n, (s^n-1)/(s-1), s, 2)$ of strength 2. Indeed, the degrees of freedom for the factors $(a_1, \dots, a_n)$ match with the degrees of freedom of interaction effects of the factors in the design s^n that correspond to nonzero coordinates $a_1, \dots, a_n$. Therefore, similarly of the proof of Theorem 6.1.1, we get that any combination of levels of two different factors $(a_1, \dots, a_n)$ and $(a'_1, \dots, a'_n)$ occurs in the design exactly s^{n-2} times. This number is the index of the orthogonal array.

Thus, we can formulate the following theorem.

Theorem 6.7.2 [13]. Let $s = p^h$ (p is prime, h is integer). Then there exists an orthogonal array $(s^n, (s^n-1)/(s-1), s, 2)$.

The described method of construction is equivalent to generating a subset of the full design s^m $(m = (s^n-1)/(s-1))$ with the following $l = (s^n-1)/(s-1) - n$ independent equations:

$$\begin{array}{l} a_{11}\chi_1 + a_{12}\chi_2 + \cdots + a_{1n}\chi_n - \chi_{n+1} = 0, \\ a_{21}\chi_1 + a_{22}\chi_2 + \cdots + a_{2n}\chi_n - \chi_{n+2} = 0, \\ \dots\dots\dots\dots\dots\dots\dots\dots \\ a_{l1}\chi_1 + a_{l2}\chi_2 + \cdots + a_{ln}\chi_n - \chi_{n+l} = 0, \end{array} \qquad (6.7.3)$$

where a_{ij} $(i = 1, \dots, l;\ j = 1, \dots, n)$ is the j-th coordinate of the i-th pencil in $PG(n, s)$ (with no pencils for main effects). Hence, the coefficients of the system (6.7.3) represent coordinates of the generators of the design.

Now it is evident that Theorem 6.6.1 is an immediate consequence of (5.2.5) and Theorem 6.7.2.

Example 6.7.2. We will illustrate the described method by the example of an orthogonal array (27, 13, 3, 2).

We will construct the array by using projective geometry $PG(3,3)$. There are 40 points in $PG(3,3)$; 13 of them are at infinity. The vertices corresponding to bundles (7.2.2) are (1, 0, 0), (0, 1,0), (0, 0, 1), (1, 1, 0), (1, 2, 0), (1, 0, 1), (1, 0, 2), (0, 1, 1), (0, 1, 2), (1, 1, 1), (1, 1, 2), (1, 2, 1), (1, 2, 2). These vertices correspond to 13 factors that we denote by $F_1, \dots, F_{13}$. If we arrange 27 finite points corresponding to 27 treatments in the matrix of size (27×3), the first column will correspond to levels of the factor F_1, the second column will correspond to levels of the factor F_2, and the third column will correspond to levels of the factor F_3. We can get the levels of the factor F_4 as the sum of the first two columns, levels of the factors F_5, as the sum of the first column and the second column multiplied by 2, etc. (addition and multiplication are performed in the field of the residue class (mod 3). The resulting design is presented in Table 6.

Table 6
Orthogonal Array (27, 13, 3, 2)

F_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8	F_9	F_{10}	F_{11}	F_{12}	F_{13}
(100)	(010)	(001)	(110)	(120)	(101)	(102)	(011)	(012)	(111)	(112)	(121)	(122)
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	1	1	1	1	0	0	1	1	1	1
2	0	0	2	2	2	2	0	0	2	2	2	2
0	1	0	1	2	0	0	1	1	1	1	2	2
1	1	0	2	0	1	1	1	1	2	2	0	0
2	1	0	0	1	2	2	1	1	0	0	1	1
0	2	0	2	1	0	0	2	2	2	2	1	1
1	2	0	0	2	1	1	2	2	0	0	2	2
2	2	0	1	0	2	2	2	2	1	1	0	0
0	0	1	0	0	1	2	1	2	1	2	1	2
1	0	1	1	1	2	0	1	2	2	0	2	0
2	0	1	2	2	0	1	1	2	0	1	0	1
0	1	1	1	2	1	2	2	0	2	0	0	1
1	1	1	2	0	2	0	2	0	0	1	1	2
2	1	1	0	1	0	1	2	0	1	2	2	0
0	2	1	2	1	1	2	0	1	0	1	2	0
1	2	1	0	2	2	0	0	1	1	2	0	1
2	2	1	1	0	0	1	0	1	2	0	1	2
0	0	2	0	0	2	1	2	1	2	1	2	1
1	0	2	1	1	0	2	2	1	0	2	0	2
2	0	2	2	2	1	0	2	1	1	0	1	0
0	1	2	1	2	2	1	0	2	0	2	1	0
1	1	2	2	0	0	2	0	2	1	0	2	1
2	1	2	0	1	1	0	0	2	2	1	0	2
0	2	2	2	1	2	1	1	0	1	0	0	2
1	2	2	0	2	0	2	1	0	2	1	1	0
2	2	2	1	0	1	0	1	0	0	2	2	1

The same design can be obtained as a subset of the full design 3^{13} by using the following system of 10 independent equations:

$$
\begin{array}{ll}
\chi_1 + \chi_2 - \chi_4 = 0, & \chi_1 + 2\chi_2 - \chi_5 = 0, \\
\chi_1 + \chi_3 - \chi_6 = 0, & \chi_1 + 2\chi_3 - \chi_7 = 0, \\
\chi_2 + \chi_3 - \chi_8 = 0, & \chi_2 + 2\chi_3 - \chi_9 = 0, \\
\chi_1 + \chi_2 + \chi_3 - \chi_{10} = 0, & \chi_1 + \chi_2 + 2\chi_3 - \chi_{11} = 0, \\
\chi_1 + 2\chi_2 + \chi_3 - \chi_{12} = 0, & \chi_1 + 2\chi_2 + 2\chi_3 - \chi_{13} = 0.
\end{array}
$$

§ 8. Construction of Compromise Designs

In this paragraph we will describe three classes of the so-called compromise symmetrical factorial designs of S. Addelman [14], which are regular geometric designs for the factorial set Ω that contains, in addition to all main effects, some two-factor interactions effects.

The first class of designs corresponds to the factorial set Ω that contains main effects of all factors and all two-factor interaction effects for given k factors.

The second class of designs corresponds to the factorial set Ω that contains main effects of all factors, all two-factor interaction effects for given k factors, and all two-factor interaction effects for the rest of factors.

The third class of designs corresponds to the factorial set Ω that contains main effects of all factors and all two-factor interaction effects for the factors that contain any one of k given factors.

It is obvious that these three types of compromise designs do not cover all cases of compromise designs, but they are important for applications and can be used in most practical situations when you want to estimate all main effects and some interaction effects of first order.

First Class

We will construct designs corresponding to the following set of pairwise orthogonal contrasts: main effects of all factors and all two-factor interaction effects for given k factors at s levels ($s = p^h$, p is prime). These given k factors are said to be interacting.

First, construct the regular symmetrical design of main effects for $(s^n - 1)/(s - 1)$ factors with s^n runs (in accordance with §7 of the chapter). Each of these $(s^n - 1)/(s - 1)$ factors corresponds to the vertex (6.7.1) of a bundle of the flats (6.7.2) in $PG(n, s)$**.** For interacting factors, we select those that correspond to the vertices of bundles satisfying the following condition: there is no nontrivial linear combination of four of them that equals zero. It is evident that main effects and interaction effects of interacting factors will form a set of pairwise orthogonal contrasts.

Delete those vertices that are represented by a linear combination of some of two vertices corresponding to the interacting factors. In this case, all main effects of the remaining noninteracting factors are pairwise orthogonal and orthogonal to main effects and interaction effects of first order of interacting factors.

Example 6.8.1. Consider regular symmetrical design for seven two-level factors in eight runs. Each of these factors corresponds to the following vertices of bundles of parallel flats:

$$F_1 \to (100),\quad F_2 \to (010),\quad F_3 \to (001),\quad F_4 \to (110)$$
$$F_5 \to (101),\quad F_6 \to (011),\quad F_7 \to (111).$$

For interacting factors, select, for example, F_4 and F_5. The sum of corresponding vertices is (011). Therefore, the vertex (011) and the corresponding factor F_6 should be deleted. The resulting design

$$\begin{array}{cccccc} F_1 & F_2 & F_3 & F_4 & F_5 & F_7 \end{array}$$
$$\left\Vert\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{array}\right\Vert$$

corresponds to the set of pairwise orthogonal main effects of the factors $F_1, F_2, F_3, F_4, F_5, F_7$ and an interaction effect of the factors F_4 and F_5.

Second Class

This class of compromise designs corresponds to the factorial set Ω containing all main effects and all two-factor interaction effects of given k factors (interaction factors of the first subset) and all two-factor interaction effects of the rest factors (interaction factors of the second subset). The number of levels of all factors is $s = p^h$ (p is prime).

First consider regular symmetrical design of main effects for $(s^n - 1)/(s - 1)$ factors in s^n runs. For interacting factors of the first subset, select those that correspond to vertices of bundles of flats satisfying the following condition: there is no nontrivial linear combination of four of them that equals zero. Then delete those vertices that are represented by a linear combination of some two vertices corresponding to the interacting factors.

Consider now the remaining vertices and select those that satisfy the following two conditions:

1) there is no nontrivial linear combination of four of them that equals zero;

2) there is no nontrivial linear combination of two of them that equals some linear combination of two vertices of interacting factors of the first subset.

Example 6.8.2. Our goal now is to construct the design for six three-level factors with 81 runs that correspond to the factorial set Ω that contains main effects of all six factors, two-factor interaction effects of one subset of three factors and two-factor interaction effects of the second subset of three remaining factors. Consider a regular symmetrical design of main effects for 40 three-level factors with 81 runs, which in accordance with §7 of this chapter is represented by 40 vertices of bundles of parallel flats. Select the vertices (1000), (0100), (0010) as factors of the first subset of interacting factors. These vertices and all their linear combinations (1100), (1200), (1010), (1020), (0110), and (0120) cannot be part of the second subset of interacting factors. At the same time, it is evident that the vertices (0001), (1110), (1121) can represent factors of the second subset. It is easy to check that no other vertex can be included in the second subset.

Third Class

This class of compromise designs corresponds to the factorial set Ω containing all main effects and all two-factor interaction effects for the factors that contain any one of k given factors. We will again start with the regular symmetrical design of main effects for $(s^n-1)/(s-1)$ factors with s^n runs. For interacting factors select those that correspond to vertices of bundles of flats satisfying the following condition: there is no nontrivial linear combination of four of them that equals zero. Delete those vertices that are represented by linear combinations of three factors of given k . Select those remaining vertices that satisfy the following condition: there is no nontrivial linear combination of two of them and two of given k vertices (factors) that equal zero. Obviously, the resulting design meets all requirements of the third class of compromise designs.

Example 6.8.3. Our goal now is to construct a two-level design with 64 runs so that all main effects and two-factor interaction effects corresponding to at least one of given four factors are pairwise orthogonal. Consider the regular symmetrical design of main effects for 63 two-level factors with 64 runs. Select the following four vertices for the given four factors: (100000), (010000), (001000), (000100). Now exclude from further consideration all vertices for which the following two conditions hold simultaneously: the last two coordinates equal zero, and among the first four coordinates there is at least one zero coordinate. Of the remaining vertices, obviously, the following seven vertices satisfy all of the requirements: (000010), (000001), 000011), (111100), (111110), (111101), and (111111).

§ 9. Two-Level Designs

Any geometric two-level design **D** (as any geometric design) is uniform. I.e., any level of any factor occurs in the design exactly $N/2$ times (N is the number of treatment combinations in the design). Hence, the Chebyshev model will be the same as the A^{Ω}-model of true effects. Then a full factorial model is

$$Ey = b_0 + b_1 x_1 + \cdots + b_m x_m + b_{12} x_1 x_2 + \cdots \\ + b_{1\ldots m} x_1 \ldots x_m, \tag{6.9.1}$$

where $x_i = 1$ for one of two levels of the factor and $x_i = -1$ for another level.

Consider two matrices of the design **D**: $\mathbf{D}_F = \{\chi_{iu}\}$ $[\chi_{iu} \in GF(2)]$ and $\mathbf{D} = \{x_{iu}\}$, where $\chi_{iu} = 0, x_{iu} = 1$ if the factor F_i occurs in the u-th treatment of the design at level 0, and $\chi_{iu} = 1, x_{iu} = -1$ if the factor F_i occurs in the u-th treatment of the design at level 1. Then, obviously, the following two equalities are equivalent:

$$\chi_{i_1 u} + \cdots + \chi_{i_r u} = 0,$$

$$x_{i_1 u} \ldots x_{i_r u} = 1.$$

Therefore, the system of the generating relations (6.3.1) for the geometric two-level design **D** is transformed as follows:

$$\begin{aligned} &x_1^{a_{11}} \ldots x_m^{a_{m1}} = 1, \\ &\ldots\ldots\ldots\ldots \\ &x_1^{a_{1l}} \ldots x_m^{a_{ml}} = 1, \end{aligned} \tag{6.9.2}$$

where $a_{ij} \in GF(2)$ $(a_{ij} = 0$ or $1)$, $l = m - k$.

The system (6.9.2) in accordance with §3 of chapter 1 corresponds to a subset of 2^k points $(k = m - l)$ of the full design 2^m.

The expressions of form $x_1^{a_1} \ldots x_m^{a_m}$ $(a_1, \ldots, a_m = 0$ or $1)$ is called an interaction (as opposed to an interaction effect), or an r-letter interaction if exactly r numbers of a_i $(i = 1, \ldots, m)$ equal 1. We will use a concept of generating, defining, independent interactions similar to a concept of generating, defining, independent flats, i.e., equalities of type (6.3.1). Generating interactions will also be called generators.

An elementary transformation of a set of interactions is multiplication of one of the interactions of the set by other interactions of the set.

Let $\mathbf{X}^f$ be the coefficient matrix of the full design 2^m (the design $\mathbf{D}^f$) for a full factorial model (6.9.1). As a simple consequence of Theorem 3.4.1 and Note 1 to the Theorem 3.4.1 we get the following theorem.

Theorem 6.9.1. The matrix $\mathbf{X}^f$ is a square matrix with elements +1 and –1; all columns of the matrix $\mathbf{X}^f$ are pairwise orthogonal; the values x_i and $x_{i_1} \dots x_{i_r}$ at the points of the design $\mathbf{D}^f$ form the vector of the main effect of the factor F_i and the vector of the interaction effect of the factors $F_{i_1}, \dots, F_{i_r}$ respectively.

Sometimes, we will use notations + and – in the design matrix and in the coefficient matrix instead of +1 and -1 respectively.

Consider the matrix of the full design 2^m (the design $\mathbf{D}^f$) and its submatrix $\mathbf{D} = \{x_{iu}\}$ defined by the following generating relations:

$$1 = R_1, \dots, 1 = R_l, \tag{6.9.3}$$

where $R_1, \dots, R_l$ are l independent interactions $(l < m)$.

In the matrix $\mathbf{X}^f$, select rows corresponding to the design **D.** Denote the resulting matrix by $\widetilde{\mathbf{X}}$. Denote by $\mathbf{X}$ the matrix composed of one representative from each set of identical columns of the matrix $\widetilde{\mathbf{X}}$.

Theorem 6.9.2. For the design **D** defined by the generating relations (6.9.3) the following statements hold:

1. The matrix $\widetilde{\mathbf{X}}$ has size $2^{m-l} \times 2^m$; 2^m columns of the matrix $\widetilde{\mathbf{X}}$ are split into 2^{m-l} alias sets, so each alias set has identical columns, columns from different alias sets are orthogonal.

2. There exist $m - l$ columns of the design **D** that form the full design 2^{m-l} (the design $\mathbf{D}_l^f$). There exist no columns of selected $m - l$ columns such that their product (in the sense of definition 3.4.1) corresponds to a defining interaction.

3. The matrix **X** is identical to the coefficient matrix of the design $\mathbf{D}_l^f$ for the full factorial model.

P r o o f. Statement 1 of the theorem follows from Theorem 6.4.1. We will prove statements 2 and 3 by induction. Let $l = 1$. Assume that $\mathbf{D}_1$ and $\mathbf{X}_1$ are the matrices that contain those row of the matrices $\mathbf{D}^f$ and $\mathbf{X}^f$ respectively that satisfy the first generating relation $1 = R_1$.

If x_i belongs to the interaction R_1, delete the column corresponding to x_i from m columns of $\mathbf{D}_1$. Then the rest $m - 1$ columns form the full design 2^{m-1} (the design $\mathbf{D}_1^f$), because these is no two identical rows in the $\mathbf{D}_1^f$. Indeed, if such two rows exist (say, the i-th and the j-th rows), the i-th and the j-th elements of the deleted column have different signs (otherwise we get two identical row in $\mathbf{D}^f$, which is a contradiction). Therefore, the i-th and the j-th elements of the column corresponding to the interaction R_1 have different signs (which is also a contradiction).

Statement 3 of the theorem for $l = 1$ is obvious, because $\mathbf{X}_1$ contains a unit column, all columns of the full design 2^{m-1}, and all possible products of $2, \ldots, m-1$ columns of the full design 2^{m-1}.

Now assume that the theorem is valid for $l = n$ for the design $\mathbf{D}_n$ defined by generating relations

$$1 = R_1, \ldots, 1 = R_n.$$

We will prove that the theorem is valid for $l = n + 1$ for the design $\mathbf{D}_{n+1}$ defined by generating relations

$$1 = R_1, \ldots, 1 = R_n, 1 = R_{n+1}.$$

Let

$$Q_1, Q_2 \ldots \tag{6.9.4}$$

be the defining interactions of the design $\mathbf{D}_n$. Then it is evident that

$$Q_1,\ Q_2, \ldots, R_{n+1},\ Q_1 R_{n+1},\ Q_2 R_{n+1} \ldots \tag{6.9.5}$$

are the defining interactions of the design $\mathbf{D}_{n+1}$. By the induction hypothesis, among selected $m - n$ columns of the design $\mathbf{D}_n$ forming the full design $\mathbf{D}_n^f$ there are no columns which product produces the defining interactions (6.9.4). Therefore, there are no columns among of them which product produces two or more defining interactions (6.9.5). Indeed, if such two interactions exist, they are interactions of type $Q_i R_{n+1}$ and $Q_j R_{n+1}$. Their product is an interaction of type Q_q, which is a contradiction. Now select the columns forming the full design $\mathbf{D}_n^f$ and consider only those columns with the product that forms an interaction from (6.9.5). Delete any of these columns. The remaining $m - n - 1$ columns, obviously, form the full design 2^{m-n-1} (the design D_{n+1}^f). Among of them, there are not columns with the product that forms an interaction of the defining relation (6.9.5).

This completes the proof of the theorem.

Example 6.9.1. Consider the matrix $\mathbf{D}^f$ of the full design 2^5. We will construct a fractional design by using the following generating relations:

$$1 = x_1 x_2 x_4,\ \ 1 = x_1 x_2 x_3 x_5. \tag{6.9.6}$$

The matrix of the fractional design 2^{5-2} is

$$\mathbf{D}_2 = \left\| \begin{matrix} + & - & + & - & - \\ - & + & + & - & - \\ - & - & - & + & - \\ + & + & - & + & - \\ + & - & - & - & + \\ - & + & - & - & + \\ - & - & + & + & + \\ + & + & + & + & + \end{matrix} \right\|.$$

The coefficient matrix $\mathbf{X}^f$ of the design $\mathbf{D}^f$ for the full factorial model has size $2^5 \times 2^5$. Applying the generating relations (6.9.6), we get the matrix $\widetilde{\mathbf{X}}$ of size $2^3 \times 2^5$. Selecting one representative from each alias set of identical columns of the matrix $\widetilde{\mathbf{X}}$, we get the matrix $\mathbf{X}$ (see Table 7). Each of the columns of this matrix in Table 7 is marked by four interactions that show which four columns of the matrix $\widetilde{\mathbf{X}}$ they represent.

Table 7
Matrix X and Alias Sets for Fractional Design 2^{5-2}

1 $x_1x_2x_4$ $x_1x_2x_3x_5$ $x_3x_4x_5$	x_1 x_2x_4 $x_2x_3x_5$ $x_1x_3x_4x_5$	x_2 x_1x_4 $x_1x_3x_5$ $x_2x_3x_4x_5$	x_3 $x_1x_2x_3x_4$ $x_1x_2x_5$ x_4x_5	x_4 x_1x_2 $x_1x_2x_3x_4x_5$ x_3x_5	x_5 $x_1x_2x_4x_5$ $x_1x_2x_3$ x_3x_4	x_1x_3 $x_2x_3x_4$ x_2x_5 $x_1x_4x_5$	x_1x_5 $x_2x_4x_5$ x_2x_3 $x_1x_3x_4$
+	+	−	+	−	−	+	−
+	−	+	+	−	−	−	+
+	−	−	−	+	−	+	+
+	+	+	−	+	−	−	−
+	+	−	−	−	+	−	+
+	−	+	−	−	+	+	−
+	−	−	+	+	+	−	−
+	+	+	+	+	+	+	+

We will use the constructive proof of Theorem 6.9.2 to select columns of the matrix $\mathbf{D}_2$ forming the full design 2^3. First, delete any column corresponding to x_i from matrix $\mathbf{D}_2$ if x_i belongs to the first generating relation of (6.9.6) (for example, x_4). Of the remaining columns, we need to delete any one that belongs to the only interaction of defining relation

$$1 = x_1x_2x_4 = x_1x_2x_3x_5 = x_3x_4x_5,$$

obtaining by multiplication of all or some of columns $x_1, x_2, x_3,$ and x_5. The required interaction is $x_1x_2x_3x_5$. Therefore, if we delete any of columns x_1, x_2, x_3, or x_5 (for example, x_5), we get the matrix of the full design 2^3:

$$\mathbf{D}_2^f = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \left\| \begin{array}{ccc} + & - & + \\ - & + & + \\ - & - & - \\ + & + & - \\ + & - & - \\ - & + & - \\ - & - & + \\ + & + & + \end{array} \right\| \end{array}.$$

The matrix $\mathbf{X}$ is identical to the coefficient matrix of the full design $\mathbf{D}_2^f$ for a full factorial model. Therefore, for constructing the design $\mathbf{D}_2$, we can start with the matrix of the full design 2^3 for variables x_1, x_2, x_3 and then add columns corresponding to x_4 and x_5 with the relations $x_4 = x_1x_2$, $x_5 = x_1x_2x_3$, resulting with the design matrix $\mathbf{D}_2$ (up to permutations of rows and columns).

The described method can be easily expanded to a general case of construction of a fractional factorial design based on the generating relations (6.9.3) by using Theorem 6.9.2.

By Theorem 6.9.2, the columns of the matrix $\widetilde{\mathbf{X}}$ split to 2^{m-l} alias sets; each alias set has identical columns; columns from different alias sets are orthogonal. It is evident that the alias set containing the interaction S can be found multiplying all interactions of the defining relation

$$1 = R_1 = R_2 = R_1R_2 = \cdots = R_1R_2 \ldots R_l$$

by S. Therefore, the alias set that contains the interaction S is

$$S,\ R_1S,\ R_2S,\ R_1R_2S, \ldots, R_1R_2 \ldots R_lS. \tag{6.9.7}$$

We cannot find unique LS estimates of parameters of the full factorial model (6.9.1) for the fractional design 2^{m-l} (the design $\mathbf{D}$), because the coefficient matrix $\widetilde{\mathbf{X}}$, obviously, contains identical columns and, therefore, the matrix $\widetilde{\mathbf{X}}^T\widetilde{\mathbf{X}}$ is singular. However, if the model contains only one interaction from each alias set, we can find unique LS estimates. Indeed, in this case the matrix $\mathbf{X}$ with orthogonal columns is the coefficient matrix of the design $\mathbf{D}$. The same is valid for the model that has not more than one representative from each alias set of interactions. Hence, the LS estimate of the vector $\widehat{\mathbf{B}}$ of parameters of the model is

$$\widehat{\mathbf{B}} = \frac{1}{2^{m-l}}\mathbf{X}^T\mathbf{y}. \tag{6.9.8}$$

Assume that we are using the design **D** for the postulated model

$$E\mathbf{y} = \mathbf{XB}$$

that contains one interaction for each alias set, but the real model

$$E\mathbf{y} = \mathbf{XB} + \mathbf{X}_0\mathbf{B}_0$$

is the full factorial model (6.9.1) (the matrix $\mathbf{X}_0$ is derived from the matrix $\widetilde{\mathbf{X}}$ by deleting of the columns included in **X**). Then the LS estimates (6.9.8) are biased. By (2.5.1),

$$E\widehat{\mathrm{B}} = \mathbf{B} + \mathbf{AB}_0, \tag{6.9.9}$$

where $\mathbf{A} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}_0$ is the bias matrix.

Put together the identical columns in $\mathbf{X}_0$. Then the matrix $\mathbf{X}^T\mathbf{X}_0$ of size $2^{m-l} \times 2^{m-l}(2^l - 1)$ is

$$\mathbf{X}^T\mathbf{X}_0 = \begin{Vmatrix} N & \dots & N & 0 & \dots & 0 & \dots & 0 & \dots & 0 \\ 0 & \dots & 0 & N & \dots & N & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 0 & \dots & 0 & \dots & N & \dots & N \end{Vmatrix},$$

where each row contains $2^l - 1$ elements equal N. Hence, the bias matrix is:

$$\begin{Vmatrix} 1 & \dots & 1 & 0 & \dots & 0 & \dots & 0 & \dots & 0 \\ 0 & \dots & 0 & 1 & \dots & 1 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 0 & \dots & 0 & \dots & 1 & \dots & 1 \end{Vmatrix}.$$

Using (6.9.9), we get the system of scalar equalities. Considering any of them, we get the following theorem.

Theorem 6.9.3. Suppose that we are using the design **D** to estimate coefficients of the postulated model that contains one interaction for each alias set, but the real model is the full factorial model (6.9.1). Then the estimate (6.9.8) of the coefficient corresponding to the interaction *S* is biased. The bias is equal to the sum of effects corresponding to all interactions (excluding *S*) that belong to the alias set containing *S*.

Hence, any estimate (6.9.8) is an unbiased estimate of the sum of effects corresponding to the interactions from one alias set. Such effects are called confounded.

In this paragraph we will discuss estimates of effects for a geometric design **D** assuming that the model contains not more than one interaction from each alias set.

Example 6.9.2. Suppose that the postulated model is

$$Ey = b_0 + b_1x_1 + b_2x_2 + b_3x_3,$$

while the real model is

$$Ey = 5 + x_1 + x_2 + 3x_3 + 0.3x_1x_2 + 0.1x_1x_3. \tag{6.9.10}$$

We will use the geometric design $2^3//4$ with the defining relation

$$1 = x_1x_2x_3 \tag{6.9.11}$$

to estimate the parameters of the postulated model. Assume that for 4 observations of the design **D**, we get the following results that presented below.

#	x_1	x_2	x_3	y
1	$-$	$-$	$+$	$6.2 + \varepsilon_1$
2	$+$	$-$	$-$	$1.6 + \varepsilon_2$
3	$-$	$+$	$-$	$1.8 + \varepsilon_3$
4	$+$	$+$	$+$	$10.4 + \varepsilon_4$

Before even trying to estimate the coefficients of the model (6.9.10), we will find the bias of the estimates by using (6.9.9).

The matrix $\widetilde{\mathbf{X}}$ (with grouped columns) is

$$\widetilde{\mathbf{X}} = \begin{array}{c} \begin{array}{cccccccc} 1 & x_1x_2x_3 & x_1 & x_2x_3 & x_2 & x_1x_3 & x_3 & x_1x_2 \end{array} \\ \left\| \begin{array}{cccccccc} + & + & - & - & - & - & + & + \\ + & + & + & + & - & - & - & - \\ + & + & - & - & + & + & - & - \\ + & + & + & + & + & + & + & + \end{array} \right\| \end{array}.$$

The matrices $\mathbf{X}$ and $\mathbf{X}_0$ in this case are identical:

$$\mathbf{X} = \mathbf{X}_0 = \left\| \begin{array}{cccc} + & - & - & + \\ + & + & - & - \\ + & - & + & - \\ + & + & + & + \end{array} \right\|.$$

Hence, (6.9.9) implies

$$E\left\| \begin{array}{c} \hat{b}_0 \\ \hat{b}_1 \\ \hat{b}_2 \\ \hat{b}_3 \end{array} \right\| = \left\| \begin{array}{c} b_0 \\ b_1 \\ b_2 \\ b_3 \end{array} \right\| + \left\| \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right\| \cdot \left\| \begin{array}{c} b_{123} \\ b_{23} \\ b_{13} \\ b_{12} \end{array} \right\|.$$

Therefore,

$$E\hat{b}_0 = b_0 + b_{123}; \quad E\hat{b}_1 = b_1 + b_{23};$$
$$E\hat{b}_2 = b_2 + b_{13}; \quad E\hat{b}_3 = b_3 + b_{12}. \tag{6.9.12}$$

We can reach the same result by using Theorem 6.9.3. To do so we need to multiply the interaction of the defining relation (6.9.11) sequentially by x_0, x_1, x_2, and x_3 and get four alias sets of interactions and corresponding effects:

$$\begin{array}{lll@{\qquad}lll} 1 & \text{and} & x_1x_2x_3, & b_0 & \text{and} & b_{123}, \\ x_1 & \text{and} & x_2x_3, & b_1 & \text{and} & b_{23}, \\ x_2 & \text{and} & x_1x_3, & b_2 & \text{and} & b_{13}, \\ x_3 & \text{and} & x_1x_2, & b_3 & \text{and} & b_{12}. \end{array}$$

Using (6.9.8), we get the estimates of the coefficients of the model (6.9.10):

$$\hat{b}_0 = 5 + \frac{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4}{4}; \qquad \hat{b}_1 = 1 + \frac{-\varepsilon_1 + \varepsilon_2 - \varepsilon_3 + \varepsilon_4}{4};$$
$$\hat{b}_2 = 1.1 + \frac{-\varepsilon_1 - \varepsilon_2 + \varepsilon_3 + \varepsilon_4}{4}; \quad \hat{b}_3 = 3.3 + \frac{\varepsilon_1 - \varepsilon_2 - \varepsilon_3 + \varepsilon_4}{4}.$$

Since $E\varepsilon_u = 0$, then $E\hat{b}_0 = 5$, $E\hat{b}_1 = 1$, $E\hat{b}_2 = 1.1$, $E\hat{b}_3 = 3.3$, which is consistent with (6.9.12) for the model (6.9.10).

Now we will focus on construction technique of a family of geometric designs, introduced by G.E.P.Box and J.S.Hunter and will give a series of theorems based on their ideas [15].

Consider l generators of the geometric design $2^m//2^{m-l}$. They can be treated as l independent interactions. Change signs of some of them. It is evident that the resulting interactions are also independent. They correspond to a geometric design that is different from the initial design. There are 2^l ways of allocating signs plus and minus to l generators. All corresponding designs are said to belong to the same family.

Definition 6.9.1. Generators of one of the design of the family are called principal generators if they have only positive signs; the corresponding defining relation is called a principal defining relation; the corresponding design is called a principal design of the family.

The whole set of defining relations of the same family can be represented by the following formal relation:

$$1 = (1 \pm R_1) \dots (1 \pm R_l),$$

where $R_1, \dots, R_l$ are the principal generators.

Lemma 6.9.1. If the interactions

$$R_1, \dots, R_n, R_{n+1}, \dots, R_l \tag{6.9.13}$$

are independent, the interactions

$$R_1, R_1R_2, \dots, R_1R_n, R_{n+1}, \dots, R_l \tag{6.9.14}$$

are also independent.

P r o o f. Suppose in the contrary that the following relationship is valid:

$$\pm 1 = R_{n+i_1} \dots R_{n+i_p} R_1 R_{j_1} \dots R_1 R_{j_r} \bar{R}_1,$$

where $0 < i_q \le l - n$, $0 < j_v \le n$, $q = 1, \dots, p$, $v = 1, \dots, r$, and $\bar{R}_1$ equal either R_1 or 1.

Then we get

$$\pm 1 = R_{j_1} \dots R_{j_r} R_{n+i_1} \dots R_{n+i_p} \bar{R}_1.$$

Since the interactions (6.9.13) are independent, we came to a contradiction. This proves the lemma.

Lemma 6.9.1 can be reformulated as follows.

Lemma 6.9.2. If (6.9.13) are generators of the design $2^m//2^{m-l}$, (6.9.14) are also generators of the design.

Lemma 6.9.3. For two designs of the same family, we can select generators in such a way that all of them are pairwise identical except one pair with the generators that have different signs.

P r o o f. Consider two designs $2^m//2^{m-l}$ of the same family. The first design has the generators (6.9.13). The generators of the second design are

$$-R_1, -R_2, \dots, -R_n, R_{n+1}, \dots, R_l. \tag{6.9.15}$$

By Lemma 6.9.2, the interactions (6.9.14) are the generators of the first design, and the interactions

$$-R_1, R_1R_2, \dots, R_1R_n, R_{n+1}, \dots, R_l \tag{6.9.16}$$

are the generators of the second design, which was to be proved.

Definition 6.9.2. The design that contains all treatments of the designs $\mathbf{D}_1, \dots, \mathbf{D}_r$ is called an aggregated design.

Note that an aggregated design is not similar to a unit of the set theory. For example, if each of two designs contains the same treatment combination, the aggregated design includes this treatment twice.

Theorem 6.9.4. The aggregated design of two geometric designs $2^m//2^{m-l}$ with the generators (6.9.13) and (6.9.15) is also a geometric design $2^m//2^{m-l+1}$ with the generators

$$R_1R_2, \dots, R_1R_n, R_{n+1}, \dots, R_l.$$

P r o o f. Since the interactions (6.9.14) and (6.9.16) are generators of the first and the second designs respectively, the aggregated design satisfies the relations

$$1 = R_1 R_2, \dots, 1 = R_1 R_n, 1 = R_{n+1}, \dots, 1 = R_l. \tag{6.9.17}$$

It is evident that the interactions of (6.9.17) are independent. Since the number of interactions in (6.9.17) is $l - 1$, these interactions are the generators of the aggregated design.

Thus, the proof is complete.

Since defining relations of two geometric designs of the same family differ only by signs, each alias set of interactions of one design corresponds to some alias set of the other design with interactions that differ only by signs.

Theorem 6.9.5. Let $\mathbf{D}_1$ and $\mathbf{D}_2$ be two geometric designs $2^m//2^{m-l}$ of the same family. Then 2^{m-l+1} estimates of the aggregated design **D** are half-sums and half-differences of 2^{m-l} pair of the unbiased estimates of sums of effects in corresponding alias sets of the designs $\mathbf{D}_1$ and $\mathbf{D}_2$.

P r o o f. Since the defining relation contains all possible products of the generators, a half of interactions (including 1) of the defining relation of the design $\mathbf{D}_1$, by Lemma 6.9.2, are identical to a half of interactions of the defining relation of the design $\mathbf{D}_2$, other interactions of the defining relation of the design $\mathbf{D}_1$ differ by signs from corresponding interactions of the defining relation of the design $\mathbf{D}_2$. Therefore, in any pair of corresponding alias sets, a half of interactions ($T_1, \dots, T_{2^{l-1}}$ in $\mathbf{D}_1$ and $\mathbf{D}_2$) are identical, and a half of interaction ($T_{2^{l-1}+1}, \dots, T_{2^l}$ in $\mathbf{D}_1$ and $-T_{2^{l-1}+1}, \dots, -T_{2^l}$ in $\mathbf{D}_2$) differ by signs. It is evident that the interactions $T_1, \dots, T_{2^{l-1}}$ belong to one alias set in **D**, and the interactions $T_{2^{l-1}+1}, \dots, T_{2^l}$ belong to other alias set. The column of the coefficient matrix of the design $\mathbf{D}_1$ corresponding to interactions $T_1, \dots, T_{2^{l-1}}, T_{2^{l-1}+1}, \dots, T_{2^l}$ denote by $\mathbf{S}_1$. The column of the coefficient matrix of the design $\mathbf{D}_2$ corresponding to interactions $T_1, \dots, T_{2^{l-1}}, -T_{2^{l-1}+1}, \dots, -T_{2^l}$ denote by $\mathbf{S}_2$. Then the column of the coefficient matrix of the design **D** corresponding to the interactions $T_1, \dots, T_{2^{l-1}}$ is

$$\mathrm{S}' = \left\| \begin{matrix} \mathrm{S}_1 \\ \mathrm{S}_2 \end{matrix} \right\|.$$

The column of the coefficient matrix of the design **D** corresponding to the interactions $T_{2^{l-1}+1}, \dots, T_{2^l}$ is

$$\mathrm{S}'' = \left\| \begin{matrix} \mathrm{S}_1 \\ -\mathrm{S}_2 \end{matrix} \right\|.$$

The estimate corresponding to the alias set $T_1, \dots, T_{2^{l-1}}$ in $\mathbf{D}$ is

$$\frac{1}{2^{m-l+1}}\mathbf{y}_D^T\mathbf{S}' = \frac{1}{2^{m-l}}\mathbf{y}_{D_1}^T\mathbf{S}_1 + \frac{1}{2^{m-l}}\mathbf{y}_{D_2}^T\mathbf{S}_2,$$

where $\mathbf{y}_D$, $\mathbf{y}_{D_1}$, and $\mathbf{y}_{D_2}$ are vector-columns of observations in the designs $\mathbf{D}$, $\mathbf{D}_1$, and $\mathbf{D}_2$ respectively.

The estimate corresponding to alias set $T_{2^{l-1}+1}, \dots, T_{2^l}$ is

$$\frac{1}{2^{m-l+1}}\mathbf{y}_D^T\mathbf{S}'' = \frac{1}{2^{m-l}}\mathbf{y}_{D_1}^T\mathbf{S}_1 - \frac{1}{2^{m-l}}\mathbf{y}_{D_2}^T\mathbf{S}_2,$$

which was to be proved.

Example 6.9.3. Consider the design $2^7//8$ (the design $\mathbf{D}'$) with the generators

$$x_1x_2x_4, \quad x_1x_3x_5, \quad x_2x_3x_6, \quad x_1x_2x_3x_7: \tag{6.9.18}$$

$$\begin{array}{ccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 \end{array}$$
$$\left\|\begin{array}{ccccccc} - & - & - & + & + & + & - \\ + & - & - & - & - & + & + \\ - & + & - & - & + & - & + \\ + & + & - & + & - & - & - \\ - & - & + & + & - & - & + \\ + & - & + & - & + & - & - \\ - & + & + & - & - & + & - \\ + & + & + & + & + & + & + \end{array}\right\|. \tag{6.9.19}$$

The defining relation of the design (6.9.19) is as follows:

$$\begin{aligned} 1 &= x_1x_2x_4 = x_1x_3x_5 = x_2x_3x_4x_5 = x_2x_3x_6 = x_1x_3x_4x_6 \\ &= x_1x_2x_5x_6 = x_4x_5x_6 == x_1x_2x_3x_7 = x_3x_4x_7 = x_2x_5x_7 \\ &= x_1x_4x_5x_7 = x_1x_6x_7 = x_2x_4x_6x_7 = x_3x_5x_6x_7 \\ &= x_1x_2x_3x_4x_5x_6x_7. \end{aligned} \tag{6.9.20}$$

By (6.9.8), we get 8 estimates

$$\hat{b}'_0 = \frac{\sum_{u=1}^8 y_u}{8}, \quad \hat{b}'_1 = \frac{\sum_{u=1}^8 x_{1u}y_u}{8}, \dots, \hat{b}'_7 = \frac{\sum_{u=1}^8 x_{7u}y_u}{8}.$$

All of them are unbiased estimates of the sums of confounded effects. For example,

$$E\hat{b}'_1 = b_1 + b_{24} + b_{35} + b_{12345} + b_{1236} + b_{346} + b_{256} + b_{1456} + b_{237} + b_{1347} + b_{1257} + b_{457} + b_{67} + +b_{12467} + b_{13567} + b_{234567}.$$

If we assume that more than two-factor interaction effects are equal to zero, the first alias set will contain only 4 interaction effects: b_1, b_{24}, b_{35},

b_{67}. Similarly, for the rest of alias sets we get the following mathematical expectations of estimates:

$$
\begin{aligned}
&E\hat{b}_0' = b_0, && E\hat{b}_4' = b_4 + b_{12} + b_{56} + b_{37},\\
&E\hat{b}_1' = b_1 + b_{24} + b_{35} + b_{67}, && E\hat{b}_5' = b_5 + b_{13} + b_{46} + b_{27},\\
&E\hat{b}_2' = b_2 + b_{14} + b_{36} + b_{57}, && E\hat{b}_6' = b_6 + b_{23} + b_{45} + b_{17},\\
&E\hat{b}_3' = b_3 + b_{15} + b_{26} + b_{47}, && E\hat{b}_7' = b_7 + b_{34} + b_{25} + b_{16}.
\end{aligned}
$$

In the defining relation of the design $\mathbf{D}'$, change signs of all interactions including x_1. Denote the resulting geometric design by $\mathbf{D}''$. Then the generators of the design $\mathbf{D}''$ are the following interactions: $-x_1x_2x_4$, $-x_1x_3x_5$, $x_2x_3x_6$, $-x_1x_2x_3x_7$. The defining relation of the design $\mathbf{D}''$ is

$$
\begin{aligned}
1 &= -x_1x_2x_4 = -x_1x_3x_5 = x_2x_3x_6 = -x_1x_2x_3x_7 = x_2x_3x_4x_5\\
&= -x_1x_3x_4x_6 = x_3x_4x_7 = -x_1x_2x_5x_6 = x_2x_5x_7 = -x_1x_6x_7\\
&= x_4x_5x_6 = -x_1x_4x_5x_7 = x_2x_4x_6x_7 = x_3x_5x_6x_7 = -x_1x_2x_3x_4x_5x_6x_7.
\end{aligned}
$$

If we assume that all interaction effects of second or more order are equal to zero, we get eight estimates $\hat{b}_0''$, $\hat{b}_1''$, ..., $\hat{b}_7''$ with the following mathematical expectations:

$$
\begin{aligned}
&E\hat{b}_0'' = b_0, && E\hat{b}_4'' = b_4 - b_{12} + b_{56} + b_{37},\\
&E\hat{b}_1'' = -b_1 + b_{24} + b_{35} + b_{67}, && E\hat{b}_5'' = b_5 - b_{13} + b_{46} + b_{27},\\
&E\hat{b}_2'' = b_2 - b_{14} + b_{36} + b_{57}, && E\hat{b}_6'' = b_6 + b_{23} + b_{45} - b_{17},\\
&E\hat{b}_3'' = b_3 - b_{15} + b_{26} + b_{47}, && E\hat{b}_7'' = b_7 + b_{34} + b_{25} - b_{16}.
\end{aligned}
$$

Combining the design $\mathbf{D}''$ with the principal design $\mathbf{D}'$ of the family, we get the aggregated design $2^7//16$ with the generators (by Theorem 6.9.4) $x_2x_5x_7$, $x_3x_4x_7$, $x_2x_3x_6$. By Theorem 6.9.5, 16 estimates of the aggregated design can be calculated as half-sums and half-differences of the corresponding estimates for the design $\mathbf{D}'$ and $\mathbf{D}''$:

$$
\begin{aligned}
&\left(\widehat{b'} - \widehat{b''}\right)/2 && \left(\widehat{b'} + \widehat{b''}\right)/2\\
&E\hat{b}_{00} = 0, && E\hat{b}_0 = b_0,\\
&E\hat{b}_1 = b_1, && E\hat{b}_{24} = b_{24} + b_{35} + b_{67},\\
&E\hat{b}_{14} = b_{14}, && E\hat{b}_2 = b_2 + b_{36} + b_{57},\\
&E\hat{b}_{15} = b_{15}, && E\hat{b}_3 = b_3 + b_{26} + b_{47},\\
&E\hat{b}_{12} = b_{12}, && E\hat{b}_4 = b_4 + b_{56} + b_{37},\\
&E\hat{b}_{13} = b_{12}, && E\hat{b}_5 = b_5 + b_{46} + b_{37},\\
&E\hat{b}_{17} = b_{17}, && E\hat{b}_6 = b_6 + b_{23} + b_{45},\\
&E\hat{b}_{16} = b_{16}, && E\hat{b}_7 = b_7 + b_{34} + b_{25}.
\end{aligned}
$$

Therefore, the estimates of the main effect of the given factor and all its two-factor interactions effects are unbiased. It is evident that for any geometric design of strength 2 (or higher) and for any given factor, there exists other design of the same family such that the aggregated design provides unbiased estimates of the main effect of this factor and all its two-factor interaction effects (assuming that all interaction effects of order two and higher are equal to zero).

