

Designs with a small number of runs for factorial experiments

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ELEMENTS OF DESIGN MATRICES

DESIGNS

WITH A SMALL NUMBER OF RUNS
FOR FACTORIAL EXPERIMENTS

P.M. UPPERMAN

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with a Small Number of Runs
for Factorial Experiments**

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de Rector Magnificus, prof. dr. J.H. van Lint,
voor een commissie aangewezen door het College
van Dekanen in het openbaar te verdedigen op
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door

Pieter Martinus Upperman

geboren te Emmen

Dit proefschrift is goedgekeurd
door de promotoren

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prof. dr .R. Doombos

en de copromotor
Dr. ir. E.E.M. van Berkum

Aan Jenny

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CHAPTER 1

Introduction

1.1. Preliminary remarks

In recent years investigators who carry out experimental work became increasingly convinced that applying statistical principles to the design and analysis of their experiments substantially improves the quality and efficiency of their efforts.

Many different designs are now available in the statistical literature from which they can choose. *Steinberg and Hunter* (1984) provide an excellent list of references.

One of the important principles of experimental design is the need to examine factors simultaneously in one experiment, in order to obtain a sound knowledge of physical and chemical mechanisms concerned.

Because the size of an experiment increases rapidly with increasing number of levels and factors, there is a need to reduce the number of treatments in order to save time and reduce the cost of experimentation.

A large number of designs have therefore been constructed in which only a subset of all possible treatments has to be used. An additional advantage of these designs is that they can be used to predict the response of a treatment which has not been used in the experiment.

A number of existing designs will be discussed in the sections 1.2, 1.3, 1.4 and 1.5. Section 1.6 reports new results on fractional replication for quantitative factors, which originated from this research.

1.2. Main-effect designs

An important group of designs with a limited number of treatments is the class of main-effect designs. These designs make it possible to estimate a relatively large number of main effects using a small number of experimental units. Interactions are ignored. These designs are very suitable as screening designs which are used to select a limited number of factors from a large number of candidates.

Addelman (1962a) gives many of these plans in which factors may have from two up to nine

levels.

To construct these plans use was made of Galois fields, the techniques of replacement and collapsing. The latter two techniques are explained in Chapter 2.

Plackett and Burman (1946) developed a set of main-effect designs for factors having two levels. These are saturated designs because the number of parameters to be estimated equals the number of experimental units.

The number of experimental units N must be a multiple of 4. These designs can be utilized to examine up to $(N - 1)$ factors. The \mathbf{X} matrices corresponding to these designs are Hadamard matrices. A Hadamard matrix \mathbf{H} of order h is a matrix consisting of -1 's and $+1$'s, such that $\mathbf{H}'\mathbf{H} = h\mathbf{I}_h$, \mathbf{I} being the identity matrix.

Raktoe and Federer (1973) develop a class of balanced saturated main-effect plans for the 2^n factorial. They use the following notations and definitions:

- (i) In a 2^n factorial experiment with n factors at two levels each, a treatment combination is an n -tuple (x_1, x_2, \dots, x_n) , with $x_i \in \{0, 1\}$.
- (ii) A set of $(n + 1)$ treatment combinations arranged in arbitrary order in an $(n + 1) \times n$ matrix \mathbf{D} (a row being a treatment combination) with the aim of estimating β , the vector of regression coefficients, consisting of the mean and the main effects (when the assumption that all other effects are negligible is justified) is called a saturated main-effect plan.
- (iii) A balanced saturated main-effect plan of the 2^n factorial is a design \mathbf{D} such that
 - (a) Each unknown parameter β is estimated with the same variance,
 - (b) the covariance between the estimates of the mean μ and a main effect is a constant, and
 - (c) the covariance between estimates of two main effects is another constant.

The plans developed are characterized by properties of the $\mathbf{D}'\mathbf{D}$ matrix. It is regrettable that no examples of plans are given and that the construction of these plans, some of which are D -optimal Hadamard designs, is left to the reader.

Taguchi (1987) strongly recommends the use of main-effect plans. He calls them orthogonal arrays and he uses a very extensive collection of these arrays, some of which are also suitable to estimate selected interactions.

Taguchi gives many interesting examples but unfortunately the numerical calculations are often difficult to understand since they do not refer to a specified model.

A very important class of main-effect designs are the Latin-, Graeco-Latin- and hyper-Graeco-Latin squares. These are designs containing k^2 experimental units suitable to examine up to $(k + 1)$ factors with k levels. *Kemphorne* (1979) shows how Galois fields can be used to construct these squares. *Box, Hunter and Hunter* (1978), *Cochran and Cox* (1957), *Johnson and Leone* (1964), *Montgomery* (1976), *Upperman* (1974), *Upperman and Dévény* (1974) give many examples of these designs. *Upperman and Dévény* (1974) treat an interesting application of a main-effect design consisting of 5 orthogonal Latin squares. These squares are used to solve a quality problem in a complicated production process.

However, main-effect designs are not always suitable since interactions may be important elements of the models under consideration. We therefore discuss some designs in the next section which allow estimation of both main effects and interactions.

1.3. Designs permitting estimation of all main effects and two-factor interactions

1.3.1. Fractions of 2^n designs

Kemphorne (1979), *Box and Hunter* (1961a, 1961b) and *Montgomery* (1976) give a sound basis of the theory to construct fractions of 2^n designs. *Kemphorne* (1979) and *Montgomery* (1976) use linear functions for this purpose.

The books of *Cochran and Cox* (1957), *Mclean and Anderson* (1984), the *Statistical Engineering Laboratory* (1957) and *Upperman* (1974) contain many fractions of 2^n designs, permitting the estimation of all main effects and two-factor interactions.

The books of *Cochran and Cox* (1957), *Upperman* (1974) and *Box, Hunter and Hunter* (1978) contain many agricultural and industrial examples. *Addelman* (1961) also provides fractions of 2^n designs. Although these designs introduce some correlations between some of the estimates, they permit the estimation of main effects and two-factor interactions with fewer trials than is required with an orthogonal plan.

It is for instance known that a $\frac{1}{2}$ replicate of the 2^7 design allows uncorrelated estimates of all main effects and two-factor interactions. This plan therefore requires 64 trials or experimental units. The plan of Addelman only requires 48 trials.

Rechtschaffner (1967) gives an algorithm to construct saturated designs for factors having two levels.

For instance the 2^7 design contains 7 main effects and 21 two-factor interactions and therefore 28 effects have to be estimated apart from the mean. *Rechtschaffner* (1967) estimates these effects using only 29 trials.

Many orthogonal fractional 2^n designs can be analyzed by using graphical methods as described by *Daniel* (1959) and *Zahn* (1975).

1.3.2. Fractions of 3^m designs

Cochran and Cox (1957), *Mclean and Anderson* (1984) and *Montgomery* (1976) give a number of useful plans. Worked examples are not provided but *Montgomery* (1976) gives some exercises with fractions of 3^m designs.

1.3.3. Fractions of $2^n 3^m$ designs

Connor (1960) explains the theoretical foundation of the methods to construct fractions of $2^n 3^m$ designs. These methods were used to develop the designs given in *Connor and Young* (1961). *Mclean and Anderson* (1984) include all the designs of *Connor and Young* (1961) and those given in the *Statistical Engineering Laboratory* (1957). *Margolin* (1969b) gives a number of plans which require far less experimental units than the corresponding designs in *Connor and Young* (1961). *Webb* (1971) provides a list of small plans but interactions cannot always be estimated. *Upperman* (1991) gives an application of a $2^n 3^m$ design to a spot-welding experiment and other examples of the application of experimental designs to industrial problems.

1.3.4. Other fractional designs

It is surprising that little attention has been paid to *Morrison* (1956). A method is described in this article which yields a $\frac{1}{2}$ replicate for factorials when some factors have more than

3 levels. All two-factor interactions can be estimated. A number of numerical examples is provided. One of these consists of a $\frac{1}{2}$ replicate of a $2^3 \times 3 \times 5$ design.

1.4. Designs for quantitative factors

Many designs have been developed for quantitative factors. They are very economical as regards the number of design points needed, especially since many of these designs, such as some response surface plans, use 5 levels for each factor.

Articles dealing with response surfaces were written by *Box and Draper* (1959, 1963), *Box and Hunter* (1957), *Lucas* (1974), *Welch* (1984) and *Myers, Khuri and Carter* (1988).

Box and Behnken (1960), *Hoke* (1974), *Mitchell and Bayne* (1978) and *Rechtschaffner* (1967) deal with designs for quantitative factors with three levels. The designs for 3, 4, 5, 6, 7, 9, 10, 11, 12 or 16 factors, of Box and Behnken, are frequently used in practical work.

Box and Draper (1974) discuss designs in which each factor has four unequally spaced levels, which may be a disadvantage in a practical situation.

There are several books dealing with response surface methodology such as *Box, Hunter and Hunter* (1978), *Box and Draper* (1987), *Cochran and Cox* (1957), *Montgomery* (1976) and *Upperman* (1974). It is mostly assumed that the response surface model can be presented by a second degree polynomial.

Box and Draper (1987) is especially useful since it incorporates many results given in articles which were previously published.

1.5. *D*-Optimal designs

Many articles and books have appeared during the last twenty years about designs for which, given the number of design points, the hyper volume of the joint confidence region of the β 's, the parameters of the regression equation, is minimized. These designs are called *D*-optimal. *Fedorov* (1972) gives an excellent treatment of the subject, *St. John and Draper* (1975) and *Oorschot* (1974) give a good review and mention further useful literature. *Mitchell* (1974a, 1974b) uses a computer algorithm to construct designs which are more or less "*D*-optimal". Although the *D*-criterion is a very useful tool to construct designs, there are a number of authors who have made some critical remarks as to the use of *D*-optimal design theory.

Welch (1984) reports that constructing D -optimal designs may be inappropriate when the number of observations is not large relative to the number of parameters.

Box, Hunter and Hunter (1978) state that in recent years the study of optimal designs has become separated from real experimentation with the predictable consequence that its limitations have not been stressed, or, often even realized (p. 472).

D -optimal designs do for instance very often not contain a center point, whereas such a point is very desirable from the experimenter's point of view.

In Chapter 5, Section 5.7, we shall see that some nearly D -optimal designs have a relatively large variance for the parameter estimates corresponding to the quadratic terms of the regression model. Box and Draper (1987) also voice some criticism as to the use of D -optimality (pp. 499, 500). Firstly because the hyper volume of the confidence region for the β 's very much depends on the range of the factor-levels chosen and secondly because D -optimality does not take into account the possible bias due to a wrong model. There are many characteristics with which a design can be judged. Two of these, D - and G -efficiency, will be discussed in Chapter 2. Some new D -optimal designs will be developed in Chapter 3.

These designs had to be constructed to be able to calculate D -efficiencies of some new designs developed in Chapters 4, 5 and 6.

1.6. The need for new designs with quantitative factors

Although an experimenter can choose from many designs for quantitative factors, our experience in statistical consultation has shown that available designs are not always satisfactory. There are three reasons:

- (i) they require that all factors have the same number of levels, mostly 3 or 5,
- (ii) the number of experimental units is rather large,
- (iii) there are only a few designs available with a small number of experimental units.

Many experimenters only want to carry out small experiments because of time and costs involved.

There is therefore a real need for a great variety of designs with quantitative factors having a small number of experimental units.

The experimenter moreover wants some freedom as to the choice of the number of levels per factor.

Especially in the preliminary stages of experimental work, for instance research concerning integrated circuits, it is desirable to carry out small experiments in which a number of quantitative factors is varied simultaneously and knowledge as regards their main effects and two-factor interactions is required.

This thesis describes some methods which enable us to construct a particular class of relatively small designs using 2^n and 3^m designs as building blocks, while maintaining as much orthogonality of the design as possible.

Three methods are discussed to construct designs for quantitative factors:

- (i) The first method constructs plans from the 2^n design using the new concept of "design generator". See Chapters 4 and 5.
- (ii) The second method also makes use of the 2^n design, but uses moreover properties of the D -optimal designs developed in Chapter 3. See Chapter 5.
- (iii) The third method, described in Chapter 6, uses orthogonal columns of some main-effect designs.

In the Appendix more than 40 plans are given, 39 of which are new, usually with the appropriate variance - covariance matrix of the parameter estimates and some additional information. Extensive use was made of the Personal Computer Package "Math Cad" to construct and evaluate these designs.

The designs developed in this thesis have been constructed using the following restrictions:

- (i) Factors have two, three or four levels.
- (ii) The two-level factors may be qualitative or quantitative.
- (iii) The three- and four-level factors are quantitative and the levels are equally spaced.
- (iv) All interactions except of the type "linear \times linear" are ignored.
- (v) The mathematical model of the observations is a second degree polynomial.

No special effort was made to construct D -optimal designs as described by *Mitchell* (1974a). We rather used the other approach namely of constructing a number of designs, then judging and comparing the designs as is done in Chapter 7, using a number of criteria. These designs have three advantages over many other designs with quantitative factors.

- (i) The number of levels for each factor varies between 2 and 4 whereas many existing designs, such as the central composite designs of *Cochran and Cox* (1957) and the *Box and Behnken* (1960) designs, require each factor to have the same number of levels.
- (ii) Many designs contain a two-level factor which may of course be either qualitative or quantitative.
- (iii) There is a great variety of small designs to choose from.

CHAPTER 2¹

Some general aspects of linear regression theory and experimental design

2.1. Introduction

Since we have to use the linear regression model and some other aspects of regression theory and experimental design, such as *D*-efficiency, *G*-efficiency, the techniques of replacement and collapsing, frequently in Chapters 3, ..., 7, we shall briefly review these in the following sections.