Example 6.9.4. We will present aggregation technique of G.E.P. Box and J.S.Hunter [15] (for the geometric designs of the same family) for constructing designs of strength 3. For the design (6.9.19) with the generators (6.9.18), add eighth variable x_8 so that the column for x_8 in the design matrix consists only of +1. Then the generating relations of the resulting design are as follows:

$$1 = x_8,\ \ 1 = x_1x_2x_4,\ \ 1 = x_1x_3x_5,$$
$$1 = x_2x_3x_6,\ \ 1 = x_1x_2x_3x_7. \tag{6.9.21}$$

Consider this design (the design $\boldsymbol{D}_1$) as a principal design of a family. Now consider the design $\boldsymbol{D}_2$ with the design matrix that has opposite signs comparing to the design matrix of $\boldsymbol{D}_1$**.** It is evident that $\boldsymbol{D}_2$ is a geometric design and its generating relations are as follows:

$$1 = -x_8,\ \ 1 = -x_1x_2x_4,\ \ 1 = -x_1x_3x_5,$$
$$1 = -x_2x_3x_6,\ \ 1 = x_1x_2x_3x_7.$$

Combine these two designs of the same family. By Theorem 6.9.4, the generating relations of the aggregated design are

$$1 = x_1x_2x_4x_8,\ \ 1 = x_1x_3x_5x_8,\ \ 1 = x_2x_3x_6x_8,\ \ 1 = x_1x_2x_3x_7.$$

It is easy to get the defining relation of the aggregated design:

$$\begin{aligned}1 &= x_1x_2x_4x_8 = x_1x_3x_5x_8 = x_2x_3x_6x_8 = x_1x_2x_3x_7\\ &= x_2x_3x_4x_5 = x_1x_3x_4x_6 = x_3x_4x_7x_8 = x_1x_2x_5x_6\\ &= x_2x_5x_7x_8 = x_1x_6x_7x_8 = x_4x_5x_6x_8 = x_2x_4x_6x_7\\ &= x_1x_4x_5x_7 = x_5x_3x_6x_7 = x_1x_2x_3x_4x_5x_6x_7x_8.\end{aligned}$$

Therefore, the aggregated design is a geometric design of strength 3. Estimates of all main effects are unbiased (assuming that all interaction effects of order two and higher are equal to zero). The aggregated design is presented in Table 8.

Table 8
Geometric Design $2^8//16$ of Strength 3

x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
−	−	−	+	+	+	−	+
+	−	−	−	−	+	+	+
−	+	−	−	+	−	+	+
+	+	−	+	−	−	−	+
−	−	+	+	−	−	+	+
+	−	+	−	+	−	−	+
−	+	+	−	−	+	−	+
+	+	+	+	+	+	+	+
+	+	+	−	−	−	+	−
−	+	+	+	+	−	−	−
+	−	+	+	−	+	−	−
−	−	+	−	+	+	+	−
+	+	−	−	+	+	−	−
−	+	−	+	−	+	+	−
+	−	−	+	+	−	+	−
−	−	−	−	−	−	−	−

The constructed design of strength 3 in 16 runs provides 16 unbiased estimates of sums of confounded effects. Mathematical expectations of these estimates (assuming that all interaction effects of order two and higher are equal to zero) are presented below:

$$
\begin{array}{ll}
E\hat{b}_0 = b_0, & E\hat{b}_8 = b_8, \\
E\hat{b}_1 = b_1, & E\hat{b}_{12} = b_{12} + b_{37} + b_{48} + b_{56}, \\
E\hat{b}_2 = b_2, & E\hat{b}_{13} = b_{13} + b_{27} + b_{58} + b_{46}, \\
E\hat{b}_3 = b_3, & E\hat{b}_{14} = b_{14} + b_{28} + b_{36} + b_{57}, \\
E\hat{b}_4 = b_4, & E\hat{b}_{15} = b_{15} + b_{38} + b_{26} + b_{47}, \\
E\hat{b}_5 = b_5, & E\hat{b}_{16} = b_{16} + b_{78} + b_{34} + b_{25}, \\
E\hat{b}_6 = b_6, & E\hat{b}_{17} = b_{17} + b_{23} + b_{68} + b_{45}, \\
E\hat{b}_7 = b_7, & E\hat{b}_{18} = b_{18} + b_{24} + b_{35} + b_{67}.
\end{array}
$$

It is evident that similar procedure can be applied for any geometric design $(2^m//2^{m-l})$ of strength 2. As a result, we get an aggregated design $2^{m+1}//2^{m-l+1}$ of strength 3.

Let $\mathbf{D}_l$ be the geometric design $2^m//2^{m-l}$ with the generators $R_1, \dots, R_l$. Assume that first n generators $(0 \le n \le l)$ do not contain variable x_r. Let $\mathbf{D}_{l-1}$ be the design $2^{m-1}//2^{m-l}$ derived from $\mathbf{D}_l$ by deleting the column x_r. Then the following theorem holds.

Theorem 6.9.6. $\mathbf{D}_{l-1}$ is a geometric design with the generators

$$R_1, R_2, \dots, R_n, R_{n+1}R_{n+2}, \dots, R_{n+1}R_l\,. \tag{6.9.22}$$

P r o o f. For the design $\mathbf{D}_{l-1}$, obviously, the following relations hold:

$$1 = R_1,\ \ 1 = R_2, \dots,\ \ 1 = R_n,\ \ 1 = R_{n+1}R_{n+2}, \dots,\ \ 1 = R_{n+1}R_l,$$

because these relations hold for the design $\mathbf{D}_l$ and interactions (6.9.22) do not contain x_r. By Lemma 6.9.1, the interactions (6.9.22) are independent. Their number equals $l-1$. Hence, they are the generators.

This completes the proof of the theorem.

Example 6.9.5. Consider the design (6.9.19) with the generators (6.9.18). After deleting, say, the column x_3, we get a new set of generators of the design (6.9.19):

$$x_1x_2x_4,\ x_1x_3x_5,\ x_1x_2x_5x_6,\ x_2x_5x_7. \tag{6.9.23}$$

The third generator in (6.9.23) is a product of the second and the third generators of (6.9.18). The fourth generator in (6.9.23) is a product of the second and the fourth generators of (6.9.18). Hence, the generators of the design for six variables x_1, x_2, x_4, x_5, x_6, and x_7 are

$$x_1x_2x_4,\ x_1x_2x_5x_6,\ x_2x_5x_7.$$

Deleting, for example, the column x_7 of the design (6.9.19), we get the following design for five variables x_1, x_2, x_4, x_5, and x_6 with the generators $x_1x_2x_4$, $x_1x_2x_5x_6$:

$$\begin{array}{ccccc} x_1 & x_2 & x_4 & x_5 & x_6 \end{array}$$
$$\left\|\begin{array}{ccccc} - & - & + & + & + \\ + & - & - & - & + \\ - & + & - & + & - \\ + & + & + & - & - \\ - & - & + & - & - \\ + & - & - & + & - \\ - & + & - & - & + \\ + & + & + & + & + \end{array}\right\|.$$

Next, we will present a few more theorems for two-factor geometric designs from the article by L.I. Brodsky and V.Z. Brodsky [16]. The theorem will be accompanied by examples from the same article. Partially, these theorems are consequences of the results of this book for the general case of geometric designs with factors at s levels. However, in [16] one can find the direct proofs of the theorems for $s = 2$, and we will present below some of them.

Theorem 6.9.7. 2^{m-l} points satisfying the system (6.3.1) contain all combinations of the levels of the factors $F_{i_1}, \dots, F_{i_t}$ with equal frequency if and only if any nontrivial linear combination of (6.3.1) contains at least one nonzero coefficient other than the i_1-th, ..., i_t-th.

The proof of Theorem 6.9.7 is similar to the proof of Theorem 6.3.1.

The set of the factors F_{i_1}, …, F_{i_t}, by Theorem 6.9.7, contains all combinations of the levels with equal frequency if and only if no defining pencil has simultaneously all nonzero coordinates other than the i_1-th, … , i_t-th. Therefore, the following theorem holds.

Theorem 6.9.8. The design **D** corresponding to the generating relations (6.9.2) contains all combinations of the levels of the factors F_{i_1}, …, F_{i_t} with equal frequency if and only if $x_{i_1}^{a_1} \ldots x_{i_t}^{a_t}$ is not a defining interaction for any $a_1, \ldots, a_t = 0$ or 1.

Example 6.9.6. Consider the design $2^4//4$ (the design **D**) corresponding to the following generating relations:

$$1 = x_1x_2x_3,\ 1 = x_2x_3.$$

The defining relation of the design is

$$1 = x_1x_2x_3 = x_2x_3 = x_1.$$

The design **D**, by Theorem 6.9.8, contains, for example, all combinations of the levels of the factors F_2 and F_4 with equal frequency, because the interactions x_2, x_4 , x_2x_4 are not defining. The set of factors F_2 and F_3 is not full in the design **D** because the interaction x_2x_3 is defining. The set of the factors F_1 and F_3 and the set F_1 are also not full, because the interaction x_1 is defining.

Following statement due to C.R.Rao [2] is a special case of Theorem 6.9.8 and restatement of Theorem 6.3.1.

Theorem 6.9.9 [2]**.** The design **D** corresponding to the generating relations (6.9.2) is a hypercube of strength t if and only if all defining interactions contain more than t letters.

Example 6.9.7. The design $2^6//8$ with the generators $x_1x_2x_3x_4$, $x_2x_3x_5x_6$, and $x_3x_4x_6$ is, by Theorem 6.9.9, a hypercube of strength 2. Indeed, all defining interactions ($x_1x_2x_3x_4$, $x_2x_3x_5x_6$, $x_3x_4x_6$, $x_1x_4x_5x_6$, $x_1x_2x_6$, $x_2x_4x_5$, and x_3x_5) contain more than 2 letters.

The following theorem is a consequence of Theorem 6.4.1 for two-level designs.

Theorem 6.9.10. For the design **D** corresponding to l generating relations (6.9.2), all $2^m - 1$ effects of the design $\mathbf{D}^f$ are split into 2^k alias sets ($k = m - l$). One of them (defining) contains $2^{m-k} - 1$ effects. Each of the rest $2^k - 1$ alias sets contains 2^{m-k} effects. Effects from different alias sets (one from each set) generate pairwise orthogonal effects in the design **D.** Effects of the same alias set generate identical effects in the design **D.**

The nature of the effects of alias sets is defined by the following theorem that is a consequence of Theorem 6.4.2.

Theorem 6.9.11. If $x_{i_1}^{a_1} \dots x_{i_t}^{a_t}$ is not a defining interaction of the design **D** for any $a_1, \dots, a_t = 0$ or 1, all main effects and interaction effects of the factors $F_{i_1}, \dots, F_{i_t}$ in the design $\mathbf{D}^f$ generate main effects and interaction effects of the same factors in the design **D**.

Let $R_1, R_2, \dots, R_{m-k}$ be the generators of the design **D**. Then the defining relation of the design **D** is

$$1 = R_1 = R_2 = R_1R_2 = \cdots = R_1R_2 \dots R_{m-k}. \tag{6.9.24}$$

Let S be some interaction. Then it follows from (6.9.24) that

$$S = SR_1 = SR_2 = SR_1R_2 = \cdots = SR_1R_2 \dots R_{m-k}. \tag{6.9.25}$$

All interactions in (6.9.25) are different and their number is equal to 2^{m-k} (including maybe 1). Hence, the following theorem holds.

Theorem 6.9.12. An alias set that includes an interaction S can be represented by the interactions of (6.9.25). If no interaction of (6.9.25) equals 1, the interactions (6.9.25) and only they form alias set including S. If one of the interactions (6.9.25) equals 1, the rest $2^{m-k} - 1$ interactions and only they form defining alias set including S.

Theorem 6.9.13. Let

$$P_{i_1}, P'_{i_1}; \dots; P_{i_r}, P'_{i_r}$$

be the pairs of confounded effects in the design **D.** Then $P'_{i_1 \dots i_r} = P'_{i_1} \dots P'_{i_r}$ is confounded with $P_{i_1 \dots i_r} = P_{i_1} \dots P_{i_r}$ (they belong to the same alias set).

P r o o f. It is evident that

$$P_{i_1} = P'_{i_1}P^o_{i_1}, \dots, P_{i_r} = P'_{i_r}P^o_{i_r},$$

where $P^o_{i_k}$ is a defining interaction of the design $\mathbf{D}'$ $(k = 1, \dots, r)$.
Hence,

$$P_{i_1 \dots i_r} = P'_{i_1 \dots i_r}P^o,$$

where P^o is, obviously, a defining interaction. This proves the theorem.

Theorem 6.9.14. Let $P_1, P_2, \dots, P_{2^{m-k}}$ be all interactions of the same alias set. Then $P_1P_2, \dots, P_1P_{2^{m-k}}$ and only they form all $2^{m-k} - 1$ defining interactions.

P r o o f. The alias set of interactions $P_1, P_2, \dots, P_{2^{m-k}}$, by Theorem 6.9.12, can be represented as P_1, P_1R_1, P_1R_2, $P_1R_1R_2$, …, $P_1R_1 \dots R_{m-k}$. This proves the theorem.

Example 6.9.8. Consider again the design $2^4//4$ from Example 6.9.6. All 15 effects in the full design 2^4 are split into 4 alias sets. The defining alias set consists of three defining interactions $x_1,\ x_2x_3,\ x_1x_2x_3$. The alias set that includes, for example, x_2 is generated by multiplying all defining interactions by x_2. It consists of the interactions x_2, x_1x_2, x_3, and x_1x_3. The values that 15 interactions take in the design 2^4 //4 is presented in the Table 9 below (they are grouped by the alias sets).

Table 9
Alias Sets of the Design $2^4//4$

x_1 x_2x_3 $x_1x_2x_3$	$\boldsymbol{x_2}$ x_1x_2 $\boldsymbol{x_3}$ x_1x_3	$\boldsymbol{x_4}$ x_1x_4 $x_2x_3x_4$ $x_1x_2x_3x_4$	$\boldsymbol{x_2x_4}$ $x_1x_2x_4$ $\boldsymbol{x_3x_4}$ $x_1x_3x_4$
+	−	+	−
+	+	−	−
+	−	−	+
+	+	+	+

The interactions marked in bold correspond to main effects and interaction effects in the design $2^4//4$. For example, the contrast corresponding to second alias set is not an interaction effect of the factors F_1 and F_3 because the interaction x_1 is defining. At the same time, this contrast is the main effect of the factor F_2 and the main effect of the factor F_3 (x_2 and x_3 are not defining interactions).

By Theorem 6.9.14, all defining interactions can be constructed only based on any alias set. For example, using the forth alias set, we get all defining interactions:

$$(x_2x_4)\,(x_1x_2x_4) = x_1,$$
$$(x_2x_4)\,(x_3x_4) = x_2x_3,$$
$$(x_2x_4)\,(x_1x_3x_4) = x_1x_2x_3.$$

If the model (part of the model (6.9.1)) contains at least two interactions that belong to the same alias set of the design **D**, coefficient matrix **X** of the design has identical columns. Therefore, the information matrix $\mathbf{X'X}$ is singular and the solution of the normal equations of the method of least squares for the parameters of the model is not unique. If the model contains not more than one interaction from each alias set, the solution of the normal equations is unique.

For a special case of the model of main effects that includes only 1-letter interactions, the solution of the normal equations is unique if and only if for the design **D** there is no alias set that contains more than one 1-letter interaction. The last condition, by Theorem 6.9.9, is equivalent to the condition that the design **D** is a hypercube of strength 2.

A case when the model contains (except all 1-letter interactions $x_1, \dots, x_m$) also some interactions $S_1, \dots, S_l$ can be reduced to the main effect model as follows. Instead of the nonsingular design **D** for the model

$$Ey = b_0 + b_1 x_1 + \dots + b_m x_m + b_{m+1} S_1 + \dots + b_{m+l} S_l \qquad (6.9.26)$$

consider the nonsingular geometric main effect design $\mathbf{D}'$ for the model

$$Ey = b_0 + b_1 x_1 + \dots + b_m x_m$$
$$+ b_{m+1} x_{m+1} + \dots + b_{m+l} x_{m+l}, \qquad (6.9.27)$$

where $x_{m+1}, \dots, x_{m+l}$ correspond to additional factors $F_{m+1}, \dots, F_{m+l}$.

Assume that for the design $\mathbf{D}'$, the following condition holds: there exist the generators $x_{m+1} S_1, \dots, x_{m+l} S_l$. Then x_{m+i} and S_i belong to the same alias set for any $i = 1, \dots, l$. However, the interactions $x_1, \dots, x_m, x_{m+1}, \dots, x_{m+l}$ belong to the different alias sets, because **D** is a nonsingular main effect design. Therefore, the interactions $x_1, \dots, x_m$, $S_1, \dots, S_l$ belong to the different alias sets. Therefore, the following theorem holds.

Theorem 6.9.15. If there exists a nonsingular geometric main effect design in *N* runs for the model (6.9.27) with the generators including $x_{m+1} S_1, \dots, x_{m+l} S_l$, then there exists a nonsingular geometric design in *N* runs for the model (6.9.26).

Theorem 6.9.16. For the design corresponding to (6.9.2), there exist such $i_1, \dots, i_{m-k}$ and nondefining interactions $P_1, \dots, P_{2^k-1}$ (unique for the given $i_1, \dots, i_{m-k}$ and one from each alias set) that no interaction of $P_1, \dots, P_{2^k-1}$ contains any of letter $x_{i_1}, \dots, x_{i_{m-k}}$.

P r o o f. It is evident that there exist such $i_1, \dots, i_{m-k}$ that the set of the generators (6.9.2) can be converted to the set of generators $R_1, \dots, R_{m-k}$ by elementary transformations and the following condition holds: the generator R_j contains x_{i_j} and does not contain x_{i_u} $(j = 1, \dots, m-k, u \neq j)$.

Consider now some interaction *S* that belongs to the alias set $\mathcal{L}_S$. Assume that *S* contains x_{i_j} $(j = l_1, \dots, l_p;\ l_1, \dots, l_p = i_1, \dots, i_{m-k})$ and does not contain x_{i_u} $(u \neq l_1, \dots, l_p)$. Then, by Theorem 6.9.12, $SR_{l_1} \dots R_{l_p} \in \mathcal{L}_S$ and has the property specified by Theorem 6.9.14. To prove that the interaction $SR_{l_1} \dots R_{l_p}$ is the only one for the given $i_1, i_2, \dots, i_{m-k}$, assume in contrary that there exist two such interactions P_1 and P_2. By Theorem 6.9.14, their product $P_1 P_2$ is a defining interaction (not containing $x_{i_1}, \dots, x_{i_{m-k}}$). On the other hand, a defining interaction should contain some of $x_{i_1}, \dots, x_{i_{m-k}}$ as a product of some generators. This contradiction proves the theorem.

Theorem 6.9.17. In the design **D** corresponding to the l generating relations (6.9.2), there exist $k = m - l$ factors (columns) forming the full design $\mathbf{D}^f$. The elements of any of remaining columns $\boldsymbol{\xi}$ are the products of the corresponding elements of some columns of $\mathbf{D}^f$ (fixed for the given $\boldsymbol{\xi}$).

Proof. Similar to the proof of Theorem 6.9.16, find such $i_1, \ldots, i_{m-k}$ and generators $R_1, \ldots, R_{m-k}$ of the design that the generator R_j contains x_{i_j} and does not contain $x_{i_u}(j = 1, \ldots, m-k; u \neq j)$. Then, obviously, any defining interaction contains at least one letter of x_{i_j} $(j = 1, \ldots, m - k)$, or (which is the same) the interactions that contain no letter of x_{i_j} $(j = 1, \ldots, m-k)$ is not defining. I.e., the interaction $x_{j_1}^{a_1} \ldots x_{j_k}^{a_k}$ $(j_1, \ldots, j_k \neq i_1, \ldots, i_{m-k})$ is not defining for any $a_1, \ldots, a_k = 0$ or 1. By Theorem 6.9.8, the design **D** contains all combinations of the levels of the factors $F_{j_1}, \ldots, F_{j_k}$ $(j_1, \ldots, j_k \neq i_1, \ldots, i_{m-k})$. These factors, obviously, form the full design. We can get the elements of columns x_{i_j} $(j = 1, \ldots, m-k)$ from the generating relations $1 = R_{i_1}, \ldots, 1 = R_{i_{m-k}}$ by using the following formula:

$$x_{i_1} = R_{i_1} x_{i_1}, \ldots, x_{i_{m-k}} = R_{i_{m-k}} x_{i_{m-k}},$$

where the generators $R_{i_1}, \ldots, R_{i_{m-k}}$ do not contain $x_{i_1}, \ldots, x_{i_{m-k}}$.

Example 6.9.9. The generators of the design $2^6//8$ of Example 6.9.7, by elementary transformations, can be converted to the following generators:

$$R_1 = x_1x_2x_3x_4,\ R_2 = x_1x_3x_5,\ R_3 = x_1x_2x_6.$$

The generator R_j contains x_{i_j} and does not contain x_{i_u} $(j = 1, 2, 3;\ i_1 = 4, i_2 = 5, i_3 = 6; u \neq j)$. Therefore, any alias set $\mathcal{L}_S$ that contains a nondefining interaction S contains also the interaction without letters x_4, x_5, and x_6. For $S = x_1x_3x_5x_6$, for example, such an interaction is $SR_2R_3 = x_1x_2$. By Theorem 6.9.17, in the design $2^6//8$, the factors F_1, F_2, and F_3 form the full design $\mathbf{D}^f$. The columns for the factors F_4, F_5, and F_6 are obtained as products (in the sense of Definition 3.4.1) of the columns of the design $\mathbf{D}^f$ as follows:

$$1 = R_1,\ 1 = R_2,\ 1 = R_3,$$

or

$$x_4 = x_1x_2x_3,\ \ x_5 = x_1x_3,\ \ x_6 = x_1x_2\,.$$

Theorem 6.9.18. There exist such representatives of all nondefining alias sets (one from each set) that their product equals either 1 or any given defining interaction.

P r o o f. By Theorem 6.9.16, we can find such $i_1, \ldots, i_k$ that there exist nondefining interactions $P_1, \ldots, P_{2^k-1}$(one from each alias set) containing only letters $x_{i_1}, \ldots, x_{i_k}$. The number of nondefining alias sets equals $2^k - 1$. The number of different interactions containing only $x_{i_1}, \ldots, x_{i_k}$ also equals $2^k - 1$. Therefore, selected nondefining interactions $P_1, \ldots, P_{2^k-1}$ include all different interactions containing only $x_{i_1}, \ldots, x_{i_k}$. It is evident that the number of the interactions including the given letter x_i $(i = i_1, \ldots, i_k)$ equals $2^k - 1$. Therefore, the product of selected nondefining interactions equals 1.

To make this product equal to the given defining interaction P_0, replace the interactions P_1 with the interaction $P_1 P_0$ (the interaction $P_1 P_0$, belongs to the alias set with the interaction P_1).

This proves the theorem.

The following theorem is a simple consequence of Theorem 6.9.18.

Theorem 6.9.19. There exist such representatives of all alias sets (one from each set) that their product equals either 1 or any given defining interaction.

Theorem 6.9.20. The product of the interactions $P_1, \ldots, P_{2^k}$ from different alias sets equals either 1 or a defining interaction.

P r o o f. By Theorem 6.9.18, we can select the representatives $P_1', \ldots, P_{2^k}'$ of alias sets so that $P_1' \ldots P_{2^k}' = 1$. However, for any representative P_i of the i-th alias set, $P_i = P_i' P_{i_0}$, where P_{i_0} is a defining interaction. Hence, $P_1 \ldots P_{2^k} = P_1' \ldots P_{2^k}' P_{1_0} \ldots P_{2^k{}_0} = P_{1_0} \ldots P_{2^k{}_0}$, which was to be proved.

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Chapter 7. Construction of Orthogonal Arrays

§ 1. Orthogonal Arrays of Strength t

In this chapter we will focus on construction of orthogonal arrays that are not geometric designs. We will start with the results of K.A.Bush on orthogonal arrays of index 1.

Orthogonal Arrays of Index 1

Theorem 7.1.1 [1]. If $s = p^h$, where p is prime and $s > t$, then there exists the orthogonal array $(s^t,\ s+1,\ s,\ t)$.

Proof. Denote the elements of the Galois field $GF(s)$ by $0, 1, \dots, s-1$. Consider the set of s^t polynomials

$$Y_i(x) = a_{t-1}^{(i)}x^{t-1} + a_{t-2}^{(i)}x^{t-2} + \cdots + a_1^{(i)}x + a_0^{(i)} \quad (i = 1, \dots, s^t),$$

where the matrix

$$\begin{Vmatrix} a_{t-1}^{(1)} & a_{t-2}^{(1)} & \dots & a_0^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{t-1}^{(s^t)} & a_{t-2}^{(s^t)} & \dots & a_0^{(s^t)} \end{Vmatrix}$$

forms the full design $\boldsymbol{D}^f$ with elements from $GF(s)$.

Now generate the matrix $\mathbf{C} = \{c_{ij}\}$ of size $(s^t \times s)$ with the elements $c_{ij} = Y_i(j)$. We will show that the matrix $\mathbf{C}$ is an orthogonal array of strength t and index 1.

Suppose in the contrary that there exist t columns with two identical rows i and i'. Let this t columns correspond to the elements $i_1, \dots, i_t$ from $GF(s)$, the i-th and the i'-th rows correspond to the polynomials

$$\begin{aligned} Y_i(x) &= a_{t-1}^{(i)}x^{t-1} + a_{t-2}^{(i)}x^{t-2} + \cdots + a_1^{(i)}x + a_0^{(i)}, \\ Y_{i'}(x) &= a_{t-1}^{(i')}x^{t-1} + a_{t-2}^{(i')}x^{t-2} + \cdots + a_1^{(i')}x + a_0^{(i')} \end{aligned} \qquad (7.1.1)$$

respectively. Substitute the element i_1 into the equations of (7.1.1) and subtract one from another. Repeat the same with all elements $i_1, \dots, i_t$. Then we get the following system:

$$\begin{array}{l} A_{t-1} i_1^{t-1} + A_{t-2} i_1^{t-2} + \cdots + A_1 i_1 + A_0 = 0, \\ \dots\dots\dots\dots\dots\dots\dots\dots \\ A_{t-1} i_t^{t-1} + A_{t-2} i_t^{t-2} + \cdots + A_1 i_t + A_0 = 0, \end{array} \qquad (7.1.2)$$

where $A_l = a_l^i - a_l^{i'}$ $(i = 0, 1, \dots, t-1)$.

Since the polynomials $Y_i(x)$ and $Y_{i'}(x)$ are different, all A_l cannot be equal to zero simultaneously. For the existence of nontrivial solution of the system (7.1.2) the determinant of the matrix of coefficients of the system

$$\begin{Vmatrix} i_1^{t-1} & i_1^{t-2} & \cdots & i_1 & 1 \\ i_2^{t-1} & i_2^{t-2} & \cdots & i_2 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ i_t^{t-1} & i_t^{t-2} & \cdots & i_t & 1 \end{Vmatrix}$$

should equal zero. However, it is Vandermonde determinant with the value

$$\prod_{u<v} (i_u - i_v),$$

which cannot be equal to zero since all $i_1, \dots, i_t$ are different. This contradiction proves that the matrix cannot contain t columns with identical rows i and i'. Therefore, the matrix **C** is an orthogonal array $(s^t,\ s,\ s,\ t)$.

We can add one more column of elements $a_{t-1}^{(i)}$ to the matrix **C**. In this case $A_{t-1} = 0$, and we get the system of $t-1$ equations with $t-1$ unknowns. For the existence of nontrivial solution, Vandermonde determinant of order $t-2$ should equal zero, which is a contradiction. Therefore, the resulting matrix $\mathbf{C}_1$ is an orthogonal array $(s^t,\ s+1,\ s,\ t)$ of strength t and index 1.

Denote by $f(N,\ s,\ t)$ the maximum number of the factors of the orthogonal arrays $(N,\ m,\ s,\ t)$. Then, by (5.2.10), (5.2.11), and Theorem 7.1.1, we get the following theorem.

Theorem 7.1.2 [1].

$$s + 1 \le f(s^t, s, t) \le s + t - 1 \ \text{ if } \ s = 2^h > t, \qquad (7.1.3)$$

$$s + 1 \le f(s^t, s, t) \le s + t - 2 \ \text{ if } \ s = p^h > t, \qquad (7.1.4)$$

where p is odd prime.

Theorem 7.1.3 [1]. If $s = p^h$, where p is prime and $s \le t$, there exists an orthogonal array $(s^t,\ t+1,\ s,\ t)$.

P r o o f . Generate the following matrix of size $[s^t \times (t+1)]$:

$$\begin{Vmatrix} a_{t-1}^{(1)} & a_{t-2}^{(1)} & \cdots & a_1^{(1)} & a_0^{(1)} & Y_1(1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{t-1}^{(s^t)} & a_{t-2}^{(s^t)} & \cdots & a_1^{(s^t)} & a_0^{(s^t)} & Y_{s^t}(t) \end{Vmatrix}.$$

This matrix, obviously, is an orthogonal array of strength t and index 1.

By (5.2.12) and Theorem 7.1.3, the following theorem holds.

Theorem 7.1.4 [1].

$$f(s^t, s, t) = t + 1 \quad \text{if } s \le t,\ s = p^h \ (p \text{ is prime}).$$

Extension of Orthogonal Arrays

Let S be an ordered set of s elements (denoted by $0, 1, \dots, s-1$). For any t, consider s^t different ordered t-dimensional vector-rows with the elements belonging to the set S. These vectors can be divided into s^{t-1} sets so that each of them consists of s t-dimensional vectors and constitutes a full set of cyclic permutations of elements S. Denote these sets by S_i $(i = 1, \dots, s^{t-1})$.

Theorem 7.1.5 [2]. Suppose that there exists a matrix consisting of r columns with the elements from S

$$\begin{Vmatrix} a_{11} & \cdots & a_{1r} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nr} \end{Vmatrix} \quad (n = \lambda s^{t-1}) \tag{7.1.5}$$

satisfying the following condition: in any its submatrix of size $(n \times t)$, the number of rows belonging to each S_i equals λ. Then there exists an orthogonal array $(\lambda s^t,\ r,\ s,\ t)$. Besides, if the matrix (7.1.5) is an orthogonal array of strength $t-1$, there exists an orthogonal array $(\lambda s^t,\ r+1, s, t)$.

P r o o f . The sets S_i $(i = 1, \dots, s^{t-1})$ can be, in particular, defined as follows. Consider s^{t-1} different $(t-1)$-dimensional vector-rows with the elements belonging to S. Let the first t-dimensional vector-rows of each set S_i be $(j, i_1, \dots, i_{t-1})$, where $(i_1, \dots, i_{t-1})$ is one of s^{t-1} different $(t-1)$-dimensional rows and j is the fixed element of S. The rest $(s-1)$ rows of each set S_i are obtained from the first by cyclic permutation of the elements of S.

Now, we will construct the orthogonal arrays $(\lambda s^t,\ r,\ s,\ t)$ as follows. The first its λs^{t-1} rows are obtained from the matrix (7.1.5) satisfying the condition of the theorem. Then we add $s-1$ matrices obtained from (7.1.5) by cyclic permutation of elements of S to the matrix (7.1.5). It can be shown that the resulting matrix is an orthogonal array $(\lambda s^t,\ r,\ s,\ t)$.

If the matrix (7.1.5) is an orthogonal array of strength $t-1$, we can add additional column with the first λs^{t-1} elements equal to 0, the second λs^{t-1} elements equal to 1, etc. to the orthogonal array $(\lambda s^t,\ r,\ s,\ t)$. The resulting matrix is an orthogonal array $(\lambda s^t,\ r+1,\ s,\ t)$.

Note to Theorem 7.1.5. It is evident that if we select the first λs^{t-1} rows and the first r columns in the constructed orthogonal array $(\lambda s^t,\ r+1,\ s,\ t)$, then we get an orthogonal array $(\lambda s^{t-1},\ r,\ s,\ t-1)$. Hence, any orthogonal array $(\lambda s^{t-1},\ r,\ s,\ t-1)$ of strength $t-1$ can be obtained (by deleting some rows and one column) from some orthogonal array $(\lambda s^t,\ r+1,\ s,\ t)$ of strength t.

§ 2. Orthogonal Arrays of Strength 2

Method of Differences

In this section we present method of differences for constructing orthogonal arrays of strength 2 due to R.C. Bose and K.A. Bush [3].

Definition 7.2.1. An orthogonal array $(\alpha\beta s^2,\ m,\ s,\ 2)$ is called β-resolvable if it is the juxtaposition of αs different arrays:

$$\mathbf{D} = \left\| \begin{matrix} \mathbf{D}_1 \\ \vdots \\ \mathbf{D}_{\alpha s} \end{matrix} \right\|,$$

where $\mathbf{D}_i\ (i = 1, \ldots, \alpha s)$ are orthogonal arrays $(\beta s,\ m,\ s,\ 1)$. A 1-resolvable array is said to be completely resolvable.

If the orthogonal array $(\alpha\beta s^2,\ m,\ s,\ 2)$ is β-resolvable, we can add at least one more column to get the orthogonal array $(\alpha\beta s^2,\ m+1,\ s,\ 2)$. This column is formed by the elements $0, 1, \ldots, s-1 \in GF(s)$, so the element 0 corresponds to $\mathbf{D}_1, \ldots, \mathbf{D}_\alpha$, the element 1 corresponds to $\mathbf{D}_{\alpha+1}, \ldots, \mathbf{D}_{2\alpha}$, and so on.

Let M be an additive group consisting of s elements $0, 1, \ldots, s-1$. Suppose the matrix (difference scheme)

$$\left\| \begin{matrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nr} \end{matrix} \right\| \qquad (7.2.1)$$

satisfies the following condition: $n = \lambda s$, $a_{ij} \in M$, among the differences of the corresponding elements of any two columns of (7.2.1), each element of M occurs exactly λ times.

Consider the addition table of M. Then replace each element of the matrix (7.2.1) with the corresponding column of the addition table. We assert that the resulting design **D** is the completely resolvable array $(\lambda s^2,\ r,\ s,\ 2)$.

s^2 different (1×2) vectors with coordinates from M can be divided into s classes. Each class corresponds to one element of M as follows. If $i - j = l$ $(i,\ j,\ l \in M)$, then the vector $(i,\ j)$ belong to the class corresponding to l. In the addition table of M the differences of the corresponding elements of two different columns remain constant. Therefore, the vectors formed from the i-th and the j-th columns of the addition table of M belong to the class that corresponds to l. In the matrix (7.2.1), among of differences of corresponding elements of any two rows, each element of M occurs exactly λ times. Hence in the design **D** each vector occurs exactly λ times.

Since the resulting orthogonal array $(\lambda s^2,\ r,\ s,\ 2)$ is completely resolvable, we can add one more column to get an orthogonal array $(\lambda s^2,\ r+1,\ s,\ 2)$.

Example 7.2.1. We will illustrate the method by the example [3] of construction of an orthogonal array (18, 7, 3, 2). For M we choose the Galois field $GF(3)$. Hence, the addition table of M is

+	0	1	2
0	0	1	2
1	1	2	0
2	2	0	1

(7.2.2)

The difference scheme (7.2.1) was obtained in [3] by trial:

$$\left\Vert \begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 2 \\ 0 & 1 & 0 & 2 & 2 & 1 \\ 0 & 2 & 2 & 0 & 1 & 1 \\ 0 & 1 & 2 & 1 & 0 & 2 \\ 0 & 2 & 1 & 1 & 2 & 0 \end{matrix} \right\Vert . \qquad (7.2.3)$$

It is easy to check that the differences of corresponding elements of any two columns are 0, 1, and 2, and each of them occurs twice. Replace each element of the matrix (7.2.3) with the corresponding column of the addition table (7.2.2). For example, we replace 1 in the matrix (7.2.3) with the column $(1,2,0)^T$. To get an orthogonal array (18, 7, 3, 2) we add one more column to the orthogonal array (18, 6, 3, 2). The resulting design is presented in the Table 10.

Table 10
Orthogonal Array (18, 7, 3, 2)

0	0	0	0	0	0	0
1	1	1	1	1	1	0
2	2	2	2	2	2	0
0	0	1	2	1	2	0
1	1	2	0	2	0	0
2	2	0	1	0	1	0
0	1	0	2	2	1	1
1	2	1	0	0	2	1
2	0	2	1	1	0	1
0	2	2	0	1	1	1
1	0	0	1	2	2	1
2	1	1	2	0	0	1
0	1	2	1	0	2	2
1	2	0	2	1	0	2
2	0	1	0	2	1	2
0	2	1	1	2	0	2
1	0	2	2	0	1	2
2	1	0	0	1	2	2

Using the method of differences, we can get the following result.

Theorem 7.2.1 [3]. If $\lambda = p^u$ and $s = p^v$ (p is prime), then there exists completely resolvable orthogonal array $(\lambda s^2,\ \lambda s,\ s,\ 2)$.

P r o o f. Consider Galois field $GF(p^h)$ $(h = u + v)$ with elements that are polynomials of degree $h - 1$ with coefficients from $GF(p)$. Denote elements of $GF(p^h)$ by $0, 1, \dots, p^h - 1$, arranging them in lexicographic order, which means the following. Denote the element of $GF(p^h)$

$$a_{h-1}\chi^{h-1} + \cdots + a_1\chi + a_0 \tag{7.2.4}$$

by i if the vector of coefficients of the polynomial (7.2.4) corresponds to the number i expressed in base p.

Consider now a subset M of elements of $GF(p^h)$ that consists of first p^v elements of $GF(p^h)$ when they are arranged in the lexicographic order. Set up a correspondence between the elements of $GF(p^h)$ and elements of M as follows. The element i of $GF(p^h)$ corresponds to one element j of M if $i \equiv j \pmod{p^v}$. Each element j of M corresponds to p^u elements of $GF(p^h)$.

Consider a multiplication table of $GF(p^h)$. Replace each of its element with the corresponding element of M. The resulting scheme has size $p^h \times p^h$. If we consider the differences of the corresponding elements of any two columns of the multiplication table, each element of $GF(p^h)$ will occur exactly once. If the elements i and i' of $GF(p^h)$ correspond to the elements j and j' of M, then the element $i - i'$ of $GF(p^h)$ corresponds to the elements $j - j'$ of M. Therefore, in the resulting scheme, each element of M occurs exactly $\lambda = p^u$ times among the differences of corresponding elements of any two columns. Replace each element the resulting scheme with the corresponding column of the addition table of M. The resulting design is, therefore, a completely resolvable orthogonal array $(\lambda s^2,\ \lambda s,\ s,\ 2)$.

Example 7.2.2. Let $p = 2,\ u = 1,\ v = 2$. Consider Galois field $GF(2^3)$. We get its elements using the irreducible polynomial $x^3 + x^2 + 1$:

$$\begin{array}{ll} 0 = P_0(x) \equiv 0, & 4 = P_4(x) \equiv x^2, \\ 1 = P_1(x) \equiv 1, & 5 = P_5(x) \equiv x^2 + 1, \\ 2 = P_2(x) \equiv x, & 6 = P_6(x) \equiv x^2 + x, \\ 3 = P_3(x) \equiv x + 1, & 7 = P_7(x) \equiv x^2 + x + 1. \end{array}$$

The correspondence between the elements of $GF(2^3)$ and M is given as follows:

$$\begin{array}{ccc} GF(2^3) & & M \\ \left.\begin{array}{c} 0,4 \\ 1,5 \\ 2,6 \\ 3,7 \end{array}\right\} & \rightarrow & \left\{\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array}\right. \end{array} \tag{7.2.5}$$

The multiplication table of $GF(2^3)$ is

x	0	1	2	3	4	5	6	7
0	0	0	0	0	0	0	0	0
1	0	1	2	3	4	5	6	7
2	0	2	4	6	5	7	1	3
3	0	3	6	5	1	2	7	4
4	0	4	5	1	7	3	2	6
5	0	5	7	2	3	6	4	1
6	0	6	1	7	2	4	3	5
7	0	7	3	4	6	1	5	2

Using (7.2.5), we get the following difference scheme:

$$\left\Vert \begin{array}{cccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\ 0 & 2 & 0 & 2 & 1 & 3 & 1 & 3 \\ 0 & 3 & 2 & 1 & 1 & 2 & 3 & 0 \\ 0 & 0 & 1 & 1 & 3 & 3 & 2 & 2 \\ 0 & 1 & 3 & 2 & 3 & 2 & 0 & 1 \\ 0 & 2 & 1 & 3 & 2 & 0 & 3 & 1 \\ 0 & 3 & 3 & 0 & 2 & 1 & 1 & 2 \end{array} \right\Vert . \tag{7.2.6}$$

To get a completely resolvable orthogonal array (32, 8, 4, 2), replace all elements of (7.2.6) with the corresponding columns of the addition table of M:

+	0	1	2	3
0	0	1	2	3
1	1	0	3	2
2	2	3	0	1
3	3	2	1	0

To get the orthogonal array (32, 9, 4, 2), add the column that consists of eight 0, eight 1, eight 2, and eight 3.

Finally, consider a procedure that adds new columns to the completely resolvable orthogonal array $(\lambda s^2,\ \lambda s,\ s,\ 2)$, where $\lambda = p^u,\ s = p^v$ (p is prime).

Let c be the integer part of u/v, i.e., $c = [u/v]$. If $c = 0$, we cannot do better after one column was added. If $c > 0$, i.e., $u \geq v$, we can use the same procedure and start from the completely resolvable orthogonal array $(\lambda s^2,\ \lambda s,\ s,\ 2)$ to get the completely resolvable orthogonal array $(\lambda_1 s^2,\ \lambda_1 s,\ s,\ 2)$, where $\lambda_1 = p^{u-v}$. Denote the first array by $\mathbf{D}_0$ and the second array, by $\mathbf{D}_1$. Since $\lambda_1 s^2 = \lambda s = p^{u+v}$, the number of rows in $\mathbf{D}_1$ is equal to the number of arrays of strength 1 composing $\mathbf{D}_0$.

Extend $\mathbf{D}_1$ by repeating each its row s times. Denote the resulting matrix by $\mathbf{D'}_1$. $\mathbf{D'}_1$ has the same number of rows as $\mathbf{D}_0$. In $\|\ \mathbf{D}_0\quad \mathbf{D'}_1\ \|$ each component of $\mathbf{D}_0$ corresponds to the same rows of $\mathbf{D}_1$ repeated s times. Since $\mathbf{D}_0$ is a completely resolvable array, then, obviously, any ordered pair of corresponding elements of rows of $\mathbf{D}_0$ and $\mathbf{D}_1$ occurs exactly λ times. Hence, $\|\ \mathbf{D}_0\quad \mathbf{D'}_1\ \|$ is the orthogonal array $(\lambda s^2,\ \lambda s + \lambda_1 s,\ s,\ 2)$ of strength 2.

Since $\mathbf{D}_1$ is completely resolvable, $\|\ \mathbf{D}_0\quad \mathbf{D'}_1\ \|$ is s-resolvable. If $c = 1$, i.e., $\lambda_1 < s$, then we have to stop after adjoining a final column that consists of λs zeros, λs units, etc. Therefore, we get the orthogonal array $(\lambda s^2,\ \lambda s + \lambda_1 s + 1,\ s,\ 2)$.

If $c > 1$, we can construct a completely resolvable orthogonal array $\mathbf{D}_2$, $(\lambda_2 s^2, \lambda_2 s,\ s,\ 2)$, where $\lambda_2 = p^{u-2v}$. By repeating each row of $\mathbf{D}_2$ s^2 times form the matrix $\mathbf{D}'_2$ and the matrix $\|\ \mathbf{D}_0\quad \mathbf{D}'_1\quad \mathbf{D}'_2\ \|$. It is evident that $\|\ \mathbf{D}_0\quad \mathbf{D}'_1\quad \mathbf{D}'_2\ \|$ is the orthogonal array of strength 2 with $\lambda s + \lambda_1 s + \lambda_2 s$ factors.

If $c = 2$, we stop the process by adding the final column. If $c > 2$, continue the procedure similarly.

Generally, the method leads to the orthogonal array $(\lambda s^2,\ \lambda s + \lambda_1 s + \cdots + \lambda_c s + 1,\ s,\ 2)$ of strength 2, where $\lambda_i = \lambda / s^i$. Therefore, the following theorem holds.

Theorem 7.2.2 [3]. Let $\lambda = p^u,\ \ s = p^v$ (p is prime). Then there exists an orthogonal array $(\lambda s^2,\ m,\ s,\ 2)$, where

$$m = \frac{\lambda(s^{c+1} - 1)}{s^c - s^{c-1}} + 1,\ \ c = [u/v].$$

Example 7.2.3 [3]**.** We will construct an orthogonal array of strength 2 in 27 runs for three-level factors. Using the results of Theorem 7.2.1 we can construct a completely resolvable orthogonal array $\mathbf{D}_0$ (27, 9, 3, 2). In this case $u = v = 1$ and $c = 1$. Hence, we can construct a completely resolvable orthogonal array $\mathbf{D}_1$, (9, 3, 3, 2). By repeating each row of this array three times, we get the 3-resolvable orthogonal array $\mathbf{D}'_1$ (27, 3, 3, 2). By adding the last column of 9 zeros, 9 units and 9 deuces to $\|\ \mathbf{D}_0\quad \mathbf{D}'_1\ \|$, we get the design that is presented in Table 11.

Table 11
Construction of Orthogonal Array (27, 13, 3, 2) by Difference Method

$$
\begin{Vmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 2 & 2 & 0 & 2 & 1 & 2 & 1 & 1 & 0 \\
1 & 2 & 1 & 2 & 0 & 0 & 1 & 0 & 2 & 2 & 1 & 1 & 0 \\
2 & 0 & 2 & 0 & 1 & 1 & 2 & 1 & 0 & 2 & 1 & 1 & 0 \\
0 & 0 & 1 & 2 & 2 & 0 & 2 & 1 & 1 & 1 & 2 & 2 & 0 \\
1 & 1 & 2 & 0 & 0 & 1 & 0 & 2 & 2 & 1 & 2 & 2 & 0 \\
2 & 2 & 0 & 1 & 1 & 2 & 1 & 0 & 0 & 1 & 2 & 2 & 0 \\
0 & 1 & 2 & 2 & 0 & 2 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\
1 & 2 & 0 & 0 & 1 & 0 & 2 & 2 & 1 & 1 & 1 & 0 & 1 \\
2 & 0 & 1 & 1 & 2 & 1 & 0 & 0 & 2 & 1 & 1 & 0 & 1 \\
0 & 2 & 2 & 0 & 2 & 1 & 1 & 0 & 1 & 0 & 2 & 1 & 1 \\
1 & 0 & 0 & 1 & 0 & 2 & 2 & 1 & 2 & 0 & 2 & 1 & 1 \\
2 & 1 & 1 & 2 & 1 & 0 & 0 & 2 & 0 & 0 & 2 & 1 & 1 \\
0 & 2 & 0 & 2 & 1 & 1 & 0 & 1 & 2 & 2 & 0 & 2 & 1 \\
1 & 0 & 1 & 0 & 2 & 2 & 1 & 2 & 0 & 2 & 0 & 2 & 1 \\
2 & 1 & 2 & 1 & 0 & 0 & 2 & 0 & 1 & 2 & 0 & 2 & 1 \\
0 & 0 & 2 & 1 & 1 & 0 & 1 & 2 & 2 & 2 & 2 & 0 & 2 \\
1 & 1 & 0 & 2 & 2 & 1 & 2 & 0 & 0 & 2 & 2 & 0 & 2 \\
2 & 2 & 1 & 0 & 0 & 2 & 0 & 1 & 1 & 2 & 2 & 0 & 2 \\
0 & 2 & 1 & 1 & 0 & 1 & 2 & 2 & 0 & 1 & 0 & 1 & 2 \\
1 & 0 & 2 & 2 & 1 & 2 & 0 & 0 & 1 & 1 & 0 & 1 & 2 \\
2 & 1 & 0 & 0 & 2 & 0 & 1 & 1 & 2 & 1 & 0 & 1 & 2 \\
0 & 1 & 1 & 0 & 1 & 2 & 2 & 0 & 2 & 0 & 1 & 2 & 2 \\
1 & 2 & 2 & 1 & 2 & 0 & 0 & 1 & 0 & 0 & 1 & 2 & 2 \\
2 & 0 & 0 & 2 & 0 & 1 & 1 & 2 & 1 & 0 & 1 & 2 & 2
\end{Vmatrix}
$$

Addelman-Kempthorne's method

Theorem 7.2.3 [4]. There exists a regular factorial design of strength 2 for

$$\frac{2(s^n-1)}{(s-1)}-1$$

factors at $s=p^h$ levels each (p is prime) in $2s^n$ runs.

The proof of this theorem is quite cumbersome and uses seven Lemmas. For the sake of simplicity, we will present only the method of construction for the case of $n=2$.

We will construct the first half of the design as follows. The first two columns (which we denote by $\mathbf{v}_1$ and $\mathbf{v}_2$) form a full design s^2. The rest of columns are as follows:

$$\mathbf{v}_1+\mathbf{v}_2,\ \mathbf{v}_1+2\mathbf{v}_2,\dots,\mathbf{v}_1+(s-1)\mathbf{v}_2,\ \mathbf{v}_1^{(2)}+\mathbf{v}_2,$$
$$\mathbf{v}_1^{(2)}+\mathbf{v}_1+\mathbf{v}_2,\ \mathbf{v}_1^{(2)}+2\mathbf{v}_1+\mathbf{v}_2,\dots,\ \mathbf{v}_1^{(2)}+(s-1)\mathbf{v}_1+\mathbf{v}_2,$$

where we denote by $\mathbf{v}_1^{(2)}$ the column with the elements that are the squares of corresponding elements of $\mathbf{v}_1$.

The following columns will form the second half of the design:

$$\mathbf{v}_1,\ \mathbf{v}_2,\ \mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\zeta}_1,\ \mathbf{v}_1+2\mathbf{v}_2+\boldsymbol{\zeta}_2,\dots,\mathbf{v}_1+(s-1)\mathbf{v}_2+\boldsymbol{\zeta}_{s-1},$$
$$k_0\mathbf{v}_1^{(2)}+\mathbf{v}_2, k_0\mathbf{v}_1^{(2)}+k_1\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_1,\ k_0\mathbf{v}_1^{(2)}+k_2\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_2,\ \dots,$$
$$k_0\mathbf{v}_1^{(2)}+k_{s-1}\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_{s-1},$$

where $\boldsymbol{\zeta}_1, \dots, \boldsymbol{\zeta}_{s-1}$ are s^2-dimensional columns consisting of elements $\zeta_1, \dots, \zeta_{s-1}$ respectively; the columns $\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_{s-1}$ consist of elements $\tau_1, \dots, \tau_{s-1}$ respectively. All parameters are defined as follows.

If s is odd, choose for the element k_0 a quadratic nonresidue in $GF(s)$. Denote by d_i i different nonzero elements of $GF(s)$ and set

$$\zeta_i=\frac{k_0-1}{4k_0d_i},\quad \mathrm{k}_i=k_0d_i,\quad \tau_i=\frac{d_i^2(k_0-1)}{4}. \tag{7.2.7}$$

If s is even, set $k_0=1$ and choose for the element ζ_i any element of $GF(s)$ that cannot be represented in the form $a^2-(1/d_i)a$, where $a\in GF(s)$. Set $k_i=d_i$ and for τ_i choose any element from $GF(s)$ that cannot be represented in the form a^2+d_i, where $a\in GF(s)$.

Using the method of S. Addelman and O. Kempthorne, we can construct the following orthogonal arrays: (18, 7, 3, 2), (32, 9, 4, 2), (50, 11, 5, 2), (128, 41, 4, 2), (250, 61, 5, 2), (54, 25, 3, 2), (98, 15, 7, 2), (128, 17, 8, 2), (162, 19, 9, 2). Only the first two of them can be constructed by using the difference method described in this section.

Example 7.2.4 [4]**.** We will illustrate the method for an orthogonal array (50, 11, 5, 2). The first half of the design in 25 runs contains 11 columns. The first two of them $\mathbf{v}_1$ and $\mathbf{v}_2$ form a full design. The rest of the columns are

$$\mathbf{v}_1+\mathbf{v}_2,\ \mathbf{v}_1+2\mathbf{v}_2,\ \mathbf{v}_1+3\mathbf{v}_2,\ \mathbf{v}_1+4\mathbf{v}_2,\ \mathbf{v}_1^{(2)}+\mathbf{v}_2,\ \mathbf{v}_1^{(2)}+\mathbf{v}_1+\mathbf{v}_2,$$
$$\mathbf{v}_1^{(2)}+2\mathbf{v}_1+\mathbf{v}_2,\ \mathbf{v}_1^{(2)}+3\mathbf{v}_1+\mathbf{v}_2,\ \mathbf{v}_1^{(2)}+4\mathbf{v}_1+\mathbf{v}_2.$$

The second half of the design also consists of 25 runs and the following columns:

$\mathbf{v}_1,\ \mathbf{v}_2,\ \mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\zeta}_1,\ \mathbf{v}_1+2\mathbf{v}_2+\boldsymbol{\zeta}_2,\ \mathbf{v}_1+3\mathbf{v}_2+\boldsymbol{\zeta}_3,\ \mathbf{v}_1+4\mathbf{v}_2+\boldsymbol{\zeta}_4,\ k_0\mathbf{v}_1^{(2)}+\mathbf{v}_2,\ k_0\mathbf{v}_1^{(2)}+k_1\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_1,\ k_0\mathbf{v}_1^{(2)}+k_2\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_2,\ k_0\mathbf{v}_1^{(2)}+k_3\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_3,\ k_0\mathbf{v}_1^{(2)}+k_4\mathbf{v}_1+\mathbf{v}_2+\boldsymbol{\tau}_4.$

For k_0 we choose a quadratic nonresidue in $GF(5)$: $k_0 = 3$. Then, by (7.2.7), we get

$$\zeta_i = 1/d_i,\quad k_i = 3\,d_i,\quad \tau_i = 3d_i^2.$$

Therefore, when d_i takes all nonzero values in $GF(5)$, $\zeta_i, \mathrm{k}_i, \tau_i$ will be as follows:

$$\begin{aligned}
&d_1 = 1,\ \zeta_1 = 1,\ k_1 = 3,\ \tau_1 = 3;\\
&d_2 = 2,\ \zeta_2 = 3,\ k_2 = 1,\ \tau_2 = 2;\\
&d_3 = 3,\ \zeta_3 = 2,\ k_3 = 4,\ \tau_3 = 2;\\
&d_4 = 4,\ \zeta_4 = 4,\ k_4 = 2,\ \tau_4 = 3.
\end{aligned}$$

Hence, 11 columns of the second half of the design are

$\mathbf{v}_1,\ \ \mathbf{v}_2,\ \ \mathbf{v}_1+\mathbf{v}_2+\mathbf{I},\ \ \mathbf{v}_1+2\mathbf{v}_2+3\mathbf{I},\ \ \mathbf{v}_1+3\mathbf{v}_2+2\mathbf{I},\ \ \mathbf{v}_1+4\mathbf{v}_2+4\mathbf{I},\ \ 3\mathbf{v}_1^{(2)}+\mathbf{v}_2,\ \ 3\mathbf{v}_1^{(2)}+3\mathbf{v}_1+\mathbf{v}_2+3\mathbf{I},\ \ 3\mathbf{v}_1^{(2)}+\mathbf{v}_1+\mathbf{v}_2+2\mathbf{I},\ 3\mathbf{v}_1^{(2)}+4\mathbf{v}_1+\mathbf{v}_2+2\mathbf{I},\ \ 3\mathbf{v}_1^{(2)}+2\mathbf{v}_1+\mathbf{v}_2+3\mathbf{I}.$

Graeco-Latin and Hyper-Graeco-Latin Squares

A set of n pairwise orthogonal Latin squares of order s is a special case of a regular factorial main effect design, i.e., a regular design for the model that contains an absolute term and main effects and do not contain interaction effects (§1 of chapter 5). Namely, this set is equivalent to a symmetrical uniform design (or an orthogonal array $(s^2,\ n+2,\ s,\ 2)$ of strength 2 and index 1).

In §7 of chapter 6, it was shown that we can construct an orthogonal array $(s^2,\ s+1,\ s,\ 2)$ (which is equivalent to a full set of pairwise orthogonal Latin squares of order s) from a finite projective geometry $PG(2,s)$. The converse is also true: if there exists a full set of pairwise orthogonal Latin squares of order s, then there exists a finite projective geometry $PG(2,s)$ [5]. Therefore, the existence of a full set of pairwise orthogonal Latin squares of order s is equivalent to the existence a finite projective geometry $PG(2,s)$. A finite projective geometry of order s exists when $s = p^h$, where p is prime (§2 of chapter 1). The method of construction of a full set of pairwise orthogonal Latin squares of order s (or an equivalent orthogonal array) was presented in §7 of chapter 6. When s is not prime power, it is unknown whether a finite projective geometry of order s (or a full set of pairwise orthogonal Latin squares of order s)

exists in a general case. It is known, for example, that there is no a full set of orthogonal Latin squares for $s = 6,\ 14,\ 21,\ 22$. In 1782, L. Euler considered the problem of 36 officers (construction of two orthogonal Latin squares of order 6) and conjectured [6] that Graeco-Latin squares of order s do not exist for any $s \equiv 2(\mathrm{mod}\ 4)$. This fact is trivial for $s = 2$. The nonexistence of Graeco-Latin squares of order 6 was confirmed in 1901 by G. Tarry [7]. In 1959, R.C. Bose and S.S. Shrikhande [8] constructed the counterexamples to Euler's conjecture for order 22. Then E.T. Parker found the following minimal counterexample of Graeco-Latin squares of order 10 [9] using a computer search:

0417298365	0786935412
8152739406	6178094523
9826374510	5027819634
5983047621	9613782045
7698415032	3902478156
6709852143	8491357260
3071986254	7859246301
1234560789	4560123789
2345601897	1234560978
4560123978	2345601897.

In 1959, R.C. Bose, S.S. Shrikhande, and E.T. Parker [10] presented their paper showing that Graeco-Latin squares exist for all orders $n \geq 3$ except $n = 6$. Therefore, Euler's conjecture was false for all $n \geq 10$.

Many articles are dedicated to the problem of construction of orthogonal Latin squares for $s \neq p^h$ (where p is prime). However, the obtained designs have too many runs comparing to a total number of main effects of factors involved. Nevertheless, we present the following five pairwise orthogonal Latin squares of order 12 from [11]:

0789TE612345	0789TE612345	0789TE612345	0789TE612345	0789TE612345
50789TE61234	123450789TE6	E6123450789T	9TE612345078	789TE6123450
450789TE6123	789TE6123450	9TE612345078	50789TE61234	23450789TE61
3450789TE612	23450789TE61	123450789TE6	E6123450789T	TE6123450789
23450789TE61	89TE61234507	6123450789TE	123450789TE6	E6123450789T
123450789TE6	6123450789TE	3450789TE612	89TE61234507	450789TE6123
6123450789TE	9TE612345078	23450789TE61	3450789TE612	89TE61234507
E6123450789T	450789TE6123	TE6123450789	450789TE6123	50789TE61234
TE6123450789	50789TE61234	789TE6123450	6123450789TE	3450789TE612
9TE612345078	TE6123450789	450789TE6123	789TE6123450	123450789TE6
89TE61234507	450789TE6123	50789TE61234	23450789TE61	9TE612345078
789TE6123450	E6123450789T	89TE61234507	TE6123450789	6123450789TE.

§ 3. Orthogonal Arrays of Strength 3

In §1 of this chapter, we presented the method of construction of an orthogonal array $(s^t,\ s+1,\ s,\ t)$ of index 1. For a special case of an orthogonal array of strength 3, we can add one more factor to the array.

Theorem 7.3.1 [1]. If $s = 2^n$ $(n > 1)$, there exists an orthogonal array $(s^3,\ s+2,\ s,\ 3)$.

P r o o f. Consider the matrix $\mathbf{C}_1$ obtained in §1 of this chapter. Using the notation of §1, add to the matrix $\mathbf{C}_1$ one more column with the elements a^i_{t-2}. It is evident that in the matrix $\mathbf{C}_2$, any t columns that include the last two columns contain any combination of the levels exactly one time. In this case $A_{t-1} = A_{t-2} = 0$, and we get a nonzero Vandermonde determinant. If t columns include only one last column, the resulting matrix is not the Vandermonde type. However, it cannot have zero determinant since it equals

$$\left\|\begin{matrix} i_1^2 & 1 \\ i_2^2 & 1 \end{matrix}\right\| = (i_1 - i_2)(i_1 + i_2). \tag{7.3.1}$$

Since $p = 2$, each element of $GF(p^h)$ is its own additive inverse, and, therefore, the matrix (7.3.1) is nonsingular.

Note that for $t = 3$, the left and right bounds in (7.1.4) are the same, and the left bound of (7.1.3), by Theorem 7.3.1, can be increased by one and then also would coincide with the right bound of this inequality. Hence, the following theorem holds.

Theorem 7.3.2 [1]. For an orthogonal array $(s^3,\ m,\ s,\ 3)$,

$$f(s^3,\ s,\ 3) = s + 1 \ \text{ if } s = p^h, \tag{7.3.2}$$

where p is prime, odd,

$$f(s^3,\ s,\ 3) = s + 2 \ \text{ if } s = 2^h. \tag{7.3.3}$$

This theorem and the method of construction of the corresponding designs imply Theorem 6.6.3.

§ 4. Two-Level Designs

Extension of Designs

We will follow E. Seiden and R. Zemach [12] and show how we can use Theorem 7.1.5 for constructing two-level designs.

Theorem 7.4.1 [12]. In an orthogonal array $(\lambda 2^t,\ t+1,\ 2,\ t)$, any two rows differing in an even number of elements occur the same number of times while any two rows differing in an odd number of elements occur together λ times.

Proof. Let $(a_1, \ldots, a_{t+1})$ be any row of the array $(\lambda 2^t, t+1, 2, t)$, where $a \in GF(2)$. Let $\mu(a_1, \ldots, a_{t+1})$ denote the number of times the row $(a_1, \ldots, a_{t+1})$ occurs in the array $(\lambda 2^t, t+1, 2, t)$. Since the array has strength 2 and index λ,

$$\mu(a_1, \ldots, a_i, \ldots, a_j, \ldots, a_{t+1}) + \mu(a_1, \ldots, a_i+1, \ldots, a_j, \ldots, a_{t+1}) = \lambda,$$
$$\mu(a_1, \ldots, a_i+1, \ldots, a_j, \ldots, a_{t+1})$$
$$+\mu(a_1, \ldots, a_i+1, \ldots, a_j+1, \ldots, a_{t+1}) = \lambda\,.$$

Then

$$\mu(a_1, \ldots, a_i, \ldots, a_j, \ldots, a_{t+1}) = \mu(a_1, \ldots, a_i+1, \ldots, a_j+1, \ldots, a_{t+1}).$$

Sequential use of similar equalities will lead to the proof of the theorem.

Theorem 7.4.2 [12]. If $t = 2u$, an orthogonal array $(\lambda 2^t, m, 2, t)$ forms a difference scheme satisfying the condition of Theorem 7.1.5 for constructing an orthogonal array $(\lambda 2^{t+1}, m+1, 2, t+1)$. If m is the maximum number of factors for the first orthogonal array of strength t, then $m+1$ is the maximum number of factors of the resulting orthogonal array of strength $t+1$.

Proof. Consider any row in the submatrix of size $\lambda 2^t \times (t+1)$ of the orthogonal array $(\lambda 2^t, m, 2, t)$. Since $t+1$ is odd,

$$\mu(a_1, \ldots, a_{t+1}) + \mu(a_1+1, \ldots, a_{t+1}+1) = \lambda.$$

Therefore, the orthogonal array $(\lambda 2^t, m, 2, t)$ forms a difference scheme satisfying the condition of Theorem 7.1.5 for constructing an orthogonal array $(\lambda 2^{t+1}, m+1, 2, t+1)$. Theorem 5.2.5 implies that the resulting orthogonal array has the maximum number of factors.

Designs of Strength 2

In this section we will focus on orthogonal arrays $(\lambda 2^2, m, 2, 2)$.

For an orthogonal array $(\lambda 2^2, m, 2, 2)$, consider the matrix

$$\| \mathbf{I}, \ \mathbf{F}_1 \ \mathbf{F}_2, \ldots, \mathbf{F}_m \|, \tag{7.4.1}$$

where $\mathbf{F}_i$ is the vector-column of the main effect of the factor F_i $(i = 1, \ldots, m)$. Remind that we assume that any matrix in (7.4.1) is normalized in such a way that sum of squares of elements of any its column is equal to $N = \lambda 2^2$. Therefore, all elements of (7.4.1) are –1 or +1.

When $\lambda = 2^n$, we can construct an orthogonal array (hypercube) $(2^{n+2}, 2^{n+2}-1, 2, 2)$. Then the matrix (7.4.1) is a square matrix with orthogonal columns and elements –1 and +1.

Definition 7.4.1. A square matrix $\mathbf{H}_N$ of order N with elements –1 and +1 is said to be a Hadamard matrix if

$$\mathbf{H}_N^T \mathbf{H}_N = N \mathbf{E}_N \tag{7.4.2}$$

($\mathbf{E}_N$ is an identity matrix of order N).

Any Hadamard matrix by multiplication of appropriate rows and columns by –1 (which again leads to a Hadamard matrix) can be brought to a normalized type, i.e., to the matrix with the first column and the first row that are consisted of +1. It is evident that a normalized Hadamard matrix $\mathbf{H}_{m+1}$ corresponds to the matrix (7.4.1) for $N = m + 1$ and, therefore, is equivalent to the orthogonal array $(m + 1,\ m,\ 2,\ 2)$. Since $N = \lambda 2^2$, for a Hadamard matrix $\mathbf{H}_N$ (for $N > 2$) the following condition holds:

$$N \equiv 0 \pmod 4. \tag{7.4.3}$$

For $N = 2$ the normalized Hadamard matrix is

$$\begin{Vmatrix} +1 & +1 \\ +1 & -1 \end{Vmatrix}.$$

Now we will focus on the problem of construction of Hadamard matrices when $N \neq 2^n$.

Theorem 7.4.3 [13]. Let $\mathbf{H}_{N_1} = \{h'_{ij}\}$ and $\mathbf{H}_{N_2} = \{h''_{ij}\}$ be Hadamard matrices of order N_1 and N_2 respectively**.** Then their direct product

$$\mathbf{H}_{N_1} \times \mathbf{H}_{N_2} = \begin{Vmatrix} h'_{11}\mathbf{H}_{N_2} & h'_{12}\mathbf{H}_{N_2} & \cdots & h'_{1N_1}\mathbf{H}_{N_2} \\ h'_{21}\mathbf{H}_{N_2} & h'_{22}\mathbf{H}_{N_2} & \cdots & h'_{2N_1}\mathbf{H}_{N_2} \\ \vdots & \vdots & \ddots & \vdots \\ h'_{N_1 1}\mathbf{H}_{N_2} & h'_{N_1 2}\mathbf{H}_{N_2} & \cdots & h'_{N_1 N_1}\mathbf{H}_{N_2} \end{Vmatrix}$$

is a Hadamard matrix of order $N_1 N_2$**.**

P r o o f. Consider the following chain of equalities:

$$\left(\mathbf{H}_{N_1} \times \mathbf{H}_{N_2}\right)\left(\mathbf{H}_{N_1} \times \mathbf{H}_{N_2}\right)^T = \left(\mathbf{H}_{N_1} \times \mathbf{H}_{N_2}\right)\left(\mathbf{H}_{N_1}^T \times \mathbf{H}_{N_2}^T\right) =$$
$$= \left(\mathbf{H}_{N_1}\mathbf{H}_{N_1}^T\right) \times \left(\mathbf{H}_{N_2}\mathbf{H}_{N_2}^T\right) = N_1 \mathbf{E}_{N_1} \times N_2 \mathbf{E}_{N_2} = N_1 N_2 \mathbf{E}_{N_1 N_2}.$$

This proves the theorem.

Theorem 7.4.4 [13]. Let $N = v + 1 = p^h + 1 \equiv 0 \pmod 4$, where p is prime. Then there exists a Hadamard matrix of order N.

P r o o f. Let $0, 1,\ \dots,\ v - 1$ be the elements of Galois field $GF(v)$. Consider the matrix $\mathbf{H} = \{h_{ij}\}$ of size $(N \times N)$:

$$h_{ij} = +1 \quad (i = v \text{ or } j = v), \quad h_{ii} = -1 \quad (0 \le i \le v - 1),$$
$$h_{ij} = \left(\frac{j - i}{v}\right) \quad (0 \le i \le v - 1 \quad 0 \le j \le v - 1,\ \ i \neq j),$$

where $\left(\frac{j-i}{v}\right)$ is the Legendre symbol.

If $i_1 \neq i_2,\ i_1 \neq v,\ i_2 \neq v$, then

$$\sum_{j=0}^{v} h_{i_1 j} h_{i_2 j} = h_{i_1 i_1} h_{i_2 i_1} + h_{i_1 i_2} h_{i_2 i_2} + h_{i_1 v} h_{i_2 v}$$
$$+ \sum_{j \neq i_1, i_2, v} \left(\frac{j-i_1}{v}\right)\left(\frac{j-i_2}{v}\right). \tag{7.4.4}$$

By (1.1.3) and (1.1.4), the first two terms of (7.4.4) have opposite signs, and their sum is equal to zero. The third term equals +1. The last sum, by (1.1.1), is –1.

Since $i_1 \neq v$,

$$\sum_{j=0}^{v} h_{vj} h_{ij} = \sum_{j=0}^{v} h_{ij} = h_{ii} + h_{iv} + \sum_{j=0}^{v-1} \left(\frac{j-i}{v}\right). \tag{7.4.5}$$

By (1.1.2), the last sum in (7.4.5) is equal to zero. The first two terms are –1 and +1 respectively. Hence, the columns of the matrix **H** are pairwise orthogonal, which was to be proved.

Theorem 7.4.5 [13]. Let $N = 2(v+1) = 2\left(p^h + 1\right) \equiv 0 \pmod 4$, p is prime. Then there exists a Hadamard matrix of order *N*.

P r o o f. Assume that $p^h \equiv 1 \pmod 4$. Otherwise, statement of the theorem is a simple consequence of Theorem 7.4.3 and Theorem 7.4.4.

Consider the matrix

$$\mathbf{S} = \begin{Vmatrix} 0 & \mathbf{I}_v^T \\ \mathbf{I}_v & \mathbf{Q} \end{Vmatrix},$$

where $\mathbf{I}_v$ is a unit vector of dimension v; $\mathbf{Q} = \{q_{ij}\}$ $(i,\ j = 0, 1,\ \dots,\ v-1)$; $q_{ii} = 0$;

$$q_{ij} = \left(\frac{i-j}{v}\right) \quad (i \neq j),$$

$0, 1,\ \dots,\ v-1$ are elements of Galois field $GF(v)$.

Following the line of the proof of Theorem 7.4.4, we can get that

$$\mathbf{S}^T\mathbf{S} = v\mathbf{E}_{v+1}.$$

Now in the matrix **S**, replace +1, –1 and 0 with the matrices

$$\begin{Vmatrix} +1 & +1 \\ +1 & -1 \end{Vmatrix}, \quad \begin{Vmatrix} -1 & -1 \\ -1 & +1 \end{Vmatrix}, \quad \begin{Vmatrix} +1 & -1 \\ -1 & -1 \end{Vmatrix}$$

respectively. It is evident that the resulting matrix is a Hadamard type.

This completes the proof of the theorem.

Theorems 6.7.2, 7.4.3, 7.4.4, and 7.4.5 provide the methods of construction of Hadamard matrices of order $4l$ up to order 88. Problems of construction of Hadamard matrices in other cases have been studied by many authors. The lowest order $N \equiv 0 \pmod 4$ for which no Hadamard matrix is presently known is 668. The more detailed presentation of the results in this area can be found, for example, in the publications [14, 15, 16].

Designs of Strength 3

By Theorems 7.1.5 and 7.4.2, the orthogonal arrays $(4\lambda,\ 4\lambda-1,\ 2,\ 2)$ of strength 2 obtained in this paragraph (and bearing the maximum number of factors) allow constructing orthogonal arrays $(8\lambda,\ 4\lambda,\ 2,\ 3)$ of strength 3 with the maximum number of factors.

The method of construction of orthogonal arrays of strength 3 with the maximum number of factors is as follows [2, 17, 18].

Let $\mathbf{D}_2 = \{a_{ij}\}$ be an orthogonal array $(4\lambda,\ 4\lambda-1,\ 2,\ 2)$, where $a_{ij} \in GF(2)$. Then

$$\mathbf{D}_3 = \begin{Vmatrix} \mathbf{D}_2 & \mathbf{0} \\ \mathbf{D}_2 + \mathbf{J} & \mathbf{I} \end{Vmatrix}$$

is an orthogonal array $(8\lambda,\ 4\lambda,\ 2,\ 3)$, where $\mathbf{I}$, $\mathbf{0}$, and $\mathbf{J}$ are a (4λ)-dimensional unit vector, a (4λ)-dimensional zero-vector, and a matrix consisting of 1's of size $(4\lambda-1)\times 4\lambda$ respectively.

Example 7.4.1. Consider the orthogonal array (4, 3, 2, 2) of strength 2 with the maximum number of factors equal 3:

$$\mathbf{D}_2 = \begin{Vmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{Vmatrix}.$$

Then

$$\mathbf{D}_3 = \begin{Vmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{Vmatrix}$$

is an orthogonal array (8, 4, 2, 3) of strength 3 with the maximum number of factors equal 4.

The results of this section implied theorem 6.6.2.

Designs of Strength 4 and 5

In this section we present methods of construction of designs of strength 4 and 5 with the maximum number of factors when the number of runs is not large.

Theorem 7.4.6 [12]. Orthogonal arrays (16, 5, 2, 4) and (48, 5, 2, 4) exist and have the maximum number of factors.

Proof. It is evident that the generator (11111) produces the orthogonal array (16, 5, 2, 4). By Theorem 5.2.4, 5 is the maximum number of factors for this array. It is also evident that the orthogonal array (48, 5, 2, 4) exists. It can be obtained by a juxtaposition of three orthogonal arrays (16, 5, 2, 4). By Theorem 5.2.6, 5 is the maximum number of factors for this array.

Theorem 7.4.7 [12]. Orthogonal arrays (32, 6, 2, 4) and (64, 8, 2, 4) exist and have the maximum number of factors.

The method of construction of the first array is given by the generator (111111). The method of construction of the second array is given by the generators (11111000) and (00011111). The proof that you cannot construct the orthogonal array with the number of factors respectively 7 and 9 used in [12] special algebraic methods and is omitted in this book.

Theorems 7.4.6, 7.4.7, 7.4.2, and 7.1.5 imply the methods of construction of the orthogonal array (32, 6, 2, 5), (64, 7, 2, 5), (96, 6, 2, 5), and (128, 9, 2, 5) with the maximum number of factors. Hence, the following theorem is a consequence of the article [12] (similar results also can be found in [19]).

Theorem 7.4.8. Orthogonal arrays (32, 6, 2, 5), (64, 7, 2, 5), (96, 6, 2, 5), and (128, 9, 2, 5) exist and have the maximum number of factors.

The results of this section imply Theorem 6.6.4.

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Chapter 8. Construction of Asymmetrical and Nonuniform Designs

§ 1. Collapsing

In this paragraph we present the technique of collapsing levels of the factors introduced by I.M. Chakravarti [1] and developed by S. Addelman [2].

Suppose that the condition of proportional frequencies (3.7.4) is satisfied for t factors $F_{i_1}, \dots, F_{i_t}$ in the design **D**. Write this condition twice for two levels j_1' and j_1'' of the factor F_{i_1} and sum up the left and the right sides. Then

$$N^{t-1}\left(w_{i_1 \dots i_t}^{j_1' \dots j_t} + w_{i_1 \dots i_t}^{j_1'' \dots j_t}\right) = \left(w_{i_1}^{j_1'} + w_{i_1}^{j_1''}\right) w_{i_2}^{j_2} \dots w_{i_t}^{j_t}. \qquad (8.1.1)$$

Consider the design $\mathbf{D}'$ with the same number of runs and the same number of factors as in the design **D**. Assume that in the design $\mathbf{D}'$ all factors except F_{i_1} (with the same notations for the factors and their levels) have the same number of levels as in the design **D**. Also assume that in the design $\mathbf{D}'$, each factor except F_{i_1} occurs at the same levels for all treatment combinations as a corresponding factor in the design **D**. The factor F_{i_1} in the design $\mathbf{D}'$ occurs at the same levels as in the design **D** except levels j_1' and j_1''. In these treatment combinations, the factor F_i occurs at one level that is different from other level. Denote this level by j_1. Then the condition (8.1.1) can be rewritten as follows:

$$N^{t-1} w_{i_1 i_2 \dots i_t}^{j_1 j_2 \dots j_t} = w_{i_1}^{j_1} w_{i_2}^{j_2} \dots w_{i_t}^{j_t}.$$

This is the condition of proportional frequencies for the j-th level of the factor F_{i_1} and for arbitrary levels of the factors $F_{i_2}, \dots, F_{i_t}$. It is evident that for the rest of levels of the factor F_{i_1}, the similar condition of proportional frequencies in the design $\mathbf{D}'$ is also satisfied. This procedure of replacement of two levels of the factor with one level is called collapsing of factor levels. Then the following theorem holds.

Theorem 8.1.1. If in the design **D** the condition of proportional frequencies is satisfied for the factors $F_{i_1}, \dots, F_{i_t}$, then this condition is satisfied for the same factors in the design **D′** that has one or more collapsed factors of the design **D**.

Theorem 8.1.2 [2]. There exists a regular main effect design for the factors F_i^j at s_i levels $(j = 1, \dots, m_i;\ i = 1, \dots, l)$ in s^n runs, where $s = p^h$ (p is prime); $s_l < \cdots < s_2 < s_1 \le s$; $\sum_{i=1}^{l} m_i \le \frac{s^n - 1}{s - 1}$.

P r o o f. By Theorem 6.7.2, it follows that there exists a regular main effect design in s^n runs for $(s^n - 1)/(s - 1)$ factors at s levels each. Collapsing some of factors and removing (if it is necessary) some of columns, we get, by Theorem 8.1.1, the required regular main effect design.

Example 8.1.1 [2]**.** To illustrate the technique of collapsing levels, construct a regular main effect design $2^2 \times 3^2//9$. Start with the regular symmetrical main effect design $3^4//9$ that can be constructed in accordance with §7 of chapter 6 (presented in the first part of Table 12).

Table 12

Construction of Design $2^2 \times 3^2//9$ from Design $3^4//9$

Design $3^4//9$				**Design $2^2 \times 3^2//9$**			
0	0	0	0	0	0	0	0
0	1	1	2	0	1	1	2
0	2	2	1	0	0	2	1
1	0	1	1	1	0	1	1
1	1	2	0	1	1	2	0
1	2	0	2	1	0	0	2
2	0	2	2	0	0	2	2
2	1	0	1	0	1	0	1
2	2	1	0	0	0	1	0

Collapse the first two factors of the design $3^4//9$ by using the following correspondence scheme:

Three-level Factor		**Two-level Factor**
0	$\longrightarrow$	0
1	$\longrightarrow$	1
2	$\longrightarrow$	0

The resulting design $3^4//9$ is presented in the second part of Table 12.

§ 2. Splitting

In this paragraph we present the technique by S. Addelman of splitting factors [2].

Let $\mathbf{D}_1$ be a regular factorial design of strength t_1 for m_1 factors $F_1, \dots, F_{m_1}$ in *N* runs. Suppose that there exists a regular factorial design $\mathbf{D}_2$ of strength t_2 in *N* runs for m_2 factors $F_{m_1+1}, \dots, F_{m_1+m_2}$ such that the following condition holds: each level of the factor F_{m_1} of the design $\mathbf{D}_1$ corresponds to only one combination of levels of the factors $F_{m_1+1}, \dots, F_{m_1+m_2}$ of the design $\mathbf{D}_2$. Then replacement of levels of the factor F_{m_1} in the design $\mathbf{D}_1$ with a corresponding combination of m_2 factors $F_{m_1+1}, \dots, F_{m_1+m_2}$ of the design $\mathbf{D}_2$ is called splitting of the factor F_{m_1} into m_2 factors of the design $\mathbf{D}_2$.