2.2. The linear regression model

The major purpose of experimental work is to find mechanisms, such as biological, physical and chemical mechanisms of products or processes.

More precisely, the effect of a number of quantitative factors or independent variables x_1, x_2, \dots, x_k on a dependent variable y has to be found.

Especially when these mechanisms are unknown, it is usually assumed that the relation between y on the one and x_1, x_2, \dots, x_k on the other hand can be described by a linear model, which is written in matrix notation as

$$y = \mathbf{f}'(\mathbf{x})\boldsymbol{\beta} + \varepsilon . \quad (2.1)$$

The vectors $\mathbf{f}'(\mathbf{x})$ and $\boldsymbol{\beta}$ are explained below.

The linear model which we shall use will be a second degree polynomial in the variables x_1, x_2, \dots, x_k .

To estimate the vector of parameters $\boldsymbol{\beta}$ we carry out observations y_1, y_2, \dots, y_N and the sampling model is written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} . \quad (2.2)$$

We use the following notation:

¹Many points discussed in Sections 2.3 and 2.4 were obtained from *Oorschot (1974)*.

- N : The number of observations y in an experiment.
- P : The number of parameters β in the linear or regression model.
- \mathbf{Y} : An $N \times 1$ vector of observations or responses y .
- \mathbf{x}_i : $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})'$ is the $k \times 1$ vector of predictor or independent variables, where \mathbf{x}_i is the i^{th} design point in the k -dimensional region R and $x_{i1}, x_{i2}, \dots, x_{ik}$ are the levels of the variables or factors x_1, x_2, \dots, x_k in the i^{th} experiment ($i = 1, 2, \dots, N$).
- \mathbf{X} : An $N \times P$ matrix (of rank P) of constants, with row i containing $\mathbf{f}'(\mathbf{x}_i)$, where $\mathbf{f}'(\mathbf{x}_i) = (f_1(\mathbf{x}_i), f_2(\mathbf{x}_i), \dots, f_P(\mathbf{x}_i))$, in which the functions f_1, f_2, \dots, f_P are known.

Therefore we have

$$\mathbf{X} = \begin{bmatrix} f_1(\mathbf{x}_1) & f_2(\mathbf{x}_1) & \cdots & f_P(\mathbf{x}_1) \\ f_1(\mathbf{x}_2) & f_2(\mathbf{x}_2) & \cdots & f_P(\mathbf{x}_2) \\ \vdots & \vdots & & \vdots \\ f_1(\mathbf{x}_N) & f_2(\mathbf{x}_N) & \cdots & f_P(\mathbf{x}_N) \end{bmatrix}.$$

- \mathbf{X}' : The transpose of \mathbf{X} .
- β : The $P \times 1$ vector of parameters to be estimated.
(The model (2.1) is called linear because it is linear in the parameters β .)
- ϵ : An $N \times 1$ vector of independently and identically distributed random variables each having mean 0 and unknown variance σ^2 .
The elements of the vector ϵ are the experimental errors.
- k : The number of independent variables or quantitative factors x .
- R : A k -dimensional experimental region in which it is feasible to perform experiments.
- c_{pq} : The elements of $(\mathbf{X}'\mathbf{X})^{-1}$, $p, q = 1, 2, \dots, P$.

The least squares estimate of β is

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}. \quad (2.3)$$

The covariance of $\hat{\beta}$ is

$$\mathcal{F}(\hat{\beta}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}. \quad (2.4)$$

At any point $\mathbf{x} \in R$, the predicted (or estimated) value of the “true” response is

$$\hat{y}(\mathbf{x}) = \mathbf{f}'(\mathbf{x})\hat{\beta} \quad (2.5)$$

with variance

$$\text{var}(\hat{y}(\mathbf{x})) = \sigma^2 \mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}). \quad (2.6)$$

The residual sum of squares is given by

$$\boldsymbol{\varepsilon}'\boldsymbol{\varepsilon} = \mathbf{Y}'\mathbf{Y} - \hat{\beta}'\mathbf{X}'\mathbf{Y}. \quad (2.7)$$

Equation (2.4) is important in the search for new designs for we want an $(\mathbf{X}'\mathbf{X})^{-1}$ matrix with the following characteristics:

- Small diagonal elements c_{pq} because they correspond with small variances of the $\hat{\beta}$'s.
- Off-diagonal elements which are preferably zero because they correspond to estimates which are mutually orthogonal. In case an off-diagonal element c_{pq} is not zero we shall calculate the corresponding correlation coefficient $\rho_{pq} = \frac{c_{pq}}{\sqrt{(c_{pp} c_{qq})}}$. We shall try to construct designs for which the ρ_{pq} are small, preferably $|\rho_{pq}| \leq 0.5$.

The term $\hat{\beta}'\mathbf{X}'\mathbf{Y}$ in Equation (2.7) can very often be divided into orthogonal segments corresponding to $\hat{\beta}$'s or to groups of $\hat{\beta}$'s which are mutually orthogonal.

2.3. *D*-optimality and *D*-efficiency

To design an experiment it is necessary to find for each of the design points $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})'$ the values of the vector elements $x_{i1}, x_{i2}, \dots, x_{ik}$.

The choice of these values has to be made in such a way that the estimators $\hat{\beta}$ have favourable properties.

There are many criteria for such properties. One of these is *D*-optimality, which is achieved

when $\det(\mathcal{F}(\hat{\beta}))$ is minimized.

This minimization is desired because $(\det(\mathcal{F}(\hat{\beta})))^{1/2}$ is proportional to the hyper volume of the joint confidence region (an ellipsoid) of the β 's .

From (2.4) it follows that

$$\det(\mathcal{F}(\hat{\beta})) = \sigma^{2P} \det((\mathbf{X}'\mathbf{X})^{-1})$$

or

$$\det(\mathcal{F}(\hat{\beta})) = \sigma^{2P} / \det(\mathbf{X}'\mathbf{X}) . \quad (2.8)$$

The minimization of $\det(\mathcal{F}(\hat{\beta}))$ therefore corresponds with the maximization of

$$\det(\mathbf{X}'\mathbf{X}) .$$

In the Appendix the expression $|\mathbf{X}\mathbf{T}\mathbf{X}|$ is used for $\det(\mathbf{X}'\mathbf{X})$.

DEFINITION 2.3.1

A D_N -optimum design is a group of design points $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ from R , such that $\det(\mathbf{X}'\mathbf{X})$ is a mazimum.

We recall that

$$\mathbf{X} = \begin{bmatrix} f_1(\mathbf{x}_1) & f_2(\mathbf{x}_1) & \cdots & f_P(\mathbf{x}_1) \\ f_1(\mathbf{x}_2) & f_2(\mathbf{x}_2) & \cdots & f_P(\mathbf{x}_2) \\ \vdots & \vdots & & \vdots \\ f_1(\mathbf{x}_N) & f_2(\mathbf{x}_N) & \cdots & f_P(\mathbf{x}_N) \end{bmatrix} ,$$

and rank \mathbf{X} is equal to P .

The matrix $\mathbf{X}'\mathbf{X}$ can now be written as

$$\mathbf{X}'\mathbf{X} = \sum_{i=1}^N \mathbf{f}(\mathbf{x}_i) \mathbf{f}'(\mathbf{x}_i) , \quad (2.9)$$

where $\mathbf{f}'(\mathbf{x}_i) = (f_1(\mathbf{x}_i), f_2(\mathbf{x}_i), \dots, f_P(\mathbf{x}_i))$ is the i^{th} row vector of \mathbf{X} .

In many cases we may have more than one observation in a certain design point \mathbf{x}_i . Then we have some identical rows in \mathbf{X} , and we can write the matrix $\mathbf{X}'\mathbf{X}$ as

$$\mathbf{X}'\mathbf{X} = \sum_{i=1}^r n_i \mathbf{f}(\mathbf{x}_i) \mathbf{f}'(\mathbf{x}_i), \quad (2.10)$$

where n_i is the number of times that design point \mathbf{x}_i is used in the design and r is equal to the number of different design points ($i = 1, 2, \dots, r$; $n_i \geq 0$; $\sum_{i=1}^r n_i = N$).

We now define

$$p_i = n_i / N.$$

Given the definition of n_i and N it follows that p_i is equal to the fraction of design points with vector

$$\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})'.$$

We may now write (2.10) as

$$\mathbf{X}'\mathbf{X} = N \sum_{i=1}^r p_i \mathbf{f}(\mathbf{x}_i) \mathbf{f}'(\mathbf{x}_i). \quad (2.11)$$

A fraction p_i of all experiments is performed in design point \mathbf{x}_i ($i = 1, 2, \dots, r$). It stands to reason that only an integer number of experiments can be carried out in design point \mathbf{x}_i .

When N is given we have the requirement that p_i is a multiple of $(1/N)$, ($i = 1, 2, \dots, r$).

We shall however drop this requirement. This simplification provides the possibility to make statements which are independent of N and to compare experiments with different values of N .

For instance the statement: "Perform $(1/3)$ of the experiment in each of the design points \mathbf{x}_1 , \mathbf{x}_2 and \mathbf{x}_3 ", only has a meaning, strictly speaking, if N is the multiple of 3.

However, such a statement gives for an arbitrary $N \geq P$ an indication about the number of experiments in each of the 3 design points. Moreover if we drop the above requirement we very often shall simplify the computational effort considerably.

We only require that $p_i \geq 0$ and $\sum_{i=1}^r p_i = 1$. We can now define an experimental design as

$$\xi = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r; p_1, p_2, \dots, p_r). \quad (2.12)$$

The design is now viewed as a probability measure on R . The fact that (2.12) does not contain N implies that the matrix $\mathbf{X}'\mathbf{X}$ no longer has its central position but a matrix \mathbf{M} has, which is defined as

$$\mathbf{M}(\xi) = \sum_{i=1}^r p_i \mathbf{f}(\mathbf{x}_i) \mathbf{f}'(\mathbf{x}_i), \quad (2.13)$$

where the symbol ξ indicates the dependence of \mathbf{M} on the choice of r different design points \mathbf{x}_i and corresponding fractions p_i . It should be noted that (2.13) does not contain N .

Note that if $\mathbf{X}'\mathbf{X}$ can be written as in (2.11), then we have $\mathbf{M}(\xi) = \mathbf{X}'\mathbf{X}/N$.

We can now define a D -optimal design as follows:

DEFINITION 2.3.2

An experimental design $\xi^0 = (\mathbf{x}_1^0, \mathbf{x}_2^0, \dots, \mathbf{x}_r^0; p_1^0, p_2^0, \dots, p_r^0)$ is D -optimal if and only if

$$\det(\mathbf{M}(\xi^0)) = \max_{\xi} \det(\mathbf{M}(\xi)). \quad (2.14)$$

DEFINITION 2.3.3

The D -efficiency of an experimental design ξ is given by the formula

$$D\text{-efficiency} = 100(\det(\mathbf{M}(\xi)) / \det(\mathbf{M}(\xi^0)))^{(1/P)}, \quad (2.15)$$

where P is equal to the number of parameters β in the regression model.

2.4. G -optimality and G -efficiency

According to equation (2.6) in Section 2.2 we found that the variance of the true response $\text{var}(\hat{y}(\mathbf{x}))$ equals

$$\text{var}(\hat{y}(\mathbf{x})) = \sigma^2 \mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}). \quad (2.16)$$

We now formulate a theorem for an experimental design

$$\xi_N = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r; n_1, n_2, \dots, n_r)$$

with design points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r$ in R , where n_1, n_2, \dots, n_r are the numbers of observations.
 $(\sum_{i=1}^r n_i = N, n_i \geq 0)$.

THEOREM 2.4.1

For the linear model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ and the design ξ_N we have

$$a) \quad \sum_{i=1}^r n_i \text{var}(\hat{y}(\mathbf{x}_i)) = P \sigma^2 . \quad (2.17)$$

(In words: The weighted sum of the variances of the estimated predicted response equals $P \sigma^2$; the summation takes place over the points of the experimental design.)

$$b) \quad \max_{\mathbf{x} \in R} \text{var}(\hat{y}(\mathbf{x})) \geq P \sigma^2 / N . \quad (2.18)$$

The largest variance of the estimated predicted response is at least equal to $P \sigma^2 / N$. It is to be noted that all the points of R are considered.

A suitable criterion for a well designed experiment could be: Choose an experimental design which minimizes the largest variance of the estimated response.

This leads to the following

DEFINITION 2.4.1

A G_N -optimal design is a group of design points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ from R , chosen in such a way that

$$\max_{\mathbf{x} \in R} \mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}) \text{ is a minimum .}$$

Since $\mathbf{M}(\xi) = \mathbf{X}'\mathbf{X}/N$ we have

$$\mathbf{M}^{-1}(\xi) = N(\mathbf{X}'\mathbf{X})^{-1} . \quad (2.19)$$

Using (2.16) we may write

$$N \text{var}(\hat{y}(\mathbf{x})) = N \sigma^2 \mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$$

or

$$N \operatorname{var}(\hat{y}(\mathbf{x})) = \sigma^2 \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}). \quad (2.20)$$

We define

$$d(\mathbf{x}, \xi) = \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}). \quad (2.21)$$

Using (2.20) and (2.21) we find

$$\operatorname{var}(\hat{y}(\mathbf{x})) = \sigma^2 d(\mathbf{x}, \xi)/N. \quad (2.22)$$

From (2.17) and (2.22) we obtain

$$\sum_{i=1}^r n_i \sigma^2 d(\mathbf{x}_i, \xi)/N = \sigma^2 \sum_{i=1}^r p_i d(\mathbf{x}_i, \xi) = P \sigma^2$$

or

$$\sum_{i=1}^r p_i d(\mathbf{x}_i, \xi) = P. \quad (2.23)$$

From (2.18) and (2.22) we derive

$$\max_{\mathbf{x} \in R} \sigma^2 d(\mathbf{x}, \xi)/N \geq P \sigma^2/N$$

or

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) \geq P. \quad (2.24)$$

In Section 2.3 we defined D -optimality independent of N . We can now likewise define G -optimality independent of N . We then have

DEFINITION 2.4.2

A design $\xi' = (\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_r; p'_1, p'_2, \dots, p'_r)$ is G -optimal if and only if

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi') = \min_{\xi} \max_{\mathbf{x} \in R} d(\mathbf{x}, \xi).$$

DEFINITION 2.4.3

The G -efficiency of a design ξ is defined as

$$G\text{-efficiency} = 100(P / \max_{\mathbf{x} \in R} d(\mathbf{x}, \xi)). \quad (2.25)$$

We shall now calculate the G -efficiency for a design with a particular N .