Consider any t_2 factors $F_{i_1}, \dots, F_{i_{t_2}}$ of the design $\mathbf{D}_2$. Each level of the factor F_{m_1} corresponds to only one combination of levels of the factors $F_{m_1+1}, \dots, F_{m_1+m_2}$ and, therefore, only one combination of levels of the factors $F_{i_1}, \dots, F_{i_{t_2}}$. However, each combination of level of the factors $F_{i_1}, \dots, F_{i_{t_2}}$, generally speaking, corresponds to a few levels of the factor F_{m_1}.

For t_2 factors of the design $\mathbf{D}_2$ (without loss of generality, take the first t_2 factors $F_{m_1+1}, \dots, F_{m_1+t_2}$), consider a combination of their levels $j_{m_1+1}, \dots, j_{m_1+t_2}$ respectively. Since $\mathbf{D}_2$ is a regular design of strength t_2,

$$N^{t_2-1} w_{m_1+1 \dots m_1+t_2}^{j_{m_1+1} \cdots j_{m_1+t_2}} = w_{m_1+1}^{j_{m_1+1}} \dots w_{m_1+t_2}^{j_{m_1+t_2}}. \tag{8.2.1}$$

Assume that the considered combination of levels of the factors $F_{m_1+1}, \dots, F_{m_1+t_2}$ corresponds to levels $j_{m_1}^1, \dots, j_{m_1}^n$ of the factor F_{m_1}, i.e.,

$$w_{m_1}^{j_{m_1}^1} + \cdots + w_{m_1}^{j_{m_1}^n} = w_{m_1+1 \dots m_1+t_2}^{j_{m_1+1} \cdots j_{m_1+t_2}}, \tag{8.2.2}$$

and

$$w_{1 \dots (t_1-1) m_1}^{j_1 \cdots j_{t_1-1} j_{m_1}^1} + \cdots + w_{1 \dots (t_1-1) m_1}^{j_1 \cdots j_{t_1-1} j_{m_1}^n}$$
$$= w_{1 \dots (t_1-1)(m_1+1) \dots (m_1+t_2)}^{j_1 \cdots j_{t_1-1} j_{m_1+1} \cdots j_{m_1+t_2}}. \tag{8.2.3}$$

(8.2.1) and (8.2.2) imply the following equality:

$$N^{t_2-1} \left(w_{m_1}^{j_{m_1}^1} + \cdots + w_{m_1}^{j_{m_1}^n} \right) = w_{m_1+1}^{j_{m_1+1}} \dots w_{m_1+t_2}^{j_{m_1+t_2}}. \tag{8.2.4}$$

Since $\mathbf{D}_1$ is a regular design of strength t_1, for $t_1 - 1$ factors of the design $\mathbf{D}_1$ (without loss of generality, take the first $t_1 - 1$ factors $F_1, \dots, F_{t_1-1}$) for any levels $j_1, \dots, j_{t_1-1}$ of these factors respectively,

$$\begin{gathered} N^{t_1-1} w_{1\dots(t_1-1)m_1}^{j_1\cdots j_{t_1-1} j_{m_1}^1} = w_1^{j_1} \dots w_{t_1-1}^{j_{t_1-1}} w_{m_1}^{j_{m_1}^1}, \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots \\ N^{t_1-1} w_{1\dots(t_1-1)m_1}^{j_1\cdots j_{t_1-1} j_{m_1}^n} = w_1^{j_1} \dots w_{t_1-1}^{j_{t_1-1}} w_{m_1}^{j_{m_1}^n}. \end{gathered} \tag{8.2.5}$$

Summing up (8.2.5), we get, by (8.2.4), that

$$\begin{aligned} N^{t_2-1} N^{t_1-1} &\left(w_{1\dots(t_1-1)m_1}^{j_1\cdots j_{t_1-1} j_{m_1}^1} + \cdots + w_{1\dots(t_1-1)m_1}^{j_1\cdots j_{t_1-1} j_{m_1}^n} \right) \\ &= w_1^{t_1} \dots w_{t_1-1}^{j_{t_1-1}} w_{m_1+1}^{j_{m_1+1}} \dots w_{m_1+t_2}^{j_{m_1+t_2}}. \end{aligned} \tag{8.2.6}$$

Using (8.2.3), we get

$$N^{t_2-1} N^{t_1-1} w_{1\dots(t_1-1)(m_1+1)\dots(m_1+t_2)}^{j_1\cdots j_{t_1-1} j_{m_1+1}\cdots j_{m_1+t_2}}$$

$$= w_1^{j_1} \dots w_{t_1-1}^{j_{t_1-1}} w_{m_1+1}^{j_{m_1+1}} \dots w_{m_1+t_2}^{j_{m_1+t_2}}.$$

Therefore, the following theorem has been proved.

Theorem 8.2.1. Splitting of the factor F_i in the regular factorial design $\mathbf{D}_1$ of strength t_1 for m_1 factors into m_2 factors of the regular factorial design $\mathbf{D}_2$ of strength t_2 results in the regular factorial design $\mathbf{D}$ of strength $t = \min(t_1,\ t_2)$ for $m_1 + m_2 - 1$ factors. Besides, the condition of proportional frequencies is satisfied for any set of factors of the design $\mathbf{D}$ that contains $t_1 - 1$ or less factors of the design $\mathbf{D}_1$ and t_2 or less factors of the design $\mathbf{D}_2$.

The regular factorial design $\mathbf{D}_2$ from Theorem 8.2.1 can be easily constructed if there exists a regular factorial design $\mathbf{D}_2'$ of strength t_2 in s_i runs and if each level of the factor F_i occurs in the design $\mathbf{D}_1$ λ_i times. Then the required design $\mathbf{D}_2$, obviously, can be constructed by a juxtaposition of λ_i designs $\mathbf{D}_2'$.

Corollary 1 to Theorem 8.2.1. Suppose that all s_i levels of the factor F_i of the regular design $\mathbf{D}_1$ of strength t in N runs for m_1 factors $F'_1, \dots, F'_{m_1}$ with $s'_1, \dots, s'_{m_1}$ levels respectively occur with equal frequency. Suppose that there exists the regular design $\mathbf{D}_2$ of strength t_2 in s_i runs for m_2 factors $F''_1, \dots, F''_{m_2}$ with $s''_1, \dots, s''_{m_2}$ levels respectively. Then there exists the regular design $\mathbf{D}$ of strength $t = \min(t_1,\ t_2)$ in N runs for $m_1 + m_2 - 1$ factors $F'_1, \dots, F'_{i-1}, F'_{i+1}, F'_{m_1}, F''_1, \dots, F''_{m_2}$ with $s'_1, \dots, s'_{i-1}, s'_{i+1}, s'_{m_1},\ s''_1, \dots, s''_{m_2}$ levels respectively. Besides, the condition of proportional frequencies is satisfied for any set of factors of the design $\mathbf{D}$ that contains $t_1 - 1$ or less factors of the design $\mathbf{D}_1$ and t_2 or less factors of the design $\mathbf{D}_2$.

Example 8.2.1. We will use Theorem 8.2.1 and Corollary 1 for the regular factorial design $4^5//16$ of strength 2 with five four-levels factors (see the first section of Table 13).

Split the first factor of the design $4^5//16$ into two two-level factors of a full design 2^2 as follows:

Four-level Factor		**Two-level Factors**
0	$\longrightarrow$	0 0
1	$\longrightarrow$	1 0
2	$\longrightarrow$	0 1
3	$\longrightarrow$	1 1

The resulting design (see the second section of Table 13) has strength 2. Hence it corresponds to pairwise orthogonal main effects of two-level and four-level factors. Besides, the condition of proportional frequencies is satisfied for any set of factors that contains two two-level factors and one four-level factor. Therefore, an interaction effect of two-level factors is orthogonal to all main effects.

Table 13
Transformations of the Design $4^5//16$

Design $4^5//16$						**Design $2^2 \times 4^4//16$**							**Design $2^6 \times 4^3//16$**								
0	0	0	0	0		0	0	0	0	0	0		0	0	0	0	0	0	0	0	0
1	0	1	1	1		1	0	0	1	1	1		1	0	1	0	0	0	1	1	1
2	0	2	2	2		0	1	0	2	2	2		0	1	1	0	0	0	2	2	2
3	0	3	3	3		1	1	0	3	3	3		1	1	0	0	0	0	3	3	3
0	1	1	2	3		0	0	1	1	2	3		0	0	0	1	0	1	1	2	3
1	1	0	3	2		1	0	1	0	3	2		1	0	1	1	0	1	0	3	2
2	1	3	0	1		0	1	1	3	0	1		0	1	1	1	0	1	3	0	1
3	1	2	1	0		1	1	1	2	1	0		1	1	0	1	0	1	2	1	0
0	2	2	3	1		0	0	2	2	3	1		0	0	0	0	1	1	2	3	1
1	2	3	2	0		1	0	2	3	2	0		1	0	1	0	1	1	3	2	0
2	2	0	1	3		0	1	2	0	1	3		0	1	1	0	1	1	0	1	3
3	2	1	0	2		1	1	2	1	0	2		1	1	0	0	1	1	1	0	2
0	3	3	1	2		0	0	3	3	1	2		0	0	0	1	1	0	3	1	2
1	3	2	0	3		1	0	3	2	0	3		1	0	1	1	1	0	2	0	3
2	3	1	3	0		0	1	3	1	3	0		0	1	1	1	1	0	1	3	0
3	3	0	2	1		1	1	3	0	2	1		1	1	0	1	1	0	0	2	1

The procedure by S. Addelman [2] that splits factor at s^n levels ($s = p^h$, p is prime) into $(s^n-1)/(s-1)$ factors at s levels can be obtain as a corollary to Theorem 8.2.1.

Let $s_i = p^h$ (p is prime). Then, by Theorem 6.7.2, there exists a regular main effect design in p^h runs for $(p^h-1)/(p-1)$ p-level factors. Suppose that in the main effect design $\mathbf{D}_1$, the uniform factor F_i has s_i levels. Then, by corollary 1 to Theorem 8.2.1, this factor can be split into $(p^h-1)/(p-1)$ p-level factors.

Corollary 2 to Theorem 8.2.1. Suppose that there exists a regular main effect design for m factors $F_1, \dots, F_m$ and the uniform factor F_i has $s_i = p^h$ (p is prime) levels. Then there exists a regular main effect design for $(p^h-1)/(p-1)$ p-level factors and factors $F_1, \dots, F_{i-1}, F_{i+1}, \dots, F_m$ with $s_1, \dots, s_{i-1}, s_{i+1}, \dots, s_m$ levels respectively.

Example 8.2.2. Consider again the regular main effect design $4^5//16$. Splitting the first and the second four-level factors into two sets of three two-level factors each can be done, by Corollary 2 to Theorem 8.2.1, as follows:

Four-level Factor		**Two-level Factors**
0	$\longrightarrow$	0 0 0
1	$\longrightarrow$	1 0 1
2	$\longrightarrow$	0 1 1
3	$\longrightarrow$	1 1 0

The resulting main effect design $2^6 \times 4^3//16$ is presented in the third section of Table 13.

§ 3. Replacement

In this paragraph we present the technique by S. Addelman [2] of replacement factors. In some sense, this method is the inverse of the splitting procedure.

By the results §7 of chapter 6, for $N = s^n$, $s = p^h$ (p is prime), there exists a regular factorial design $\mathbf{D}_N$ of strength 2 in N runs for $(s^n-1)/(s-1)$ s-level factors. For lN runs, a regular factorial design $\mathbf{D}_{lN}$ of strength 2 for $(s^n-1)/(s-1)$ s-level factors can be obtained by a juxtaposition of l designs $\mathbf{D}_N$. Set up a one-to-one correspondence between all combinations of all factors of the design $\mathbf{D}_{lN}$ and levels of some N-level factor F.

Suppose that a part of columns of a regular factorial design $\mathbf{D}$ of strength 2 forms the design $\mathbf{D}_{lN}$. Then all main effects corresponding to these columns are orthogonal to any other effects of the design $\mathbf{D}$. Replace the columns of the design **D** that constitute the design $\mathbf{D}_{lN}$ with the column corresponding to the factor *F*. In the design $\mathbf{D}_N$, by the results of §1 of chapter 6, any contrast can be obtained as a linear combination of main effects of its $(s^n-1)/(s-1)$ s-level factors. Therefore, any main effect of the factor *F* is orthogonal to any other main effects of the resulting design **D**.

This procedure involved the design $\mathbf{D}_{lN}$ and the factor *F* is called a replacement.

Example 8.3.1 [2]**.** Consider the regular factorial design 2^7 of strength 2 in 8 runs (see the first section of Table 14). The last three columns of the design form a regular factorial design $2^3//8$ of strength 2 that is the juxtaposition of two designs $2^3//4$ of strength 2:

$$\left\|\begin{matrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{matrix}\right\|.$$

Therefore, we can use the procedure of replacement to obtain four-level factor with the following correspondence:

Two-level Factors		**Four-level Factor**
0 0 0	$\longrightarrow$	0
1 1 0	$\longrightarrow$	1
1 0 1	$\longrightarrow$	2
0 1 1	$\longrightarrow$	3

As a result, we get the regular factorial design $2^4 \times 4//8$ of strength 2 (see the second section of Table 14).

Table 14

Construction of Design $2^4 \times 4//8$ from Design $2^7//8$

Design $2^7//8$		**Design $2^4 \times 4//8$**
0 0 0 0 0 0 0		0 0 0 0 0
1 0 0 1 1 1 0		1 0 0 1 1
0 1 0 1 1 0 1		0 1 0 1 2
1 1 0 0 0 1 1		1 1 0 0 3
0 0 1 1 0 1 1		0 0 1 1 3
1 0 1 0 1 0 1		1 0 1 0 2
0 1 1 0 1 1 0		0 1 1 0 1
1 1 1 1 0 0 0		1 1 1 1 0

The replacement procedure can be used in a more general situation. Suppose that the design **D** corresponds to the full set of pairwise orthogonal main effects and interaction effects of two factors F_1 and F_2 with s_1 and s_2 levels respectively. Now consider the factor F such that there is a one-to-one correspondence between its levels and combinations of levels of the factors F_1 and F_2. It is evident that any main effects of the factors F_1 and F_2 and also any interaction effects of these factors are main effects of the factor F. Total number of pairwise orthogonal main effects and interaction effects of the factors F_1 and F_2 equals $(s_1 - 1) + (s_2 - 1) + (s_1 - 1)(s_2 - 1) = s_1 s_2 - 1$. A full set of pairwise orthogonal main effects of the factor F is also equals $s_1 s_2 - 1$ (since the number of levels of the factor F equals $s_1 s_2$). Therefore, any main effect of the factor F is a linear combination of main effects and interaction effects of the factors F_1 and F_2. Hence, if main effects and interaction effects of the factors F_1 and F_2 for the design **D** are orthogonal to some effects of other factors, then all main effects of the factor F are orthogonal to the same effects of other factors.

Consider, for example, a regular main effect design in which interaction effects of the factors F_1 and F_2 are orthogonal to all main effects of all factors of the design. Then, using the replacement procedure, i.e., replacing factors F_1 and F_2 with the factor F, we get a regular main effect design.

Similar construction can be used for a full set of pairwise orthogonal main effects and all interaction effects of several factors. Therefore, the following theorem holds.

Theorem 8.3.1. Suppose that the design corresponds to a set of pairwise orthogonal effects consisting of all main effects and all interaction effects of the factors $\mathrm{F}_1, \dots, \mathrm{F}_\mathrm{r}$ and also effects of a factorial set Ω consisting of main effects and some interaction effects of the factors $F_{r+1}, \dots, F_m$. Then substituting factor F obtained by the replacement procedure for factors $\mathrm{F}_1, \dots, \mathrm{F}_\mathrm{r}$ leads to the design that corresponds to the set of pairwise orthogonal effects consisting of all main effects of the factor F and all effects of the set Ω.

If a procedure of replacement is used for a geometric design, the resulting design is also called geometric.

§ 4. Production of Designs

In this paragraph we will develop the technique of production of designs introduced by I.M. Chakravarti [1]. We will also see how it can be used in combination with the replacement procedure.

Production Technique

Theorem 8.4.1. Suppose that there exist n regular factorial designs D_i $(i = 1, \dots, n)$ of strength t_i in N_i runs for m_i factors F_j^i $(j = 1, \dots, m_i)$ with $s_j^{(i)}$ level respectively. Then there exists a regular factorial design **D** of strength $t = \min(t_1, \dots, t_n)$ in $N = \prod_{i=1}^{n} N_i$ runs for $m = \sum_{i=1}^{n} m_i$ factors F_j^i with $s_j^{(i)}$ levels respectively. Besides, in the design **D** the condition of proportional frequencies holds for any set of factors including t_i or less factors from the set of factors F_j^i.

Proof. Consider two designs $\mathbf{D}_1$ and $\mathbf{D}_2$ that satisfy the condition of the theorem. Now construct the design $\mathbf{D}_{12}$ by using the following procedure. Repeat N_2 times each row of the design $\mathbf{D}_1$. Denote the resulting matrix by $\mathbf{D}_1'$. Repeat N_1 times the design $\mathbf{D}_2$. Denote the resulting matrix by $\mathbf{D}_2'$. Now generate the design $\mathbf{D}_{12}$ (consisting of N_1N_2 rows) as follows:

$$\mathbf{D}_{12} = \| \ \mathbf{D}_1' \quad \mathbf{D}_2' \ \|.$$

Consider any combination of levels any t_1 factors of the design $\mathbf{D}_1$. Assume that this combination occurs in the design $\mathbf{D}_1$ w^1 times and corresponding levels of the factors occur $w_1^1, \dots, w_{t_1}^1$ respectively. We will keep similar notation for the design $\mathbf{D}_2$. By virtue of the hypothesis of the theorem, the condition of proportional frequencies holds for any set of t_1 and t_2 factors of the designs $\mathbf{D}_1$ and $\mathbf{D}_2$ respectively. Therefore,

$$N_1^{t_1-1} w^1 = w_1^1 \dots w_{t_1}^1, \tag{8.4.1}$$
$$N_2^{t_2-1} w^2 = w_1^2 \dots w_{t_2}^2. \tag{8.4.2}$$

We will use similar notation for the design $\mathbf{D}_{12}$ using a letter W. Then, it is evident that

$$W_i^1 = w_i^1 N_2, \quad W_i^2 = w_i^2 N_1. \tag{8.4.3}$$

Let W denote the number of occurrence together (in the design $\mathbf{D}_{12}$) all levels of t_1 selected factors of the design $\mathbf{D}_1$ and all levels of t_2 selected factors of the design $\mathbf{D}_2$. Then

$$W = w^1 w^2. \tag{8.4.4}$$

Multiplying left and right sides of (8.4.1) and (8.4.2), we get

$$N_1^{t_1-1} N_2^{t_2-1} w^1 w^2 = w_1^1 \dots w_{t_1}^1 w_1^2 \dots w_{t_2}^2. \tag{8.4.5}$$

Substitute (8.4.3) and (8.4.4) into (8.4.5). Then

$$N_1^{t_1-1}N_2^{t_2-1}W = N_1^{-t_2}N_2^{-t_1}W_1^1 \dots W_{t_1}^1 W_1^2 \dots W_{t_2}^2,$$

or

$$N_{12}^{t_1+t_2-1}W = W_1^1 \dots W_{t_1}^1 W_1^2 \dots W_{t_2}^2, \tag{8.4.6}$$

(where $N_{12} = N_1N_2$), which is the condition of proportional frequencies for the considered two sets of the factors (t_1 factors from D_1 and t_2 factors from D_2). The proof for the general case of n designs is simple.

The theorem that is similar to Theorem 8.4.1 for a special case of orthogonal arrays has been proved by I.M. Chakravarti [1].

Theorem 8.4.1 shows that the design $\mathbf{D}$ of strength $t = \min(t_1, \dots, t_n)$ corresponds to pairwise orthogonal effects of two types. The first type consists of main effects and interaction effects that belong to the sets of pairwise orthogonal effects of all designs $\mathbf{D}_i$. The second type consists of interaction effects of factors such that not more than $[t_i/2]$ of them correspond to the design $\mathbf{D}_i$.

Production-Replacement Combination

A combination of procedures of production and replacement might lead to useful results.

Let $\mathbf{D}_1$ and $\mathbf{D}_2$ be two regular factorial designs of strength 2. Generate a production $\mathbf{D}_{12}$ of these designs, which is also a regular factorial design of strength 2. The design $\mathbf{D}_{12}$ in addition to orthogonal main effects of all factors corresponds to orthogonal interaction effects of several pair factors with one factor from the design $\mathbf{D}_1$ and the other factor from the design $\mathbf{D}_2$. These two-factor interaction effects are orthogonal to all main effects. By the results of §3 of this chapter, we can use a procedure of replacement that replace any such a pair of factors having, say, s_1 and s_2 levels with the (s_1s_2)-level factor. The procedure of replacement may be used several times for all such pairs of factors with an obvious limitation: each step of replacement should not include factors that were used in the previous steps.

Consider one special case of the method when the design $\mathbf{D}_1$ includes only one factor F. Then the design $\mathbf{D}_{12}$ is formed by repeating the design $\mathbf{D}_2$ with the each level of the factor F. The procedure of replacement for pair of factors F and F' (F' is any factor from $\mathbf{D}_2$) leads to the design, which is a juxtaposition of the following designs: $\mathbf{D}_2$; $\mathbf{D}_2$ with a substitute the levels $s', s'+1, \dots, 2s'-1$ for the levels $0, 1, \dots, s'-1$ of the factor F'; $\mathbf{D}_2$ with a substitute the levels $2s', 2s'+1, \dots, 3s'-1$ for the levels $0, 1, \dots, s'-1$ of the factor F'; etc. The last design $\mathbf{D}_2$ replaces the levels $0, 1, \dots, s'-1$ of the factor with the levels $(s-1)s', (s-1)s'+1, \dots, ss'-1$.

Example 8.4.1 [2]. To construct a regular main effect design $2 \times 3^2 \times 5//18$, first generate a regular symmetrical design $3^4//9$ of strength 2 in accordance with the results of §7 of chapter 6. Denote the factors of this design by $F_1,\ F_2,\ F_3,$ and F_4. Repeat all 9 treatments replacing the levels 0, 1, and 2 of the factor F_4 with 3, 4, and 5 respectively. In the resulting design $3^3 \times 6//18$, split factors F_1 and F_4. As a result, we get the regular main effect design $2 \times 3^2 \times 5//18$.

Another special case of the described procedure is a method of B.H. Margolin [3] of construction of a regular factorial design $r \times 2^n$ of strength 3 in $r(n+1)$ runs $(r = 2l)$ from the regular main effect design in $n+1$ runs for n two-level factors. Let $\mathbf{D} = \{a_{ij}\}$ $\left(a_{ij} \in GF(2)\right)$ be an orthogonal array $(n+1,\ n,\ 2,\ 2)$. Then using a method of construction of the two-level design of strength 3 (see §4 of chapter 7) and applying the described in this section procedure, we get the design

$$\left\|\begin{matrix} \mathbf{D} & \mathbf{0} \\ \mathbf{D}+\mathbf{J} & \mathbf{I} \\ \vdots & \vdots \\ \mathbf{D} & (r-2)\mathbf{I} \\ \mathbf{D}+\mathbf{J} & (r-1)\mathbf{I} \end{matrix}\right\| \tag{8.4.7}$$

that is a required regular design $r \times 2^n$ of strength 3 (where $\mathbf{J}$ is the matrix consisting of +1). It follows from (5.2.2) that the number of runs in such a design should be at least $r(n+1)$. Therefore, the number of runs of the design (8.4.7) is minimal.

Example 8.4.2. Consider two regular main effect designs: the first design $\mathbf{D}_1$ for four three-level factors $F_1,\ F_2,\ F_3,$ and F_4 in 9 runs; the second design $\mathbf{D}_2$ for three two-level factors $F_5,\ F_6,$ and F_7 in 4 runs. Production of these designs $\mathbf{D}_{12}$ corresponds to pairwise orthogonal main effects of four three-level and three two-level factors and also all two-factor interaction effects of a two-level and a three-level factors. Use a procedure of replacement for the following pairs of factors: F_1 and F_5, F_2 and F_6, F_3 and F_7. As a result, we get a regular main effect design $3 \times 6^3//36$. This design can be regarded as two orthogonal F-squares $F(6;\ 1^6)$ and $F(6;\ 2^3)$.

§ 5. Orthogonal *F*-squares

As it follows from Theorem 5.1.3, the set of pairwise of orthogonal Latin squares of order s is a special case of a regular factorial design of strength 2 in s^2 runs. Therefore, for $s = p^h$ (p is prime) construction of orthogonal F-squares can be made by using the methods described above. For $s \neq p^h$ the most important for application is the case of $s = 6$, which was studied by D.J. Finney [4]. In this paragraph we will present some of his results.

Start with an example of a Latin square of order 6 and its orthogonal partition $F(6;\ 1^4,\ 2)$:

$$\begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 3 & 5 & 2 & 4 \\ 2 & 5 & 0 & 4 & 1 & 3 \\ 3 & 4 & 1 & 0 & 5 & 2 \\ 4 & 3 & 5 & 2 & 0 & 1 \\ 5 & 2 & 4 & 1 & 3 & 0, \end{array} \qquad (8.5.1)$$

$$\begin{array}{cccccc} 0 & 2 & 4 & 4 & 3 & 1 \\ 4 & 3 & 1 & 0 & 2 & 4 \\ 1 & 4 & 4 & 2 & 0 & 3 \\ 2 & 1 & 3 & 4 & 4 & 0 \\ 4 & 0 & 2 & 3 & 1 & 4 \\ 3 & 4 & 0 & 1 & 4 & 2. \end{array} \qquad (8.5.2)$$

Using a procedure of collapsing, we can transform the F-square (8.5.2) to the following orthogonal partitions of the Latin square (8.5.1): $F(6;\ 2^3)$, $F(6;\ 3^2)$, $F(6;\ 1^2,\ 2,\ 2)$, etc. Various sets of two F-squares of order 6 can be obtained similarly. The orthogonal F-squares (8.5.1) and (8.5.2) correspond to the regular main effect design $5 \times 6^3//36$.

Present here a set of two mutually orthogonal partitions of the Latin square

$$\begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & 5 \\ 1 & 2 & 5 & 0 & 3 & 4 \\ 2 & 5 & 1 & 4 & 0 & 3 \\ 3 & 0 & 4 & 1 & 5 & 2 \\ 4 & 3 & 0 & 5 & 2 & 1 \\ 5 & 4 & 3 & 2 & 1 & 0 \end{array} \qquad (8.5.3)$$

of type $F(6;\ 1^3,\ 3)$:

$$\begin{array}{cccccc} 0 & 3 & 3 & 3 & 1 & 2 \\ 3 & 0 & 1 & 2 & 3 & 3 \\ 1 & 3 & 2 & 3 & 3 & 0 \\ 2 & 3 & 0 & 1 & 3 & 3 \\ 3 & 1 & 3 & 0 & 2 & 3 \\ 3 & 2 & 3 & 3 & 0 & 1, \end{array} \quad \begin{array}{cccccc} 0 & 3 & 3 & 1 & 3 & 2 \\ 1 & 2 & 3 & 3 & 3 & 0 \\ 3 & 1 & 0 & 3 & 2 & 3 \\ 3 & 3 & 1 & 2 & 0 & 3 \\ 2 & 0 & 3 & 3 & 1 & 3 \\ 3 & 3 & 2 & 0 & 3 & 1. \end{array} \qquad (8.5.4)$$

F-squares (8.5.3) and (8.5.4) correspond to the regular main effect design $4^2 \times 6^3//36$.

§ 6. Other Methods

Starks' method

Series of regular designs of main effects $2^n \times 3^m$ $(n+m \le 7)$ in 16 runs was constructed by T.H. Starks [5]. The method of construction is based on the regular design $2^7//8$ of strength 2:

$$\mathbf{D}_1 = \left\| \begin{matrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{matrix} \right\|. \tag{8.6.1}$$

The matrix is transformed (by trial) to the matrix

$$\mathbf{D}_2 = \left\| \begin{matrix} 2 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 2 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 2 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 2 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 2 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 2 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 2 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{matrix} \right\|,$$

so that

$$\mathbf{D} = \left\| \begin{matrix} \mathbf{D}_2 \\ 2\mathbf{J} - \mathbf{D}_2 \end{matrix} \right\|$$

is a regular main effect design $3^7//16$. Any column of this design can be split into a uniform two-level factor.

Margolin's method

One more method of construction of main effect designs for factors with two and three levels is due to B.H. Margolin [6].

Let $\mathbf{D} = \| \; \mathbf{D}', \quad \mathbf{D}'' \; \|$ be an orthogonal array $(n,\ n-1, 2, 2)$, where elements of the first column $\mathbf{D}'$ are 0 and 2, and elements of the submatrix

$\mathbf{D}''$ are 0 and 1. Then the design $2^{2n-4} \times 3//2n$ is given by the following matrix with addition in Galois field $GF(2)$:

$$\left\| \begin{matrix} \mathbf{D}' & \mathbf{D}'' & \mathbf{D}'' \\ \mathbf{I} & \mathbf{D}'' & \mathbf{D}'' + \mathbf{J} \end{matrix} \right\|, \tag{8.6.2}$$

where $\mathbf{I}$ is a unit vector, $\mathbf{J}$ is a matrix of 1.

To prove that the matrix (8.6.2) is a regular design of strength 2, we have to check whether main effects of the design are pairwise orthogonal. The matrix (with addition in a class of integer numbers)

$$\left\| \begin{matrix} \mathbf{D}' - 1 & \mathbf{I} & 2\mathbf{D}'' - \mathbf{J} & 2\mathbf{D}'' - \mathbf{J} \\ \mathbf{0} & -\mathbf{I} & 2\mathbf{D}'' - \mathbf{J} & \mathbf{J} - 2\mathbf{D}'' \end{matrix} \right\|$$

contains all vectors of main effects. Their orthogonality follows from the properties of the original orthogonal array of strength 2.

Using the method of B.H.Margolin, we can construct, for example, regular main effect designs $2^{20} \times 3//24$, $2^{36} \times 3//40$, $2^{44} \times 3//48$, and $2^{52} \times 3//56$.

A combination of different techniques of this paragraph allows obtaining other regular main effect designs. B.H.Margolin reported [6] but did not present regular main effect designs $2^{16} \times 3^7//32$ and $2^{48} \times 3^7//64$. A method of their construction is presented in the article of S. Addelman [7].

Some of the designs that were constructed by S.Addelman were also obtained by E.V. Markova and A.N. Lisenkov [8] with a different technique and were called the complex combined designs.

Augmenting Designs of Addelman-Kempthorne

In this section we consider a method of augmenting regular symmetrical main effect designs with one additional two-level factor [9].

Each design of Addelman-Kempthorne considered in §2 of chapter 7 can be represented in the following form:

$$\left\| \begin{matrix} \mathbf{A}_1 \\ \mathbf{A}_2 \end{matrix} \right\|.$$

The number of rows of the submatrix A_1 equals the number of rows of the submatrix A_2 and equals s^l. Let l columns $\mathbf{v}_1, \dots, \mathbf{v}_l$ form the full design s^l. Then any column of A_1 and A_2 can be represented as follows:

$$q\mathbf{v}_1^{(2)} + q_1\mathbf{v}_1 + q_2\mathbf{v}_2 + \cdots + q_s\mathbf{v}_s + \mathbf{b}, \tag{8.6.3}$$

where $\boldsymbol{b}^T = (b, \dots, b)$; $q, q_1, \dots, q_s$, b and elements of columns $\mathbf{v}_1, \dots, \mathbf{v}_s$ belong to Galois field $GF(s)$; $\mathbf{v}_i^{(2)}$ is obtained by squaring the levels of $\mathbf{v}_i$.

Using lemma 4 of article [10], it is easy to show that the column (8.6.3) contains each of s elements of GF(s) exactly s^{l-1} times. It follows that the design

$$\left\| \begin{matrix} 0 \; \dots \; 0 & 1 \; \dots \; 1 \\ \mathbf{A}_1 & \mathbf{A}_2 \end{matrix} \right\|^T .$$

is a regular asymmetrical factorial main effect design. This statement can be proved based on properties (8.6.3) of the columns of submatrix A_1 and A_2 and by using the condition of proportional frequencies.

Example 8.6.1. The orthogonal arrays (18, 7, 3, 2) and (50, 11, 5, 2) can be transformed to the regular main effect designs $2 \times 3^7//18$ and $2 \times 5^{11}//50$ respectively. The first of them (the design $2 \times 3^7//18$) is presented below:

$$\left\| \begin{matrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\
0 & 2 & 2 & 2 & 2 & 2 & 2 & 0 \\
0 & 0 & 1 & 0 & 2 & 2 & 1 & 1 \\
0 & 1 & 2 & 1 & 0 & 0 & 2 & 1 \\
0 & 2 & 0 & 2 & 1 & 1 & 0 & 1 \\
0 & 0 & 1 & 2 & 1 & 0 & 2 & 2 \\
0 & 1 & 2 & 0 & 2 & 1 & 0 & 2 \\
0 & 2 & 0 & 1 & 0 & 2 & 1 & 2 \\
1 & 0 & 0 & 1 & 2 & 1 & 2 & 0 \\
1 & 1 & 1 & 2 & 0 & 2 & 0 & 0 \\
1 & 2 & 2 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 2 & 2 & 0 & 1 & 1 & 1 \\
1 & 1 & 0 & 0 & 1 & 2 & 2 & 1 \\
1 & 2 & 1 & 1 & 2 & 0 & 0 & 1 \\
1 & 0 & 2 & 1 & 1 & 2 & 0 & 2 \\
1 & 1 & 0 & 2 & 2 & 0 & 1 & 2 \\
1 & 2 & 1 & 0 & 0 & 1 & 2 & 2
\end{matrix} \right\|$$

The design $2 \times 5^{11}//50$ is included into the Catalog of the book (the design $\mathbf{D}_{50}$, #50).

Asymmetrical Main Effect Designs $2^l \times 4^n \times 8^m//64$

A series of designs $2^l \times 4^n \times 8^m//64$ was obtained in [9] based on a special representation of a finite projective geometry $PG(5, 2)$.

Consider the full design $2^6//64$. Each treatment combination of this design corresponds to a point $(x_1, \ldots, x_6)$ of finite space $EG(6,2)$. Coordinates of the points belong to Galois field $GF(2)$. Denote these coordinates by 0 and 1. Consider a hyperplane

$$a_0 + a_1 x_1 + \cdots + a_6 x_6 = 0 \tag{8.6.4}$$

in $EG(6,2)$ ($a_i \in GF(2)$ and are not equal simultaneously to zero). If a_0 takes in (8.6.4) two different values from $GF(2)$, we get a pencil $P(a_1, \ldots, a_6)$ of two parallel flats in $EG(6,2)$ as a solution of (8.6.4). The numbers $a_1, \ldots, a_6$ are coordinates of the pencil $P(a_1, \ldots, a_6)$. There is one-to-one correspondence between the set of pencils $P(a_1, \ldots, a_6)$ and the set of their coordinates $a_1, \ldots, a_6$. Therefore, the set all pencils $P(a_1, \ldots, a_6)$ is a finite projective geometry $PG(5,2)$. There are 63 points in $PG(5,2)$ and, therefore, 63 different pencils of parallel flats in $EG(6,2)$. Each of the pencils $P(a_1, \ldots, a_6)$, or the point $(a_1, \ldots, a_6)$ of the projective geometry $PG(5,2)$, corresponds to the two-level factor that we also denote by $(a_1, \ldots, a_6)$. . A set of all such 63 two-level factors forms an orthogonal array (64, 63, 2, 2), or a regular factorial main effect design $2^{63}//64$ (see §7 of chapter 6).

Points $\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_v$ of the projective geometry $PG(5,2)$ ($v \le 6$) is called linearly independent if

$$Rg\|\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_v\| = v.$$

Denote the points (1, 0, …, 0), (0, 1, …, 0), …, (0, 0, …, 1) of the projective geometry $PG(5,2)$ by 1, 2, …, 6 respectively. These points are linearly independent. Any point $(a_1, \ldots, a_6)$ in $PG(5,2)$ can be represented by a linear combination of the points 1, 2, …, 6:

$$(a_1, \ldots, a_6) = \lambda_1(1, 0, \ldots, 0) + \cdots + \lambda_6(0, 0, \ldots, 1), \tag{8.6.5}$$

where $\lambda_i = 0$ or 1 and are not equal simultaneously to zero.

Denote the point (8.6.5) by $1^{\lambda_1} 2^{\lambda_2} \ldots 6^{\lambda_6}$. For example, the point (1, 1, 1, 0, 1, 0) will be denoted by 1235. In these notations, all 63 points of $PG(5,2)$ presented in Figure 8 are split into 9 subset (displayed as triangles) of 9 points each. Each subset has three linearly independent points. Therefore, seven points of subset (triangle) belong to 2-flat. In 2-flat, seven points belong to seven lines (1-flats). In Figure 8 these lines passing through three points in each 2-flat, are displayed as one circle and six line segments.

For example, the upper left triangle in Figure 8 is 2-flat containing seven points: 5, 35, 3, 135, 15, 13, and 1. The points, for example, 1, 3, and 5 are linearly independent. Seven points of the upper left triangle belong to seven lines: 15-35-13, 13-3-1, 15-5-1, 13-135-5, 15-135-3, 1-135-35, and 3-5-35.

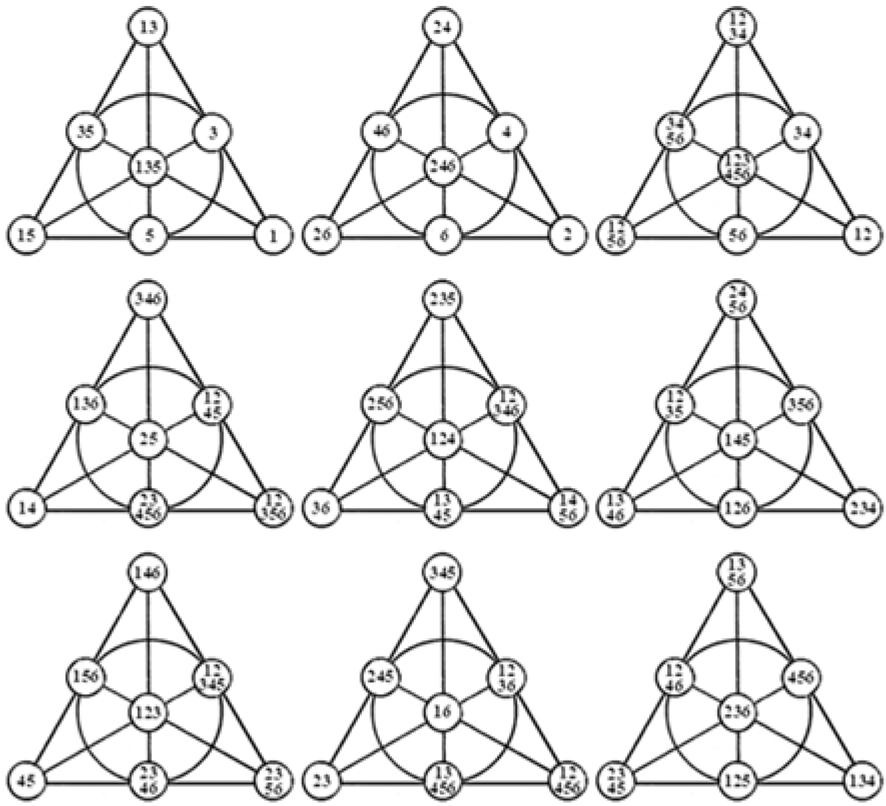

Figure 8. Magic finite projective geometry $PG(5,2)$

Note one additional property of $PG(5,2)$ in Figure 8. Consider any three triangles (2-flats) displayed in Figure 8 in the one row. Three corresponding points of these triangles belong to one line (1-flat). For example, three central points 25, 124, and 145 of three triangles of the second row belong to one line. We will call it a horizontal line. Similarly, we can define vertical lines, however, we are not going to use them. Such representation of the finite projective geometry $PG(5,2)$ reminds a magic square. So we will call it a magic finite projective geometry $PG(5,2)$.

It follows from the method of replacement that any three points (three two-level factors) belonging to one line of $PG(5,2)$ can be used to form one four-level factor. Similarly, any seven points (seven two-level factors) belonging to one 2-flat can be used to form one eight-level factor.

Based on the magic finite projective geometry $PG(5,2)$ (Figure 8) in [9] were constructed new regular main effect designs $4^7 \text{x}\, 8^6//64$ and $4^{14}\text{ x}\, 8^3//64$. The design $4^7\text{x}\, 8^6//64$ can be constructed, for example, by using six triangles (2-flats) from the second and the third rows and seven horizontal lines of the first row of Figure 8. The resulting design is shown below (in the transposed form):

```
0123103210320123321023012301321023013210321023011032012301231032
0231132002311320132002311320023120133102201331023102201331022013
0321210312303012123030120321210312303012032121030321210312303012
0202020213131313131313020202023131313120202020202020202031313131
0011110022333322223333220011110000111100223333222233332200111100
0213312013022031021331201302203120311302312002132031130231200213
0330122121123003300321121221033012210330300321122112300303301221
0011001122332233001100112233223377667766554455447766776655445544
0101232301012323767654547676545401012323010123237676545476765454
0110233223320110766754455445766776675445544576670110233223320110
0312657430215647120374652130475656473021657403124756213074651203
0536142763507241271436054172506314270536724163503605271450634172
0312746565741203564721303021475621305647475630217465031212036574
```

The design $4^{14}\text{ x}\, 8^3//64$ can be constructed, for example, by using three triangles (2-flats) of the third row and 14 horizontal lines of the first and second rows of Figure 8.

The list of the main effect designs that can be constructed by using the magic finite projective geometry $PG(5,2)$ is presented in Table 15.

The design of Table 15 can be augmented with two-level factors by using points of $PG(5,2)$ that do not belong to 1-flats and 2-flats, which form four-level and eight-level factors. This procedure leads to construction of the following regular uniform main effect designs: 4^{21}, $2^8\text{ x}\, 4^{16}\text{ x}\, 8$, $2^4\text{ x}\, 4^{15}\text{ x}\, 8^2$, $4^{14}\text{ x}\, 8^3$, $2^8\text{ x}\, 4^9\text{ x}\, 8^4$, $2^4\text{ x}\, 4^8\text{ x}\, 8^5$, $4^7\text{ x}\, 8^6$,

$2^8 \times 4^2 \times 8^7$, $2^4 \times 4 \times 8^8$.

Table 15

Construction of Designs $4^n \times 8^m//64$ from Magic Finite Projective Geometry $PG(5,2)$.

Design	Construction of 4-Level Factors	Construction of 8-Level Factors
4^{21}	21 horizontal lines	
$4^{16} \times 8$	14 horizontal lines of the first six triangles, any line of the 7-th triangle and any line of the 8-th triangle	the 9-th triangle
$4^{15} \times 8^2$	14 horizontal lines of the first six triangles and any line of the 7-th triangle	the 8-th and 9-th triangles
$4^{14} \times 8^3$	14 horizontal lines of the first six triangles	the 7-th, 8-th, and 9-th triangles
$4^9 \times 8^4$	7 horizontal lines of the 1-st, 2-nd, and 3-rd triangles, any line of the 4-th triangle, and any line of the 5-th triangle	the 6-th, 7-th, 8-th, and 9-th triangles
$4^8 \times 8^5$	7 horizontal lines of the 1-st, 2-nd, and 3-rd triangles and any line of the 4-th triangle	the 5-th, 6-th, 7-th, 8-th, and 9-th triangles
$4^7 \times 8^6$	7 horizontal lines of the 1-st, 2-nd, and 3-rd triangles	the 4-th, 5-th, 6-th, 7-th, 8-th, and 9-th triangles
$4^2 \times 8^7$	Any line of the 1-st triangle and any line of the 2-nd triangle	All triangles, except the 1-st and 2-nd
4×8^8	Any line of the 1-st triangle	All triangles, except the 1-st
8^9		All 9 triangles

After publication of the article [9], the following question remained open. What is the maximum value of m in geometric main effect designs $4^m \times 8^n//64$ for given n? The solution of this problem was found by I.E. Boguslavsky [11]. Further, up to the end of §6, we will present his results.

Lemma 8.6.1 [11]. The following two conditions are necessary for the existence of a geometric main effect design $4^m \times 8^n//64$:

1. $7n + 3m \leq 63$;
2. $7n + 3m \neq 62; 7n + 3m \neq 61$.

Proof. It is evident that the first statement of the theorem holds.

Now we will prove that the second statement of the theorem also holds.

The sum of all points of any line, the sum of any 2-flat, and the sum of the whole $PG(5,2)$ are a zero-vector. Therefore, the sum of all points of $PG(5,2)$ that are not in use for constructing four-level and eight-level factors of the design 4^m x $8^n//64$ is equal to a zero-vector. Since all points of $PG(5,2)$ are nonzero and different, the number of points that are not in use for constructing four-level and eight-level factors cannot be 2 or 1. I.e., $7n+3m \neq 62,\ 7n+3m \neq 61,$ which was to be proved.

In Table 16 below, the designs obtained from the magic projective geometry are comparing with the designs that do not exist by Lemma 8.6.1.

Table 16
Designs that do not Exist by Lemma 8.6.1.

Designs Obtained From Magic Finite Projective Geometry	Designs that do not Exist by Lemma 8.6.1
4^{21} x $8^0//64$	4^{22} x $8^0//64$
4^{16} x $8^1//64$	4^{18} x $8^1//64$
4^{15} x $8^2//64$	4^{16} x $8^2//64$
4^{14} x $8^3//64$	4^{15} x $8^3//64$
4^9 x $8^4//64$	4^{11} x $8^4//64$
4^8 x $8^5//64$	4^9 x $8^5//64$
4^7 x $8^6//64$	4^8 x $8^6//64$
4^2 x $8^7//64$	4^4 x $8^7//64$
4 x $8^8//64$	4^2 x $8^8//64$
$8^9//64$	4 x $8^9//64$
	$8^{10}//64$

Therefore, there is only an open question about the existence of the designs 4^{17} x $8//64$, 4^{10} x $8^4//64$, and 4^3 x $8^7//64$.

Theorem 8.6.1 [11]. There exist geometrical main effect designs 4^{17} x $8//64$ and 4^{10} x $8^4//64$.

The existence of a design 4^{17} x $8//64$ is confirmed by the following subsets in $PG(5,2)$: one 2-flat 1-2-12-3-13-23-123 and 17 lines: 12456-24-156, 146-3456-135, 25-2356-36, 4-46-6, 246-35-23456, 1246-15-2456, 13456-256-1234, 1356-245-12346, 134-16-346, 1256-2346-1345, 234-1456-12356, 356-235-26, 1236-12345-456.

The existence of a design 4^{10} x $8^4//64$ is confirmed by the following subset in $PG(5,2)$: four 2-flats: 1246-136-234-2456-15-12345-356, 14-25-1245-1346-36-123456-2356, 1-2-12-3-13-23-123, 4-5-

45-6-46-56-456 and 10 lines: 1236-345-12456, 134-16-346, 246-13456-1235, 145-125-24, 35-256-236, 23456-1234-156, 1456-235-12346, 2345-124-135, 2346-34-26, 1256-245-146.

Theorem 8.6.1 [11]. A geometric main effect design $4^3 \times 8^7//64$ does not exist.

The proof of the Theorem 8.6.1 in the original article [11] includes six Lemmas and is very cumbersome. So we omit it here.

Finally, we present the list of the main effect designs $2^l \times 4^n \times 8^m//64$ that contain the maximal number n of four-level factors for the given number m of eight-level factors (and that contain the maximal number l of two-level factors for the given n and m):

$4^{21}//64$
$2^5 \times 4^{17} \times 8//64$
$2^4 \times 4^{15} \times 8^2//64$
$4^{14} \times 8^3//64$
$2^5 \times 4^{10} \times 8^4//64$
$2^4 \times 4^8 \times 8^5//64$
$4^7 \times 8^6//64$
$2^8 \times 4^2 \times 8^7//64$
$2^4 \times 4 \times 8^8//64$
$8^9//64$

§ 7. Blocking

We will start this paragraph with an example that explains how the problem of blocking of geometric designs can be reduced to the problem of construction of compromise asymmetrical (generally speaking) regular designs.

Suppose that we need to construct a design in 16 runs for 8 two-level factors $F_1, \dots, F_8$ that corresponds to pairwise orthogonal effects of all main effects and two-level interaction effects any of the factors F_1, F_2, F_3, and F_4. We assume that there is some restriction on the design: all 16 experiments cannot be performed in homogeneous environments. Homogeneous environments can be only kept in a series of 8 experiments. Therefore, we need to divide the design into two blocks. For orthogonal blocking the problem is reduced, by the results of §14 of chapter 3, to the problem of construction of a geometric compromise design in 16 runs for 9 two-level factors (denote additional blocking factor by F_9) that corresponds to pairwise orthogonal main effects of all factors and two-factor interaction effects of factors F_1, F_2, F_3, and F_4.

It follows from the results of §8 of chapter 6 that such a design exists and its factors are defined by the vertices of bundles of parallel flats in $PG(4,\ 2)$: (1000), (0100), (0010), (0001), (1110), (1101), (1011), (0111), (1111). Arrange all treatments of the design in such a way that the blocking factor F_9 appears in the first eight treatments at level 0 and in the second eight treatments, at level 1. Then the design will be as follows:

$$
\begin{array}{cc}
\text{First Block} & \text{Second Block} \\
\begin{array}{cccccccc} F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & F_7 & F_8 \end{array} & \begin{array}{cccccccc} F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & F_7 & F_8 \end{array} \\
\begin{Vmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\
0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{Vmatrix} &
\begin{Vmatrix}
1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\
1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\
0 & 1 & 1 & 1 & 0 & 0 & 0 & 1
\end{Vmatrix}.
\end{array}
$$

Further, in this paragraph, we will present the results on blocking for geometric factorial designs [12-17] starting with the blocking concept by R.C.Bose [17].

Consider a full design for m factors with the levels that are the elements of the field $GF\left(p^h\right)$. All points of the full design are the finite points of $PG\left(m,\ p^h\right)$. Consider n independent pencils in $PG\left(m,\ p^h\right)$:

$$P_i = P(a_{i1}, \dots, a_{im}) \quad (i = 1, \dots, n). \tag{8.7.1}$$

Consider degrees of freedom carried by the pencils (8.7.1) as degrees of freedoms carried by main effects of certain virtual factors $\Phi_1, \dots, \Phi_n$. Different levels of these factors correspond to different flats of the pencils (8.7.1).

The pencil

$$P(\lambda_1 a_{11} + \dots + \lambda_n a_{n1}, \dots, \lambda_1 a_{1m} + \dots + \lambda_n a_{nm})$$

carries degrees of freedoms of interaction effects of factors $\Phi_{i_1}, \dots, \Phi_{i_r}$ belonging to the set of the factors $\Phi_1, \dots, \Phi_n$ if and only if coefficients $\lambda_{i_1}, \dots, \lambda_{i_r}$ (and only they) are nonzero. Let $S_{i_1}, \dots, S_{i_n}$ be flats belonging to the pencils (8.7.1). These flats pass through a common $(m-n)$-flat $S_{i_1 \dots i_n}$. Since each pencil has $s = p^h$ flats, all s^m treatments is divided into s^n sets of type $S_{i_1 \dots i_n}$. It is evident that degrees of freedom carried by contrasts between these sets are identical to the degrees of freedom carried by main effects and interaction effects of the factors $\Phi_1, \dots, \Phi_n$. The latest degrees of freedom, by Theorem 8.3.1, are identical to degrees of freedom carried by main effects of s^n-level block factor F obtained by the technique of replacement for the factors $\Phi_1, \dots, \Phi_n$.

Now consider a design **D** with the block factor F and other factors that correspond to vertices of bundles of parallel flats in $PG(m, s)$.

Definition 8.7.1. If some main effect or interaction effect of the design **D** is represented by a linear combination of main effects of the block factor, the corresponding main effect or interaction effect is called confounded (with blocks). Other contrasts are called unconfounded.

Similarly, we can define confounded and unconfounded degrees of freedoms.

Finding confounded contrasts (as well as finding alias sets for geometric designs) is important from two points of view. First, it is necessary to determine a portion of a full factorial model for which this design is nonsingular. Second, it is necessary to determine the bias of LS estimates of parameters of the model (see §9 of Chapter 6).

The vertices of bundles $P_1, \dots, P_n$ have a common $(m-n-1)$-flat at infinity. Denote this flat by S. Then the flats $S_{i_1}, \dots, S_{i_n}$ when extended at infinity pass through S so that $S_{i_1 \dots i_n}$ passes through S. Therefore, all s^n extended at infinity flats of type $S_{i_1 \dots i_n}$ form a bundle of parallel flats with the vertex S.

It is evident that confounded degrees of freedom are carried by those and only those pencils (8.7.1) with the vertex that passes through S. Hence, there are exactly $(s^n-1)/(s-1)$ $(m-n)$-flats at infinity that pass through S. These flats correspond to all confounded degrees of freedom. Denote by (s^m, s^n) a regular design in s^m runs divided into s^n orthogonal blocks of size s^{m-n} each. Such a design will be determined by the $(m-n-1)$-flat S at infinity.

The nature of the degrees of freedom carried by any bundle, by Theorem 6.2.2, depends on the relation in which the vertex of the bundle stands to the fundamental simplex. Therefore, the nature of the design (s^m, s^n) depends on the relation in which the flat S defining the design stands to the fundamental simplex. That allows enumerating the designs (s^m, s^n).

Consider, for example, designs (s^3, s^2). The flat S has dimension $m-n-1=0$. Therefore, each design corresponds to the point S in a flat at infinity. There are only three possible relations S to the fundamental simplex: 1) the point S is a vertex of the fundamental simplex; 2) the point S lies on a side of the fundamental simplex (except a vertex); 3) the point S does not lie on any side of the fundamental simplex.

For the first case, consider $s+1$ lines passing through S. Two of them coincide with the sides of the fundamental simplex. The others pass through the vertex S without coinciding with a side of the fundamental simplex. Therefore, $s-1$ degrees of freedom for each main effect of two factors and $(s-1)^2$ degrees of freedom carried by interaction effects of these factors are confounded.

For the second case, consider again $s+1$ lines passing through *S*. One of them coincides with the side of the fundamental simplex that contains *S*. Other passes through opposite vertex of the fundamental simplex. The rest do not pass through any vertex of the fundamental simplex. Therefore, $s-1$ degrees of freedom carried by the main effects of one factor, $s-1$ degrees of freedom carried by interaction effects of the two other factors, and $(s-1)^2$ degrees of freedom carried by three-factor interaction effects are confounded..

For the third case, consider again $s+1$ lines passing through *S*. Three of them join *S* to the vertices of the fundamental simplex. No other passes through any vertex of the fundamental simplex. Therefore, $s-1$ degrees of freedom for each of three two-factor interaction effects and $(s-1)(s-2)$ degrees of freedom carried by three-factor interaction effects are confounded.

Enumeration of the various designs of the classes (s^4, s^3) and $(s^4,\ s^2)$ can be found in [14, 17].

Now an important question arises. How many factors can be accommodated in the experiment so that all main effects and interaction effects up to *t*-factor are not confounded in the design $(s^m,\ s^n)$ for given size of blocks s^{m-n}?

The $(m-n-1)$-flat *S* at infinity that defines confounding of the design can be represented by means of $m-n$ independent points $L_1, \dots, L_{m-n}$ c with coordinates

$$
\begin{aligned}
&(0,\ a_{11}, \dots, a_{1m}),\\
&(0,\ a_{21}, \dots, a_{2m}),\\
&\dots\dots\dots\dots\dots\\
&(0,\ a_{m-n,1}, \dots, a_{m-n,m}).
\end{aligned}
$$

The equations of any $(m-t)$-cell of the fundamental simplex are

$$\chi_0 = 0, \chi_{i_1} = 0, \chi_{i_2} = 0, \dots, \chi_{i_t} = 0. \tag{8.7.2}$$

Any $(m-2)$-flat at infinity that passes through the cell (8.7.2) is represented by the following equations:

$$\chi_0 = 0, \quad \lambda_{i_1}\chi_{i_1} + \cdots + \lambda_{i_t}\chi_{i_t} = 0. \tag{8.7.3}$$

The necessary and sufficient condition that (8.7.3) passes through *S* are

$$
\begin{aligned}
&\lambda_{i_1} a_{1i_1} + \lambda_{i_2} a_{1i_2} + \cdots + \lambda_{i_t} a_{1i_t} = 0,\\
&\lambda_{i_1} a_{2i_1} + \lambda_{i_2} a_{2i_2} + \cdots + \lambda_{i_t} a_{2i_t} = 0,\\
&\dots\dots\dots\dots\dots\dots\dots\dots\dots\\
&\lambda_{i_1} a_{m-n,i_1} + \lambda_{i_2} a_{m-n,i_2} + \cdots + \lambda_{i_t} a_{m-n,i_t} = 0.
\end{aligned}
$$

It is equivalent to the condition that the i_1-th, i_2-th, …, i_t-th columns of the matrix

$$\begin{Vmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m-n,1} & a_{m-n,2} & \cdots & a_{m-n,m} \end{Vmatrix} \tag{8.7.4}$$

are dependent. Therefore, the following theorem holds.

Theorem 8.7.1 [17]. The maximum number of factors that can be accommodated in the design $(s^m,\ s^n)$ for the given size of blocks s^{m-n} without confounding any degrees of freedom carried by main effects and interaction effects up to t-factor is equal to the maximum number of columns of the matrix (8.7.4) with elements from $GF(s)$ such that no t its columns are dependent.

Theorem 8.7.1 can be stated by using terminology of projective geometries as follows.

Theorem 8.7.2 [17]. The maximum number of factors that can be accommodated in the design $(s^m,\ s^n)$ for the given size of blocks s^{m-n} without confounding any degrees of freedom carried by main effects and interaction effects up to t-factor is equal to the maximum number of points in $PG(m-n-1, s)$ such that no t of them lie on a flat of dimension $t-2$ or less.

This maximum number in §6 of chapter 6 is denoted by $m_t(m-n, s)$ and corresponds to complete (m, t)-set in $PG(m-n-1,\ s)$.

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Chapter 9. Irregular Main Effect Designs

§ 1. Transformation of Regular Designs

In this paragraph we consider a generalization of the method of S. Addelman of splitting of factor levels (see §2 of chapter 8) when the resulting factors are not necessarily orthogonal [1, 2].

Let $\overline{\mathbf{D}}$ be a nonsingular main effect design in *N* runs for *n* factors $F_1, \dots, F_n$ at $s_1, \dots, s_n$ levels respectively. Denote by $\overline{\mathbf{F}}_i$ a matrix that consists of $s_i - 1$ linearly independent vectors of main effects of the factor F_i of the design $\overline{\mathbf{D}}$. Scalar squares of the columns of the matrix $\overline{\mathbf{F}}_i$ equal *N*. Regardless of the type of a model of main effects, necessary and sufficient condition that the plan is nonsingular for the given model is that

$$\overline{\mathbf{X}} = \| \ \mathbf{I}, \quad \overline{\mathbf{F}}_1, \dots, \overline{\mathbf{F}}_n \ \|$$

is a full rank matrix (see §12 of chapter 3), or

$$\det(\overline{\mathbf{X}}^T \overline{\mathbf{X}}) \neq 0. \tag{9.1.1}$$

Consider the following method of construction a new main effect design $\mathbf{D}$ based on the design $\overline{\mathbf{D}}$. In the design $\overline{\mathbf{D}}$ replace the factor F_i (with s_i levels) with the factors $F_i^1, \dots, F_i^{m_i}$ (with $s_i^{(1)}, \dots, s_i^{(m_i)}$ levels respectively) such that

$$\left(s_i^{(1)} - 1\right) + \dots + \left(s_i^{(m_i)} - 1\right) = S_i - 1 \leq s_i - 1, \tag{9.1.2}$$

and a given level of the factor F_i in the design $\overline{\mathbf{D}}$ corresponds only to one combination of levels of the factors $F_i^1, \dots, F_i^{m_i}$ in the design $\mathbf{D}$. Therefore, as a result, each level of the factors F_i corresponds to a row of the auxiliary design $\mathbf{D}_i$:

$$\begin{array}{c} F_i \\ \left\| \begin{array}{c} 0 \\ \vdots \\ s_i - 1 \end{array} \right\| \end{array} \rightarrow \begin{array}{c} \begin{array}{ccc} F_i^1 & \dots & F_i^{m_i} \end{array} \\ \left\| \begin{array}{ccc} F_i^1(0) & \dots & F_i^{m_i}(0) \\ \vdots & \ddots & \vdots \\ F_i^1(s_i - 1) & \dots & F_i^{m_i}(s_i - 1) \end{array} \right\| \end{array} = \mathbf{D}_i.$$

Hence, a main effect of any factor of $F_i^1, \dots, F_i^{m_i}$ in the design $\mathbf{D}$ is a main effect of the factor F_i in the design $\overline{\mathbf{D}}$.

Let $\mathbf{D}^f$ be the full design in $N^f = s_1^{(1)} \dots s_1^{(m_1)} \dots s_n^{(1)} \dots s_n^{(m_n)}$ runs for the factors $F_1^1, \dots, F_1^{m_1}, \dots, F_n^1, \dots, F_n^{m_n}$; $\mathbf{D}_i^f$ be the full design in $n_i^f = s_i^{(1)} \dots s_i^{(m_i)}$ runs for the factors $F_i^1, \dots, F_i^{m_i}$. Hence, $N^f = \prod_{i=1}^n n_i^f$.

Denote by $\mathbf{F}_i^j$ a matrix of main effects of the factor F_i^j of the design $\mathbf{D}$. Denote by $\mathbf{x}_i^T = \mathbf{x}_i^T\left(j_i^1, \dots, j_i^{m_i}\right)$ a row of the matrix

$$\mathbf{F}_i = \| \; \mathbf{F}_i^1, \dots, \mathbf{F}_i^{m_i} \; \|$$

corresponding to the levels $j_i^1, \dots, j_i^{m_i}$ of the factors $F_i^1, \dots, F_i^{m_i}$ respectively. Each treatment of the design $\mathbf{D}^f$ with the levels $j_1^1, \dots, j_1^{m_1}, \dots, j_n^1, \dots, j_n^{m_n}$ of the factors $F_1^1, \dots, F_1^{m_1}, \dots, F_n^1, \dots, F_n^{m_n}$ respectively correspond to the vector

$$\mathbf{x}^T = \mathbf{x}^T\left(j_1^1, \dots, j_1^{m_1}, \dots, j_n^1, \dots, j_n^{m_n}\right) = (1, \mathbf{x}_1^T, \dots, \mathbf{x}_n^T).$$

Regardless of the type of a model of main effects for the nonsingular design $\mathbf{D}$, variance σ_x^2 of estimate of the regression function at the point $\left(j_1^1, \dots, j_1^{m_1}, \dots, j_n^1, \dots, j_n^{m_n}\right)$ of the design $\mathbf{D}^f$, by the results of §12 of chapter 3, is

$$\sigma_x^2 = \mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}\sigma^2, \tag{9.1.3}$$

where $\mathbf{X} = \| \; \mathbf{I}, \mathbf{F}_1, \dots, \mathbf{F}_n \; \|$.

It is easy to show that for $s_i^{(1)}, \dots, s_i^{(m_i)}$ satisfying the condition $S_i = s_i$ the levels $F_i^1, \dots, F_i^{m_i}$ can be arranged in such a way that

$$\operatorname{Rg} \mathbf{F}_i = S_i - 1. \tag{9.1.4}$$

Indeed, the following transformation

$$\left\| \begin{matrix} 0 \\ 1 \\ 2 \\ \vdots \\ s_i - 2 \\ s_i - 1 \end{matrix} \right\| \to \left\| \begin{matrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 1 & \cdots & 1 \\ 1 & 1 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 1 \end{matrix} \right\| = \mathbf{D'}_i \tag{9.1.5}$$

shows how we can arrange the levels of $s_i - 1$ two-level factors $F_i^1, \dots, F_i^{s_i - 1}$ to satisfy the condition (9.1.4). If there is a factor with l levels among of factors $F_i^1, \dots, F_i^{m_i}$, we need to combine any $l - 1$ columns for two-level factors from $\mathbf{D'}_i$. For example, we arrange a three-level factor combining two two-levels factors as follows:

$$\begin{Vmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 1 \\ \vdots & \vdots \\ 1 & 1 \\ 1 & 1 \end{Vmatrix} \rightarrow \begin{Vmatrix} 0 \\ 1 \\ 2 \\ \vdots \\ 2 \\ 2 \end{Vmatrix}.$$

If $S_i = s_i - q \quad (q > 0)$, we need to use the matrix $\mathbf{D}'_i$ deleting q its columns.

If the condition (9.1.4) holds, the matrices $\bar{\mathbf{F}}_i$ and $\mathbf{F}_i$ are related by a nonsingular linear transformation. Hence the design $\mathbf{D}$ is also (as the design $\bar{\mathbf{D}}$) the main effect design, i.e., the matrix $\mathbf{X}^T\mathbf{X}$ is nonsingular.

Even though the transformations similar to (9.1.5) lead to nonsingular designs, they are not, generally speaking, optimal. However, it is possible to find such transformations that the resulting designs will have some optimal properties.

If $\bar{\mathbf{D}}$ is a regular main effect design, then any column of $\bar{\mathbf{F}}_i$ is orthogonal to any column of $\bar{\mathbf{F}}_j$ and, therefore, any column of $\mathbf{F}_i$ is orthogonal to any column of $\mathbf{F}_j$. Hence, the matrix $\mathbf{X}^T\mathbf{X}$ is block diagonal:

$$\mathbf{X}^T\mathbf{X} = \begin{Vmatrix} N & & & \mathbf{0} \\ & \mathbf{F}_1^T\mathbf{F}_1 & & \\ & & \ddots & \\ \mathbf{0} & & & \mathbf{F}_n^T\mathbf{F}_n \end{Vmatrix}.$$

It follows from (9.1.3) that

$$\sigma_{\mathbf{x}}^2 = \mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}\sigma^2 = \left\{\frac{1}{N} + \sum_{i=1}^{n} \mathbf{x}_i^T\left(\mathbf{F}_i^T\mathbf{F}_i\right)^{-1}\mathbf{x}_i\right\}\sigma^2.$$

An average variance over treatment of the full design $\mathbf{D}^f$ is

$$\begin{aligned} \sigma_a^2 &= \frac{\sigma^2}{N^f}\sum_{\mathbf{x}\in\mathbf{D}^f}\left\{\frac{1}{N} + \sum_{i=1}^{n} \mathbf{x}_i^T\left(\mathbf{F}_i^T\mathbf{F}_i\right)^{-1}\mathbf{x}_i\right\} \\ &= \sigma^2\left\{\frac{1}{N} + \frac{1}{N^f}\sum_{i=1}^{n}\sum_{\mathbf{x}\in\mathbf{D}^f} \mathbf{x}_i^T\left(\mathbf{F}_i^T\mathbf{F}_i\right)^{-1}\mathbf{x}_i\right\} \\ &= \sigma^2\left\{\frac{1}{N} + \sum_{i=1}^{n}\frac{1}{N^f}\sum_{\mathbf{x}\in\mathbf{D}^f} \mathbf{x}_i^T\left(\mathbf{F}_i^T\mathbf{F}_i\right)^{-1}\mathbf{x}_i\right\}. \end{aligned}$$

By the results §4 of chapter 4,

$$\sigma_a^2 = \sigma^2\left\{\frac{1}{N} + \sum_{i=1}^{n}\sum_{j=1}^{S_i-1} c_{jj}^i\right\}, \tag{9.1.6}$$

where $\left(\mathbf{F}_i^T\mathbf{F}_i\right)^{-1} = \{c_{jl}^i\}$.

Let $\{\bar{c}_{jl}^i\}\sigma^2$ be a covariance matrix for the design $\mathbf{D}_i$ for a model of main effects. Then, it is evident that

$$c_{jl}^{i}\frac{N}{s_i} = \bar{c}_{jl}^{i}.$$

If the design $\bar{\mathbf{D}}$ is uniform, then

$$\begin{aligned}\sigma_{ia}^2 &= \frac{\sigma^2}{s_i}\left\{1 + \frac{N}{n_i^f}\sum_{\mathbf{x}\in\mathbf{D}^f}\mathbf{x}_i^T\left(\mathbf{F}_i^T\mathbf{F}_i\right)^{-1}\mathbf{x}_i\right\} \\ &= \sigma^2\left\{\frac{1}{s_i} + \frac{N}{s_i}\sum_{j=1}^{S_i-1} c_{jj}^i\right\} = \sigma^2\sum_{j=1}^{S_i}\bar{c}_{jj}^i\end{aligned} \tag{9.1.7}$$

is an average (over $\mathbf{D}_i^f$) variance of the estimate of the regression function for the design $\mathbf{D}_i$. It follows from (9.1.6) and (9.1.7) that

$$\sigma_a^2 = \frac{\sigma^2}{N}\left(1 - n + \sum_{i=1}^{n}\frac{\sigma_{ia}^2 s_i}{\sigma^2}\right).$$

Therefore, minimum of σ_a^2 is reached if and only if σ_{ia}^2 reaches minimum for any $i = 1, \ldots, n$. Therefore, the problem of getting an optimal (in sense of minimization of σ_a^2) design $\mathbf{D}$ from the design $\bar{\mathbf{D}}$ is equivalent to the problem of getting optimal (in the same sense) designs $\mathbf{D}_i$.

Analogously, it is easy to show that the problem of getting of *D*-optimal design $\mathbf{D}$ is reduced to the problem of getting *D*-optimal designs $\mathbf{D}_i$.

Denote by σ_n^2 and σ_{in}^2 normalized (per one observation and per one parameter) variances σ_a^2 and σ_{ia}^2 respectively:

$$\sigma_n^2 = \sigma_a^2\frac{N}{k};\;\; \sigma_{in}^2 = \sigma_{ia}^2\frac{s_i}{S_i}$$

(k is the number of parameters in the model). Then, it follows from (9.1.6) and (9.1.7) that

$$\sigma_n^2 = \frac{\sigma^2}{k}\left(1 + N\sum_{i=1}^{n}A_i\right), \quad \sigma_{in}^2 = \frac{\sigma^2}{s_i}\left(1 + NA_i\right),$$

where $A_i = \sum_{j=1}^{S_i-1} c_{jj}^i$.

A function of effectiveness related to an average variance is often represented as a ratio of a variance σ^2 and a normalized average variance of the regression function over the points of the full design. I.e., an effectiveness function (or just effectiveness) of the design $\mathbf{D}$ is

$$\varphi = \frac{\sigma^2}{\sigma_n^2} = \frac{k}{1+\sum_{i=1}^{n}NA_i}.$$

Effectiveness of the design $\mathbf{D}_i$ (or the transformation $\mathbf{D}_i$) is

$$\varphi_i = \frac{\sigma^2}{\sigma_{in}^2} = \frac{S_i}{1+NA_i}.$$

It is evident that for the identical transformation $\varphi_i = 1$. Hence, effectiveness of the design **D** can be expressed in terms of effectiveness of all designs $\mathbf{D}_i$ corresponding to the design **D**:

$$\varphi = k/(1 - n + \textstyle\sum_{i=1}^{n} S_i/\varphi_i) \qquad (9.1.8)$$

It follows from the results of §5 of chapter 4 that effectiveness of a design $\varphi \leq 1$.

The problem of optimal transformations (designs $\mathbf{D}_i$) can be solved for all important for applications cases numerically [2]. In this book, optimal (in the sense of minimization of average variance) transformations for factors up to seven-levels are presented in the Catalog as follows. Section III contains matrices of basic transformations. For each basic transformation, there are several information rows that show how to obtain an optimal transformation from the basic one.

Example 9.1.1. Consider basic transformation №11 of the Catalog:

0 0 0
0 1 1
1 1 0
1 0 1
2 0 0
3 1 1

This basic transformation allows constructing three optimal transformations: $4 \times 2^2//6$, $4 \times 2//6$, and $4//6$. The first optimal transformation of six-level factor to two two-level factors and one four-level factor contains all three columns of basic transformation. Its effectiveness equal 67%. The second transformation contains the first two column of the basic transformation. Its effectiveness equal 74%. The third transformation consists of the first column of the basic transformation. Its effectiveness equal 89%.

The optimal transformations 14a, 15a, and 16a are found by projection method as follows. The optimal transformation 14a ($2^6//7$) are chosen among matrices that have the first five columns identical to the transformation 14b ($2^5//7$). The transformation 15a ($3 \times 2^4//7$) and 16a ($3^2 \times 2^2//7$) are obtained from the transformations 15b ($3 \times 2^3//7$) and 16b ($3^3 \times 2//7$) respectively.

In Appendix 2 we will present a more general class of transformations that includes also interaction effects.

§ 2. Incomplete Block Design

Often a large number of experiments arises due to the fact that two or more factors $F_1, \dots, F_r$ (with levels $s_1, \dots, s_r$ respectively) form a large number of treatment combinations. When all these experiments cannot be performed in homogeneous environments, we may have an assumption that high-order interaction effects equal zero. Then we can divide a design into homogeneous blocks so that block effect will be confounded with these high-order interaction effects (§7 of chapter 8).

If we cannot sacrifice any interaction effects of these factors or if a large number of experiments arises due to the fact that there is one factor with a large number s of levels, we have to design the experiment using so-called an incomplete block design (or just block design). Actually, it is easy to see that these two cases are equivalent if $s = s_1 \dots s_r$. So hereafter, we will consider just one factor with a large number of levels. In this case the model is

$$Ey = \beta_0 + \beta_1^{(0)} x_1^{(0)} + \cdots + \beta_1^{(s_1-1)} x_1^{(s_1-1)}$$
$$+\beta_2^{(0)} x_2^{(0)} + \cdots + \beta_2^{(s_2-1)} x_2^{(s_2-1)} \tag{9.2.1}$$

with the restrictions

$$\sum_{i=1}^{s_j-1} \beta_j^{(i)} = 0 \quad (j = 1, 2), \tag{9.2.2}$$

where $\beta_1^{(i)}$ are effects of the levels of the blocking factor; $\beta_2^{(i)}$ are effects of the levels of main factor.

Therefore, (9.2.1) is a model of main effects, and incomplete block designs are factorial main effect designs. A system with several blocks will also lead to the model of main effects. The corresponding designs are called multi-dimensional incomplete block designs.

Incomplete block designs were first used for the design of experiments by F. Yates [3, 4], though they were studied as combinatorial constructions back in the XIX century.

In this book we are not going to pay much attention to this issue traditionally considered separately from the problem of factorial design of experiments. However, we will introduce here balanced incomplete block designs (BIB-designs), which we are going to use in the next chapter.

For a set V, an incidence structure is defined as a set of nonempty subsets of the set V.

Definition 9.2.1. Let a set V contains v different elements $a_1, \dots, a_v$; assume that B is a set of subset of the set V: $B_1, \dots, B_b$ (called blocks). Then an incidence structure generated by B and V is called a block design.

In this case, therefore, there is established relation of incidence $a_i \in B_j$ meaning that an element a_i of the set V belongs to the block B_j.

Definition 9.2.2. A matrix

$$\begin{Vmatrix} n_{11} & \cdots & n_{1\mathrm{b}} \\ \vdots & \ddots & \vdots \\ n_{v1} & \cdots & n_{v\mathrm{b}} \end{Vmatrix}$$

is called an incidence matrix of a block design if n_{ij} is the number of elements a_i belonging to the block B_j.

Definition 9.2.3. A block design is called a balanced incomplete block design with parameters $v,\ b,\ k,\ r,\ \lambda$, or BIB-design $(v,\ b,\ k,\ r,\ \lambda)$ if the number of the blocks of the design is equal to b, each block contains k elements, the number of elements in V equals v, each element from V occurs in r blocks, and any pair of elements from V belongs to λ blocks.

Hence, the incidence matrix of a BIB-design is a matrix of 0 and 1, and

$$n_{ij} = \begin{cases} = 1 & \text{if } \ a_i \in B_j, \\ = 0 & \text{if } \ a_i \notin B_j. \end{cases}$$

Example 9.2.1. BIB-design (6, 10, 3, 5, 2) can be represented by the following blocks:

$B_1 = (1{,}2{,}3);\ \ B_2 = (1{,}2{,}4);\ \ B_3 = (1{,}3{,}5);\ \ B_4 = (2{,}4{,}5);$
$B_5 = (3{,}4{,}5);\ \ B_6 = (2{,}3{,}6);\ \ B_7 = (1{,}4{,}6);\ \ B_8 = (3{,}4{,}6);$
$B_9 = (1{,}5{,}6);\ \ B_{10} = (2{,}5{,}6).$

The incidence matrix of this design is

$$\begin{Vmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \end{Vmatrix}.$$

It follows from the definition BIB-design that for an incidence matrix of a design $(v,\ b,\ k,\ r,\ \lambda,)$, the number of units in each column equals k, the number of units in each row equals r, and any two rows contains λ units in common columns.

Two trivial necessary conditions of the existence of a BIB-design $(v,\ b,\ k,\ r,\ \lambda)$ are

$$vr = bk, \quad \lambda(v-1) = r(k-1). \tag{9.2.3}$$

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Chapter 10. Two-Level Irregular Main Effect Designs

§ 1. Connection with Weighing Designs

We will consider a problem of construction of effective irregular (generally speaking) two-level main effect factorial designs for the A^{Ω}-model of true effects for quantitative factors. This problem is, obviously, equivalent to the problem of construction of first order designs, i.e., nonsingular designs for the model

$$Ey = b_0 + b_1x_1 + \cdots + b_mx_m \tag{10.1.1}$$

defined in the domain

$$x_i = \pm 1. \tag{10.1.2}$$

The problem has a close connection to the weighing problem (proposed by H. Hotelling [1]) – the design of experiments for estimating the unknown weights of m given objects by means of a specified number of weighing. There are two different statements of the problem: the chemical balance problem (when the objects may be placed in either of the two pans of the balance) and the spring balance problem (when the objects may be placed in only one pan).

The chemical balance problem corresponds to a design matrix $\mathbf{D} = \{d_{iu}\}$ with the elements –1, 0, and +1, where the u-th row corresponds to the u-th measurement and the i-th column corresponds to the i-th object; $d_{iu} = -1$ if the i-th object in the u-th measurement is placed in the left pan of the balance, $d_{iu} = 0$ if the i-th object in the u-th measurement is neither in the left nor the right pan; $d_{iu} = +1$ if the i-th object in the u-th measurement is placed in the right pan of the balance.

For the chemical balance problem, there are two types of a model: with an unknown absolute term, i.e., the model 10.1.1, and with a known absolute term (which without loss of generality can be assumed to be zero), i.e., the model

$$Ey = b_1x_1 + \cdots + b_mx_m. \tag{10.1.3}$$

The model (10.1.3) is not factorial. However, we will consider this model because the results on design construction for the models (10.1.3) and (10.1.1) are interrelated.

A zero absolute term in the model corresponds to measurements without bias (when it is known that measurement without any objects will be zero). An unknown absolute term in the model corresponds to measurements with a bias.

A design for the chemical balance problem is factorial if the design matrix does not contain zero. Further, we will focus on construction of the factorial type of designs for the chemical balance problem. Nevertheless, we will get effective designs for the models (10.1.1) and (10.1.3) not only for the domain (10.1.2) but also for the domain

$$x_i = -1, 0, +1. \tag{10.1.4}$$

The spring balance problem corresponds to a design matrix $\mathbf{D} = \{d_{iu}\}$ with elements –1 and +1; $d_{iu} = +1$ or $d_{iu} = -1$ if the i-th object in the u-th measurement is placed or not placed in the pan respectively. Hence, the spring balance problem is equivalent to the problem of construction of factorial designs for the model (10.1.1) in the domain (10.1.2).

It is obvious that the coefficient b_i $(i = 1, \dots, m)$ of the model (10.1.1) for the spring balance problem equals half of the weight of the i-th object unlike the chemical balance problem, where the coefficient equals the weight of the object.

For the spring balance problem, there are also two cases. The first case corresponds to designs in the domain (10.1.2) for the model (10.1.1) without restrictions. The second case corresponds to designs in the domain (10.1.2) for the model (10.1.1) with the restriction $b_0 = \sum_{i=1}^{m} b_i + c$. For the second case, a measurement with no objects is equal to c. Without loss of generality, we can assume that $c = 0$. We will call the first and the second cases weighing with a bias and with no bias respectively. The second case we will also call the model with the fixed point.

It is evident that for any design $\mathbf{D}_1$ in the domain (10.1.2) and the model (10.1.1), a coefficient matrix $\mathbf{X} = \| \ \mathbf{I}, \quad \mathbf{D}_1 \ \|$, and for any design $\mathbf{D}$ in the domain (10.1.2) and the model (10.1.3), a coefficient matrix $\mathbf{X} = \mathbf{D}$. Multiplication of any row in the design $\mathbf{D}$ for the model (10.1.3) by –1 does not change the matrix $\mathbf{X}^T\mathbf{X}$. Therefore, for the optimality criteria depending only on $\mathbf{X}^T\mathbf{X}$ we can assume (without loss of generality) that the design $\mathbf{D}$ is brought into a form $\mathbf{X} = \| \ \mathbf{I}, \quad \mathbf{D}_I \ \|$.

Now consider the design $\mathbf{D}_I$ for the model

$$Ey = b_0 + b_1 x_1 + \cdots + b_{m-1} x_{m-1}. \tag{10.1.5}$$

It is evident that a coefficient matrix of the design $\mathbf{D}_I$ for the model (10.1.5) is $\| \ \mathbf{I}, \quad \mathbf{D}_I \ \|$, i.e., identical to the coefficient matrix of the design

D for the model (10.1.3). Therefore, if the design **D** has some optimal properties for the model (10.1.3), then the design $\mathbf{D}_I$ has similar optimal properties for the model (10.1.5). In particular, the following theorem holds.

Theorem 10.1.1. If the design **D** in the domain (10.1.2) is an *A*- (*D*-, *E*-) optimal design with *N* runs for the model (10.1.3), then the design $\mathbf{D}_I$ in the domain (10.1.2) is an *A*- (*D*-, *E*-) optimal design respectively with *N* runs for the model (10.1.5).

Similar results hold if there are some additional restrictions on a set of designs, for example, restrictions on a number of runs, a form of a moment matrix, etc.

In §2-6 we will consider *A*-, *D*-, *E*-optimal weighing designs for the chemical balance problem with no bias for the model (10.1.3). Since these designs satisfy (10.1.2), they will be *A*-, *D*-, *E*-optimal weighing designs for the chemical balance problem with a bias for the model (10.1.1) and, therefore, *A*-, *D*-, *E*-optimal weighing designs for the spring balance problem with a bias for the model (10.1.1) without restrictions. In §7 we will consider the model with the fixed point corresponding to weighing designs for the spring balance problem with no bias.

§ 2. Designs $[m,\ v,\ \lambda]$

Our first goal is to find optimal weighing designs for the chemical balance problem for the model (10.1.3). We will focus on the designs satisfying (10.1.2) that is optimal for the domain (10.1.4). We will consider criteria *A*-, *D*-, *E*-optimality, which for weighing designs are called Kishen's, Mood's, and Ehrenfeld's criteria respectively.