According to (2.22) we may write

$$d(\mathbf{x}, \xi) = N \text{var}(\hat{y}(\mathbf{x})) / \sigma^2$$

and therefore we have

$$G\text{-efficiency} = 100(P \sigma^2 / N \max_{\mathbf{x} \in R} \text{var}(\hat{y}(\mathbf{x}))) \quad (2.26)$$

or

$$G\text{-efficiency} = 100P / (N \max_{\mathbf{x} \in R} (\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))). \quad (2.27)$$

From (2.25) it follows that a design has a G -efficiency of 100% if $\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = P$.

2.5. The general equivalence theorem

If we assume that p_i ($i = 1, 2, \dots, r; \sum_{i=1}^r p_i = 1$) can have any value between 0 and 1, the general equivalence theorem applies, which states that the design

$$\xi^0 = (\mathbf{x}_1^0, \mathbf{x}_2^0, \dots, \mathbf{x}_r^0; p_1^0, p_2^0, \dots, p_r^0),$$

which is D -optimal (see (2.14)), coincides with the design

$$\xi' = (\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_r; p'_1, p'_2, \dots, p'_r),$$

which is G -optimal.

This theorem, due to *Kiefer and Wolfowitz* (1960), can be summarized as follows

THEOREM 2.5.1

(The general equivalence theorem)

The following assertions are equivalent.

$$\det(\mathbf{M}(\xi')) = \max_{\xi} \det(\mathbf{M}(\xi)) . \quad (2.28)$$

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi') = \min_{\xi} \max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) . \quad (2.29)$$

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi') = P . \quad (2.30)$$

It means that design ξ' is D -optimal and G -optimal.

It is to be noted that such a design ξ' is, generally speaking, not exact but approximate, since it can only be realized in practice, if each p_i is a multiple of $1/N$.

COROLLARY 2.5.1

We can use (2.30) to verify whether a particular design is D -optimal. If (2.30) is satisfied, then the design is D -optimal.

Note that D -optimality is essentially a parameter estimation criterion whereas G -optimality is a response estimation criterion. The equivalence theorem states that these two design criteria are identical when the design is expressed as a probability measure on R .

It is generally speaking, difficult to find a D -optimal design. In practice a certain design, which is likely to be D -optimal, is constructed. Afterwards the value $\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi)$ is calculated. If this value equals P , we have found a D -optimal design.

If this value is not equal to P , we add points to the design where $d(\mathbf{x}, \xi)$ obtains its maximum. The design will then have a better D -efficiency.

As an example we shall construct a D -optimal design in the next section.

2.6. The construction of a D -optimal design with three factors

It is required to construct a D -optimal design for the linear model

$$\mathbf{y} = \beta_0 x_0 + \beta_{11} x_1^2 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \varepsilon . \quad (2.31)$$

Therefore 3 factors have linear terms, all first order interactions are present and one of the 3 factors has a quadratic term.

The ranges of the x 's are scaled to a common interval $-1 \leq x_i \leq +1$ and the three-dimensional region R is therefore a cube.

In Section 2.2 we defined

$$\mathbf{f}'(\mathbf{x}_i) = (f_1(\mathbf{x}_i), f_2(\mathbf{x}_i), \dots, f_p(\mathbf{x}_i)),$$

the i^{th} row of the matrix X . According to (2.31) we have

$$f_1(\mathbf{x}_i) = f_1(x_{i1}, x_{i2}, x_{i3}) = x_0 = 1$$

$$f_2(\mathbf{x}_i) = f_2(x_{i1}, x_{i2}, x_{i3}) = x_{i1}^2,$$

$$f_3(\mathbf{x}_i) = f_3(x_{i1}, x_{i2}, x_{i3}) = x_{i1}$$

$$f_4(\mathbf{x}_i) = f_4(x_{i1}, x_{i2}, x_{i3}) = x_{i2}$$

(2.32)

$$f_5(\mathbf{x}_i) = f_5(x_{i1}, x_{i2}, x_{i3}) = x_{i3}$$

$$f_6(\mathbf{x}_i) = f_6(x_{i1}, x_{i2}, x_{i3}) = x_{i1}x_{i2}$$

$$f_7(\mathbf{x}_i) = f_7(x_{i1}, x_{i2}, x_{i3}) = x_{i1}x_{i3}$$

$$f_8(\mathbf{x}_i) = f_8(x_{i1}, x_{i2}, x_{i3}) = x_{i2}x_{i3}.$$

In our effort to find a D -optimal design we use an intuitive approach.

We define an experimental design by choosing levels, -1 , 0 and $+1$ for x_1 , levels -1 and $+1$ for x_2 and x_3 and choose as design points the $3 \times 2 \times 2$ factor-level combinations.

We assume that a fraction α of the observations takes place in each of the 2^3 design points where the factors have the levels -1 or $+1$. A fraction β of the observations is carried out in each of the four design points where x_1 has the level 0 and the two other factors have levels -1 or $+1$.

The design matrix \mathbf{DM} can now be written as

$$\mathbf{DM} = \begin{array}{cccc}
& x_1 & x_2 & x_3 & \text{fraction} \\
\left[\begin{array}{l}
-1 & -1 & -1 \\
-1 & 1 & -1 \\
-1 & -1 & 1 \\
-1 & 1 & 1 \\
1 & -1 & -1 \\
1 & 1 & -1 \\
1 & -1 & 1 \\
1 & 1 & 1 \\
0 & -1 & -1 \\
0 & 1 & -1 \\
0 & -1 & 1 \\
0 & 1 & 1
\end{array} \right] & \begin{array}{l}
\alpha \\
\alpha \\
\alpha \\
\alpha \\
\alpha \\
\alpha \\
\alpha \\
\alpha \\
\beta \\
\beta \\
\beta \\
\beta
\end{array}
\end{array} \tag{2.33}$$

The matrix \mathbf{X} can now be written as

$$\mathbf{X} = \begin{array}{cccccccc}
x_{0i} & x_{i1}^2 & x_{i1} & x_{i2} & x_{i3} & x_{i1}x_{i2} & x_{i1}x_{i3} & x_{i2}x_{i3} & \text{fraction } p_i \\
\left[\begin{array}{l}
1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & \alpha \\
1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & \alpha \\
1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & \alpha \\
1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & \alpha \\
1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & \alpha \\
1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & \alpha \\
1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & \alpha \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & \alpha \\
1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & \beta \\
1 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & \beta \\
1 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & \beta \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & \beta
\end{array} \right]
\end{array} \tag{2.34}$$

Using (2.13) we have

$$\mathbf{M}(\xi) = \sum_{i=1}^r p_i \mathbf{f}(\mathbf{x}_i) \mathbf{f}'(\mathbf{x}_i).$$

We find

$$\mathbf{M}(\xi) = \begin{bmatrix} 8\alpha + 4\beta & 8\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 8\alpha & 8\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8\alpha + 4\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8\alpha + 4\beta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8\alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8\alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8\alpha + 4\beta \end{bmatrix}. \quad (2.35)$$

Since $8\alpha + 4\beta = 1$ we can easily find that

$$\det(\mathbf{M}(\xi)) = (8\alpha)^4 (1 - 8\alpha). \quad (2.36)$$

This value reaches a maximum for $\alpha = 0.1$ and since $8\alpha + 4\beta = 1$ we have $\beta = 0.05$.

Substituting $\alpha = 0.1$ in (2.36) we find

$$\max \det(\mathbf{M}(\xi)) = 0.08192.$$

We now have to prove that (2.33) is a D -optimal design.

We shall use the equivalence theorem and therefore calculate, see also (2.21)

$$d(\mathbf{x}, \xi) = \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}). \quad (2.37)$$

We have

$$\mathbf{f}'(\mathbf{x}) = (1, x_1^2, x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3). \quad (2.38)$$

To find $\mathbf{M}^{-1}(\xi)$ we first calculate $\mathbf{M}(\xi)$ by substituting $\alpha = 0.1$ and $\beta = 0.05$ in (2.35).

Omitting ξ , we obtain

$$\mathbf{M} = \begin{bmatrix} 1 & 0.8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.8 & 0.8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad (2.39)$$

$$\mathbf{M}^{-1} = \begin{bmatrix} 5 & -5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -5 & 6.25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.25 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.25 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad (2.40)$$

$$\mathbf{M}^{-1} \mathbf{f}(\mathbf{x}) = \begin{bmatrix} 5 - 5x_1^2 \\ -5 + 6.25x_1^2 \\ 1.25x_1 \\ x_2 \\ x_3 \\ 1.25x_1x_2 \\ 1.25x_1x_3 \\ x_2x_3 \end{bmatrix}$$

$$\mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}) = 5 - 5x_1^2 - 5x_1^2 + 6.25x_1^4 + 1.25x_1^2 + x_2^2 + x_3^2 + 1.25x_1^2x_2^2 + 1.25x_1^2x_3^2 + x_2^2x_3^2$$

or

$$\mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}) = 5 - 8.75x_1^2 + 6.25x_1^4 + x_2^2 + x_3^2 + 1.25x_1^2x_2^2 + 1.25x_1^2x_3^2 + x_2^2x_3^2. \quad (2.41)$$

The fourth degree polynomial (2.41) reaches a maximum for

$$x_1 = x_2 = x_3 = \pm 1 \text{ but also for } x_1 = 0, x_2 = x_3 = \pm 1 .$$

Substituting each set of values into (2.41) we obtain

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = \max_{\mathbf{x} \in R} \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}) = 8 = P . \quad (2.42)$$

According to the equivalence theorem we now have proved that design (2.33) is D -optimal. Since $\alpha = 0.1$ and $\beta = 0.05$ we can realize this design in practice when we take $N = 20$, because for $N = 20$ we have that α and β are a multiple of $(1/N)$ since $\alpha = 2/N$ and $\beta = 1/N$. The D -optimum design therefore has 2 observations in each of the 8 design points where the factors have the levels -1 or $+1$ and one observation in each of the 4 design points where x_1 has the level 0 and the two other factors have levels -1 or $+1$.

A graphical presentation of the design points in R , a 3-dimensional region, is given in Figure 2.1.

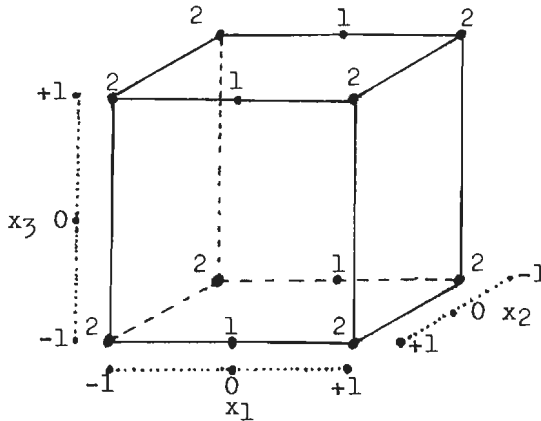


Figure 2.1. A D -optimal design with three factors.

It is interesting to know the value of the D -efficiency of the $3 \times 2 \times 2$ factorial design if one observation is taken in each of the 12 factor-level combinations.

We then have $p_i = 1/12$ ($i = 1, 2, \dots, 12$) or $\alpha = \beta = 1/12$.

Substituting this value in (2.36) we find

$$\det(\mathbf{M}) = (8/12)^4 (1 - 8/12) = 0.0658436214 .$$

We found $\max \det(\mathbf{M}(\xi)) = 0.08192$.

Therefore, using (2.15)

$$D\text{-efficiency} = 100(0.0658436214/0.08192)^{(1/8)} = 97.31\% .$$

To calculate the G -efficiency of the same design we first of all compute

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = \max_{\mathbf{x} \in R} \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}) .$$

See also (2.21) and (2.25).

To calculate $\mathbf{M}^{-1}(\xi)$ we substitute $\alpha = \beta = 1/12$ in (2.35) and we find

$$\mathbf{M}^{-1}(\xi) = \begin{bmatrix} 3 & -3 & 0 & 0 & 0 & 0 & 0 & 0 \\ -3 & 4.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} .$$

We already know, see (2.38),

$$\mathbf{f}'(\mathbf{x}) = (1, x_1^2, x_1, x_2, x_3, x_1 x_2, x_1 x_3, x_2 x_3) .$$

After some calculations we find

$$\begin{aligned} d(\mathbf{x}, \xi) &= \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}) \\ &= 3 - 4.5x_1^2 + 4.5x_1^4 + x_2^2 + x_3^2 + 1.5(x_1^2 x_2^2 + x_1^2 x_3^2) + x_2^2 x_3^2 . \end{aligned} \quad (2.43)$$

It can easily be seen that $d(\mathbf{x}, \xi)$ reaches a maximum for $x_1 = x_2 = x_3 = \pm 1$.