It follows from the results of §4 of chapter 7 that *A*-, *D*-, *E*-optimal designs can be constructed when the number of runs *N* is a Hadamard number, i.e., when there exists a Hadamard matrix of order N. For $2 < N < 668$, any number divisible by 4 is a Hadamard number. Hence, we will focus on construction of effective saturated designs for $N = m \neq 4l$. We will construct the designs with the moment matrix of the form

$$\mathbf{X}^T\mathbf{X} = \begin{Vmatrix} r & \lambda & \cdots & \lambda \\ \lambda & r & \cdots & \lambda \\ \vdots & \vdots & \ddots & \vdots \\ \lambda & \lambda & \cdots & r \end{Vmatrix} = (r-\lambda)\mathbf{E}_m + \lambda\mathbf{J}_m, \qquad (10.2.1)$$

where $\mathbf{E}_m$ and $\mathbf{J}_m$ are respectively a unit matrix and a matrix of units of order m. Denote these designs by $[m,\ v,\ \lambda]$, where v is the number of zeros in each column. Designs of type $[m,\ 0,\ \lambda]$ are of special interest.

The inverse of the matrix (10.2.1) is

$$(\mathbf{X}^T\mathbf{X})^{-1} = (r^* - \lambda^*)\mathbf{E}_m + \lambda^*\mathbf{J}_m, \tag{10.2.2}$$

where

$$r^* = \frac{r + \lambda(m-2)}{(r-\lambda)[r+\lambda(m-1)]}; \quad \lambda^* = \frac{\lambda}{(r-\lambda)[r+\lambda(m-1)]}.$$

It follows from (10.2.2) that estimates of coefficient of the model for the design $[m,\ v,\ \lambda]$ have equal variances and equal covariances.

Let us write down an efficiency function for the designs satisfying (10.2.1). Kishen's efficiency [2] is

$$\varphi_A(r,\lambda) = \left(\sum_{i=1}^{m} c_{ii}\right)^{-1} = \frac{(r-\lambda)[r+\lambda(m-1)]}{m[r+\lambda(m-2)]}, \tag{10.2.3}$$

where $(\mathbf{X}^T\mathbf{X})^{-1} = \{c_{ij}\}$.

Mood's efficiency [3] is

$$\varphi_D(r,\lambda) = \det(\mathbf{X}^T\mathbf{X}) = (\det\mathbf{X})^2$$
$$= (r-\lambda)^{m-1}[r+\lambda(m-1)]. \tag{10.2.4}$$

Since

$$(\det\mathbf{X})^2 > 0,$$

we get that

$$r > \lambda, \quad r + \lambda(m-1) > 0. \tag{10.2.5}$$

The inequalities (10.2.5) hold only for $\lambda = -1$ or $\lambda \geq 0$. In case $\lambda = -1$ it is necessary that $m = r$.

Ehrenfeld's efficiency [4] is

$$\varphi_E(r,\ \lambda) = {z_{\min}}/{m} = \begin{cases} \frac{r-\lambda}{m} & \text{if } r > \lambda \geq 0, \\ \frac{1}{m} & \text{if } \lambda = -1,\ r = m, \end{cases} \tag{10.2.6}$$

where $z_{\min}$ is minimum eigenvalue of the matrix $\mathbf{X}^T\mathbf{X}$.

Indeed, find the roots of the equation

$$\det(\mathbf{X}^T\mathbf{X} - z\mathbf{E}_m) = 0,$$

or

$$\det[(r-\lambda-z)\mathbf{E}_m + \lambda\mathbf{J}_m] = 0.$$

For $\lambda \neq 0$ the equation has a root $r-\lambda$ of multiplicity $m-1$ and a simple root $r+\lambda(m-1)$. For $\lambda = 0$ the equation have the only root r of multiplicity m. The minimum root is $r-\lambda$ except a case when $\lambda = -1$, $r = m$, $z_{\min} = 1$.

§ 3. Existence Theorems for Designs $[m,\ v,\ \lambda]$

Theorem 10.3.1 [5]. A necessary condition for the existence of a design $[m,\ v,\ \lambda]$ is that

$$m - v + (m-1)\lambda \tag{10.3.1}$$

is a perfect square.

P r o o f. It follows from (10.2.4) that

$$\begin{aligned}\det \mathbf{X} &= \pm(\det \mathbf{X}^T\mathbf{X})^{1/2} \\ &= \pm(m - v - \lambda)^{(m-1)/2}[m - v + (m-1)\lambda]^{1/2}.\end{aligned}$$

Since $\det \mathbf{X}$ is integer, (10.3.1) is a perfect square, which was to be proved.

It follows from Theorem 10.3.1 that several types of designs $[m,\ v,\ \lambda]$ do not exist. Let m be odd. Then cases when a design $[m,\ v,\ \lambda]$ does not exist are as follows:

1. $m \equiv 1 (\mathrm{mod}\ 4)$, $\mathrm{v} \equiv 2 (\mathrm{mod}\ 4)$;
2. $m \equiv 1 (\mathrm{mod}\ 4)$, $\mathrm{v} \equiv 3 (\mathrm{mod}\ 4)$;
3. $m \equiv 3 (\mathrm{mod}\ 4)$, $\mathrm{v} \equiv 0 (\mathrm{mod}\ 4)$, $\lambda \equiv 0 (\mathrm{mod}\ 2)$;
4. $m \equiv 3 (\mathrm{mod}\ 4)$, $\mathrm{v} \equiv 1 (\mathrm{mod}\ 4)$, $\lambda \equiv 0 (\mathrm{mod}\ 2)$;
5. $m \equiv 3 (\mathrm{mod}\ 4)$, $\mathrm{v} \equiv 2 (\mathrm{mod}\ 4)$, $\lambda \equiv 1 (\mathrm{mod}\ 2)$;
6. $m \equiv 3 (\mathrm{mod}\ 4)$, $\mathrm{v} \equiv 3 (\mathrm{mod}\ 4)$, $\lambda \equiv 1 (\mathrm{mod}\ 2)$.

For the cases 1, 3, and 5, (10.3.1) satisfies the congruence

$$m - v + (m-1)\lambda \equiv 3 (\mathrm{mod}\ 4)$$

and, therefore, cannot be a perfect square.

For the cases 2, 4, and 6, (10.3.1) satisfies the congruence

$$m - v + (m-1)\lambda \equiv 2 (\mathrm{mod}\ 4)$$

and, therefore, cannot be a perfect square.

The special case of Theorem 10.3.1 is the following statement.

Theorem 10.3.2 [6]. A necessary condition for the existence of a design $[m,\ 0,\ 1]$ is

$$m = (d^2 + 1)/2, \tag{10.3.2}$$

where d is odd.

The following theorem can be proved similarly to Theorem 10.3.1.

Theorem 10.3.3 [7]. A necessary condition for the existence of a design $[m,\ 0,\ 2]$ is

$$m = 1/3\left[4 + (3d^2 + 4)^{1/2}\right], \tag{10.3.3}$$

where d is integer.

Theorem 10.3.4 [6]. If $v = 0$ or $v = 1$, a necessary condition for the existence of a design $[m,\ v,\ \lambda]$ is that $m - \lambda$ is even.

P r o o f. For $v = 0$ the proof is evident. Consider case when $v = 1$.

Let $\boldsymbol{\xi}_i$ and $\boldsymbol{\xi}_j$ be any two columns of the matrix **X**. $\boldsymbol{\xi}_i^T \boldsymbol{\xi}_j$ has m terms (+1, 0, and –1). Since $\boldsymbol{\xi}_i^T \boldsymbol{\xi}_j = \lambda \ (i \neq j)$, there exist $m - \lambda$ terms with the sum equal zero. Suppose that $m - \lambda$ is odd. Then among selected $m - \lambda$ terms, there is a single zero term. That can be only if the columns $\boldsymbol{\xi}_i$ and $\boldsymbol{\xi}_j$ have a common row with zeros. That is also the case for any two columns of the matrix **X**. Therefore, we get a zero-row in **X** and the singular matrix $\mathbf{X}^T\mathbf{X}$, which is a contradiction. This proves the theorem.

Other theorems on the existence of the designs $[m,\ v,\ \lambda]$ are obtained in the [5] by special algebraic methods. Two statements below follow from these results and Theorem 10.3.1. We present them omitting the proofs.

Theorem 10.3.5 [5]. 1. Let $m \equiv 3 (\mathrm{mod}\ 4)$, then designs $[m,\ v,\ \lambda]$ for $-1 < v + \lambda < 3$ and [15, 0, 3] do not exist. 2. Let $m \equiv 1 (\mathrm{mod}\ 4)$, then designs $[m,\ v,\ \lambda]$ for $v + \lambda < 5$ (except $v = 0, \lambda = 1$) do not exist.

Theorem 10.3.6 [5]. A necessary condition for the existence of a design $[m,\ 0,\ \lambda]$ $(m \neq 2)$ is

$$m - \lambda \equiv 0 (\mathrm{mod}\ 4). \tag{10.3.4}$$

It is evident that the necessary condition (7.4.3) for the existence of Hadamard matrices is a special case of the condition (10.3.4).

§ 4. Sufficient Conditions of Optimality of Designs $[m,\ v,\ \lambda]$

Lemma 10.4.1 [7]. For $r > \lambda \geq 0$, $\varphi_D(r, \lambda)$ (10.2.4) is a monotonic increasing function in r for a fixed λ and is a monotonic decreasing function in λ for a fixed r.

The lemma can be proved by partially differentiating $\varphi_D(r, \lambda)$ with respect to r and λ.

Theorem 10.4.1 [6, 7]. Let $\mathbf{X} = \mathbf{D}$ be a coefficient matrix of the design **D** for the model (10.1.3), m is odd, and

$$\mathbf{X}^T\mathbf{X} = (m-1)\mathbf{E}_m + \mathbf{J}_m.$$

Then **D** is an *A*-, *D*-, *E*-optimal design $[m,\ 0,\ 1]$ on a set of saturated designs $[m,\ v,\ \lambda]$ for the domain (10.1.4).

P r o o f. First, prove the theorem for Kishen's criterion of optimality (10.2.3). For $r > \lambda \geq 0$ or $r = m,\ \lambda = -1$ the following equality holds:

$$\varphi_A(m, 1) - \varphi_A(r, \lambda) = \frac{2m-1}{2m} - \frac{(r-\lambda)[r+\lambda(m-1)]}{m[r+\lambda(m-2)]}$$

$$= \frac{(m-1)\lambda(2m-2r-2\lambda-1)+(2m-2r-1)(r-\lambda)}{2m[r+\lambda(m-2)]}.$$

Note that $\varphi_A(m,1)-\varphi_A(r,\lambda)>0$ when $r<m$. If $r=m$, then

$$\varphi_A(m,1)-\varphi_A(r,\lambda)=\frac{\lambda(\lambda-1)(m-2)+m(\lambda^2-1)}{2m[r+\lambda(m-2)]}. \qquad (10.4.1)$$

Since m is odd, $\lambda \neq 0$, by Theorem 10.3.4. For $\lambda \neq 0$, (10.4.1) is strictly positive. This proves an A-optimality of the design.

An E-optimality of the design **D** follows from efficiency function (10.2.6) and Theorem 10.3.4.

Now we will prove a D-optimality of the design **D**.

It is evident that

$$\varphi_D(m,1)-\varphi_D(m-1,0)=m(m-1)^{m-1}>0. \qquad (10.4.2)$$

Then

$$\varphi_D(m,1)-\varphi_D(m,-1)=(m-1)^{m-1}(2m-1)-(m+1)^{m-1}$$
$$=2\left\{m^{m-3}\left[(m-1)\binom{m-1}{2}-\binom{m-1}{3}\right]\right.$$
$$+m^{m-5}\left[(m-1)\binom{m-1}{4}-\binom{m-1}{5}\right]+\cdots$$
$$\left.+m^2\left[(m-1)\binom{m-3}{m-1}-\binom{m-2}{m-1}\right]+(m-1)\right\}.$$

However, $(m-1)\binom{m-1}{i}>\binom{m-1}{i+1}$.

Therefore,

$$\varphi_D(m,1)>\varphi_D(m,-1). \qquad (10.4.3)$$

Since m is odd, $\lambda \neq 0$. Now a D-optimality of the design **D** follows from (10.4.2), (10.4.3), and Lemma 10.4.1.

Thus, the proof is complete.

Theorem 10.4.2 [7]. Let $\mathbf{X}=\mathbf{D}$ be a coefficient matrix of the design **D** for the model (10.1.3), $m\equiv 2 (\mathrm{mod}\ 4)$, $m\neq 2$, and

$$\mathbf{X}^T\mathbf{X}=(m-2)\mathbf{E}_m+2\mathbf{J}_m.$$

Then **D** is a D-optimal design $[m,\ 0,\ 2]$ on a set of saturated designs $[m,\ v,\ \lambda]$ for the domain (10.1.4).

P r o o f. It is evident that

$$\varphi_D(m,2)-\varphi_D(m-1,0)$$
$$=(m-1)\left\{\left[1-\frac{1}{m-1}\right]^{m-1}\left[3+\frac{1}{m-1}\right]-1\right\}. \qquad (10.4.4)$$

Substitute $a=1/(m-1)$ into the inequality

$$a < -\ln(1-a) < a/(1-a) \quad (0 < a < 1).$$

Then

$$\left(1-\frac{1}{m-1}\right)^{m-1} > \exp\left(-\frac{m-1}{m-2}\right).$$

Therefore, (10.4.4) is greater than zero if

$$3exp\left(-\frac{m-1}{m-2}\right) - 1 > 0.$$

This inequality holds for $m > 11$. It is easy to check that

$$\varphi_D(m,2) > \varphi_D(m-1,0)$$

for $m = 5, \dots, 11$. Hence,

$$\varphi_D(m,2) > \varphi_D(m-1,0) \quad (m \geq 5). \tag{10.4.5}$$

It follows from Theorem 10.4.1 that $\lambda \neq \pm 1$ if $r = m \equiv 2(\text{mod } 4)$. Besides, no Hadamard matrices exists in this case. Therefore, $\lambda \neq 0$. Now the statement of the theorem follows from (10.4.5) and Lemma 10.4.1.

Theorem 10.4.3 [5]. Let $\mathbf{X} = \mathbf{D}$ be a coefficient matrix of the design $\mathbf{D}$ for the model (10.1.3), $m \equiv 3(\text{mod } 4)$, and

$$\mathbf{X}^T\mathbf{X} = (m-3)\mathbf{E}_m + 3\mathbf{J}_m.$$

Then $\mathbf{D}$ is an A- and E-optimal design $[m,\ 0,\ 3]$ on a set of saturated designs $[m,\ v,\ \lambda]$ for the domain (10.1.4).

P r o o f. The following equality follows from (10.2.3):

$$\begin{aligned} &\varphi_A(m,3) - \varphi_A(m-v,\lambda) \\ &= (m-v-\lambda)[m(4v+4\lambda-9) - 6v - 6\lambda + 9] \\ &+ \frac{\lambda[(4v+4\lambda-13)m^2 + (4-v-\lambda)\,6m - 9]}{m(4m-6)[m-v+(m-2)\lambda]}. \end{aligned} \tag{10.4.6}$$

It is evident that (10.4.6) is positive if $\lambda = -1$ and $m > 3$ and also if $v + \lambda > 3$. If $v + \lambda = 3$, then (10.4.6) is transformed to

$$\frac{(m-3)^2(3-\lambda)}{m(4m-6)[m-3+(m-1)\lambda]},$$

which is nonnegative, since $\lambda \leq 3$. Therefore, (10.4.6) is positive if $v + \lambda \geq 3$. Therefore we have proved that the design $\mathbf{D}$ is A-optimal, because, by the statement 1 of Theorem 10.3.5, designs $[m,\ v,\ \lambda]$ for $v + \lambda = 0$, 1, 2 and $m \equiv 3(\text{mod } 4)$ do not exist. Further, using the efficiency function (10.2.6), we get that the design $\mathbf{D}$ is E-optimal.

Thus, the proof is complete.

Theorem 10.4.4 [5]. Let $\mathbf{X} = \mathbf{D}$ be a coefficient matrix of the design $\mathbf{D}$ for the model (10.1.3), and $m \equiv 3(\text{mod } 4)$. Suppose that

$$\mathbf{X}^T\mathbf{X} = (m-3)\mathbf{E}_m + 3\mathbf{J}_m \quad \text{for } m > 15$$

and

$$\mathbf{X}^T\mathbf{X} = (m+1)\mathbf{E}_m - \mathbf{J}_m \quad \text{for } m \leq 15.$$

Then the design **D** is *D*-optimal on a set of saturated designs $[m,\ v,\ \lambda]$ in the domain (10.1.4).

P r o o f. Consider the following difference:

$$\varphi_D(m,3) - \varphi_D(m-v,\lambda) = m(m-3)^{m-1}\left\{4 - \frac{3}{m} - \left(\lambda + 1 - \frac{v+\lambda}{m}\right)\left(1 - \frac{v+\lambda-3}{m-3}\right)^{m-1}\right\}. \tag{10.4.7}$$

It can be shown that (10.4.7) is positive for $m > 3,\ v+\lambda \geq 3,\ \lambda \geq 0$. It follows from the statement 1 of Theorem 10.3.5 that $[m,\ v,\ \lambda]$ do not exist for $-1 < v+\lambda < 3$. Hence, we only need to consider the case $v + \lambda = -1 \quad (v = 0,\ \lambda = -1)$. It follows from (10.4.7) that

$$\varphi_D(m,3) - \varphi_D(m,-1) = (m-3)^{m-1}\left\{(4m-3) - \left[1 + \frac{4}{m-3}\right]^{m-1}\right\}. \tag{10.4.8}$$

Evidently, (10.4.8) is positive for $m > 14$ and negative for $3 \leq m \leq 14$. It follows from statement 1 of Theorem 10.3.5 that $[15, 0, 3]$ does not exist.

Thus, the proof is complete.

Theorem 10.4.5 [5]. Let $\mathbf{X} = \mathbf{D}$ be a coefficient matrix of the design **D** for the model (10.1.3), $m \equiv 1 (\mathrm{mod}\ 4)$, $m > 5$, and

$$\mathbf{X}^T\mathbf{X} = (m-5)\mathbf{E}_m + \mathbf{J}_m.$$

Suppose that $[m,\ 0,\ 1]$ does not exist. Then **D** is *A*-, *D*-, *E*-optimal design $[m,\ 0,\ 5]$ on a set of saturated designs $[m,\ v,\ \lambda]$ in the domain (10.1.4).

P r o o f. For $m > 5$ and $v + \lambda \geq 5$

$$\varphi_A(m,5) - \varphi_A(m-v,\lambda) = \frac{(m-v-\lambda)[(6m-10)(v+\lambda) - 25(m-1)]}{m(6m-10)[m-v+(m-2)\lambda]} + \frac{\lambda[m(6m-10)(v+\lambda) - 31m^2 + 60m - 25]}{m(6m-10)[m-v+(m-2)\lambda]} \tag{10.4.9}$$

and, as can be shown, is positive.

$$\varphi_D(m,5) - \varphi_D(m-v,\lambda)$$

$$= m(m-5)^{m-1}\left\{\left(6-\frac{5}{m}\right) - \left(\lambda+1+\frac{v+\lambda}{m}\right)\left[1-\frac{v+\lambda-5}{m-5}\right]^{m-1}\right\} \qquad (10.4.10)$$

and, as can be shown, is also positive.

It follows from statement 2 of Theorem 10.3.5 that $[m,\ v,\ \lambda]$ does not exist for $v+\lambda<5$ except a case $v=0,\ \lambda=1$, i.e., a design $[m,\ 0,\ 1]$. This proves *A*- and *D*-optimality of the design **D**. *E*-optimality of the design follows from the expression of an efficiency function (10.2.6).

§ 5. Construction of Designs $[m,\ v,\ \lambda]$

In this paragraph we will focus on the problem of construction designs with the moment matrices that satisfy some of sufficient conditions corresponding to the results of the previous paragraph, namely:$[m,0,-1]$, $[m,0,1]$, $[m,0,2]$, $[m,0,3]$, and $[m,0,5]$.

A general method of construction of the designs $[m,0,\lambda]$ uses a balanced incomplete block designs.

Theorem 10.5.1 [5]. If there exists BIB-design with parameters $v^*,\ b^*,\ k^*,\ r^*,\ \lambda^*$, satisfying the equalities $v^*=b^*$, $k^*=r^*$, then there exists the design $[m,0,\lambda]$, where

$$m=v^*=b^*,\quad \lambda=b^*-4r^*+4\lambda^*. \qquad (10.5.1)$$

P r o o f. We will construct a matrix $\mathbf{D}=\mathbf{X}$ of the design $[m,0,\lambda]$ from BIB-design replacing its zeros with -1. The resulting matrix **D** will be square matrix of order *m* with elements –1 and +1. A scalar product of the *i*-th and the *j*-th columns of **D**, by the definition of BIB-design, will contain $2(r^*-\lambda^*)$ negative terms and $b^*-2(r^*-\lambda^*)$ positive terms. Therefore,

$$\lambda=b^*-4r^*+4\lambda^*,$$

which was to be proved.

It follows from (9.2.3) that

$$\lambda^*=\frac{r^*(r^*-1)}{b^*-1}. \qquad (10.5.2)$$

Substituting (10.5.2) into (10.5.1), we get

$$r=\frac{m\pm\sqrt{\lambda m-\lambda+m}}{2}. \qquad (10.5.3)$$

That allows calculating parameters of a BIB-design for a given design $[m,0,\lambda]$ by using (10.5.2) and (10.5.3).

Example 10.5.1. Consider a method of construction designs $[m, 0, 1]$ and $[m, 0, 2]$. By Theorem 10.3.2, a necessary condition for the existence of a design $[m, 0, 1]$ is given by (10.3.2). The first three value $m > 1$ satisfying (10.3.2) is 5, 13, and 25. Calculation by (10.5.2) and (10.5.3) leads to the task of construction balanced incomplete block designs with the following parameters:

$v^* = b^*$	$k^* = r^*$	λ^*
5	1	0
13	4	1
25	9	3.

It is known that such BIB-designs exist [8]. Therefore, designs $[5, 0, 1]$, $[13, 0, 1]$, and $[25, 0, 1]$ can be constructed. For example, an incidence matrix of BIB-design with parameters $v^* = b^* = 5$, $k^* = r^* = 1$, $\lambda^* = 0$ is

$$\begin{Vmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{Vmatrix}.$$

Replacement of zeros of the incidence matrix with –1 leads to the design [5, 0, 1]

$$\begin{Vmatrix} 1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 \\ -1 & -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & -1 & 1 \end{Vmatrix}.$$

By Theorem 10.3.3, a necessary condition for the existence of a design $[m, 0, 2]$ is given by (10.3.3). The values m satisfying (10.3.3) are fairly rare. For $m < 200$ there are only two of them: $m = 6$ and $m =66$. The BIB-design that leads to construction of the design $[6, 0, 2]$ does exist and has the following parameters: $v^* = b^* = 6$, $k^* = r^* = 1$, $\lambda = 0$. Construction of the design $[6, 0, 2]$ is similar to construction of the design $[5, 0, 1]$.

Denote

$$\mathbf{S}_m = 2\mathbf{E}_m - \mathbf{J}_m. \tag{10.5.4}$$

Since $\mathbf{S}_m^T \mathbf{S}_m = 4\mathbf{E}_m + (m-4)\mathbf{J}_m$, the matrix $\mathbf{S}_m$ leads to the design $[m,\ 0,\ m-4]$. Consider the most important for applications cases when m is small.

Theorem 10.5.2. Let $\mathbf{X} = \mathbf{D} = \mathbf{S}_m$ be a coefficient matrix of the design $\mathbf{D}$ for the model (10.1.3), $m = 3, \dots, 9$. Then $\mathbf{D}$ is a *A*-, *D*-, *E*-

optimal design $[m,\ 0,\ m-4]$ on a set of saturated designs $[m,\ v,\ \lambda]$ in the domain (10.1.4) with the exception of cases of A- and E-optimality for $m=6$ and D-optimality for $m=7$ and $m=8$.

Proof. For $m=3$, as it is easy to show, there exist only one (up to permutations of rows and columns and multiplication by -1) design for each set of designs $[3,0,\lambda]$, $[3,1,\lambda]$, and $[3,2,\lambda]$: $[3,0,-1]$, $[3,1,1]$, and $[3,2,0]$ respectively. A direct calculation of the efficiency functions (10.2.3), (10.2.4), and (10.2.5) for these designs proves that $[3,0,-1]$ (i.e., $\mathbf{S}_3=2\mathbf{E}_3-\mathbf{J}_3$) is an A-, D-, E-optimal design.

For $m=4$, a design $\mathbf{S}_4=2\mathbf{E}_4-\mathbf{J}_4$ is identical to a Hadamard matrix $\mathbf{H}_4$ and, therefore, A -, D -, E -optimal.

For $m=5$, $\mathbf{S}_5=2\mathbf{E}_5-\mathbf{J}_5$ is a design $[5,0,1]$, which is A-, D-, E-optimal (by Theorem 10.4.1).

For $m=6$, $\mathbf{S}_6=2\mathbf{E}_6-\mathbf{J}_6$ is a design $[6,0,2]$. Its D-optimality follows from Theorem 10.4.2. Besides, A- and E-optimal designs $[6,0,\lambda]$ on a set of $[6,v,\lambda]$ designs do not exist. Indeed, it is follows from Theorem 10.3.4 that $[6,0,2]$ is the only representative of a set of designs $[6,0,\lambda]$. However, the design $[6,1,0]$ is better in the sense of efficiencies (10.2.3) and (10.2.5).

For $m=7$, $\mathbf{S}_7=2\mathbf{E}_7-\mathbf{J}_7$ is a design $[7,0,3]$, which is A- and E-optimal (by Theorem 10.4.3). The design $[7,0,-1]$ is D-optimal. Besides, $\varphi_D(7,\ 3)<\varphi_D(7,-1)$ (see the proof of Theorem 10.4.4).

For $m=8$, a design that corresponds to Hadamard matrix $\mathbf{H}_8$ is A-, D-, E-optimal.

For $m=9$, $\mathbf{S}_9=2\mathbf{E}_9-\mathbf{J}_9$ is a design $[9,0,5]$, which is A-, D-, E-optimal (by Theorems 10.3.2 and 10.4.5).

Therefore, for $m=3,\dots,9$ all optimal designs $[m,0,\lambda]$ can be easily constructed. A method of construction of the designs $\mathbf{S}_m$ is given by (10.5.4). The design $[7,0,-1]$, as any other design $[m,0,-1]$, where $m+1$ is a Hadamard number, can be constructed by deleting the first column and the first row of a normalized Hadamard matrix of corresponding order. The designs $[4,0,0]$ and $[8,0,0]$ are given by Hadamard matrices $\mathbf{H}_4$ and $\mathbf{H}_8$ respectively.

§ 6. Saturated *D*-optimal Designs of First Order

In this paragraph we will consider a problem of construction of D-optimal designs for the model (10.1.3) on a set of saturated designs with the domain

$$-1\le x_i\le 1. \tag{10.6.1}$$

This problem leads to the factorial designs. It is well known the following theorem.

Theorem 10.6.1. There exists a saturated design satisfying the condition (10.1.2) that is *D*-optimal for the model (10.1.3) on a set of saturated designs with the domain (10.6.1).

P r o o f. Let *D* be a saturated design that is *D*-optimal for the model (10.1.3) on a set of saturated designs with the domain (10.6.1). Show that the value x_{iu} of the variable x_i in the u-th points of **D** can be replaced with +1 or –1 without decreasing a criterion of *D*-optimality. Indeed, since the design **D** is saturated, a coefficient matrix **X** is square and

$$\det(\mathbf{X}^T\mathbf{X}) = (\det \mathbf{X})^2.$$

Now replace x_{iu} with –1 if a cofactor of element x_{iu} in the matrix **D** less than zero and replace x_{iu} with +1 if a cofactor is more or equal zero. It is obvious that this replacement does not decrease $\det \mathbf{X}$ and, therefore, $\det(\mathbf{X}^T\mathbf{X})$, which was to be proved.

From Theorem 10.6.1 follows that the problem of construction of *D*-optimal designs for the model (10.1.3) on a set of saturated designs with the domain (10.6.1) is equivalent to the problem of construction matrices with elements +1 and –1 with a maximal determinant. The last problem is called a determinant Hadamard problem.

Denote by d_m maximal value of a determinant of a matrix with elements +1 and -1 of order *m*. The problem of finding d_m, upper bounds for d_m, and construction of corresponding matrix are considered in articles of many authors. We will give in Table 17 the upper bounds d_m for $m = 3, \dots, 9$ from the article [9]:

Table 17.
Upper Bound in Determinant Hadamard Problem

m	3	4	5	6	7	8	9
d_m	2^2	2^4	2^5+2^4	2^7+2^5	2^9+2^6	2^{12}	$2^{14}-2^{11}$

The values of upper bounds d_m for $m = 3, 4, 5,$ and 8 from Table 17 are reached on *D*-optimal designs on a set of saturated designs $[m, 0, \lambda]$, i.e., on the designs $\mathbf{S}_3$, $\mathbf{S}_4 = \mathbf{H}_4$, $\mathbf{S}_5$, and $\mathbf{H}_8$ respectively. The values of the upper bounds d_m for $m = 6, 7,$ and 9 from Table 17 are not reached on the designs $[m, 0, \lambda]$.

To find designs corresponding to the upper bounds from Table 17, we can use the following simple computer algorithm. Each element of an initial matrix is selected randomly (for example, using uniform random numbers on the segment [–1, +1]). Then each element is replaced sequentially with –1 if its cofactor is negative, and replaced with +1 if its cofactor is nonnegative. It is evident that on each step of this procedure the determinant of the matrix is not decreasing.

Following this procedure, it is easy to get the matrices for $m = 6, 7,$ and 9 with the determinant equal to upper bound from Table 17. For $m = 6$, for example, the design matrix and the moment matrix respectively are as follows:

$$\left\|\begin{matrix} 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 \end{matrix}\right\|, \quad \left\|\begin{matrix} 6 & -2 & -2 & 0 & 0 & 0 \\ -2 & 6 & 2 & 0 & 0 & 0 \\ -2 & 2 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & -2 & -2 \\ 0 & 0 & 0 & -2 & 6 & 2 \\ 0 & 0 & 0 & -2 & 2 & 6 \end{matrix}\right\|.$$

§ 7. Model with Fixed Point

Now we will focus on the problem of construction of *D*-optimal designs for the model (10.1.1) with the restrictions

$$b_0 = b_1 + \cdots + b_m \tag{10.7.1}$$

in the domain

$$-1 \le x_i \le 1 \quad (i = 1, \dots, m). \tag{10.7.2}$$

We will see that a solution of the problem, obtained by V.Z.Brordsky and T.I.Golikova [10, 11], leads to the designs satisfying the condition (10.1.2). Note that the model (10.1.1) with the restriction (10.7.1) for the design in the domain (10.1.2) is not factorial However, we will consider this model because the results of this paragraph are related to other results of this chapter.

Substitute (10.7.1) into the model (10.1.1). Then

$$Ey = b_1' x_1' + \cdots + b_m' x_m', \tag{10.7.3}$$

where $x_i' = (1 + x_i)/2, \quad b_i' = 2b_i.$

The set (10.7.2) and (10.1.2) are transformed respectively into the sets

$$0 \le x_i' \le 1 \tag{10.7.4}$$

and

$$x_i' = 0, 1. \tag{10.7.5}$$

Therefore, the problem is reduced to the problem of construction *D*-optimal designs for the model (10.7.3) with the domain (10.7.4).

Theorem 10.7.1. A design **D** for the model (10.7.3) with the domain (10.7.4) is *D*-optimal if and only if its normalized information matrix

$$\bar{\mathbf{M}} = \begin{cases} \frac{n}{2(2n-1)}(\mathbf{E}_m + \mathbf{J}_m) \text{ if } m = 2n-1, \\ \frac{n+1}{2(2n+1)}(\mathbf{E}_m + \mathbf{J}_m) \text{ if } m = 2n. \end{cases} \tag{10.7.6}$$

Proof. First, prove that the condition (10.7.6) is sufficient for D-optimality of the design $\mathbf{D}$. The necessity of the condition (10.7.6) for D-optimality of the design $\mathbf{D}$ follows from the Theorem 4.3.2.

A normalized covariance matrix $\bar{\mathbf{\Gamma}}$ of the design $\mathbf{D}$ is

$$\frac{\bar{\mathbf{\Gamma}}}{\sigma^2} = \begin{cases} \frac{2n-1}{n^2}(2n\mathbf{E}_m - \mathbf{J}_m) \text{ if } m = 2n-1, \\ \frac{2}{n+1}[(2n+1)\mathbf{E}_m - \mathbf{J}_m] \text{ if } m = 2n. \end{cases}$$

$\bar{\mathbf{\Gamma}}$ is a positive definite matrix. Therefore, a normalized variance $\bar{d}(\mathbf{D},\mathbf{x})$ of an estimate of a regression function at the point $\mathbf{x} = (x_1', \dots, x_m')$ is a strictly convex function in $\mathbf{x}$. Hence, $\bar{d}(\mathbf{D}, \mathbf{x})$ in the domain (10.7.4) reaches its maximum on the vertex. Any vertex of the hypercube (10.7.4) can be represented as a point with l units and $m-l$ zeros ($l = 0, 1, \dots, m$). At this vertex

$$\bar{d}(\mathbf{D},\mathbf{x}) = \begin{cases} \frac{2n-1}{n^2} l(2n-l) \text{ if } m = 2n-1, \\ \frac{2}{n+1} l(2n-l+1) \text{ if } m = 2n. \end{cases}$$

The maximum of this function equals m and is reached for $l = n$ if $m = 2n-1$ and is also reached for $l = n+1$ if $m = 2n$.

The existence of the design $\mathbf{D}$ with the normalized information matrix (10.7.6) is based on the following considerations. By Theorem 4.3.2, the maximum of $(\mathbf{D}, \mathbf{x})$ is reached at points of the design. Therefore, a D-optimal design may include only those vertices of the hypercube (10.7.4) for which $l = n$ for $m = 2n-1$, or $l = n+1$ for $m = 2n$. It is easy to show that a normalized information matrix of the design that consists of all such vertices has the form (10.7.6).

This completes the proof of the theorem.

Now we will focus on construction of D-optimal designs with a minimal number of runs for the model (10.7.3). First, get some necessary conditions for the number N of runs in a D-optimal design. Let $m = 2n - 1 > 1$. For a D-optimal design, $nN/(2n-1)$ is the number of units in any column of the design matrix, and $nN/2(2n-1)$ is a scalar product of its any two columns. Since the elements of the columns equal only 0 or 1, these ratios are integers. The numbers n and $2n-1$ have no common divisors except 1. Therefore, in a D-optimal design $N \geq 2n-1 = m$ for $n = 2k$ and $N \geq 2(2n-1) = 2m$ for $n = 2k-1$.

Similarly, we can show that for $m = 2n$ the following inequalities hold: $N \geq m + 1$ if $n = 2k - 1$ and $N \geq 2(m + 1)$ if $n = 2k$. Therefore, we have proved the following theorem.

Theorem 10.7.2. For *D*-optimal design for the model (10.7.3) in the domain (10.7.4) the following inequalities hold:

1) $N \geq 2m + 2 \quad \text{for} \quad m \equiv 0(\text{mod } 4)$,
2) $N \geq 2m \quad \text{for} \quad m \equiv 1(\text{mod } 4) \quad (m > 1)$,
3) $N \geq m + 1 \quad \text{for} \quad m \equiv 2(\text{mod } 4)$,
4) $N \geq \text{m} \quad \text{for} \quad m \equiv 3(\text{mod } 4)$.

Theorem 10.7.3. There exists a *D*-optimal design for the model (10.7.3) in the domain (10.7.4) with the minimal number of runs $N = m$ if $(m + 1)$ is Hadamard number.

Proof. Let $\mathbf{H}_{m+1}$ be a normalized Hadamard matrix of order $(m + 1)$. In the matrix $-\mathbf{H}_{m+1}$ (like in the matrix $\mathbf{H}_{m+1}$), by (7.4.2), each column, except the first one, has $(m + 1)/2$ elements –1 and $(m + 1)/2$ elements +1. Since the proportional frequency condition holds, combinations (+1, +1), (–1, –1), (+1, –1), and (–1, +1) in any pair of columns (except the first one) occur the same number of times, namely, $(m + 1)/4$. Now remove the first column and the first row of the matrix $-\mathbf{H}_{m+1}$, and replace elements –1 with zeros. The resulting matrix of order $m \equiv 3(\text{mod } 4)$ is a *D*-optimal design. Indeed, it is easy to show that this design has normalized information matrix of the form (10.7.6). Besides, by theorem 10.7.2, the design contains the minimal number of runs.

This completes the proof of the theorem.

Theorem 10.7.4. If $m = p^h \equiv 1(\text{mod } 4)$, where p is prime, h is integer, then there exists *D*-optimal design for the model (10.7.3) in the domain (10.7.4) with the minimal number of runs $N = 2m$.

Proof. Let elements of the matrices $\mathbf{X}' = \{x'_{ij}\}$ and $\mathbf{X}'' = \{x''_{ij}\}$ $(i, j = 1, \ldots, m)$ are

$$x'_{ii} = 1; \; x'_{ij} = \frac{1}{2}\left[1 + \left(\frac{a_j - a_i}{p^h}\right)\right] \text{ for } i \neq j;$$

$$x''_{ii} = 1; \; x''_{ij} = \frac{1}{2}\left[1 - \left(\frac{a_j - a_i}{p^h}\right)\right] \text{ for } i \neq j,$$

where $a_i, a_j \in GF(p^h)$ and parentheses means the Legendre symbol. Let $\mathbf{X} = \|\mathbf{X}', \; \mathbf{X}''\|^T$. We will show that $\mathbf{X}$ is a matrix of the *D*-optimal design. Since $\mathbf{X}$ has the size $2m \times m$, we need to prove that the diagonal elements of the matrix $\mathbf{X}^T\mathbf{X}$ equal $m + 1$ and off-diagonal elements equal $(m + 1)/2$.

Any diagonal element of the matrix $\mathbf{X}^T\mathbf{X}$ is

$$(x'_{1j} + \cdots + x'_{mj}) + (x''_{1j} + \cdots + x''_{mj}) = m + 1.$$

Using (1.1.1), we get the following relationship:

$$\sum_{i=1}^{m} x'_{ik}x'_{il} + \sum_{i=1}^{m} x''_{ik}x''_{il}$$
$$= x'_{kk}x'_{kl} + x'_{lk}x'_{ll} + x''_{kk}x''_{kl} + x''_{lk}x''_{ll}$$
$$+\frac{1}{4}\sum_{\substack{i\neq k\\ i\neq l}}\left[1+\left(\frac{a_k-a_i}{p^h}\right)\right]\left[1+\left(\frac{a_l-a_i}{p^h}\right)\right]$$
$$+\frac{1}{4}\sum_{\substack{i\neq k\\ i\neq l}}\left[1-\left(\frac{a_k-a_i}{p^h}\right)\right]\left[1-\left(\frac{a_l-a_i}{p^h}\right)\right]=\frac{1}{2}(m+1).$$

Thus, the proof is complete.

Theorem 10.7.5. There exists *D*-optimal design for the model (10.7.3) in the domain (10.7.4) with the minimal number of runs $N = m + 1$ if $(m + 2)$ is a Hadamard number.

P r o o f. It follows from Theorem 10.7.3 that if $(m + 2)$ is a Hadamard number, then there exists *D*-optimal design with the minimal number of runs for $m' = m + 1 = 2n - 1$ variables (factors). We will show that by removing any column of this design we get *D*-optimal design with the minimal numbers of runs for *m* factors. A normalized information matrix of the resulting design has the size $m \times m$; its diagonal and off-diagonal elements are respectively

$$\frac{(n-1)+1}{2(n-1)+1} \quad \text{and} \quad \frac{(n-1)+1}{2[2(n-1)+1]},$$

i.e., the resulting design for $m = 2(n - 1)$ is *D*-optimal. Since $m \equiv 2 (\mathrm{mod}\ 4)$, by Theorem 10.7.2, this design has a minimal number of runs.

This completes the proof of the theorem.

Theorem 10.7.6. Let $m = p^h - 1 \equiv 0 (\mathrm{mod}\ 4)$, where p is prime, h is integer. Then there exists *D*-optimal design for the model (10.7.3) in the domain (10.7.4) with a minimal number of runs $N = 2m + 2$.

P r o o f. It follows from Theorem 10.7.4 that if $m = p^h - 1 \equiv 0 (\mathrm{mod}\ 4)$, then there exists *D*-optimal design for $m' = m + 1 = 2n - 1$ factors. Similarly, Theorem 10.7.5, it can be proved that by removing any column of the design, we get *D*-optimal design for $m = 2(n - 1)$ factors with a minimal number of runs.

Using the theorems of this paragraph, we can construct all *D*-optimal designs with a minimal number of runs for $m < 20$.

For $m = 3, 7, 11, 15, 19$ a corresponding matrix **X** of a *D*-optimal design is a square matrix of order *m* derived from a Hadamard matrix. It can be obtained by a cyclic permutation of elements of the first row: (110) for $m = 3$, (1110100) for $m = 7$, (11011100010) for $m = 11$, and (1100111101010000110) for $m = 19$.

For $m = 15$ the matrix is presented in Table 18.

Table 18
***D*-optimal Design for $m = 15$**

1	1	1	1	0	0	0	0	0	0	1	1	1	1	0
0	1	1	1	1	1	1	0	0	0	0	0	0	1	1
1	0	1	1	1	0	0	1	1	0	0	0	1	0	1
0	0	1	1	0	1	1	1	1	0	1	1	0	0	0
1	1	0	1	0	1	0	1	0	1	0	1	0	0	1
0	1	0	1	1	0	1	1	0	1	1	0	1	0	0
1	0	0	1	1	1	0	0	1	1	1	0	0	1	0
0	0	0	1	0	0	1	0	1	1	0	1	1	1	1
1	1	1	0	0	0	1	0	1	1	1	0	0	0	1
0	1	1	0	1	1	0	0	1	1	0	1	1	0	0
1	0	1	0	1	0	1	1	0	1	0	1	0	1	0
0	0	1	0	0	1	0	1	0	1	1	0	1	1	1
1	1	0	0	0	1	1	1	1	0	0	0	1	1	0
0	1	0	0	1	0	0	1	1	0	1	1	0	1	1
1	0	0	0	1	1	1	0	0	0	1	1	1	0	1

For $m = 2, 6, 10, 14, 18$ the matrix $\mathbf{X}$ of a *D*-optimal design can be obtained respectively from the designs for $m = 3, 7, 11, 15, 19$ by removing any column.

For $m = 5, 9, 13, 17$ the design matrix has the size $2m \times m$. It can be represented in a form $\| \mathbf{X}', \mathbf{X}'' \|^T$, where $\mathbf{X}'' = \mathbf{E}_m + \mathbf{J}_m - \mathbf{X}'$. For $m = 5, 13, 17$ a square matrix $\mathbf{X}'$ of order m can be obtained by a cyclic permutation of elements of the first row: (11001) for $m = 5$, (1101100001101) for $m = 13$, (11101000110001011) for $m = 17$.

For $m = 9$ the matrix $\mathbf{X}'$ is

$$\mathbf{X}' = \left[\mathbf{E}_3 \circledast \left(\mathbf{J}_3 - \frac{1}{2}\mathbf{E}_3\right)\right] + \left[\left(\mathbf{J}_3 - \frac{1}{2}\mathbf{E}_3\right) \circledast \mathbf{E}_3\right],$$

where $\circledast$ is the symbol of Kronecker product.

For $m = 4, 8, 12, 16$ a matrix $\mathbf{X}$ of *D*-optimal design can be obtained from the designs for $m = 5, 9, 13, 17$ respectively by removing any column.

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Chapter 11. Irregular Designs of Resolution 4, 5 and Compromise Designs

§ 1. Designs of Resolution 4

Minimal Designs

In this section we will consider two types of designs of resolution 4: 2^n and $2^n \times 3^m$. We will also answer a question: what is a minimum number of runs for such designs for the given number of factors.

Suppose that we are using the design **D** to estimate parameters of postulated A$^{\Omega}$-model of true effects

$$E\mathbf{y}^f = b_0\mathbf{I} + \textstyle\sum_{i=1}^{n} \mathbf{F}_i^f \mathbf{B}_i. \tag{11.1.1}$$

Suppose that a real model is

$$E\mathbf{y}^f = b_0\mathbf{I} + \textstyle\sum_{i=1}^{n} \mathbf{F}_i^f \mathbf{B}_i + \sum_{i>j} \mathbf{F}_{ij}^f \mathbf{B}_{ij}.$$

Lemma 11.1.1 [1]**.** A necessary and sufficient condition for the design $2^n//N$ (the design **D**) to be of resolution 4 is that in the set of vectors from $\mathbf{I}, \mathbf{F}_i^{fD}, \mathbf{F}_{i_1 i_2}^{fD}$ $(i,\ i_1,\ i_2 = 1, \dots, n)$, there be no linear dependency involving vectors from $\mathbf{F}_i^{fD}$.

P r o o f. Suppose that the condition of the lemma does not hold. Then without loss of generality, the following equality is true for the factor F_1:

$$\mathbf{F}_1^{fD} = c_0\mathbf{I} + \textstyle\sum_{i=1}^{n} c_i \mathbf{F}_i^{fD} + \sum_{i_1>i_2} c_{i_1 i_2} \mathbf{F}_{i_1 i_2}^{fD}. \tag{11.1.2}$$

There exists the matrix $\mathbf{W}_1$ such that

$$\widehat{\mathbf{B}}_1 = \mathbf{W}_1^T \mathbf{y} \quad \text{and} \quad E\widehat{\mathbf{B}}_1 = \mathbf{B}_1.$$

Then

$$E\widehat{\mathbf{B}}_1 = E(\mathbf{W}_1^T \mathbf{y}) = \mathbf{W}_1^T \mathbf{I} b_0 + \mathbf{W}_1^T \textstyle\sum_{i=1}^{n} \mathbf{F}_i^{fD} \mathbf{B}_i + \mathbf{W}_1^T \sum_{i_1>i_2} \mathbf{F}_{i_1 i_2}^{fD} \mathbf{B}_{ij}.$$

Therefore,

$$\mathbf{W}_1^T \mathbf{F}_1^{fD} = \mathbf{I}, \quad \mathbf{W}_1^T \mathbf{I} = \mathbf{W}_1^T \mathbf{F}_i^{fD} = \mathbf{W}_1^T \mathbf{F}_{i_1 i_2}^{fD} = 0$$
$$(i,\ i_1,\ i_2 = 1, \dots, n).$$

However, by (11.1.2),

$$\mathbf{W}_1^T\mathbf{F}_1^{fD} = c_0\mathbf{W}_1^T\mathbf{I} + \sum_{i=1}^{n} c_i\mathbf{W}_1^T\mathbf{F}_1^{fD} + \sum_{i_1>i_2} c_{i_1 i_2}\mathbf{W}_1^T\mathbf{F}_{i_1 i_2}^{fD} = 0.$$

The obtained contradiction proves the necessity of the assertion of the lemma.

Now suppose that the condition of the lemma holds. Then a matrix **A** that contains all vectors of the matrices $\mathbf{F}_i^{fD}$ $(i = 1, \dots, n)$ has rank $q\sum_{i=1}^{n}(s_i - 1)$. Suppose that rank of the matrix of vectors **I** and $\mathbf{F}_{i_1 i_2}^{fD}$ $(i_1,$ $i_2 = 1, \dots, n)$ equals *r*. From this set, choose a submatrix **B** of r columns that has rank r. By virtue of the assumption, Rg $\| \ \mathbf{A}, \mathbf{B} \ \| = q + r$. Each LS estimate $\hat{b}_i$ is determined by a linear function of observations with a vector of coefficients that has to be orthogonal to any vector from **B**. This orthogonality extends to all linear combinations of *r* columns of the matrix **B** and, therefore, to all column-vectors of two-factor interaction effects and the mean.

This completes the proof of Lemma 11.1.1.

Theorem 11.1.1 [1, 2]. A design 2^n of resolution 4 for *n* factors contains at least $2n$ runs.

P r o o f. A set of vectors from $\mathbf{F}_1^{fD}, \dots, \mathbf{F}_n^{fD}$ is linearly independent. Then a set of vectors from $\mathbf{I}, \mathbf{F}_{12}^{fD}, \dots, \mathbf{F}_{1n}^{fD}$ is also linearly independent. Since resolution of the design is 4, by Lemma 11.1.4, we get that a set of vectors from $\mathbf{F}_1^{fD}, \dots, \mathbf{F}_n^{fD}, \mathbf{I}, \mathbf{F}_{12}^{fD}, \dots, \mathbf{F}_{1n}^{fD}$ is also linearly independent. Since the number of vectors of the set is equal to $2n$, the number of runs of the design should be at least $2n$, which was to be proved.

The next theorem uses the method of proof of Theorem 11.1.1.

Theorem 11.1.2 [2]. A design 2^n of resolution 4 is nonsingular for the $\mathbf{A}^{\Omega}$-model that includes main effects of all factors and all two-factor interactions of a given factor.

The next theorem can be proved by using Lemma 11.1.1. The proof is omitted here and can be found in the original paper [1].

Theorem 11.1.3 [1]. A design $2^n \times 3^m$ $(m > 0)$ of resolution 4 contains at least $3(n + 2m - 1)$ runs.

Construction of Minimal Designs

A minimal design 2^n of resolution 4, i.e., a design with $N = 2n$ runs, can be constructed by using technique by G.E.P.Box and J.S.Hunter [3] that similar to the method of chapter 7. In chapter 7 regular designs of resolution 3 were constructed from regular designs of resolution 2 by using technique known as a fold-over method. This technique can be used for construction of designs of resolution 4 from designs of resolution 3. Effectiveness φ of designs $2^n//2n$ of resolution 4 obtained from the designs $2^{n-1}//n$ of resolution 3 is presented in Table 19. The last row of Table 19 contains a reference to the work where the corresponding design $2^{n-1}//n$ of resolution 3 has been constructed.

Table 19
Effectiveness of Minimal Designs [1]

n	3	5	6	7	10	13	14	18	25	26
Effectiveness	0.67	0.90	0.83	0.65	0.90	0.96	0.93	0.94	0.98	0.96
Reference	[4]	[4]	[4]	[2]	[5]	[6]	[5]	[5]	[6]	[5]

Estimating Parameters and Blocking

We will describe a simple method of estimating parameters [7] for fold-over designs.

Let a coefficient matrix of the design $2^{n-1}//n$ of resolution 3 for the model (11.1.1) be $\mathbf{X}_1$. Then a coefficient matrix of the fold-over design $\mathbf{D}$ of resolution 4 constructed from the initial design for the model (11.1.1) is

$$\mathbf{X} = \begin{Vmatrix} \mathbf{I} & \mathbf{X}_1 \\ \mathbf{I} & -\mathbf{X}_1 \end{Vmatrix}.$$

Since the first column of $\mathbf{X}$ is orthogonal to all other columns, vector of LS estimates is

$$\widehat{\mathbf{B}} = \frac{1}{2}(\mathbf{X}_1^T\mathbf{X}_1)^{-1}\mathbf{X}_1^T(\mathbf{y}_1 - \mathbf{y}_2), \tag{11.1.3}$$

where $\mathbf{y}_1$ and $\mathbf{y}_2$ are vectors of observations for the first and second half of the design $\mathbf{D}$ respectively. Since $\mathbf{X}_1$ is a square nonsingular matrix, (11.1.3) is equivalent to the equality

$$\widehat{\mathbf{B}} = \frac{1}{2}\mathbf{X}_1^{-1}(\mathbf{y}_1 - \mathbf{y}_2). \tag{11.1.4}$$

It follows from (11.1.3) and (11.1.4) that the design can be divided into blocks of size 2. Each block consists of some treatment and its fold-over treatment. The estimate $\widehat{\mathbf{B}}$ is clear of block effects and two-factor interaction effects.

§ 2. Compromised Designs and Designs of Resolution 5

In this paragraph, we will consider methods of construction nonsingular compromised irregular designs 2^n that lead to the designs that are less efficient than regular ones but consist of much lower number of runs.

Combination of Fractional Geometric Designs

In this section we will describe the method of S.Addelman [8] of construction of nongeometric designs by using a combination of geometric designs of the same family.

Consider four fractional geometric designs $2^5//8$ corresponding to the following four defining relations:

$$\begin{aligned} 1 &= -x_1x_2x_3 = -x_1x_4x_5 = x_2x_3x_4x_5, \\ 1 &= -x_1x_2x_3 = x_1x_4x_5 = -x_2x_3x_4x_5, \\ 1 &= x_1x_2x_3 = -x_1x_4x_5 = -x_2x_3x_4x_5, \\ 1 &= x_1x_2x_3 = x_1x_4x_5 = x_2x_3x_4x_5. \end{aligned} \quad (11.2.1)$$

The designs corresponding to the defining relations (11.2.1) form the full set of fractional designs of the same family with the principal generators $x_1x_2x_3$ and $x_1x_4x_5$. These designs are presented in Table 20 with the signs of all defining interactions.

Table 20
Combination of Designs of the Same Family

Defining Relations	Designs of Family			
	1	2	3	4
$x_1x_2x_3$	–	–	+	+
$x_1x_4x_5$	–	+	–	+
$x_2x_3x_4x_5$	+	–	–	+

The treatment combinations that constitute the nongeometric design $2^5//24$ (the design **D**) may be obtained by combining any three of four fractions of Table 20.

Definition 11.2.1. Let $\mathbf{F}_P^{fD}$ and $\mathbf{F}_Q^{fD}$ be two effects generated by the design **D** and corresponding to interaction effects P and Q. We shall say that $\mathbf{F}_P^{fD}$ is completely confounded with $\mathbf{F}_Q^{fD}$ if $\mathbf{F}_P^{fD} = \mathbf{F}_Q^{fD}$ or $\mathbf{F}_P^{fD} = -\mathbf{F}_Q^{fD}$; $\mathbf{F}_P^{fD}$ is not confounded with $\mathbf{F}_Q^{fD}$ if $\mathbf{F}_P^{fD}$ is orthogonal to $\mathbf{F}_Q^{f\mathrm{D}}$; $\mathbf{F}_P^{fD}$ is partially confounded with $\mathbf{F}_Q^{f\mathrm{D}}$ if $\mathbf{F}_P^{f\mathrm{D}}$ is not orthogonal to $\mathbf{F}_P^{fD}$, $\mathbf{F}_P^{f\mathrm{D}} \neq \mathbf{F}_Q^{f\mathrm{D}}$, and $\mathbf{F}_P^{f\mathrm{D}} \neq -\mathbf{F}_Q^{f\mathrm{D}}$.

If all signs for the given interaction R in the defining relations of Table 20 are equal, $\mathbf{F}_R^{fD}$ is completely confounded with **I**. In this case, for any interaction S, effects $\mathbf{F}_{RS}^{fD}$ and $\mathbf{F}_{S}^{fD}$ are completely confounded. If not all signs are equal, $\mathbf{F}_{R}^{fD}$ is partially confounded with $\mathbf{I}$. Also, $\mathbf{F}_{RS}^{fD}$ and $\mathbf{F}_{S}^{fD}$ are partially confounded.

Consider k designs $2^n//2^{n-m}$ of the same family (similar to designs of Table 20). Then consider A^{Ω}-model of true effects containing the terms corresponding to unconfounded and partially confounded effects.

Sort all terms of the model into groups so that partially confounded effects were adjacent. Then an information matrix will be block diagonal with the blocks corresponding to partially confounded effects. Suppose that t of k signs corresponding to some interaction of the defining relation be pluses and $k-t$ signs be minuses. Then off-diagonal elements of the corresponding block of the information matrix equal $(2t-k)2^{n-m}$. For $2t-k=-1$, a diagonal block of the information matrix of the design $2^n//3\cdot 2^{n-m}$ is

$$2^{n-m+2}\mathbf{E}_p - 2^{n-m}\mathbf{J}_p.$$

Since all off-block elements equal zero, a covariance matrix can be calculated by finding inverse matrices separately for all blocks. Therefore, a covariance matrix is block diagonal with the blocks

$$2^{-n+m-2}\left\| \ \mathbf{E}_p + \frac{1}{4-p}\mathbf{J}_p \ \right\| \tag{11.2.2}$$

(for the sake of simplicity, assume that $\sigma^2 = 1$).

When $p=2$, the diagonal block of the covariance matrix is

$$2^{-n+m-3}\| \ 2\mathbf{E}_p + \mathbf{J}_p \ \| = 2^{-n+m-3}\left\| \begin{matrix} 3 & 1 \\ 1 & 3 \end{matrix} \right\|.$$

When $p=3$, the block is

$$2^{-n+m-2}\| \ \mathbf{E}_3 + \mathbf{J}_3 \ \| = 2^{-n+m-2}\left\| \begin{matrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{matrix} \right\|.$$

It is easy to show [8] that LS estimates for the design $2^n//3\cdot 2^{n-m}$ depend on the type of confounding and are as follows:

1. If $\mathbf{F}_{P}^{fD}, \mathbf{F}_{Q}^{fD}$, and $\mathbf{F}_{R}^{fD}$ are effects that are partially confounded with each other, estimates $\hat{b}_P, \hat{b}_Q$, and $\hat{b}_R$ are given by

$$\left\| \begin{matrix} \hat{b}_P \\ \hat{b}_Q \\ \hat{b}_R \end{matrix} \right\| = 2^{-n+m-1}\left\| \begin{matrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{matrix} \right\| \cdot \left\| \begin{matrix} \mathbf{y}^T\mathbf{F}_{P}^{fD} \\ \mathbf{y}^T\mathbf{F}_{Q}^{fD} \\ \mathbf{y}^T\mathbf{F}_{R}^{fD} \end{matrix} \right\|$$

and

$$\sigma^2\{\hat{b}_P\} = \sigma^2\{\hat{b}_Q\} = \sigma^2\{\hat{b}_R\} = 2^{-n+m-1}\sigma^2.$$

2. If $\mathbf{I}$, $\mathbf{F}_P^{fD}$, and $\mathbf{F}_Q^{fD}$ are partially confounded effects, then estimates $\hat{b}_P, \hat{b}_Q,$ and $\hat{b}_0$ are given by

$$\left\| \begin{matrix} 2\hat{b}_0 \\ \hat{b}_P \\ \hat{b}_Q \end{matrix} \right\| = 2^{-n+m-1} \left\| \begin{matrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{matrix} \right\| \cdot \left\| \begin{matrix} \mathbf{y}^T\mathbf{I} \\ \mathbf{y}^T\mathbf{F}_P^{fD} \\ \mathbf{y}^T\mathbf{F}_Q^{fD} \end{matrix} \right\|$$

and

$$\sigma^2\{\hat{b}_P\} = \sigma^2\{\hat{b}_Q\} = 2^{-n+m-1}\sigma^2.$$

3. If $\mathbf{F}_P^{fD}$ and $\mathbf{F}_Q^{fD}$ are partially confounded with one another and with no others, then

$$\left\| \begin{matrix} \hat{b}_P \\ \hat{b}_Q \end{matrix} \right\| = 2^{-n+m+2} \left\| \begin{matrix} 3 & 1 \\ 1 & 3 \end{matrix} \right\| \cdot \left\| \begin{matrix} \mathbf{y}^T\mathbf{F}_P^{fD} \\ \mathbf{y}^T\mathbf{F}_Q^{fD} \end{matrix} \right\|$$

and

$$\sigma^2\{\hat{b}_P\} = \sigma^2\{\hat{b}_Q\} = 3 \cdot 2^{-n+m-1}\sigma^2.$$

4. If $\mathbf{I}$ and $\mathbf{F}_P^{fD}$ are partially confounded with one another and with no others, then

$$\left\| \begin{matrix} 2\hat{b}_0 \\ \hat{b}_P \end{matrix} \right\| = 2^{-n+m+2} \left\| \begin{matrix} 3 & 1 \\ 1 & 3 \end{matrix} \right\| \cdot \left\| \begin{matrix} \mathbf{y}^T\mathbf{I} \\ \mathbf{y}^T\mathbf{F}_P^{fD} \end{matrix} \right\|$$

and

$$\sigma^2\{2\hat{b}_0\} = \sigma^2\{\hat{b}_P\} = 3 \cdot 2^{-n+m-1}\sigma^2.$$

It is evident from (11.2.2) that a block for $p = 4$ has to be singular.

We present below Table 21 [8] that includes some useful for applications designs described in this section. In all cases except the first one, it is assumed that the model contains an absolute term and terms corresponding to all main effects and all two-factor interaction effects. For the first design, it is assumed that the model contains an absolute term and terms corresponding to all main effects and only two two-factor interaction effects.

Table 21
Index of Useful Nongeometric Fractional Designs 2^n

Design	Generators	Designs of Family		
		1	2	3
$2^3//6$	x_1x_2	+	−	−
	x_1x_3	−	−	+
$2^4//12$	$x_1x_2x_3$	−	−	+
	$x_1x_2x_4$	−	+	−
$2^5//24$	$x_1x_2x_3$	−	−	+
	$x_1x_4x_5$	−	+	−
$2^6//24$	$x_1x_2x_3x_4x_5$	+	+	+
	$x_1x_2x_6$	−	−	+
	x_1x_5	+	−	−
$2^6//48$	$x_1x_2x_3x_4$	+	−	−
	$x_1x_2x_5x_6$	−	−	+
$2^7//48$	$x_1x_2x_3x_4x_5$	+	+	+
	$x_1x_2x_6$	−	−	+
	$x_1x_5x_7$	−	+	−
$2^8//48$	$x_1x_2x_3x_4x_5$	+	+	+
	$x_1x_2x_6x_7x_8$	+	+	+
	$x_1x_3x_6$	−	−	+
	$x_2x_5x_7$	−	+	−
$2^9//96$	$x_1x_2x_3x_4x_5$	+	+	+
	$x_1x_2x_6x_7x_8$	+	+	+
	$x_1x_3x_6$	−	−	+
	$x_2x_5x_7x_9$	+	−	−

Augmenting Designs

P.W.M. John [9] introduced an idea of a special type of a sequential design when an initial fractional factorial experiment $2^n//2^{n-1}$ is carried out and then information from it is used to augment the initial design by an additional fraction $2^n//2^{n-m}$.

Consider first augmenting a geometric design $2^n//2^{n-1}$ by a design $2^n//2^{n-3}$. Suppose that the initial design $\mathbf{D}_1$ is given by the defining relation

$$1 = -\mathrm{P}$$

and an additional fraction $\mathbf{D}_2$ is given by the defining relation

$$1 = P = Q = PQ = R = PR = QR = PQR.$$

The effects of $\mathbf{F}_S^{fD_1}$, $\mathbf{F}_{PS}^{fD_1}$, $\mathbf{F}_{QS}^{fD_1}$, $\mathbf{F}_{PQS}^{fD_1}$,$\mathbf{F}_{RS}^{fD_1}$,$\mathbf{F}_{PRS}^{fD_1}$,$\mathbf{F}_{QRS}^{fD_1}$,$\mathbf{F}_{PQRS}^{fD_1}$ are confounded in the alias set of the design $\mathbf{D}_1$. Pairs $\mathbf{F}_S^{fD_2}$ and $\mathbf{F}_{PS}^{fD_2}$, $\mathbf{F}_{QS}^{fD_1}$ and $\mathbf{F}_{PQS}^{fD_2}$, etc. are confoundedd in the alias sets of the design $\mathbf{D}_2$. Grouping effects appropriately, we get (as in the previous section) that an information matrix has a block diagonal type. Each block is

$$\mathbf{U} = \left\| \begin{array}{cccccccc} 5 & -3 & 1 & 1 & 1 & 1 & 1 & 1 \\ -3 & 5 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 5 & -3 & 1 & 1 & 1 & 1 \\ 1 & 1 & -3 & 5 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 5 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & -3 & 5 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 5 & -3 \\ 1 & 1 & 1 & 1 & 1 & 1 & -3 & 5 \end{array} \right\| 2^{n-3}.$$

It is evident that Rg $\mathbf{U} = 5$. We cannot, however, obtain a nonsingular matrix of order five and, therefore, find a unique solution for estimates of the remaining five effects assuming that any three of the effects are zero. A nonsingular matrix of order five can be obtained by deleting one row (and column) from any three of the four pairs. I.e., the design $\mathbf{D}_1$ splits the effects into pairs. Each alias set of the design $\mathbf{D}_2$ consists of four pairs. If we assume that three of the pairs have zero members then the remaining two effects in the other pair can be estimated. If, however, there are two pairs in an alias set with both nonzero members, these effects cannot be estimated (we cannot find unique LS solution), no matter how many of the remaining four effects are zero.

Eliminating one member from each of the last three pairs, we get information matrix

$$2^{n-3} \left\| \begin{array}{cc} 8\mathbf{E}_2 - 3\mathbf{J}_2 & \mathbf{J}_{2,3} \\ \mathbf{J}_{3,2} & 4\mathbf{E}_3 + \mathbf{J}_3 \end{array} \right\|$$

and its inverse

$$2^{-n} \left\| \begin{array}{cc} \mathbf{E}_2 + 3\mathbf{J}_2 & -\mathbf{J}_{2,3} \\ -\mathbf{J}_{3,2} & 2\mathbf{E}_3 \end{array} \right\|.$$

In a general case, consider augmenting a geometric design $2^n//2^{n-1}$ by a design $2^n//2^{n-m}$.

Suppose that the initial design $\mathbf{D}_1$ is given by the defining relation

$$1 = -\mathrm{P}$$

and an additional fraction $\mathbf{D}_2$ is given by the defining relation

$$1 = P = Q = PQ = \cdots$$

Matrices $\mathbf{U}$ of order 2^m contain submatrices $2^m\mathbf{E}_2 - (2^{m-1} - 1)\mathbf{J}_2$ along the main diagonal and 1's elsewhere. It can be shown that in each alias set of the design $\mathbf{D}_1$, only one pair of effects can be nonzero.

If in the alias set of the design $\mathbf{D}_1$, there is one pair with two nonzero effects and $p > 0$ pairs with one nonzero effect, then after removing corresponding row and columns we get a reduced matrix

$$\mathbf{U} = 2^{n-m} \left\| \begin{array}{cc} 2^m\mathbf{E}_2 - (2^{m-1} - 1)\mathbf{J}_2 & \mathbf{J}_{2,p} \\ \mathbf{J}_{p,2} & 2^{m-1}\mathbf{E}_n - \mathbf{J}_p \end{array} \right\|.$$

Then

$$\mathbf{U}^{-1} = 2^{-n} \left\| \begin{array}{cc} \mathbf{E}_2 + \frac{1}{2}(2^{m+1} - 1 + p)\mathbf{J}_2 & -\mathbf{J}_{2,p} \\ -\mathbf{J}_{p,2} & 2\mathbf{E}_p \end{array} \right\|.$$

The only nonzero effect in the pair is estimated from the design $\mathbf{D}_1$. Suppose that the pair of nonzero effects is $\mathbf{F}_S^{fD}$ and $\mathbf{F}_{PS}^{fD}$. Let $\hat{b}_S^h$ and $\hat{b}_S^l$ be an estimates respectively from the designs $\mathbf{D}_1$ and $\mathbf{D}_2$. Then it can be shown that

$$\hat{b}_S = \frac{\hat{b}_S^* + \hat{b}_S^h}{2},$$

where $\hat{b}_S^* = \hat{b}_S^l - \left(\hat{b}_{QS}^h + \hat{b}_{RS}^h + \cdots\right)$ and the terms in brackets correspond to the remaining nonzero effects.

If in the alias set for the design $\mathbf{D}_2$, there is no pair with two nonzero effects, then

$$\mathbf{U} = 2^{n-m}\| \; 2^{m-1}\mathbf{I}_p - \mathbf{J}_p \; \|,$$
$$\mathbf{U}^{-1} = 2^{-n+1}\| \; \mathbf{I}_p - (p + 2^{m-1})^{-1}\mathbf{J}_p \; \|.$$

Parameter estimates can be found by the following formula:

$$\hat{b}_S = (p + 2^{m-1})^{-1}\left[\hat{b}_S^* + (p + 2^{m-1} - 1)\hat{b}_S^h\right],$$

where $b_S^* = b_S^l - \left(b_{QS}^h + \cdots\right)$ and brackets includes $p - 1$ terms.

These designs may be divided into blocks [10].

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Appendix 1. The Catalog

The catalogue includes important for applications factorial designs for various types of models. There potentially exists an enormous number of factorial designs, so it is difficult to include all of them in the catalog directly. We give economical way of indirect representation of factorial designs by using the following three sections of the catalog.

Section I contains auxiliary matrices that can be transformed to various factorial designs. Section II describes how to get regular uniform designs using the auxiliary matrices of section I. The designs of section II, in accordance with § 5 of Chapter 4, are the D- and Q-optimal (with the efficiency function φ = 1).

As an example of using sections I and II of the catalog, consider construction of a regular uniform main effect design $4^6//16$. Based on the symmetrical design of the table of section II, we can construct the design using columns from 16-th to 20-th of the auxiliary matrix $\mathbf{D}_{16}$. This design is a part of Table 22 (the first section).

Table 22
Construction of Designs from Catalog

Design $4^5//16$					**Irregular Design K_1 $2^4 \times 3 \times 4^2//16$**							**Regular Design K_2 $2^4 \times 3 \times 4^2//16$**						
0	0	0	0	0	0	1	1	0	0	0	0	0	1	1	0	0	0	0
2	0	2	1	3	1	1	0	0	0	1	3	1	1	0	0	1	1	3
3	0	3	3	1	0	0	0	0	0	3	1	0	0	0	0	0	3	1
1	0	1	2	2	1	0	1	0	0	2	2	1	0	1	0	1	2	2
0	2	2	3	2	0	1	1	1	0	3	2	0	1	1	1	1	3	2
2	2	0	2	1	1	1	0	1	0	2	1	1	1	0	1	0	2	1
3	2	1	0	3	0	0	0	1	0	0	3	0	0	0	1	1	0	3
1	2	3	1	0	1	0	1	1	0	1	0	1	0	1	1	0	1	0
0	3	3	2	3	0	1	1	2	1	2	3	0	1	1	2	0	2	3
2	3	1	3	0	1	1	0	2	1	3	0	1	1	0	2	1	3	0
3	3	0	1	2	0	0	0	2	1	1	2	0	0	0	2	0	1	2
1	3	2	0	1	1	0	1	2	1	0	1	1	0	1	2	1	0	1
0	1	1	1	1	0	1	1	0	1	1	1	0	1	1	0	1	1	1
2	1	3	0	2	1	1	0	0	1	0	2	1	1	0	0	0	0	2
3	1	2	2	0	0	0	0	0	1	2	0	0	0	0	0	1	2	0
1	1	0	3	3	1	0	1	0	1	3	3	1	0	1	0	0	3	3

Now consider Section III of the catalog. It contains matrices of transformations of regular uniform designs for constructing various regular and irregular designs. The transformations were obtained in [1] (see their description in §1 of Chapter 9). A transformation of any factor to l new factors leads to regular design if and only if $l = 1$ or (for $l > 1$) the efficiency $\varphi = 1$. The efficiency of resulting design (after transformation) can be calculated by (9.1.8).

As an example of transformations, consider a method of construction of a main effect design $2^4 \times 3 \times 4^2//16$ from a regular main effect design $4^5//16$. We can use the following two options for transformations.

For the first choice, we replace the first four-level factor with three two-level factors using the transformation 2a, and replace the second four-level factor with a two-level and a three-level factors using transformation 3a:

2a **3a**

$$\left.\begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix}\right\} \rightarrow \left\{\begin{matrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{matrix}\right., \qquad \left.\begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix}\right\} \rightarrow \left\{\begin{matrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 2 & 1 \end{matrix}\right..$$

Then we delete the third four-level factor of the design $4^5//16$, leaving the fourth and fifth factors unchanged. As a result, we get a factorial main effect design $\mathbf{K}_1$: $2^4 \times 3 \times 4^2//16$ (the middle section of Table 22). Since the efficiency of the transformation 3a is less than 100% ($\varphi < 1$), the resulting design $\mathbf{K}_1$ is irregular.

However, it is possible to construct a regular main effect design, using the second choice of transformations of the design $4^5//16$. Transformations for the first, fourth and fifth factors are the same as for the first choice. The second four-level factor is replaced with a three-level factor using transformation 3b. The third four-level factor is replaced with a two-level factor using transformation 2c. As a result, we get a factorial main effect design $\mathbf{K}_2$ (regular but nonuniform): $2^4 \times 3 \times 4^2//16$ (the last section of Table 22).

The efficiencies of the resulting designs $\mathbf{K}_1$ and $\mathbf{K}_2$ can be calculated by (9.1.8). Details of calculations are presented below:

	k	n	S_1	S_2	S_3	S_4	S_5	φ_1	φ_2	φ_3	φ_4	φ_5	φ
$\mathbf{K}_1$	13	4	4	4	–	4	4	1	0,60	–	1	1	0,83
$\mathbf{K}_2$	13	5	4	3	2	4	4	1	0,90	1	1	1	0,98

Further, in this catalog, we will present three section: I. Auxiliary matrices; II. Regular uniform designs; III. Optimal transformations of regular uniform designs.

I. Auxiliary Matrices

$$\mathrm{D}_4 = \begin{array}{r} 123 \\ \left\| \begin{array}{l} 000 \\ 101 \\ 011 \\ 110 \end{array} \right\| \end{array} \qquad \mathrm{D}_8 = \begin{array}{r} 12345678 \\ \left\| \begin{array}{l} 00000000 \\ 10011011 \\ 01010112 \\ 11001103 \\ 00101113 \\ 10110102 \\ 01111001 \\ 11100010 \end{array} \right\| \end{array} \qquad \mathrm{D}_9 = \begin{array}{r} 1234 \\ \left\| \begin{array}{l} 0000 \\ 1011 \\ 2022 \\ 0112 \\ 1120 \\ 2101 \\ 0221 \\ 1202 \\ 2210 \end{array} \right\| \end{array}$$

$$\mathbf{D}_{12} = \begin{array}{r} 11111 \\ 12345678901234 \\ \left\| \begin{array}{l} 11011100010000 \\ 01101110001011 \\ 10110111000110 \\ 01011011100101 \\ 00101101110002 \\ 00010110111013 \\ 10001011011112 \\ 11000101101103 \\ 11100010110004 \\ 01110001011015 \\ 10111000101114 \\ 00000000000105 \end{array} \right\| \end{array} \qquad \mathbf{D}_{16} = \begin{array}{r} 111111111122 \\ 123456789012345678901 \\ \left\| \begin{array}{l} 000000000000000000000 \\ 100011100011101202131 \\ 010010011011011303312 \\ 110001111000110101223 \\ 001001010110111022324 \\ 101010110101010220215 \\ 011011001101100321036 \\ 111000101110001123107 \\ 000100101101111033230 \\ 100111001110010231301 \\ 010110110110100330122 \\ 110101010101001132013 \\ 001101111011000011114 \\ 101110011000101213025 \\ 011111100000011312206 \\ 111100000011110110337 \end{array} \right\| \end{array}$$

$$\mathbf{D}_{18} = \begin{array}{r} 111 \\ 123456789012 \\ \left\| \begin{array}{c} 000000000000 \\ 011111100111 \\ 022222200222 \\ 100121201120 \\ 111202001201 \\ 122010101012 \\ 001022112210 \\ 012100212021 \\ 020211012102 \\ 102201110003 \\ 110012210114 \\ 121120010225 \\ 001210221123 \\ 012021021204 \\ 020102121015 \\ 102112022213 \\ 110220122024 \\ 121001222105 \end{array} \right\| \end{array} \qquad \mathbf{D}_{20} = \begin{array}{r} 1111111111 \\ 1234567890123456789 \\ \left\| \begin{array}{c} 1100111101010000110 \\ 0110011110101000011 \\ 1011001111010100001 \\ 1101100111101010000 \\ 0110110011110101000 \\ 0011011001111010100 \\ 0001101100111101010 \\ 0000110110011110101 \\ 1000011011001111010 \\ 0100001101100111101 \\ 1010000110110011110 \\ 0101000011011001111 \\ 1010100001101100111 \\ 1101010000110110011 \\ 1110101000011011001 \\ 1111010100001101100 \\ 0111101010000110110 \\ 0011110101000011011 \\ 1001111010100001101 \\ 0000000000000000000 \end{array} \right\| \end{array}$$

$$
\begin{array}{rl}
 & \begin{array}{l}
1111111111222222222\\
1234567890123456789012345678
\end{array}\\[6pt]
\mathbf{D}_{24} = & \left\|\begin{array}{l}
1111101011001100101000000000\\
0111110101100110010100010011\\
0011111010110011001010001021\\
0001111101011001100101011030\\
0000111110101100110010100131\\
1000011111010110011001010120\\
0100001111101011001100101110\\
1010000111110101100110011101\\
0101000011111010110011000002\\
0010100001111101011001110013\\
1001010000111110101100101023\\
1100101000011111010110011032\\
0110010100001111101011000133\\
0011001010000111110101110122\\
1001100101000011111010101112\\
1100110010100001111101011103\\
0110011001010000111110100004\\
1011001100101000011111010015\\
0101100110010100001111101025\\
1010110011001010000111111034\\
1101011001100101000011100135\\
1110101100110010100001110124\\
1111010110011001010000101114\\
0000000000000000000000011105
\end{array}\right\|
\end{array}
\qquad
\begin{array}{rl}
 & \begin{array}{l}123456\end{array}\\[6pt]
\mathbf{D}_{25} = & \left\|\begin{array}{l}
000000\\
101111\\
202222\\
303333\\
404444\\
011234\\
112340\\
213401\\
314012\\
410123\\
022413\\
123024\\
224130\\
320241\\
421302\\
033142\\
134203\\
230314\\
331420\\
432031\\
044321\\
140432\\
241043\\
342104\\
443210
\end{array}\right\|
\end{array}
$$

$$\mathbf{D}_{27} = \begin{array}{c} 11111 \\ 12345678901234 \\ \left\| \begin{array}{c} 00000000000000 \\ 10011110011111 \\ 20022220022222 \\ 01012001112123 \\ 11020111120204 \\ 21001221101015 \\ 02021002221216 \\ 12002112202027 \\ 22010222210108 \\ 00100121211220 \\ 10111201222001 \\ 20122011200112 \\ 01112122020013 \\ 11120202001124 \\ 21101012012205 \\ 02121120102106 \\ 12102200110217 \\ 22110010121028 \\ 00200212122110 \\ 10211022100221 \\ 20222102111002 \\ 01212210201203 \\ 11220020212014 \\ 21201100220125 \\ 02221211010026 \\ 12202021021107 \\ 22210101002218 \end{array} \right\| \end{array}$$

$$\mathbf{D}_{28} = \begin{array}{r}
111111111122222222 \\
123456789012345678901234567 \\
\left\| \begin{array}{c}
101111000010001001110101101 \\
110111000001100100011110110 \\
011111000100010010101011011 \\
000101111001010001101110101 \\
000110111100001100110011110 \\
000011111010100010011101011 \\
111000101001001010101101110 \\
111000110100100001110110011 \\
111000011010010100011011101 \\
010001001110101101101111000 \\
001100100011110110110111000 \\
100010010101011011011111000 \\
001010001101110101000101111 \\
100001100110011110000110111 \\
010100010011101011000011111 \\
001001010101101110111000101 \\
100100001110110011111000110 \\
010010100011011101111000011 \\
110101101101111000010001001 \\
011110110110111000001100100 \\
101011011011111000100010010 \\
101110101000101111001010001 \\
110011110000110111100001100 \\
011101011000011111010100010 \\
101101110111000101001001010 \\
110110011111000110100100001 \\
011011101111000011010010100 \\
000000000000000000000000000
\end{array} \right\|
\end{array}$$

$$
\begin{array}{rr}
 & 11111111112222222222333333333344 \\
 & 12345678901234567890123456789012345678901 \\
\mathbf{D}_{32} = & \left\|\begin{array}{l}
00000000000000000000000000000000000000000 \\
10000111100000011111100001111010220222311 \\
01000100011100011100011101110110102211122 \\
11000011111100000011111100001100322033233 \\
00100010010011010011011011101110011120224 \\
10100101110011001100111010010100231302135 \\
01100110001110011110001100110001133331306 \\
11100001101111010000100111100010333113017 \\
00010001001010101010110111011112212310010 \\
10010110101010110101010110100102032132301 \\
01010101010110110110101010101002310101132 \\
11010010110110101001001011010012130323223 \\
00110011011001111001101100110002203230234 \\
10110100111001100110001101001012023012125 \\
01110111000101100101110001000112301021316 \\
11110000100101111010010000111102121203007 \\
00001000100101100101101110111111121130110 \\
10001111000101111010001111000101301312201 \\
01001100111001111001110011001001023321032 \\
11001011011001100110010010110011203103323 \\
00101010110110110110110101010001130010334 \\
10101101010110101001010100101011310232025 \\
01101110101010101010101000100111032201216 \\
11101001001010110101001001011101212023107 \\
00011001101111001111011001100003333220100 \\
10011110001111010000111000011013113002211 \\
01011101110011010011000100010113231031022 \\
11011010010011001100100101101103011213333 \\
00111011111100011100000010001113322300324 \\
10111100011100000011100011110103102122035 \\
01111111100000000000011111111003220111206 \\
11111000000000011111111110000013000333117
\end{array}\right\|
\end{array}
$$

$$\mathbf{D}_{36} = \begin{array}{c} 123456 \\ \left\| \begin{array}{c} 000000 \\ 011101 \\ 211202 \\ 210303 \\ 101404 \\ 100505 \\ 210011 \\ 100110 \\ 101213 \\ 001315 \\ 011412 \\ 210514 \\ 101022 \\ 210125 \\ 200220 \\ 011324 \\ 010421 \\ 101523 \\ 001033 \\ 111134 \\ 100231 \\ 200330 \\ 210435 \\ 011532 \\ 210044 \\ 000143 \\ 011245 \\ 101342 \\ 100440 \\ 211541 \\ 111055 \\ 201152 \\ 010254 \\ 110351 \\ 201453 \\ 000550 \end{array} \right\| \end{array}$$

$$\mathbf{D}_{49} = \begin{array}{c} 12345678 \\ \left\| \begin{array}{c} 00000000 \\ 10111111 \\ 20222222 \\ 30333333 \\ 40444444 \\ 50555555 \\ 60666666 \\ 01123456 \\ 11234560 \\ 21345601 \\ 31456012 \\ 41560123 \\ 51601234 \\ 61012345 \\ 02246135 \\ 12350246 \\ 22461350 \\ 32502461 \\ 42613502 \\ 52024613 \\ 62135024 \\ 03362514 \\ 13403625 \\ 23514036 \\ 33625140 \\ 43036251 \\ 53140362 \\ 63251403 \\ 04415263 \\ 14526304 \\ 24630415 \\ 34041526 \\ 44152630 \\ 54263041 \\ 64304152 \\ 05531642 \\ 15642053 \\ 25053164 \\ 35164205 \\ 45205316 \\ 55316420 \\ 65420531 \\ 06654321 \\ 16065432 \\ 26106543 \\ 36210654 \\ 46321065 \\ 56432106 \\ 66543210 \end{array} \right\| \end{array}$$

$$\mathbf{D}_{50} = \begin{array}{r} 111 \\ 123456789012 \\ \left\| \begin{array}{c} 000000000000 \\ 001123411111 \\ 002241322222 \\ 003314233333 \\ 004432144444 \\ 010111112340 \\ 011234023401 \\ 012302434012 \\ 013420340123 \\ 014043201234 \\ 020222241302 \\ 021340102413 \\ 022413013024 \\ 023031424130 \\ 024104330241 \\ 030333342031 \\ 031401203142 \\ 032024114203 \\ 033142020314 \\ 034210431420 \\ 040444410432 \\ 041012321043 \\ 042130232104 \\ 043203143210 \\ 044321004321 \\ 100132403223 \\ 101200314334 \\ 102323220440 \\ 103441131001 \\ 104014042112 \\ 110243034143 \\ 111311440204 \\ 112434301310 \\ 113002212421 \\ 114120123032 \\ 120304121124 \\ 121422032230 \\ 122040443341 \\ 123113304402 \\ 124231210013 \\ 130410224211 \\ 131033130322 \\ 132101041433 \\ 133224402044 \\ 134342313100 \\ 140021333414 \\ 141144244020 \\ 142212100131 \\ 143330011242 \\ 144403422303 \end{array} \right\| \end{array}$$

II. Regular Uniform Designs

Designs of Strength 2 (Main Effect Designs)

Symmetrical Designs

#	Design	Method of Construction	
		Auxiliary Matrix	# of Columns of Auxiliary Matrix
1	$2^3//4$	$\mathbf{D}_4$	1-3
2	$2^7//8$	$\mathbf{D}_8$	1-7
3	$2^{11}//12$	$\mathbf{D}_{12}$	1-11
4	$2^{15}//16$	$\mathbf{D}_{16}$	1-15
5	$2^{19}//20$	$\mathbf{D}_{20}$	1-19
6	$2^{23}//24$	$\mathbf{D}_{24}$	1-23
7	$2^{27}//28$	$\mathbf{D}_{28}$	1-27
8	$2^{31}//32$	$\mathbf{D}_{32}$	1-31
9	$3^4//9$	$\mathbf{D}_9$	1-4
10	$3^{13}//27$	$\mathbf{D}_{27}$	1-13
11	$4^5//16$	$\mathbf{D}_{16}$	16-20
12	$5^6//25$	$\mathbf{D}_{25}$	1-6
13	$6^3//36$	$\mathbf{D}_{36}$	4-6
14	$7^8//49$	$\mathbf{D}_{49}$	1-8

Asymmetrical Designs

#	Design	Method of Construction	
		Auxiliary Matrix	# of Columns of Auxiliary Matrix
15	$2^4 \times 4//8$	$\mathbf{D}_8$	1-3, 7, 8
16	$2^2 \times 6//12$	$\mathbf{D}_{12}$	12-14
17	$2^8 \times 8//16$	$\mathbf{D}_{16}$	4, 7, 9, 10, 12-15, 21
18	$2 \times 3^7//18$	$\mathbf{D}_{18}$	1-8
19	$3^3 \times 6//18$	$\mathbf{D}_{18}$	9-12
20	$2^3 \times 4 \times 6//24$	$\mathbf{D}_{24}$	24-28
21	$3^9 \times 9//27$	$\mathbf{D}_{27}$	3, 6-14
22	$2^6 \times 4^6 \times 8//32$	$\mathbf{D}_{32}$	18, 19, 21-23, 31-37, 41
23	$2^4 \times 4^9//32$	$\mathbf{D}_{32}$	3, 16, 19, 22, 32-40
24	$2^2 \times 6^3//36$	$\mathbf{D}_{36}$	2-6
25	$3 \times 6^3//36$	$\mathbf{D}_{36}$	1, 3-6
26	$2 \times 5^{11}//50$	$\mathbf{D}_{50}$	1-12

Designs of Strength 3

#	Design	Method of Construction
27	$2^4//8$	Columns 1 – 3, 7 of the Auxiliary Matrix $\mathbf{D}_8$
28	$2^8//16$	Columns 1 – 4, 11 – 14 of the Auxiliary Matrix $\mathbf{D}_{16}$
29	$2^{12}//24$	$\left\Vert \begin{matrix} \mathbf{0}_{12} & \mathbf{D}_{12}(11) \\ \mathbf{I}_{12} & \mathbf{D}_{12}(11) \end{matrix} \right\Vert$
30	$2^{16}//32$	Columns 1 – 5, 16 – 25, 31 of the Auxiliary Matrix $\mathbf{D}_{32}$
31	$2^{20}//40$	$\left\Vert \begin{matrix} \mathbf{0}_{20} & \mathbf{D}_{20} \\ \mathbf{I}_{20} & \mathbf{D}_{20} \end{matrix} \right\Vert$
32	$2^{24}//48$	$\left\Vert \begin{matrix} \mathbf{0}_{24} & \mathbf{D}_{24}(23) \\ \mathbf{I}_{24} & \mathbf{D}_{24}(23) \end{matrix} \right\Vert$
33	$3^4//27$	Columns 1 – 3, 10 of the Auxiliary Matrix $\mathbf{D}_{27}$

* $\mathbf{0}_N$ and $\mathbf{I}_N$ are N-dimensional vector-columns that consist of 0 and 1 respectively; $\mathbf{D}_N(N-1)$ is a matrix that includes the first $N-1$ columns of auxiliary matrix $\mathbf{D}_N$.