Substituting these values into (2.43) we find

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = 9 .$$

Using (2.25) we obtain

$$G\text{-efficiency} = 100 \times 8/9 = 88.9\% .$$

The $3 \times 2 \times 2$ factorial design is therefore very satisfactory, if it is used to estimate a linear regression model, because it has a high D - and G -efficiency.

2.7. The value of $d(\mathbf{x}, \xi)$ for D -optimal designs

In the previous section we found that the value of $d(\mathbf{x}, \xi)$ was equal to P for all design points. This is not a coincidence but stems from the following Theorem 2.7.1.

THEOREM 2.7.1

The condition $\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = P$ is satisfied by all the design points of a D -optimal design.

Proof

According to (2.23) we have

$$\sum_{i=1}^r p_i d(\mathbf{x}_i, \xi) = P .$$

Since $\sum_{i=1}^r p_i = 1$, we may write

$$\sum_{i=1}^r p_i d(\mathbf{x}_i, \xi) = P \sum_{i=1}^r p_i = \sum_{i=1}^r p_i P$$

or

$$\sum_{i=1}^r p_i (d(\mathbf{x}_i, \xi) - P) = 0 . \tag{2.44}$$

Because $\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = P$, since we have a D -optimal design, it follows that each $d(\mathbf{x}_i, \xi) \leq P$ and each value $d(\mathbf{x}_i, \xi) - P$ is either negative or zero.

However, it is obvious that (2.44) can only be satisfied if for all $i = 1, 2, \dots, r$, we have

$$d(\mathbf{x}_i, \xi) - P = 0$$

or

$$d(\mathbf{x}_i, \xi) = P \quad \text{q.e.d.}$$

2.8. The 2^2 design

Because we will use the 2^n designs for constructing other designs we first give the usual 2^2 design in Table 2.1. This particular design shall also be used to introduce the techniques of replacement and collapsing.

The levels of the factors A and B have been given in three different ways as indicated in Table 2.1.

	A		(1)	a
		A	-1	+1
B		x_A	0	1
	B	x_B		
(1)	-1	0	y_1	y_2
b	+1	1	y_3	y_4

Table 2.1. The 2^2 design.

For the time being we assign the variables A and B to the factors A and B . These variables take on the value -1 or $+1$.

We then have the following well known mathematical model for the observations y_i which are normally distributed mutually independent variables with common variance σ^2 and

$$E(y_i) = \beta_0 x_{0i} + \beta_1 A_i + \beta_2 B_i + \beta_{12} A_i B_i$$

or in matrix notation

$$E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta},$$

where

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}, \quad \mathbf{X} = \begin{array}{cccc} x_{0i} & A_i & B_i & A_i B_i \\ +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & +1 & +1 & +1 \end{array}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{12} \end{bmatrix}.$$

Using Equation (2.3) we may write

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}.$$

In the case of a 2^2 design we therefore find the following estimator for $\boldsymbol{\beta}$.

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_{12} \end{bmatrix} = \begin{bmatrix} (y_1 + y_2 + y_3 + y_4)/4 \\ (-y_1 + y_2 - y_3 + y_4)/4 \\ (-y_1 - y_2 + y_3 + y_4)/4 \\ (y_1 - y_2 - y_3 + y_4)/4 \end{bmatrix}$$

and $\text{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ with

$$(\mathbf{X}'\mathbf{X}) = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix} \quad \text{and} \quad (\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{bmatrix}.$$

Therefore

$$\begin{bmatrix} \sigma_{\hat{\beta}_0}^2 \\ \sigma_{\hat{\beta}_1}^2 \\ \sigma_{\hat{\beta}_2}^2 \\ \sigma_{\hat{\beta}_{12}}^2 \end{bmatrix} = \begin{bmatrix} \sigma^2/4 \\ \sigma^2/4 \\ \sigma^2/4 \\ \sigma^2/4 \end{bmatrix}.$$

The 2^2 design has some nice properties.

- The design is D - and G -optimal.
- It is efficient because all the observations are being used to estimate each parameter.
- The matrix $(\mathbf{X}'\mathbf{X})^{-1}$ is diagonal and that means that all the estimates $\hat{\beta}$ are uncorrelated and have, given the numbers of observations, minimum variance.

We shall therefore always try to construct designs with a diagonal $(\mathbf{X}'\mathbf{X})^{-1}$ matrix or if that is not possible to obtain an $(\mathbf{X}'\mathbf{X})^{-1}$ matrix with many off-diagonal elements equal to zero.

2.9. The technique of replacement

If we employ a 2^2 design, we have four treatments as shown in the preceding section. If we use a four-level factor we also have four treatments.

We can therefore associate the treatments of the 2^2 design with the treatments of the four-level factor and establish a one-to-one correspondence between them.

This correspondence is given in Table 2.2, where the four equally spaced levels of P are indicated with $x_P = 0, 1, 2$ and 3 .

A	(1)		a	
A	-1		+1	
x_A	0		1	
B	(1)	b	(1)	b
B	-1	+1	-1	+1
x_B	0	1	0	1
obs.	y_1	y_3	y_2	y_4
value				
of x_P	0	1	2	3

Table 2.2. The 2^2 design with four-level factor P .

The relation given in Table 2.2 has a great practical value, because it is now possible to take two factors out of a 2^n design or a fraction thereof and replace these two factors by an equally spaced four-level factor P .

This technique is called replacement. See *Addelman* (1962a, 1963).

We are now able to use a 2^n design as a building block for designs with a number of quantitative factors having four levels. We shall develop these designs in Chapter 4 and 5. In Section 1.6 we stipulated that the mathematical model of the observations can be described by a second degree polynomial. We can therefore represent the effect of P with a second degree polynomial in x_P .

However, to ensure orthogonality as much as possible, which means many zeros in the $\mathbf{X}'\mathbf{X}$ matrix, we shall employ orthogonal polynomials to represent the P -effect.

The first and second degree orthogonal polynomials of an equally spaced four-level factor are

$$P \text{ (linear)} \quad = Pl = -3 + 2x_P$$

$$P \text{ (quadratic)} \quad = Pq = 1 - 3x_P + x_P^2 .$$

The values of these polynomials can be calculated from

$$P \text{ (linear)} \quad = Pl_i = -3 + 2x_{P_i} \tag{2.45}$$

$$P \text{ (quadratic)} \quad = Pq_i = 1 - 3x_{P_i} + x_{P_i}^2 , \tag{2.46}$$

where x_P can take on the values $x_{P_i} = 0, 1, 2$ or 3 .

Since the polynomials are orthogonal we have

$$\sum_{i=1}^4 Pl_i Pq_i = 0 .$$

The method to calculate these orthogonal polynomials is described in *Addelman* (1962a) and Appendix 6A. This method is also applicable when the levels of P are not equally spaced or do not occur with equal frequency.

Substituting the values $x_{P_i} = 0, 1, 2$ and 3 in (2.45) and (2.46) we obtain orthogonal polynomial values for a four-level factor: See Table 2.3.

x_{P_i}	Pl_i	Pq_i
0	-3	+1
1	-1	-1
2	+1	-1
3	+3	+1

Table 2.3. Orthogonal polynomial values for a four-level factor.

Replacing the two-level factors A and B by one four-level factor is equivalent to replacing the column vectors \mathbf{A} , \mathbf{B} and \mathbf{AB} in the \mathbf{X} matrix by the column vectors \mathbf{Pl} and \mathbf{Pq} of Table 2.3.

To facilitate the construction of new designs later on it is necessary to find the relation between the elements of the set of column vectors $(\mathbf{A}, \mathbf{B}, \mathbf{AB})$ and $(\mathbf{Pl}, \mathbf{Pq})$.

These sets are, together with x_{P_i} , again given in Table 2.4. Note that the x_{P_i} values are not in their natural order.

x_{P_i}	A_i	B_i	$A_i B_i$	Pl_i	Pq_i
0	-1	-1	+1	-3	+1
2	+1	-1	-1	+1	-1
1	-1	+1	-1	-1	-1
3	+1	+1	+1	+3	+1

Table 2.4. Values of x_{P_i} and column vectors \mathbf{A} , \mathbf{B} , \mathbf{AB} , \mathbf{Pl} and \mathbf{Pq} .

Some elementary algebra gives the following relations:

$$\left. \begin{aligned} Pl_i &= 2A_i + B_i \\ Pq_i &= A_i B_i \end{aligned} \right\} \quad (2.47)$$

The formulae (2.45), (2.46) and (2.47) are such that

$$\sum_{i=1}^4 Pl_i = \sum_{i=1}^4 Pq_i = \sum_{i=1}^4 Pl_i Pq_i = 0. \quad (2.48)$$

When we define:

$$Pl = \lambda_1(2A + B) = \lambda_1(-3 + 2x_P)$$

$$Pq = \lambda_2 AB = \lambda_2(1 - 3x_P + x_P^2),$$

where λ_1 and λ_2 are constants, we still have that (2.48) is true and the set (Pl, Pq) still consists of two orthogonal polynomials.

In order to compare designs later on we shall, for a number of designs, standardize the \mathbf{X} matrix in such a way, that the sum of squares of the elements of the columns in the \mathbf{X} matrix equals N , the number of experimental units in the experiment.

The diagonal elements of $\mathbf{X}'\mathbf{X}$ will then be equal to N . This procedure also has the advantage that the variances of the $\hat{\beta}$'s are equal for an orthogonal design and nearly equal if the design is nearly orthogonal.

Hence for the \mathbf{X} matrix corresponding to Table 2.2 we have

$$\sum_{i=1}^4 Pl_i^2 = \sum_{i=1}^4 \lambda_1^2(2A_i + B_i)^2 = 4 = 2^2$$

or

$$\lambda_1^2(3^2 + 1^2 + 1^2 + 3^2) = 4,$$

hence

$$\lambda_1 = \frac{1}{\sqrt{5}}.$$

Likewise we find from

$$\sum_{i=1}^4 Pq_i^2 = 4$$

that $\lambda_2 = 1$. We now summarize the results in Table 2.5.

x_{P_i}	A_i	B_i	$A_i B_i$	$Pl_i = (2A_i + B_i)/\sqrt{5}$	$Pq_i = A_i B_i$
0	-1	-1	+1	$-3/\sqrt{5}$	+1
1	-1	+1	-1	$-1/\sqrt{5}$	-1
2	+1	-1	-1	$+1/\sqrt{5}$	-1
3	+1	+1	+1	$+3/\sqrt{5}$	+1

Table 2.5. Values of x_{P_i} and column vectors **A**, **B**, **AB**, **Pl** and **Pq**.

The following relations now hold.

$$\left. \begin{aligned} Pl_i &= (2A_i + B_i)/\sqrt{5} = (-3 + 2x_{P_i})/\sqrt{5} \text{ or } x_{P_i} = (3 + Pl_i \sqrt{5})/2 \\ Pq_i &= A_i B_i = 1 - 3x_{P_i} + x_{P_i}^2 \end{aligned} \right\} \quad (2.49)$$

We shall frequently use these formulae when constructing new designs.

2.10. The technique of collapsing

In the preceding section it was shown that the 2^n design can be used to construct designs of which some quantitative factors have four equally spaced levels. The factors in the 2^n design which have not been used for replacement will still have two levels.

This replacement technique therefore generates designs with some or all quantitative factors having four equally spaced levels and the remaining factors having two levels.

A number of these designs will be discussed in Chapter 4 and 5. It was however pointed out in Section 1.6 that experimenters want some freedom as to the choice of the number of levels. It is therefore logical that they may wish to have designs, in which some quantitative factors have three levels.

This can be achieved by making use of the technique of collapsing. See *Addelman* (1962a, 1962b), *Margolin* (1969b).

This technique establishes for our purpose a correspondence between the levels of the four-level factor and the levels of a three-level factor.

The following correspondence schemes give two methods to achieve collapsing:

Four-level factor	→	Three-level factor	→	Four-level factor	→	Three-level factor
0	→	0	→	0	→	0
1	→	1	→	1	→	1
2	→	2	→	2	→	2
3	→	1	→	3	→	2

These two schemes are further developed in Table 2.6 and 2.7 where the values of the first and second degree orthogonal polynomials, Pl_i (linear) and Pq_i (quadratic) respectively, are given, together with the relations of these values with the column elements of the 2^2 design and the levels $x_P = 0, 1, 2$ of the three-level factor P .

In Section 5.3 we shall use a third collapsing method using the following correspondence scheme:

Four-level factor	→	Three-level factor
0	→	0
1	→	1
2	→	1
3	→	2

The advantage of this procedure is that zero elements of the $X'X$ matrix remain, for most designs, zero after collapsing. For further details we refer to Section 5.3.

Four-level factor		Three-level factor						
x'_{P_i}		x_{P_i}	A_i	B_i	$A_i B_i$	Pl_i	Pq_i	
0	→	0	-1	-1	+1	$-\sqrt{2}$	+1	
2	→	2	+1	-1	-1	$+\sqrt{2}$	+1	
1	→	1	-1	+1	-1	0	-1	
3	→	1	+1	+1	+1	0	-1	

Table 2.6. Collapsing a four-level factor to a three-level factor with relevant column vectors.

The quantities in Table 2.6 are related as follows

$$Pl_i = (A_i - A_i B_i) / \sqrt{2} \quad (2.50)$$

$$Pq_i = -B_i \quad (2.51)$$

$$Pl_i = (-1 + x_{P_i}) \sqrt{2} \rightarrow x_{P_i} = 1 + Pl_i / \sqrt{2} \quad (2.52)$$

$$Pq_i = 1 - 4x_{P_i} + 2x_{P_i}^2. \quad (2.53)$$

Pl_i and Pq_i are the values of the first and second degree orthogonal polynomials such that

$$\sum_{i=1}^4 Pl_i^2 = \sum_{i=1}^4 Pq_i^2 = 4.$$

Four-level factor		Three-level factor					
x'_{P_i}		x_{P_i}	A_i	B_i	$A_i B_i$	Pl_i	Pq_i
0	→	0	-1	-1	+1	$-5/\sqrt{11}$	$+2\sqrt{(2/11)}$
2	→	2	+1	-1	-1	$+3/\sqrt{11}$	$+1\sqrt{(2/11)}$
1	→	1	-1	+1	-1	$-1/\sqrt{11}$	$-4\sqrt{(2/11)}$
3	→	2	+1	+1	+1	$+3/\sqrt{11}$	$+1\sqrt{(2/11)}$

Table 2.7. Collapsing a four-level factor to a three-level factor with relevant column vectors.

The quantities in Table 2.7 are related as follows

$$Pl_i = (3A_i + B_i - A_i B_i) / \sqrt{11} \quad (2.54)$$

$$Pq_i = (A_i - 3(B_i - A_i B_i) / 2) \sqrt{(2/11)} \quad (2.55)$$

$$Pl_i = (-5 + 4x_{P_i}) / \sqrt{11} \longrightarrow x_{P_i} = (Pl_i \sqrt{11} + 5) / 4 \quad (2.56)$$

$$Pq_i = (+2 - (23/2)x_{P_i} + (11/2)x_{P_i}^2) \sqrt{(2/11)}. \quad (2.57)$$

Equations (2.52), (2.53), (2.56) and (2.57) have been computed using again the method described in *Addelman* (1962a) and Appendix 6A.

Again we have:

$$\sum_{i=1}^4 Pl_i^2 = \sum_{i=1}^4 Pq_i^2 = 4.$$

Equations (2.48), (2.49), (2.52) and (2.53) shall be used in Chapter 4 and 5 because they will turn out to be useful in the search for new designs.

CHAPTER 3

The construction of D -optimal designs for an incomplete quadratic model.¹

3.1. Introduction

It was stated in Chapter 1 and 2 that our regression model will be a second degree polynomial. Since however many of the designs to be constructed have one or more factors with only two levels, see for example Section 2.6, an incomplete quadratic model has to be considered in the sense that d variables have linear and quadratic terms, but the other $(k - d)$ variables have only linear terms. All $\binom{k}{2}$ linear \times linear interactions are however included in the model. So we have the model

$$y = \beta_0 + \beta_{11}x_1^2 + \dots + \beta_{dd}x_d^2 + \beta_1x_1 + \dots + \beta_kx_k + \beta_{12}x_1x_2 + \dots + \beta_{k-1,k}x_{k-1}x_k + \varepsilon, \quad (3.1)$$

where y is the response and $1 \leq d \leq k$.

For the vector of predictor variables

$$\mathbf{x} = (x_1, x_2, \dots, x_k)', \text{ we have, } -1 \leq x_m \leq 1, \quad m = 1, 2, \dots, k.$$

Hence the experimental region R is a k -dimensional cube. The experiment consists of N runs with the values of the predictor variables given by the vectors

$$\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})', \quad i = 1, 2, \dots, N.$$

The i^{th} row of the matrix $\mathbf{X}_{N \times P}$ equals

$$\mathbf{f}'(\mathbf{x}_i) = (1, x_{i1}^2, \dots, x_{id}^2, x_{i1}, x_{i2}, \dots, x_{ik}, x_{i1}x_{i2}, \dots, x_{i,k-1}x_{i,k}).$$

The number of elements in this row equals P , the number of β 's in (3.1) and

$$P = 1 + d + k + \binom{k}{2} = 1 + d + \frac{1}{2}k(k + 1).$$

¹This chapter was written in cooperation with E.E.M. van Berkum, Technical University Eindhoven. See also Van Berkum and Upperman (1991).

In our effort to find a D -optimal design corresponding to model (3.1) we shall use an intuitive strategy as in Section 2.6. This strategy and the relevant calculations will be explained in the next sections.

3.2. The construction of the designs

DEFINITION 3.2.1

We define a design $\xi(\alpha, \beta, \gamma)$ consisting of three subsets from R as follows.

- i) The 2^k vertices of the k -dimensional cube with weights α . This means we choose 2^k design points where the factors have the level $+1$ or -1 .
- ii) The $d2^{k-1}$ design points where one of the d quadratic variables has the value zero and all other variables have the value -1 or $+1$. These points are given weights β ; the points are in the middle of some edges, but not all edges.
- iii) The $\binom{d}{2} 2^{k-2}$ design points where two of the d quadratic variables have the value zero and all other variables have the value -1 or $+1$; these points are given weights γ and are at the center of some two dimensional faces. If $d = 1$ this set is empty.

From i), ii) and iii) above it follows that

$$2^{k-3}(8\alpha + 4d\beta + d(d-1)\gamma) = 1. \quad (3.2)$$

We define

$$u = 2^k\alpha + (d-1)2^{k-1}\beta + \frac{1}{2}(d-1)(d-2)2^{k-2}\gamma, \quad (d \geq 1) \quad (3.3)$$

$$v = 2^k\alpha + (d-2)2^{k-2}\beta + \frac{1}{2}(d-2)(d-3)2^{k-2}\gamma, \quad (d \geq 2). \quad (3.4)$$

Since iii) is empty for $d = 1$, we have for $d = 1$

$$2^{k-3}(8\alpha + 4\beta) = 1 \quad (3.5)$$

$$u = 2^k\alpha \quad (3.6)$$

or

$$\alpha = u/2^k . \tag{3.7}$$

Combining (3.5) and (3.7) we find

$$\beta = (1 - u)/2^{k-1} . \tag{3.8}$$

First we consider for $d > 1$ the matrix $\mathbf{M}(\xi)$, see equation (2.13) of Chapter 2, equal to

$$\mathbf{M}(\xi) = \left[\begin{array}{c|c|c} \mathbf{A} & & \\ \hline & u\mathbf{I}_d & \\ & & \mathbf{I}_{k-d} \\ \hline & & v\mathbf{I}_{\frac{1}{2}d(d-1)} \\ & & & u\mathbf{I}_{d(k-d)} \\ & & & & \mathbf{I}_{\frac{1}{2}(k-d)(k-d-1)} \end{array} \right] , \tag{3.9}$$

where

$$\mathbf{A} = \left[\begin{array}{c|ccc} 1 & u & \dots & u \\ \hline u & & & \\ \vdots & & & \\ u & & & \end{array} \right] .$$

\mathbf{I}_s is the identity matrix of size $s \times s$, \mathbf{J}_s is a matrix of size $s \times s$ with $J_{ij} = 1$ for all i and j .

The determinant of $\mathbf{M}(\xi)$ is equal to

$$\text{Det}(\mathbf{M}(\xi)) = D = u^{d(k-d+1)} v^{\binom{d}{2}} (u - v)^{d-1} (u + (d - 1)v - du^2) . \tag{3.10}$$

The maximum value of (3.10) is determined by differentiating with respect to u and v and putting the result equal to zero. We find

$$\begin{aligned} \frac{\partial D}{\partial u} &= (k - d + 2) u^2 + (d - 2)(k - d + 2) uv - (d(k - d) + 2d + 1) u^3 \\ &\quad - (d - 1)(k - d + 1) v^2 + (d(k - d + 1) + 2) u^2 v = 0 \end{aligned} \tag{3.11}$$

$$\frac{\partial D}{\partial v} = u^2 + (d-2)uv - du^3 - (d+1)v^2 + (d+2)u^2v = 0. \quad (3.12)$$

Eliminating v^2 from (3.11) and (3.12) yields an expression for v as a function of u . This value of v is substituted into (3.12). After some algebraic calculations we find

$$u_0 = \frac{(2k-d+3)[2k(d+1)+d+7+(d-1)\sqrt{4k^2+12k+17}]}{4(k+2)(2dk-d^2+3d+2)} \quad (3.13)$$

$$v_0 = \frac{(2k-d+3)[(4k^2+8k+9)d+2k-5+(2dk+d+3)\sqrt{4k^2+12k+17}]}{8(k+2)^2(2dk-d^2+3d+2)}. \quad (3.14)$$

Solving (3.2), (3.3) and (3.4) for α , β and γ yields

$$\alpha_0 = \frac{1}{2^{k+1}} [(d-2)(d-1) - 2d(d-2)u_0 + d(d-1)v_0] \quad (3.15)$$

$$\beta_0 = \frac{1}{2^{k-1}} [(2d-3)u_0 - (d-1)v_0 - (d-2)] \quad (3.16)$$

$$\gamma_0 = \frac{1}{2^{k-2}} [1 + v_0 - 2u_0]. \quad (3.17)$$

So far we have dealt with the case for $d > 1$. For $d = 1$ we have

$$M(\xi) = \left[\begin{array}{cc|c|c} 1 & u & & \\ u & u & & \\ \hline & u & & \\ & \mathbf{I}_{(k-1)} & & \\ \hline & & u\mathbf{I}_{k-1} & \\ & & & \mathbf{I}_{\frac{1}{2}(k-1)(k-2)} \end{array} \right]$$

and

$$D = \det(M(\xi)) = u^{k+1}(1-u).$$

$$\frac{dD}{dk} = (k+1)(1-u)u^k - u^{k+1} = 0$$

or

$$u_0 = (k + 1) / (k + 2) . \quad (3.18)$$

Using (3.7) and (3.8) we have for $d = 1$

$$\alpha_0 = u_0 / 2^k \quad (3.19)$$

$$\beta_0 = (1 - u_0) / 2^{k-1} . \quad (3.20)$$

3.3. D -optimality of the designs

Although we have found the values of u and v for which $\det(\mathbf{M}(\xi))$ reaches a maximum, we have not proved that the design $\xi(\alpha, \beta, \gamma)$ considered in Section 3.2 is D -optimal, because it might be possible to use other points of the experimental region R , such that $\det(\mathbf{M}(\xi))$ will be larger than the value we found.

We shall however prove the D -optimality of the design $\xi(\alpha, \beta, \gamma)$ through the use of the general equivalence theorem given in Section 2.5.

We therefore shall, as in Section 2.6 calculate

$$\mathbf{d}(\mathbf{x}, \xi) = \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x}) , \quad (3.21)$$

where

$$\mathbf{f}'(\mathbf{x}) = (1, x_1^2, x_2^2, \dots, x_d^2, x_1, x_2, \dots, x_k, x_1 x_2, x_1 x_3, \dots, x_{k-1} x_k) .$$

We have to prove that

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) \leq P \quad (3.22)$$

or

$$\max_{\mathbf{x} \in R} d(\mathbf{x}, \xi) = P ,$$

where $P = 1 + d + k + \binom{k}{2}$.

Using (3.9) we find

$$\mathbf{M}^{-1}(\xi) = \left[\begin{array}{c|c|c} \mathbf{A}^{-1} & & \\ \hline & \frac{1}{u_0} \mathbf{I}_d & \\ \hline & & \mathbf{I}_{k-d} \\ \hline & & \frac{1}{v_0} \mathbf{I}_{\frac{1}{2}d(d-1)} \\ & & \frac{1}{u_0} \mathbf{I}_{d(k-d)} \\ & & \mathbf{I}_{\frac{1}{2}(k-d)(k-d-1)} \end{array} \right], \quad (3.23)$$

with

$$\mathbf{A}^{-1} = \frac{1}{u_0 + (d-1)v_0 - du_0^2} \left[\begin{array}{c|ccc} u_0 + (d-1)v_0 & -u_0 & \dots & -u_0 \\ \hline -u_0 & & & \\ \vdots & & & \\ -u_0 & & & \end{array} \middle| \begin{array}{c} \frac{u_0 + (d-1)v_0 - du_0^2}{u_0 - v_0} \mathbf{I}_d - \frac{v_0 - u_0^2}{u_0 - v_0} \mathbf{J}_d \end{array} \right]. \quad (3.24)$$

For $d(\mathbf{x}, \xi) = \mathbf{f}'(\mathbf{x}) \mathbf{M}^{-1}(\xi) \mathbf{f}(\mathbf{x})$ we obtain

$$\begin{aligned} d(\mathbf{x}, \xi) &= \frac{u_0 + (d-1)v_0}{u_0 + (d-1)v_0 - du_0^2} + \frac{u_0 + (d-1)v_0 - du_0^2 - v_0 + u_0^2}{(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} \sum_{i=1}^d x_i^4 + \\ &+ \frac{-2u_0}{u_0 + (d-1)v_0 - du_0^2} \sum_{i=1}^d x_i^2 - 2 \frac{v_0 - u_0^2}{(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} \sum_{1 \leq i < j \leq d} x_i^2 x_j^2 + \\ &+ \frac{1}{u_0} \sum_{i=1}^d x_i^2 + \sum_{j=d+1}^k x_j^2 + \frac{1}{v_0} \sum_{1 \leq i < j \leq d} x_i^2 x_j^2 + \frac{1}{u_0} \sum_{i=1}^d \sum_{j=d+1}^k x_i^2 x_j^2 + \sum_{d+1 \leq i < j \leq k} x_i^2 x_j^2. \end{aligned} \quad (3.25)$$

Since $-1 \leq x_m \leq +1$ for $m = 1, 2, \dots, k$ we have that the x_i^2 and x_j^2 are at most equal to 1.

The maximum value of $\sum_{j=d+1}^k x_j^2$ therefore equals $(k-d)$.

The maximum value of $\frac{1}{u_0} \sum_{i=1}^d \sum_{j=d+1}^k x_i^2 x_j^2$ therefore equals $\frac{k-d}{u_0} \sum_{i=1}^d x_i^2$.