Designs of Strength 4

#	Design	Method of Construction	
		Auxiliary Matrix	# of Columns Of Auxiliary Matrix
34	$2^2//4$	$\mathbf{D}_4$	1, 2
35	$2^3//8$	$\mathbf{D}_8$	1-3
36	$2^5//16$	$\mathbf{D}_{16}$	1-4, 15
37	$2^6//32$	$\mathbf{D}_{32}$	1-5, 31
38	$3^2//9$	$\mathbf{D}_9$	1, 2
39	$3^3//27$	$\mathbf{D}_{27}$	1-3

Compromise Designs

#	Design	Interaction Effects to be Estimated	Method of Construction: Auxiliary Matrix	Method of Construction: # of Columns of Auxiliary Matrix
40	$2^6//8$	F_{12}	$\mathbf{D}_8$	1-3, 5-7
41	$2^4//8$	F_{12}, F_{13}, F_{14}	$\mathbf{D}_8$	1-3, 6
42	$2^4//8$	F_{12}, F_{13}, F_{23}	$\mathbf{D}_8$	1-3, 7
43	$2^{14}//16$	F_{12}	$\mathbf{D}_{16}$	1-4, 6-15
44	$2^{12}//16$	F_{12}, F_{13}, F_{23}	$\mathbf{D}_{16}$	1-7, 7, 9-15
45	$2^9//16$	F_{12}, F_{13}, F_{14} F_{23}, F_{24}, F_{34}	$\mathbf{D}_{16}$	1-4, 11-15
46	$2^8//16$	F_{12}, F_{13}, F_{14} $F_{15}, F_{16}, F_{17}, F_{18}$	$\mathbf{D}_{16}$	1-4, 8-10, 14
47	$2^{30}//32$	F_{12}	$\mathbf{D}_{32}$	1-5, 7-31
48	$2^{28}//32$	F_{12}, F_{13}, F_{23}	$\mathbf{D}_{32}$	1-5, 8, 9, 11-31
49	$2^{25}//32$	F_{12}, F_{13}, F_{14} F_{23}, F_{24}, F_{34}	$\mathbf{D}_{32}$	1-5, 9, 12, 14-31
50	$2^{21}//32$	$F_{12}, F_{13}, F_{14}, F_{15}, F_{23}$ $F_{24}, F_{25}, F_{34}, F_{35}, F_{45}$	$\mathbf{D}_{32}$	1-5, 16-31
51	$2^{16}//32$	$F_{12}, F_{13}, F_{14}, F_{15}, F_{16}$ $F_{23}, F_{24}, F_{25}, F_{26}, F_{34}$ $F_{35}, F_{36}, F_{45}, F_{46}, F_{56}$	$\mathbf{D}_8$	1-3, 5-7
52	$2^7//32$	$F_{34}, F_{35}, F_{36}, F_{37}, F_{45}$ $F_{46}, F_{47}, F_{56}, F_{57}, F_{67}$	$\mathbf{D}_8$	1-3, 6
53	$2^7//32$	$F_{12}, F_{13}, F_{23}, F_{45}, F_{46}$ $F_{47}, F_{56}, F_{57}, F_{67}$	$\mathbf{D}_8$	1-3, 7
54	$2^{16}//32$	$F_{12}, F_{13}, F_{14}, F_{15}, F_{16}$ $F_{17}, F_{18}, F_{19}, F_{1\,10}, F_{1\,11}$ $F_{1\,12}, F_{1\,13}, F_{1\,14}, F_{1\,15}, F_{1\,16}$	$\mathbf{D}_{16}$	1-4, 6-15
55	$2^9//32$	$F_{12}, F_{13}, F_{14}, F_{15}, F_{16}$ $F_{17}, F_{18}, F_{19}, F_{23}, F_{24}$ $F_{25}, F_{26}, F_{27}, F_{28}, F_{29}$ $F_{34}, F_{35}, F_{36}, F_{37}, F_{38}, F_{39}$	$\mathbf{D}_{32}$	1-5, 15, 26, 27, 31
56	$2^7//32$	$F_{12}, F_{13}, F_{14}, F_{15}, F_{16}, F_{17}$ $F_{23}, F_{24}, F_{25}, F_{26}, F_{27}, F_{34}$ $F_{35}, F_{36}, F_{37}, F_{45}, F_{46}, F_{47}$	$\mathbf{D}_{32}$	1-5, 26, 31
57	$3^{11}//27$	F_{12}	$\mathbf{D}_{27}$	1-3, 6-13
58	$3^7//27$	F_{12}, F_{13}, F_{23}	$\mathbf{D}_{27}$	1-3, 10-13
59	$3^5//27$	$F_{12}, F_{13}, F_{14}, F_{15}$	$\mathbf{D}_{32}$	1-3, 8, 9

III. Optimum Transformations of Regular Uniform Designs

№1 a) $2^2//3$ b) $2//3$	0 0 0 1 1 0 * * 67% * 89%
№2 a) $2^3//4$ b) $2^2//4$ c) $2//4$	0 1 1 1 0 1 1 1 0 0 0 0 * * * 100% * * 100% * 100%
№3 a) $3 \times 2//4$ b) $3//4$	0 0 0 1 1 0 2 1 * * 60% * 90%
№4 a) $2^4//5$ b) $2^3//5$ c) $2^2//5$ d) $2//5$	0 1 1 1 1 0 1 1 1 1 0 1 1 1 1 0 0 0 0 0 * * * * 90% * * * 91% * * 93% * 96%
№5 a) $3 \times 2^2//5$ b) $3 \times 2//5$ c) $3//5$	0 0 0 0 1 1 1 0 1 1 1 0 2 0 0 * * * 75% * * * 80% * * * 90%

№6 $3^2//5$	0 0 0 1 1 0 1 2 2 0 * * 53%
№7 a) $4 \times 2//5$ b) $4//5$	0 0 0 1 1 0 2 0 3 1 * * 57% * 91%
№8 a) $2^5//6$ b) $2^4//6$ c) $2^3//6$ d) $2^2//6$ e) $2//6$	0 1 0 1 1 0 1 1 1 0 1 1 0 1 0 1 1 1 0 1 0 0 0 0 0 1 0 1 1 1 * * * * * 83% * * * * 85% * * * 89% * * 92% * 100%
№9 a) $3 \times 2^3//6$ b) $3 \times 2^2//6$ c) $3 \times 2//6$ d) $3//6$	0 0 0 0 0 1 1 0 1 1 0 0 1 0 1 1 2 0 1 0 2 1 0 1 * * * * 83% * * * * 95% * * * * 100% * * * * 100%
№10 a) $3^2 \times 2//6$ b) $3^2//6$	0 0 1 1 0 0 0 1 0 2 1 1 1 2 1 2 2 0 * * * 82% * * 79%

№11 a) $4 \times 2^2//6$ b) $4 \times 2//6$ c) $4//6$	0 0 0 0 1 1 1 1 0 1 0 1 2 0 0 3 1 1 * * * 67% * * 74% * 89%
№12 $4 \times 3//6$	0 0 0 1 0 2 1 0 2 1 3 2 * * 50%
№13 a) $5 \times 2//6$ b) $5//6$	0 0 0 1 1 0 2 0 3 1 4 1 * * 56% * 93%
№14 a) $2^6//7$ b) $2^5//7$	0 0 0 0 0 0 0 0 1 1 1 0 0 1 0 0 1 1 0 1 1 1 0 0 1 0 0 1 0 1 1 0 1 0 0 1 1 1 0 0 1 0 * * * * * * 78% * * * * * 81%

№14 (continued) c) $2^4//7$ d) $2^3//7$ e) $2^2//7$ f) $2//7$	1 0 0 0 0 0 1 0 0 1 0 0 1 1 1 0 1 0 0 1 0 0 1 1 0 1 0 1 * * * * 86% * * * 91% * * 95% * 98%
№15 a) $3 \times 2^4//7$ b) $3 \times 2^3//7$ c) $3 \times 2^2//7$ d) $3 \times 2//7$ e) $3//7$	0 0 0 1 1 0 1 1 0 0 1 0 1 1 0 1 1 0 0 1 2 0 1 0 1 2 0 0 0 0 2 1 0 1 1 * * * * * 83% * * * * 88% * * * 93% * * 95% * 96%
№16 a) $3^2 \times 2^2//7$ b) $3^2 \times 2//7$ c) $3^2//7$	0 0 0 1 0 1 0 0 0 2 1 0 1 0 0 0 1 1 1 1 2 0 1 0 2 2 0 1 * * * * 81% * * * 83% * * 82%
№17 $3^3//7$	0 2 2 1 2 1 2 2 0 0 1 0 2 1 2 2 0 1 1 0 0 * * * 75%

№18 a) $4 \times 2^3//7$ b) $4 \times 2^2//7$ c) $4 \times 2//7$ d) $4//7$	0 1 0 1 0 0 1 0 1 1 0 0 1 0 1 1 2 0 0 0 2 1 1 0 3 1 0 1 * * * * 70% * * * 81% * * 86% * 91%
№19 a) $4 \times 3 \times 2//7$ b) $4 \times 3//7$	0 0 1 0 2 0 1 0 0 1 1 1 2 1 0 2 2 1 3 2 0 * * * 68% * * 68%
№20 $4^2//7$	0 0 1 0 0 1 2 1 0 2 3 2 0 3 * * 47%

№21 a) $5 \times 2^2//7$ b) $5 \times 2//7$ c) $5//7$	0 1 0 0 0 1 1 0 0 1 1 1 2 0 1 3 1 1 4 1 0 * * * 62% * * 71% * 89%
№22 $5 \times 3//7$	0 0 0 1 1 0 1 2 2 0 3 0 4 0 * * 48%
№23 a) $6 \times 2//7$ b) $6//7$	0 0 0 1 1 0 2 0 3 0 4 1 5 1 * * 55% * 94%

References

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Appendix 2. Computer Algorithm of Construction of Factorial Designs

In this chapter we describe a computer algorithm [1] of construction of factorial designs (with blocking) that are close to Q-optimal for a model that contains main effects of two-level and multi-level factors and interaction effects of two-level factors. The algorithm includes two basic modules and is based on a combination of analytical methods, a catalog of basic designs, and numerical procedures.

§ 1. Preliminary examples

There exist many methods leading to construction of effective designs for different types of factorial models. However, it is relatively easy to construct a design using a given method, but it is much more difficult to solve the inverse problem, namely, the task of finding method of construction leading to the requested design.

Consider two examples.

Example A2.1.1. Let

$$x_1x_3x_4x_6, x_2x_3x_5x_7, x_1x_2x_3x_8, x_1x_2x_4x_9, x_1x_2x_5x_{10},$$
$$x_1x_5x_{11}, x_2x_3x_4x_{12}, x_1x_3x_5x_{13}, x_2x_4x_5x_{14} \qquad \text{(A2.1.1)}$$

be the generators of a geometric design $2^{14}//32$ for 14 two-level factors in 32 runs.

Anyone familiar with a methodology of geometric designs can easily construct the design and the alias sets for the given generators (A2.1.1). An analysis of the alias sets shows that the design is nonsingular (and therefore has a wide range of optimal properties) for the model that includes absolute term, main effects of all 14 factors $F_1, \ldots, F_{14}$, all two-factor interaction effects of factors $F_3, \ldots, F_7$ and three two-factor interaction effects of the following pairs of factors: $F_1 - F_2$, $F_{11} - F_{12}$, and $F_{13} - F_{14}$. A pair of main effects of two-level factors together with interaction effects of these factors is equivalent to main effects of a four-level factors. Therefore, instead of 14 two-level factors we can construct a design for 8 two-level factors and 3 four-level factors. One of these four-level factor can be treated as block factor (with the block size

8), and two other four-level factors can be treated as two qualitative factors. Therefore, the geometric design defined by the generators (A2.1.1) can be transformed to a nonsingular design in four blocks (size 8 each). The model will include absolute term, effects of levels of two qualitative four-level factors, effects of levels of a block factor, main effects of eight two-level factors and all two-factor interaction effects between the first five of them.

Now consider the inverse problem, which actually occurs in practice. Suppose that we need to estimate parameters of the model that includes absolute term, effects of levels of two qualitative four-level factors, main effects of eight two-level factors and all two-factor interaction effects between the first five of them. Besides, the number of experiments that have to be conducted in homogeneous environments shall not exceed eight. The problem of finding generators that lead to a nonsingular design for the model specified above is a very laborious task. It presents a significant challenge even for experts in the theory of factorial designs.

Example A2.1.2. Suppose that we need to estimate parameters of the model of main effects in the experiment that includes five two-level quantitative factors and four three-level qualitative factors. Besides, the number experiments that have to be conducted in homogeneous environments shall not exceed four. With this goal, we will use the catalog of regular uniform designs and their optimal transformations (see chapter 12).

By using the method of optimal transformations for the regular uniform design $2^6 \text{ x } 4^6 \text{ x } 8//32$ (see design #22 of section II of the Catalog), we can easily get a main effect design $2^5 \text{ x } 3^4 \text{ x } 8//32$ for five two-level and four three-level factors in 8 blocks (size 4 each) in 32 runs. To do that, we have to remove one two-level and two four-level factors. Then, we need to transform the remaining four-level factors into three-level factors. An efficiency of the resulting design is 94.0%. However, there is no certainty that the initial design and the chosen transformations of this design are best suited for this case. And really, we can take a regular uniform design $3^9 \text{ x } 9//27$ as the initial one (see design #21 of section II of Catalog) and then construct the required design transforming five three-level factors into two-level factors. The resulting design will have better efficiency (94,7%) with only 27 runs. Besides, the 9-level factor allows dividing the experiment into 9 blocks (size 3 each). In order to make sure that the latest plan is the best, you need to loop through all the regular designs and all valid transformations, which is a very laborious task.

Therefore, we are often faced with a problem intractable without a computer: to construct an optimal factorial design with the required properties while navigating through a huge amount of methods of construction. The most sensible approach in this situation is the creation of an elaborate computer algorithm for the construction of effective designs.

§ 2. General Considerations and Problem Statement

The application of general numerical procedures for constructing an optimal design seems appropriate only for relatively small dimensions. This is true not only because they lead to time consuming calculations for large dimensions but mostly because they do not give the factorial structure of the designs, so essential for a clear interpretation of the results of experiments. That is why the described algorithm has been chosen as a combination of analytical techniques and numerical procedures.

The algorithm is based on a criterion of *Q*-optimality, because this criterion is the most convenient for numerical procedures. On the other hand, as it has been shown in [2] (where criteria of *D*-, *E*-, *Q*-optimality are considered), for the most of practical applications, the design that is optimal in the sense of one criterion of optimality is also optimal in the sense of other criteria of optimality.

Often, the described procedure allows constructing the designs that are *Q*-optimal. The examples of such designs are geometric designs. That means that these designs will be optimal in a wider sense. In other cases, the described procedure results in the designs that are close to *Q*-optimal. Then, as we assume, they will be close to optimal designs for other criteria of optimality.

The described algorithm works for the factorial model that includes main effects of quantitative and/or qualitative factors, two-factor interaction effects of two-level factors, and also all interaction effects of sets of three two-level factors.

Input data are supposed to include the following information:

1. The number of factors and the numbers of their levels.
2. Required interactions of two-level factors.
3. The maximal number of experiments.
4. A size of the maximal block.

§ 3. Idea of Algorithm

The algorithm generates the designs that are obtained as transformations of some class of regular uniform (nongeometric) designs (with the number of runs $N \leq 100$) or as transformations of three types of geometric designs $2^n//16, 2^m//32, 2^q//64$.

A general scheme of a choice of the design based on input information is as follows.

On the first step of algorithm, we calculate the number of degrees of freedom for the model based on formula

$$v = k - r,$$

where k is the number of parameters of the model, r is the number of linearly independent equalities (3.10.12).

On the next step, for the i-th design of the set of regular uniform designs and/or three geometric designs with the number of runs N_i ($v \le N_i \le N$), we choose the optimal transformation that convert the design into required one. The designs are transformed in ascending order of N_i.

The algorithm provides the splitting of all input two-level factors into disjoint sets with the following property: there is no interaction effect of factors from different sets. The set is called minimal if it cannot be split into two sets with the same property. It is obvious that splitting factors into minimal sets is unique. Table 23 includes four types of minimal sets of factors. All minimal sets not included into Table 23 have, by definition, type 5.

If the model contains only minimal sets of type 1, only nongeometric designs are transformed. If the model contains at least one set of type 5, only geometric designs are transformed. If the model does not contain a set of type 5 and it does contain at least one set of types 2, 3, or 4, then both geometric and nongeometric designs are transformed.

Table 23
Minimal Sets of Factors

Type of Set	Factors	Interaction Effects	Terms in Model
1	F_1, F_2	F_{12}	Φ_1
2	F_1, F_2, F_3	F_{12}, F_{13}, F_{23}	Φ_2
3	F_1, F_2, F_3	F_{12}, F_{13}	Φ_3
	F_1, F_2, F_3	F_{12}, F_{13}, F_{14}	Φ_4
	F_1, F_2, F_3, F_4	F_{12}, F_{23}, F_{34}	Φ_5
4	F_1, F_2, F_3, F_4	$F_{12}, F_{23}, F_{34}, F_{14}$	Φ_6
	F_1, F_2, F_3, F_4	$F_{12}, F_{23}, F_{34}, F_{24}$	Φ_7

§ 4. Transformations of Nongeometric Designs

Let $\overline{\mathbf{D}}$ be a regular uniform main effect design in N runs for n factors $F_1, \dots, F_n$ with $s_1, \dots, s_n$ levels respectively. Consider a method of construction of a design $\mathbf{D}$ for a factorial model M from the design $\overline{\mathbf{D}}$ for the model $\overline{M}$. Replace the factor F_i (with s_i levels) in the design $\overline{\mathbf{D}}$ with factors $F_i^1, \dots, F_i^{m_i}$ (with $s_i^1, \dots, s_i^{m_i}$ level respectively) so that for equal levels of the factor F_i, factors $F_i^1, \dots, F_i^{m_i}$ have the same combinations of levels and

$$1 + r + \sum_{j=1}^{m_i}(s_i^{(j)} - 1) = S_i \le s_i, \qquad \text{(A2.4.1)}$$

where r is the number of two-factor interaction effects of two-level factors (of factors $F_i^1, \dots, F_i^{m_i}$) included into the model M.

Therefore, as a results of the replacement (transformation) of the factor F_i, each its level corresponds to the row of auxiliary design $\mathbf{D}_i$:

$$\begin{array}{c} F_i \\ \left\| \begin{matrix} 0 \\ \vdots \\ s_i - 1 \end{matrix} \right\| \end{array} \rightarrow \begin{array}{c} \begin{matrix} F_i^1 & \cdots & F_i^{m_i} \end{matrix} \\ \left\| \begin{matrix} F_i^1(0) & \cdots & F_i^{m_i}(0) \\ \vdots & \ddots & \vdots \\ F_i^1(s_i - 1) & \cdots & F_i^{m_i}(s_i - 1) \end{matrix} \right\| \end{array} = \mathbf{D}_i.$$

This is a more general class of transformations (comparing to transformations of §1 of chapter 9) that includes also interaction effects.

We shall say that for the given design $\overline{\mathbf{D}}$, we define

a) a skeleton of the transformation if for each factor F_i with s_i levels of the design $\overline{\mathbf{D}}$, we set the levels $s_i^{(1)}, \dots, s_i^{(m_i)}$ of factors $F_i^1, \dots, F_i^{m_i}$ with the given interaction effects in the design $\mathbf{D}$ $(i = 1, \dots, n)$, i.e., if we set the following mapping:

$$\begin{aligned} & s_1 \rightarrow s_1^{(1)}, \dots, s_1^{(m_1)}, \\ & s_2 \rightarrow s_2^{(1)}, \dots, s_2^{(m_2)}, \\ & \quad \cdots\cdots\cdots \\ & s_n \rightarrow s_n^{(1)}, \dots, s_n^{(m_n)}; \end{aligned} \qquad \text{(A2.4.2)}$$

b) a structure of transformation if we set a skeleton of the transformation and the design $\mathbf{D}_i$ (the i-th structure) is defined for each factor F_i $(i = 1, \dots, n)$ of the design $\overline{\mathbf{D}}$,

c) a scale of transformation if for each design $\mathbf{D}_i$ for any levels of the factors F_i^j $(j = 1, \dots, m_i)$, we set the values of corresponding quantitative variables $X_i^{(j)}$.

A skeleton of the transformation (A2.4.2) will be called admissible if (A2.4.1) holds and the set $s_1^{(1)}, \dots, s_1^{(m_1)}, s_2^{(1)}, \dots, s_2^{(m_2)}, \dots, s_n^{(1)}, \dots, s_n^{(m_n)}$ matches (up to a reorder) with the input set of levels.

Let $\mathbf{D}^f$ be the full design in $N^f = s_1^{(1)} \dots s_1^{(m_1)} \dots s_n^{(1)} \dots s_n^{(m_n)}$ runs for factors $F_1^1, \dots, F_1^{m_1}, \dots, F_n^1, \dots, F_n^{m_n}$; $\mathbf{D}_i^f$ be the full design in $n_i^f = s_i^{(1)}, \dots, s_i^{(m_i)}$ runs for factors $F_i^1, \dots, F_i^{m_i}$. Hence, $N^f = \prod_{i=1}^n n_i^f$.

It follows from the results of §12 of chapter 3 that a variance of the estimate of the regression function at point of $\mathbf{D}^f$ for the model M depends neither on the type of the model (i.e., on quantitative or qualitative structure of factors) nor on values of variables X_i in the design $\mathbf{D}$ (i.e., on a scale of the transformation).

Denote by M_i a factorial model for the design $\mathbf{D}_i$ that contains main effects of factors $F_i^1, \dots, F_i^{m_i}$ and two-factor interaction effects some of these factors with two levels, providing that the condition (A2.4.1) is met. Denote by σ_{ia}^2 an average variance over points $\mathbf{D}_i^f$ for the model M_i and the design $\mathbf{D}_i$. Denote by σ_a^2 an average variance over points of $\mathbf{D}^f$ for the model M of main effects and the design $\mathbf{D}$. We have to choose an admissible skeleton and structure of the transformation to minimize an average variance σ_a^2. It follows from the results of §1 of chapter 9 that an average variance σ_a^2 for the given skeleton and the structure of the transformation is

$$\sigma_a^2 = \frac{\sigma^2}{N}\left(1 - n + \sum_{i=1}^n \sigma_{ia}^2 \, {}^{s_i}\!/_{\sigma^2}\right).$$

Therefore, minimum of σ_a^2 is reached if and only if σ_{ia}^2 are minimal for all $i = 1, \dots, n$. That means that for the given skeleton of the transformation, the problem of construction of an optimal design $\mathbf{D}$ is reduced to the problem of construction of optimal designs $\boldsymbol{D}_i$. In other words, the problem of construction of an optimal design $\mathbf{D}$ is reduced to the problem of construction of optimal structures of the transformation.

We will represent a function of effectiveness related to an average variance (as in §1 of chapter 9) as a ratio of a variance σ^2 and a normalized (per one observation and one parameter) average variance of the regression function over the points of the full design:

$$\varphi = {}^{k\sigma^2}\!/_{N\sigma_a^2},$$

where $k = 1 - n + \sum_{i=1}^m S_i$. Effectiveness of the design $\mathbf{D}_i$ (or the structure $\mathbf{D}_i$)

$$\varphi_i = {S_i\sigma^2}\Big/{s_i\sigma_a^2}\,. \qquad \text{(A2.4.3)}$$

Effectiveness of the design $\mathbf{D}$ can be expressed via effectiveness of each of the designs $\mathbf{D}_i$ that correspond to the design $\mathbf{D}$:

$$\varphi = k/(1 - n + \textstyle\sum_{i=1}^{n} S_i/\varphi_i). \qquad \text{(A2.4.4)}$$

Effectiveness of the design

$$\varphi \le 1. \qquad \text{(A2.4.5)}$$

For the implementation of the described algorithm, optimal structures of transformations for up to seven-level factors (without interaction effects) of Chapter 12 were augmented by optimal structures of transformations for eight-level and nine-level factors. All admissible (satisfying to (A2.4.1)) skeletons of transformations with up to nine-level factors and with two-factor interaction effects of two-level factors were included into the basic set of transformations. These structures are optimal for any regular uniform design and for any selection of a skeleton of the transformation.

Now consider the problem of a selection of an optimal skeleton of the transformation of the design $\overline{\mathbf{D}}$. We will show how this problem can be reduced to the problem of the integer linear programming.

Consider a parameter Δ_i for the given design $\mathbf{D}_i$:

$$\Delta_i = \left(\frac{\sigma_{ia}^2}{\sigma^2}\right) s_i - S_i.$$

Then, by (A2.4.3),

$$\varphi_i = S_i/(S_i + \Delta_i).$$

By (A2.4.5), we get that $\Delta_i \ge 0$. Besides, $\Delta_i = 0$ if and only if $\varphi_i = 1$. It follows from (A2.4.4) that

$$\varphi = k/(k + \textstyle\sum_{i=1}^{n} \Delta_i).$$

A selection of the skeleton that maximizes φ is equivalent to a selection of the skeleton that minimizes

$$\frac{1}{\varphi} = 1 + \frac{\sum_{i=1}^{n} \Delta_i}{k},$$

or just minimizes

$$K = \textstyle\sum_{i=1}^{n} \Delta_i.$$

Now sort all optimal structures in an ascending order of s_i. Let z_i be the number of structures with the sequence number i in the given skeleton of the transformation (A2.4.2). Denote by $k_s^{(i)}$ the number of s-level factors that are result of the transformation with the i-th structure. For the admissible skeleton of the transformation

$$\sum_{i=1}^{l} k_s^{(i)} z_i = n_s^{\text{inp}} \ (s = 2, \dots, 9), \tag{A2.4.6}$$

where n_s^{inp} is the number of input s-level factors, l is the sequence number of the last structure.

The count of the number of s-level factors n_s in the resulting (after transformation) design leads to inequality

$$\sum_{i=l_{s-1}+1}^{l_s} z_i \le n_s \ (s = 2, \dots, 9), \tag{A2.4.7}$$

where l_s is the sequence number of the last structure for s-level factor ($l_1 = 0$).

The optimal skeleton of the transformation is determined by minimization of a functional

$$K = \sum_{i=1}^{n} \Delta_i = \sum_{i=1}^{l} z_i \Delta_i.$$

The problem of minimization of the functional K for the given $\overline{\mathbf{D}}$ with the restrictions (A2.4.6) and (A2.4.7) is a task of integer linear programming.

An optimal scale of the transformation is determined for the given skeleton and structure of the transformation. An information matrix of the resulting regular design for the model of main effects can be reduced to a block diagonal type. Therefore, the task of the choice of an optimal scale of transformation is reduced to the task of the choice an optimal scale of the designs $\mathbf{D}_i$.

§ 5. Blocking for Designs Generated from Geometric Ones

We need to divide a factorial design into blocks when not more than n^{inp} experiments can be performed in homogeneous environments. In such cases we actually have one more factor, which is called a block factor.

The size of maximal block is not determined by only the number of levels s_{bl} of block factor F_{bl} and the number of runs N but also by frequency of occurrence of levels of block factors F_{bl}. The later depends on the structure of the $\mathbf{D}_i$ that is used for the block factor. For the given number s row in the $\mathbf{D}_i$, a size of the maximal block is determined by the distribution of levels of the block factor. For example, if $(0\ 0\ 0\ 1\ 2)^T$ is the column of the structure $\mathbf{D}_i$ corresponding to the block factor, then the distribution of all N experiments in the three blocks are as follows. The first block (corresponding to level 0) contains $3N/5$ runs, the second and the third blocks (corresponding to levels 1 and 2 respectively) contain $N/5$ runs each. Hence, a size of a maximal block equals $3N/5$.

It is obvious that for the column $(0\ 0\ 1\ 1\ 2)^T$, the first and the second blocks contain $2N/5$ runs each, the third block contains $N/5$ runs. Hence, a size of a maximal block equals $2N/5$.

In case of uniform distribution of levels of the block factor, a size n_{max} of a maximal block is

$$n_{max} = -\frac{N}{s}\left[-\frac{s}{s_{bl}}\right], \tag{A2.5.1}$$

where $[-\, s/s_{bl}]$ is the integer part of $(-\, s/s_{bl})$.

With few exceptions, the found optimal structures let us to choose the block column with an uniform distribution of levels. In other words, most of the created structures produce a maximal size of the block defined by (A2.5.1). The exceptions are some structures, such as $5 \text{ x } 3//7$, $3^2 \text{x } 2^3//8$, $3^2 \text{x } 2^2//8$, $3^2 \text{x } 2//8$, $3^3 \text{x } 2//8$. For the first one, the three-level block factor has a maximal size of the block equal to $5N/7$. For the rest cases, the two-level block factor has a maximal size of the block that equals $5N/8$.

Therefore, the size of a maximal block is the following function of N, s, s_{bl} and the type of the structure:

$$n_{max} = \begin{cases} 5N/7 & \text{for the structure } 5 \text{ x } 3//7 \text{ and } s = 7, s_{bl} = 3, \\ 5N/8 & \text{for the structures } 3^2 \text{ x } 2^3//8,\ 3^2 \text{ x } 2^2//8, \\ & \qquad 3^2 \text{ x } 2//8, \text{ and } s = 8, s_{bl} = 2 \\ \cdots & \cdots \\ -\dfrac{N}{s}\left[-\dfrac{s}{s_{bl}}\right] & \text{in other cases for } s, s_{bl} = 2, \dots, 9; s_{bl} \le s. \end{cases}$$

For given N and s_{bl} we will call block structures those $\mathbf{D}_i$ for which the following inequality holds:

$$n_{max} \le n^{\text{inp}}. \tag{A2.5.2}$$

The algorithm of blocking is as follows. For given N (the given regular uniform design $\overline{\mathbf{D}}$), we fix consequently values s_{bl}. Add a qualitative s_{bl}-level factor F_{bl}. By (A2.5.2), mark a set of blocking structure and add one more restriction

$$\textstyle\sum_i z_i \ge 1 \tag{A2.5.3}$$

with summation over all block structures. After that, we solve the task of integer linear programming with the restrictions (A2.4.6), (A2.4.7), and (A2.5.3). The result of the procedure is an optimal design that depends on

s_{bl} and N. This procedure is repeated for all values s_{bl} for which at least one blocking structure exists.

§ 6. Transformation of Geometric Designs

Denote the input model *M* by
$2^{n_2}, 3^{n_3}, \dots, 8^{n_8}, \Pi_1, \Pi_2 \dots,$

where

n_2 is the total number of two-level qualitative factors and quantitative variables with the maximal degree of model equal to 1;

n_3 is the total number of three-level qualitative factors and quantitative variables with the maximal degree of model equal to 2;

…

n_8 is the total number of eight-level qualitative factors and quantitative variables with the maximal degree of model equal to 7;

Π_1, Π_2 ... are interaction effects of two-level factors.

The algorithm of construction of the design **D** for the model *M* consists of two steps.

Step 1. Construction of an auxiliary regular uniform design $\overline{\mathbf{D}}$ for the model $\overline{M}$.

Step 2. Optimal transformation of the regular design $\overline{\mathbf{D}}$ into a design **D** for the input model *M*.

In step 1, the model *M* is replaced with the model $\overline{M}'$ for two-, four-, and eight-level factors with a set of interaction effects of two-level factors. Then the model $\overline{M}'$ is replaced with the model $\overline{M}$, where each four-level factor is replaced with two two-level factors and their interaction and each eight-level factor is replaced with three two-level factors and all their interactions.

Since the model $\overline{M}$ includes only two-level factors and their interactions, the regular uniform design $\overline{\mathbf{D}}$ can be constructed as a geometric design $2^n//2^k$ for the given number *k*. Consider a procedure of construction of the geometric design $\overline{\mathbf{D}}$ in more detail.

A set of points of the design $\overline{\mathbf{D}}$ is a subset of the full design $\mathbf{D}^f$ in 2^n runs. Coordinates χ_i of the points $(\chi_1, \dots, \chi_n)$ of this subset satisfy $n-k$ linearly independent equations with coefficients from $GF(2)$. These equations are the generating relations. In the design $\mathbf{D}^f$, any main effect or interaction effect is defined as contrast between two flats of some pencil. For given generating relations, all pencils are divided into alias sets that generate identical pencils in the design $\overline{\mathbf{D}}$. It was shown in article [3] that for the given generators of the design $\overline{\mathbf{D}}$, there exist one representative from each alias set such that some fixed $n-k$ coordinates are zero. Conversely, if some main effects and interaction effects correspond to pencils with fixed $n-k$ zero coordinates (for example, the last ones), then there exist $n-k$ generating relations with all these effects belonging to different alias sets.

Therefore, we have to set up a correspondence between main effects and interaction effects, and pencils with zero coordinates in the last $n-k$ positions in such a way that all main effects and interaction effects correspond to different pencils with at least one nonzero coordinate. Besides, the pencil corresponding to interaction effect is a sum of the pencils corresponding to main effects. If that is possible, the required design $\overline{\mathbf{D}}$ exists.

Now we will describe an algorithm of obtaining the required correspondence. For the sake of simplicity, consider an example. The general case will be clear from this.

Suppose that we have 10 two-level factors $F_1, \dots, F_{10}$. We need to construct a geometric design $\overline{\mathbf{D}}$ in 2^4 runs, i.e., a design $2^{10}//2^4$ such that all 10 main effects and 5 interaction effects F_{12}, F_{34} F_{56} F_{78} $F_{9,10}$ have unique LS estimates.

Set up a correspondence between the main effect of the factor F_1 and the first (in the lexicographic order) pencil $P(0\ 0\ 0\ 1)$ (for the sake of simplicity, we omit the last six 0's). Set up a correspondence between the main effect of the factor F_2 and the next pencil $P(0\ 0\ 1\ 0)$. Then the interaction effect of factors F_1 and F_2 will correspond to the pencil $P(0\ 0\ 1\ 1\ )$.

Set up a correspondence between the next (in the lexicographic order) pencil $P(0\ 1\ 0\ 0)$ and the main effect of the factor F_3, and set up a correspondence between the pencil $P(1\ 0\ 0\ 0)$ and the main effect of the factor F_4. Then the interaction effect of factors F_3 and F_4 will correspond to the pencil $P(1\ 1\ 0\ 0\ )$.

Set up a correspondence between the next pencil $P(0\ 1\ 0\ 1)$ and the main effect of the factor F_5. Then $P(0\ 1\ 1\ 0)$ cannot be the pencil that corresponds to the main effect of the factor F_6, because interaction effect of the factors F_5 and F_6 will correspond to the pencil $P(0\ 0\ 1\ 1)$, which is already taken for the interaction effect of the factors F_1 and F_2 .

The first suitable pencil for the factor F_6 is $P(1\ 0\ 1\ 0)$. Then the interaction effect of the factors F_5 and F_6 will correspond to the pencil $P(1\ 1\ 1\ 1)$.

Set up a correspondence between the main effect of the factor F_7 and the first of remaining pencils, i.e., $P(0\ 1\ 1\ 0)$. Then the first suitable pencil for the factor F_8 is $P(1\ 0\ 1\ 1)$. The interaction effect of the factors F_7 and F_8 will correspond to the pencil $P(1\ 1\ 0\ 1)$.

Set up a correspondence between the main effect of the factor F_9 and the pencil $P(0\ 1\ 1\ 1)$. Then the main effect of the factor F_{10} will correspond to the pencil $P(1\ 0\ 0\ 1)$. The effect of interaction of the factors F_9 and F_{10} will correspond to the pencil $P(1\ 1\ 1\ 0)$.

This concludes the work of the algorithm for this example.

However, the matter may be not this simple for another situation. It may happen that we cannot set up a correspondence between the main effect of some factor F_i and any pencil. Then we have to come back to the factor F_{i-1} and try to set up a correspondence between its main effect and the next (in the lexicographic order) pencil and then repeat the choice for the main effect of the factor F_i.

We have to do analogously in a general situation, but at the end, we have to set up a correspondence between factors without interaction effects and the remaining pencils.

A similar algorithm was also presented in [4].

The most successful implementation of the algorithm described above was demonstrated to the author of this book by I. Boguslavsky. His program found a solution for the design $2^q//64$ within a fraction of a second (on pre-2000 computers). That included the most complicated case: computer proof of the nonexistence of the design 4^3 x $8^7//64$. That, by the way, confirms the analytical result of I. Boguslavsky (see Theorem 8.6.1). I. Boguslavsky has never published a description of his program. Apparently, he has never used his software commercially or for any research.

Note that time-consuming calculations for the program of construction of geometric designs might be a serious disadvantage of the software, since in a general procedure, this part of the algorithm is used repeatedly.

Blocking for the designs generated from the geometric ones is similar to blocking for nongeometric designs.

More details on the described algorithm can be found in [1].

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