The maximum value of $\sum_{d+1 \leq i < j \leq k} x_i^2 x_j^2$ equals $\binom{k-d}{2}$ since this sum contains $\binom{k-d}{2}$ terms which are all at most equal to 1.

We therefore have

$$\begin{aligned}
d(\mathbf{x}, \xi) &\leq \frac{u_0 + (d-1)v_0}{u_0 + (d-1)v_0 - du_0^2} + \frac{u_0 + (d-1)v_0 - du_0^2 - v_0 + u_0^2}{(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} \sum_{i=1}^d x_i^4 \\
&\quad - \frac{2u_0}{u_0 + (d-1)v_0 - du_0^2} \sum_{i=1}^d x_i^2 - 2 \frac{v_0 - u_0^2}{(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} \sum_{1 \leq i < j \leq d} x_i^2 x_j^2 \\
&\quad + \frac{1}{u_0} \sum_{i=1}^d x_i^2 + (k-d) + \frac{1}{v_0} \sum_{1 \leq i < j \leq d} x_i^2 x_j^2 + \frac{k-d}{u_0} \sum_{i=1}^d x_i^2 + \binom{k-d}{2}. \quad (3.26)
\end{aligned}$$

The coefficient of $\sum_{1 \leq i < j \leq d} x_i^2 x_j^2$ in (3.26) equals

$$\begin{aligned}
&\frac{-2v_0^2 + 2v_0u_0^2 + u_0^2 + du_0v_0 - u_0v_0 - du_0^3 - u_0v_0 - dv_0^2 + v_0^2 + du_0^2v_0}{v_0(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} = \\
&= \frac{u_0^2 + u_0v_0(d-2) - du_0^3 - v_0^2(d+1) + u_0^2v_0(d+2)}{v_0(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} = 0,
\end{aligned}$$

because the nominator of this expression equals (3.12).

The coefficient of $\sum_{i=1}^d x_i^2$ in (3.26) equals

$$c_1 = \frac{-2u_0}{u_0 + (d-1)v_0 - du_0^2} + \frac{1}{u_0} + \frac{k-d}{u_0} = \frac{-2u_0^2 + (k-d+1)(u_0 + (d-1)v_0 - du_0^2)}{u_0(u_0 + (d-1)v_0 - du_0^2)}.$$

The coefficient of $\sum_{i=1}^d x_i^4$ in (3.26) equals

$$c_2 = \frac{u_0 + (d-1)v_0 - du_0^2 - v_0 + u_0^2}{(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)}.$$

After some calculations we find

$$\begin{aligned}
c_1 + c_2 &= \frac{u_0^2(k-d+2) + (d-2)(k-d+2)u_0v_0 - (d(k-d) + 2d+1)u_0^3}{u_0(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)} \\
&\quad + \frac{-(d-1)(k-d+1)v_0^2 + (d(k-d+1) + 2)u_0^2v_0}{u_0(u_0 - v_0)(u_0 + (d-1)v_0 - du_0^2)}.
\end{aligned}$$

Using (3.11) it follows that $c_1 + c_2 = 0$ or $-c_1 = c_2$. Hence

$$d(\mathbf{x}, \xi) \leq \frac{u_0 + (d-1)v_0}{u_0 + (d-1)v_0 - du_0^2} + (k-d) + \binom{k-d}{2} + c_1 \sum_{i=1}^d (x_i^2 - x_i^4). \quad (3.27)$$

Since $0 \leq x_i^2 \leq 1$, and

$$c_1 = \frac{-2u_0^2 + (k-d+1)(u_0 + (d-1)v_0 - du_0^2)}{u_0(u_0 + (d-1)v_0 - du_0^2)} < 0,$$

verified after some computer calculations, for all the sets (k, d, u_0, v_0) of Table 3.1a, it follows that the maximum value of $c_1 \sum_{i=1}^d (x_i^2 - x_i^4)$ equals zero. Hence

$$d(\mathbf{x}, \xi) \leq \frac{u_0 + (d-1)v_0}{u_0 + (d-1)v_0 - du_0^2} + (k-d) + \binom{k-d}{2}. \quad (3.28)$$

Finally substituting the expressions (3.13) and (3.14) for u_0 and v_0 in (3.28) we obtain after some calculations

$$d(\mathbf{x}, \xi) \leq 1 + d + k + \binom{k}{2} = P, \quad (3.29)$$

and we have shown that (3.22) is true for $d > 1$. We now have to prove that $d(\mathbf{x}, \xi) \leq P$ for $d = 1$. For $d = 1$ we find

$$\begin{aligned} d(\mathbf{x}, \xi) &= \frac{1}{1-u_0} - \frac{x_1^2}{1-u_0} - \frac{x_1^2}{1-u_0} + \frac{x_1^4}{u_0(1-u_0)} + \frac{x_1^2}{u_0} + \sum_{i=2}^k x_i^2 + \\ &+ \frac{1}{u_0} x_1^2 \sum_{i=2}^k x_i^2 + \sum_{2 \leq i < j \leq k} x_i^2 x_j^2. \end{aligned}$$

An upper bound for $\sum_{i=2}^k x_i^2$ equals $(k-1)$, an upper bound for $\sum_{2 \leq i < j \leq k} x_i^2 x_j^2$ is $\binom{k-1}{2}$.

The coefficient of x_1^2 is equal to

$$c_1 = \left[\frac{-2}{1-u_0} + \frac{k}{u_0} \right] = \frac{-2u_0 + k - ku_0}{u_0(1-u_0)} = \frac{-u_0(k+2) + k}{u_0(1-u_0)},$$

but $u_0 = (k+1)/(k+2)$ according to (3.18). Hence

$$c_1 = \frac{-(k+1)+k}{u_0(1-u_0)} = \frac{-1}{u_0(1-u_0)}.$$

Then we have

$$d(\mathbf{x}, \xi) \leq \frac{1}{1-u_0} - \frac{1}{u_0(1-u_0)} (x_1^2 - x_1^4) + (k-1) + \binom{k-1}{2}.$$

Since $-\frac{1}{u_0(1-u_0)} (x_1^2 - x_1^4)$ is at most equal to zero, we have

$$d(\mathbf{x}, \xi) \leq \frac{1}{1-u_0} + (k-1) + \binom{k-1}{2} = k+2 + k-1 + \frac{1}{2}(k-1)(k-2)$$

using $\frac{1}{1-u_0} = k+2$.

Finally $d(\mathbf{x}, \xi) \leq \frac{1}{2}k^2 + \frac{1}{2}k + 2$.

For $d = 1$ we have

$$P = 1 + 1 + k + \binom{k}{2} = 2 + k + \frac{1}{2}k(k-1)$$

or

$$P = \frac{1}{2}k^2 + \frac{1}{2}k + 2$$

and $d(\mathbf{x}, \xi) \leq P$ for $d = 1$ q.e.d.

We can now formulate

THEOREM 3.3.1

If α_0, β_0 and γ_0 as given in (3.15), (3.16), (3.17) or in (3.19), (3.20) are positive then the design $\xi(\alpha_0, \beta_0, \gamma_0)$ of Definition 3.1 is D -optimal for model (3.1).

For $d = 1$ we have the design $\xi(\alpha_0, \beta_0)$. We shall prove that $\xi(\alpha_0, \beta_0)$ is always D -optimal.

The formulae (3.18), (3.19) and (3.20) are applicable if $d = 1$.

It is easily seen from (3.18) that $0 < u_0 < 1$ for $d = 1$.

It is then obvious from (3.19) and (3.20) that $\alpha > 0$ and $\beta > 0$.

If follows that the design $\xi(\alpha_0, \beta_0)$ is always D -optimal for $d = 1$ q.e.d.

The weights α_0, β_0 and γ_0 of (3.15), (3.16) and (3.17) are positive when $1 \leq d \leq k \leq 5$, $k = 6, 7$ and $d \leq k - 1$, $8 \leq k \leq 10$ and $d \leq k - 2$. See also *Van Berkum* and *Upperman* (1991).

No weights were computed for $k > 10$.

In Table 3.1a and 3.1b some design characteristics for $1 \leq d \leq k \leq 5$ are given.

k	d	u_0	v_0	α_0	β_0	γ_0
1	1	0.66667	–	1/3	1/3	–
2	1	0.75000	–	0.187500	0.125000	–
	2	0.74349	0.58316	0.145791	0.080161	0.096193
3	1	0.80000	–	0.100000	0.050000	–
	2	0.79699	0.65489	0.081861	0.035526	0.030451
	3	0.79302	0.65162	0.071976	0.018953	0.032792
4	1	0.83333	–	0.052083	0.020833	–
	2	0.83171	0.70549	0.049093	0.015777	0.010518
	3	0.82969	0.70378	0.038892	0.010189	0.011100
	4	0.82710	0.70158	0.037042	0.003845	0.011844
5	1	0.85714	–	0.026786	0.008929	–
	2	0.85617	0.74316	0.023224	0.007063	0.003853
	3	0.85500	0.74215	0.020670	0.005045	0.004018
	4	0.85358	0.74091	0.019276	0.002823	0.004219
	5	0.85181	0.73938	0.019268	0.000324	0.004469

Table 3.1a. Design characteristics of D -optimal designs.

k	d	Fraction of points with weight α_0 $2^k \alpha_0$	Fraction of points with weight β_0 $d2^{k-1} \beta_0$	Fraction of points with weight γ_0 $d(d-1)2^{k-3} \gamma_0$	$\text{Max}(\det(\mathbf{M}(\xi)))$
1	1	2/3	1/3	-	4/27
2	1	0.75000	0.2500	-	0.105469
	2	0.58316	0.32064	0.09619	0.0114270
3	1	0.80000	0.20000	-	0.0819200
	2	0.65489	0.28421	0.06090	0.00681453
	3	0.57581	0.22743	0.19675	0.000578313
4	1	0.83333	0.16667	-	0.0669796
	2	0.70549	0.25244	0.04207	0.00453077
	3	0.62227	0.24453	0.13320	0.000310235
	4	0.59268	0.12305	0.28427	2.157234 E-005
5	1	0.85714	0.14286	-	0.0566528
	2	0.74316	0.22602	0.03082	0.00323170
	3	0.66143	0.24215	0.09642	0.000185864
	4	0.61682	0.18068	0.20249	1.079587 E-005
	5	0.61658	0.02590	0.35752	6.34783 E-007

Table 3.1b. Design characteristics of D -optimal designs.

The case when $d = 1$ and $k = 3$ has already been dealt with in Section 2.6 and we saw that this design with $\alpha = 0.1$ and $\beta = 0.05$ can be realized in practice if $N = 20$ or a multiple of 20. For $k = d = 1$ we also have simple values for α and β .

Since $\alpha = \beta = 1/3$ and we can construct a 100% D -efficient design if N is a multiple of 3.

The model for $k = d = 1$ is a parabola and is written as

$$y = \beta_0 + \beta_{11}x_1^2 + \beta_1x_1 + \varepsilon. \quad (3.30)$$

According to Definition 3.2.1 in Section 3.2 we then have three different design points namely $x_1 = -1$, $x_1 = 0$ and $x_1 = +1$ and because $\alpha = \beta = 1/3$ the number of observations in each point has to be equal to $N/3$.

In Section 2.3 we defined the D -efficiency of an arbitrary design ξ_1 as

$$D\text{-efficiency} = 100(\det(\mathbf{M}(\xi_1)) / \max(\det(\mathbf{M}(\xi)))^{1/P}). \quad (3.31)$$

See (2.14) and (2.15).

The denominator of (3.31) has been given in Table 3.1b for $1 \leq k \leq d \leq 5$.

Many of these values shall be used in the next chapters to calculate the D -efficiencies of the designs to be developed.

CHAPTER 4

The 2^3 design as a building block for other designs

4.1. Main-effect designs

The 2^3 design has a well-known structure as given in Table 4.1.

		<i>A</i>		(1)		<i>a</i>	
		<i>A</i>		-1		+1	
		<i>B</i>		(1)	<i>b</i>	(1)	<i>b</i>
		<i>B</i>		-1	+1	-1	+1
<i>C</i>		<i>C</i>					
(1)		-1		y_1	y_3	y_2	y_4
<i>c</i>		+1		y_5	y_7	y_6	y_8

Table 4.1. 2^3 design.

The X matrix of column vectors corresponding to the 2^3 design is given in Table 4.2.

Experimental

unit	x_{0i}	A_i	B_i	C_i	$A_i B_i$	$A_i C_i$	$B_i C_i$	$A_i B_i C_i$
1	1	-1	-1	-1	+1	+1	+1	-1
2	1	+1	-1	-1	-1	-1	+1	+1
3	1	-1	+1	-1	-1	+1	-1	+1
4	1	+1	+1	-1	+1	-1	-1	-1
5	1	-1	-1	+1	+1	-1	-1	+1
6	1	+1	-1	+1	-1	+1	-1	-1
7	1	-1	+1	+1	-1	-1	+1	-1
8	1	+1	+1	+1	+1	+1	+1	+1

Table 4.2. The X matrix of column vectors for the 2^3 design.

The \mathbf{X} matrix of Table 4.2 has excellent properties because $\mathbf{X}'\mathbf{X}$ is orthogonal which means that the inner product of two different column vectors always equals zero. Each column vector with the exception of column \mathbf{x}_o has four values -1 and four values $+1$. This means that this \mathbf{X} matrix can be used as a design matrix for experimental designs with 3, 4, ..., 7 two-level factors. In this way a number of small (8 experimental units) main-effect designs for two-level factors can and have been constructed. See *Addelman* (1962b, 1963). In the next section we shall investigate whether it is possible to construct a $4 \times 2 \times 2$ design with eight experimental units from the \mathbf{X} matrix of Table 4.2, using the restrictions mentioned in Section 1.6.

Such a design shall be indicated as a $4 \times 2 \times 2/8$ design.

4.2. The $4 \times 2 \times 2$ design in eight experimental units

The factors to be used are the following.

P : A quantitative factor with four equally spaced levels 0, 1, 2 and 3.

Q : A two-level factor with levels $Q_1 = -1$ and $Q_2 = +1$ or $x_{Q1} = 0$ and $x_{Q2} = 1$.

R : A two-level factor with levels $R_1 = -1$ and $R_2 = +1$ or $x_{R1} = 0$ and $x_{R2} = 1$.

Using the orthogonal polynomials Pl and Pq as defined in Section 2.9, see (2.49), we have the following mathematical model

$$y_i = \beta_0 x_{oi} + \beta_1 Pl_i + \beta_{23} Q_i R_i + \beta_{11} Pq_i + \beta_2 Q_i + \beta_{13} Pl_i R_i + \beta_3 R_i + \beta_{12} Pl_i Q_i + \varepsilon_i, \quad (4.1)$$

$$(i = 1, 2, \dots, 8).$$

Since (4.1) contains 8 parameters β it must be possible to employ an experiment with 8 experimental units to estimate these parameters.

To find the column vector elements $Pl_i, R_i, \dots, Pl_i Q_i$ we use the \mathbf{X} matrix of Table 4.2.

We use the technique of replacement as in Section 2.9 and replace the column vector elements A_i, B_i and $A_i B_i$ by Pl_i and Pq_i using formula (2.49) namely

$$Pl_i = (2A_i + B_i)/\sqrt{5}$$

$$Pq_i = A_i B_i.$$

As to the choice of Q_i and R_i from Table 4.2 we can choose two elements from the set $C_i, A_iC_i, B_iC_i, A_iB_iC_i$.

We therefore can construct $\binom{4}{2} = 6$ possible designs.

These are presented in Table 4.3.

Nr. of design **Column vector elements**

	Q_i	R_i	\longrightarrow	Q_iR_i	
1	C_i	A_iC_i	\longrightarrow	A_i	since $C_i^2 = 1$
2	C_i	B_iC_i	\longrightarrow	B_i	since $C_i^2 = 1$
3	C_i	$A_iB_iC_i$	\longrightarrow	A_iB_i	since $C_i^2 = 1$
4	A_iC_i	B_iC_i	\longrightarrow	A_iB_i	since $C_i^2 = 1$
5	A_iC_i	$A_iB_iC_i$	\longrightarrow	B_i	since $A_i^2C_i^2 = 1$
6	B_iC_i	$A_iB_iC_i$	\longrightarrow	A_i	since $B_i^2C_i^2 = 1$

Table 4.3. Six possible $4 \times 2 \times 2/8$ designs.

Designs 3 and 4 cannot be used since $Q_iR_i = A_iB_i = Pq_i$. This means that $\hat{\beta}_{23}$ will be confounded with $\hat{\beta}_{11}$.

For **design 1** we have

$$x_{oi} = 1$$

$$Pl_i = (2A_i + B_i)/\sqrt{5}$$

$$Q_iR_i = A_i$$

$$Pq_i = A_iB_i$$

$$Q_i = C_i$$

$$Pl_iR_i = (2A_i + B_i)(A_iC_i)/\sqrt{5} = (2C_i + A_iB_iC_i)/\sqrt{5}$$

$$R_i = A_i C_i$$

$$Pl_i Q_i = (2A_i + B_i) (C_i) / \sqrt{5} = (2A_i C_i + B_i C_i) / \sqrt{5} .$$

The design matrix and the \mathbf{X} matrix of column vectors can now be derived from Table 4.2 and are presented in Table 4.4a and 4.4b.

Exp. unit	x_P	x_Q	x_R	x_{oi}	Pl_i	$Q_i R_i$	Pq_i	Q_i	$Pl_i R_i$	R_i	$Pl_i Q_i$
1	$\begin{bmatrix} 0 & 0 & 1 \\ 2 & 0 & 0 \\ 1 & 0 & 1 \\ 3 & 0 & 0 \\ 0 & 1 & 0 \\ 2 & 1 & 1 \\ 1 & 1 & 0 \\ 3 & 1 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & -3/\sqrt{5} & -1 & 1 & -1 & -3/\sqrt{5} & 1 & 3/\sqrt{5} \\ 1 & 1/\sqrt{5} & 1 & -1 & -1 & -1/\sqrt{5} & -1 & -1/\sqrt{5} \\ 1 & -1/\sqrt{5} & -1 & -1 & -1 & -1/\sqrt{5} & 1 & 1/\sqrt{5} \\ 1 & 3/\sqrt{5} & 1 & 1 & -1 & -3/\sqrt{5} & -1 & -3/\sqrt{5} \\ 1 & -3/\sqrt{5} & -1 & 1 & 1 & 3/\sqrt{5} & -1 & -3/\sqrt{5} \\ 1 & 1/\sqrt{5} & 1 & -1 & 1 & 1/\sqrt{5} & 1 & 1/\sqrt{5} \\ 1 & -1/\sqrt{5} & -1 & -1 & 1 & 1/\sqrt{5} & -1 & -1/\sqrt{5} \\ 1 & 3/\sqrt{5} & 1 & 1 & 1 & 3/\sqrt{5} & 1 & 3/\sqrt{5} \end{bmatrix}$	$\begin{bmatrix} 1 & -3/\sqrt{5} & -1 & 1 & -1 & -3/\sqrt{5} & 1 & 3/\sqrt{5} \\ 1 & 1/\sqrt{5} & 1 & -1 & -1 & -1/\sqrt{5} & -1 & -1/\sqrt{5} \\ 1 & -1/\sqrt{5} & -1 & -1 & -1 & -1/\sqrt{5} & 1 & 1/\sqrt{5} \\ 1 & 3/\sqrt{5} & 1 & 1 & -1 & -3/\sqrt{5} & -1 & -3/\sqrt{5} \\ 1 & -3/\sqrt{5} & -1 & 1 & 1 & 3/\sqrt{5} & -1 & -3/\sqrt{5} \\ 1 & 1/\sqrt{5} & 1 & -1 & 1 & 1/\sqrt{5} & 1 & 1/\sqrt{5} \\ 1 & -1/\sqrt{5} & -1 & -1 & 1 & 1/\sqrt{5} & -1 & -1/\sqrt{5} \\ 1 & 3/\sqrt{5} & 1 & 1 & 1 & 3/\sqrt{5} & 1 & 3/\sqrt{5} \end{bmatrix}$								
2											
3											
4											
5											
6											
7											
8											

Table 4.4a. Design

Table 4.4b. \mathbf{X} matrix of design 1.

matrix nr. 1

We can of course calculate $\mathbf{X}'\mathbf{X}$ easily from the \mathbf{X} matrix of Table 4.4b. It is, however, more elegant and we obtain more insight into the structure of $\mathbf{X}'\mathbf{X}$ when the expressions for Pl_i , $Q_i R_i$, etc. are used.

We shall also make use of the following properties of 2^n designs

I $A_i^2 = B_i^2 = A_i^2 B_i^2 = \dots = A_i^2 B_i^2 C_i^2 = 1.$

II The inner product of any two different vectors in a 2^n design equals zero, i.e.

$$\begin{aligned} \sum_{i=1}^8 A_i B_i &= (\mathbf{A}, \mathbf{B}) = \sum_{i=1}^8 A_i C_i = (\mathbf{A}, \mathbf{C}) = \dots = \sum_{i=1}^8 (B_i C_i) (A_i B_i C_i) = \\ &= (\mathbf{BC}, \mathbf{ABC}) = 0 . \end{aligned}$$

III The inner product of a column vector in \mathbf{X} with the same vector equals 2^n in a 2^n design.

For a 2^3 design we therefore have:

$$\sum_{i=1}^8 (A_i)^2 = (\mathbf{A}, \mathbf{A}) = \sum_{i=1}^8 (B_i)^2 = (\mathbf{B}, \mathbf{B}) = \dots = \sum_{i=1}^8 (A_i B_i C_i)^2 = (\mathbf{ABC}, \mathbf{ABC}) = 8.$$

The inner product of \mathbf{x}'_0 with any other column vector of \mathbf{X} equals zero.

We may now write, using the elements of the $\mathbf{X}'\mathbf{X}$ matrix and known properties of vectors:

$$\begin{aligned} (\mathbf{P1}, \mathbf{P1}) &= ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, (2\mathbf{A} + \mathbf{B})/\sqrt{5}) = (1/5) \{4(\mathbf{A}, \mathbf{A}) + 4(\mathbf{A}, \mathbf{B}) + (\mathbf{B}, \mathbf{B})\} = \\ &= (4 \times 8 + 0 + 8)/5 = 8 \end{aligned}$$

$$(\mathbf{P1}, \mathbf{QR}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, \mathbf{A}) = (1/\sqrt{5}) \{2(\mathbf{A}, \mathbf{A}) + (\mathbf{A}, \mathbf{B})\} = (2 \times 8 + 0)/\sqrt{5} = 16/\sqrt{5}$$

$$(\mathbf{P1}, \mathbf{Pq}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, \mathbf{AB}) = (1/\sqrt{5}) \{2(\mathbf{A}, \mathbf{AB}) + (\mathbf{B}, \mathbf{AB})\} = 0 + 0 = 0$$

$$(\mathbf{P1}, \mathbf{Q}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, \mathbf{C}) = (1/\sqrt{5}) \{2(\mathbf{A}, \mathbf{C}) + (\mathbf{B}, \mathbf{C})\} = 0 + 0 = 0$$

$$(\mathbf{P1}, \mathbf{PIR}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, (2\mathbf{C} + \mathbf{ABC})/\sqrt{5}) = (1/5) (0 + 0 + 0 + 0) = 0$$

$$(\mathbf{P1}, \mathbf{R}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, \mathbf{AC}) = (1/\sqrt{5}) \{2(\mathbf{A}, \mathbf{AC}) + (\mathbf{B}, \mathbf{AC})\} = 0 + 0 = 0$$

$$(\mathbf{P1}, \mathbf{PIQ}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, (2\mathbf{AC} + \mathbf{BC})/\sqrt{5}) = (1/5) (0 + 0 + 0 + 0) = 0$$

$$(\mathbf{QR}, \mathbf{QR}) = (\mathbf{A}, \mathbf{A}) = 8$$

$$(\mathbf{QR}, \mathbf{Pq}) = (\mathbf{A}, \mathbf{AB}) = 0$$

$$(\mathbf{QR}, \mathbf{Q}) = (\mathbf{A}, \mathbf{C}) = 0$$

$$(\mathbf{QR}, \mathbf{PIR}) = (\mathbf{A}, (2\mathbf{C} + \mathbf{ABC})/\sqrt{5}) = 0 + 0 = 0$$

$$(\mathbf{QR}, \mathbf{R}) = (\mathbf{A}, \mathbf{AC}) = 0$$

$$(\mathbf{QR}, \mathbf{PIQ}) = (\mathbf{A}, (2\mathbf{AC} + \mathbf{BC})/\sqrt{5}) = 0 + 0 = 0$$

$$(\mathbf{Pq}, \mathbf{Pq}) = (\mathbf{AB}, \mathbf{AB}) = 8$$

$$(\mathbf{Pq}, \mathbf{Q}) = (\mathbf{AB}, \mathbf{C}) = 0$$

$$(\mathbf{Pq}, \mathbf{PIR}) = (\mathbf{AB}, (2\mathbf{C} + \mathbf{ABC})/\sqrt{5}) = 0 + 0 = 0$$

$$(\mathbf{Pq}, \mathbf{R}) = (\mathbf{AB}, \mathbf{AC}) = 0$$

$$(\mathbf{Pq}, \mathbf{PIQ}) = (\mathbf{AB}, (2\mathbf{AC} + \mathbf{BC})/\sqrt{5}) = 0 + 0 = 0$$

$$(\mathbf{Q}, \mathbf{Q}) = (\mathbf{C}, \mathbf{C}) = 8$$

$$\begin{aligned} (\mathbf{Q}, \mathbf{PIR}) &= (\mathbf{C}, (2\mathbf{C} + \mathbf{ABC})/\sqrt{5}) = (1/\sqrt{5}) \{2(\mathbf{C}, \mathbf{C}) + (\mathbf{C}, \mathbf{ABC})\} = (2 \times 8 + 0)/\sqrt{5} = \\ &= 16/\sqrt{5} \end{aligned}$$

$$(\mathbf{Q}, \mathbf{R}) = (\mathbf{C}, \mathbf{AC}) = 0$$

$$(\mathbf{Q}, \mathbf{PIQ}) = (\mathbf{C}, (2\mathbf{AC} + \mathbf{BC})/\sqrt{5}) = 0 + 0 = 0$$

$$\begin{aligned} (\mathbf{PIR}, \mathbf{PIR}) &= ((2\mathbf{C} + \mathbf{ABC})/\sqrt{5}, (2\mathbf{C} + \mathbf{ABC})/\sqrt{5}) = \{4(\mathbf{CC}) + 4(\mathbf{C}, \mathbf{ABC}) + \\ &+ (\mathbf{ABC}, \mathbf{ABC})\}/5 = (4 \times 8 + 0 + 8)/5 = 8 \end{aligned}$$

$$(\mathbf{PIR}, \mathbf{R}) = ((2\mathbf{C} + \mathbf{ABC})/\sqrt{5}, \mathbf{AC}) = (1/\sqrt{5}) (0 + 0) = 0$$

$$(\mathbf{PIR}, \mathbf{PIQ}) = (2\mathbf{C} + \mathbf{ABC}, 2\mathbf{AC} + \mathbf{BC})/5 = (0 + 0 + 0 + 0)/5 = 0$$

$$(\mathbf{R}, \mathbf{R}) = (\mathbf{AC}, \mathbf{AC}) = 8$$

$$\begin{aligned} (\mathbf{R}, \mathbf{PIQ}) &= (\mathbf{AC}, (2\mathbf{AC} + \mathbf{BC})/\sqrt{5}) = \{2(\mathbf{AC}, \mathbf{AC})\}/\sqrt{5} = (2 \times 8 + 0)/\sqrt{5} = \\ &= 16/\sqrt{5} \end{aligned}$$

$$\begin{aligned} (\mathbf{PIQ}, \mathbf{PIQ}) &= (2\mathbf{AC} + \mathbf{BC}, 2\mathbf{AC} + \mathbf{BC})/5 = (4(\mathbf{AC}, \mathbf{AC}) + 4(\mathbf{AC}, \mathbf{BC}) + (\mathbf{BC}, \mathbf{BC}))/5 = \\ &= (4 \times 8 + 0 + 8)/5 = 8 . \end{aligned}$$

These calculations may seem cumbersome, but once some experience has been obtained all necessary inner products can quickly be computed.

We now have all the elements of $\mathbf{X}'\mathbf{X}$ and we find

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} x_{oi} & Pl_i & Q_i R_i & Pq_i & Q_i & Pl_i R_i & R_i & Pl_i Q_i \\ 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 16/\sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & 16/\sqrt{5} & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 16/\sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 16/\sqrt{5} & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 16/\sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 & 16/\sqrt{5} & 8 \end{bmatrix}$$

and

$$(\mathbf{X}'\mathbf{X})^{-1} = (1/8) \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & -2\sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & -2\sqrt{5} & 5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & -2\sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & -2\sqrt{5} & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5 & -2\sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 & -2\sqrt{5} & 5 \end{bmatrix}$$

Although a large measure of orthogonality is maintained, because $(\mathbf{X}'\mathbf{X})^{-1}$ contains many off-diagonal elements equal to zero, we shall not use design nr. 1 since the non-zero off-diagonal elements of $(\mathbf{X}'\mathbf{X})^{-1}$ are all equal to $(-2\sqrt{5})/8$ and this covariance value corresponds to a correlation coefficient between two $\hat{\beta}$'s of

$$\frac{-2\sqrt{5}}{\sqrt{(5 \times 5)}} = -0.89 .$$

This value is very high and it means that the pairs $(\hat{\beta}_1, \hat{\beta}_{23})$, $(\hat{\beta}_2, \hat{\beta}_{13})$ and $(\hat{\beta}_3, \hat{\beta}_{12})$ are highly correlated, which is undesirable.

It appears that design nr. 6 leads to the same $(\mathbf{X}'\mathbf{X})^{-1}$ matrix and it will therefore not be used.

We shall now explore design nr. 2 where we had the following choice

$$Q_i = C_i \quad R_i = B_i C_i \longrightarrow Q_i R_i = B_i .$$

Using the same method as already described, we can find the design matrix and the \mathbf{X} matrix of column vectors. See Table 4.5a and 4.5b.

Exp. unit	x_P	x_Q	x_R	x_{oi}	Pl_i	$Q_i R_i$	Pq_i	Q_i	$Pl_i R_i$	R_i	$Pl_i Q_i$
1	0	0	1	1	$-3/\sqrt{5}$	-1	1	-1	$-3/\sqrt{5}$	1	$3/\sqrt{5}$
2	2	0	1	1	$1/\sqrt{5}$	-1	-1	-1	$1/\sqrt{5}$	1	$-1/\sqrt{5}$
3	1	0	0	1	$-1/\sqrt{5}$	1	-1	-1	$1/\sqrt{5}$	-1	$1/\sqrt{5}$
4	3	0	0	1	$3/\sqrt{5}$	1	1	-1	$-3/\sqrt{5}$	-1	$-3/\sqrt{5}$
5	0	1	0	1	$-3/\sqrt{5}$	-1	1	1	$3/\sqrt{5}$	-1	$-3/\sqrt{5}$
6	2	1	0	1	$1/\sqrt{5}$	-1	-1	1	$-1/\sqrt{5}$	-1	$1/\sqrt{5}$
7	1	1	1	1	$-1/\sqrt{5}$	1	-1	1	$-1/\sqrt{5}$	1	$-1/\sqrt{5}$
8	3	1	1	1	$3/\sqrt{5}$	1	1	1	$3/\sqrt{5}$	1	$3/\sqrt{5}$

Table 4.5a. Design matrix nr. 2.

Table 4.5b. \mathbf{X} matrix of design 2.

Using

$$x_{oi} = 1$$

$$Pl_i = (2A_i + B_i)/\sqrt{5}$$

$$Q_i R_i = B_i$$

$$Pq_i = A_i B_i$$

$$Q_i = C_i$$

$$Pl_i R_i = (2A_i B_i C_i + C_i)/\sqrt{5}$$

$$R_i = B_i C_i$$

$$Pl_i Q_i = (2A_i C_i + B_i C_i)/\sqrt{5} ,$$

we find

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} x_{0i} & Pl_i & Q_i R_i & Pq_i & Q_i & Pl_i R_i & R_i & Pl_i Q_i \\ 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 8/\sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & 8/\sqrt{5} & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 8/\sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 8/\sqrt{5} & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 8/\sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 & 8/\sqrt{5} & 8 \end{bmatrix}$$

and

$$(\mathbf{X}'\mathbf{X})^{-1} = (1/8) \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5/4 & -(1/4)\sqrt{5} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -(1/4)\sqrt{5} & 5/4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5/4 & -(1/4)\sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -(1/4)\sqrt{5} & 5/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5/4 & -(1/4)\sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 & -(1/4)\sqrt{5} & 5/4 \end{bmatrix}$$

The matrix $(\mathbf{X}'\mathbf{X})^{-1}$ again contains many zero's, in fact the same elements are zero as for design nr. 1, but the correlation coefficients between two $\hat{\beta}$'s within the pairs $(\hat{\beta}_1, \hat{\beta}_{23})$, $(\hat{\beta}_2, \hat{\beta}_{13})$ and $(\hat{\beta}_3, \hat{\beta}_{12})$ is now equal to

$$\frac{-(1/4) (1/8)\sqrt{5}}{\sqrt{[(1/8) (5/4) (1/8) (5/4)]}} = -\frac{1}{\sqrt{5}} = -0.45 .$$

This is only half the value found previously for design 1. Design nr. 2 therefore appears to be better than design nr. 1.

When we examine $(\mathbf{X}'\mathbf{X})^{-1}$ in more detail it appears that the estimated values $\hat{\beta}$ can be divided into 5 groups, namely

$$\hat{\beta}_0, (\hat{\beta}_1, \hat{\beta}_{23}), \hat{\beta}_{11}, (\hat{\beta}_2, \hat{\beta}_{13}), (\hat{\beta}_3, \hat{\beta}_{12}) .$$

It is striking that all linear effects belong to different groups; $\hat{\beta}$'s belonging to different groups are orthogonal estimates and therefore uncorrelated. Some authors call this clumpwise orthogonality (see *Margolin, 1969b*).

A large measure of orthogonality is therefore maintained.

Another important advantage of design 2 is the fact that the variances of $\hat{\beta}_1, \hat{\beta}_{23}, \hat{\beta}_2, \hat{\beta}_{13}, \hat{\beta}_3$ and $\hat{\beta}_{12}$ are only (1/4)th of the corresponding variances in design nr. 1.

To examine this difference in variance and also the already mentioned decrease of the correlation coefficient in absolute value from 0.89 to 0.45, we compare the $\mathbf{X}'\mathbf{X}$ matrices of both designs.

These matrices differ only in the values of three off-diagonal elements which have the value $16/\sqrt{5}$ for design 1 and the value $8/\sqrt{5}$ for design 2.

There are in fact 6 such values but since $\mathbf{X}'\mathbf{X}$ is symmetric we only have to consider three of them.

These values are three inner products of vectors. For design 1 we have:

$$(\mathbf{P1}, \mathbf{QR}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, \mathbf{A}) = 16/\sqrt{5} = 2(\mathbf{A}, \mathbf{A})/\sqrt{5}$$

$$(\mathbf{PIR}, \mathbf{Q}) = ((2\mathbf{C} + \mathbf{ABC})/\sqrt{5}, \mathbf{C}) = 16/\sqrt{5} = 2(\mathbf{C}, \mathbf{C})/\sqrt{5}$$

$$(\mathbf{PIQ}, \mathbf{R}) = ((2\mathbf{AC} + \mathbf{BC})/\sqrt{5}, \mathbf{AC}) = 16/\sqrt{5} = 2(\mathbf{AC}, \mathbf{AC})/\sqrt{5}.$$

For design 2 we have

$$(\mathbf{P1}, \mathbf{QR}) = ((2\mathbf{A} + \mathbf{B})/\sqrt{5}, \mathbf{B}) = 8/\sqrt{5} = (\mathbf{B}, \mathbf{B})/\sqrt{5}$$

$$(\mathbf{PIR}, \mathbf{Q}) = ((2\mathbf{ABC} + \mathbf{C})/\sqrt{5}, \mathbf{C}) = 8/\sqrt{5} = (\mathbf{C}, \mathbf{C})/\sqrt{5}$$

$$(\mathbf{PIQ}, \mathbf{R}) = ((2\mathbf{AC} + \mathbf{BC}), \mathbf{BC}) = 8/\sqrt{5} = (\mathbf{BC}, \mathbf{BC})/\sqrt{5}.$$

From these expressions we can see how the value of $16/\sqrt{5}$ arose. It originated from the term $2\mathbf{A}$ in $\mathbf{P1} = (2\mathbf{A} + \mathbf{B})/\sqrt{5}$. We also had $\mathbf{Pq} = \mathbf{AB}$. We can now formulate an important rule *Having once chosen $\mathbf{P1} = (2\mathbf{A} + \mathbf{B})/\sqrt{5}$ and $\mathbf{Pq} = \mathbf{AB}$ it is necessary not to equate the \mathbf{A} and \mathbf{AB} columns of the 2^3 design to any of the columns for \mathbf{Q}, \mathbf{R} and \mathbf{QR} .*

Using an \mathbf{A} column produces a high covariance of $16/\sqrt{5}$, while using the \mathbf{AB} column causes

confounding between $\hat{\beta}$'s.

Applying this rule indicates that, apart from design 2, only design 5, see Table 4.3, is a suitable design. It turns out that it has the same $X'X$ matrix as design 2.

Comparing the $(X'X)^{-1}$ matrices of design 1 and 2 shows that the decrease of the three off-diagonal elements from $16/\sqrt{5}$ to $8/\sqrt{5}$ had a large effect since the three covariances decreased by a factor 8 and the variances of $\hat{\beta}_1, \hat{\beta}_{23}, \hat{\beta}_2, \hat{\beta}_{13}, \hat{\beta}_3$ and $\hat{\beta}_{12}$ decreased by a factor 4.

The variances of $\hat{\beta}_0$ and $\hat{\beta}_{11}$ remained unchanged.

Using the designs 2 and 5 we obtain the designs given in Table 4.6a and Table 4.6b. Table 4.6a has also been presented in design 8.1 of the Appendix. Design 8.1 also contains $X'X, (X'X)^{-1}$ and some other particulars to be explained in the next section, Chapter 5 and Chapter 7.

Exp. unit	x_P	x_Q	x_R
1	0	0	1
2	2	0	1
3	1	0	0
4	3	0	0
5	0	1	0
6	2	1	0
7	1	1	1
8	3	1	1

	x_Q	0		1	
	x_R	0	1	0	1
x_P					
0			1	5	
1		3			7
2			2	6	
3		4			8

Design matrix

Experimental design

Table 4.6a. A $4 \times 2 \times 2/8$ design (Design nr. 2).

Exp. unit	x_P	x_Q	x_R
1	0	1	0
2	2	0	1
3	1	1	1
4	3	0	0
5	0	0	1
6	2	1	0
7	1	0	0
8	3	1	1

		x_Q		0		1	
		x_R		0	1	0	1
x_P	0			5	1		
	1	7					3
	2		2	6			
	3	4					8

Design matrix

Experimental design

Table 4.6b. A $4 \times 2 \times 2/8$ design (Design nr. 5).

Comparing the experimental designs in Table 4.6a and Table 4.6b shows that they are identical. It therefore appears that there is only one suitable $4 \times 2 \times 2$ design in 8 runs.

4.3. A measure of nonorthogonality

It is useful and interesting to consider the matrices $\mathbf{X}'\mathbf{X}$ of design 1 and 2 in more detail. If we ignore the zero's in $\mathbf{X}'\mathbf{X}$ we see that it consists of 5 submatrices, two of which consist of the scalar 8, whereas the remaining three have the following structure

$$\begin{bmatrix} \sum_{i=1}^8 X_{ip}^2 & \sum_{i=1}^8 X_{ip}X_{iq} \\ \sum_{i=1}^8 X_{ip}X_{iq} & \sum_{i=1}^8 X_{iq}^2 \end{bmatrix} = \begin{bmatrix} a & b \\ b & c \end{bmatrix} = \mathbf{W} .$$

X_{ip} and X_{iq} are elements of the p^{th} and q^{th} column of the \mathbf{X} matrix.

For design 1 we have: $a = c = 8$, $b = 16/\sqrt{5}$.

For design 2 we have: $a = c = 8$, $b = 8/\sqrt{5}$.

To invert $\mathbf{X}'\mathbf{X}$ we simply can take the inverse of 8 twice and invert \mathbf{W} three times.

We have

$$\mathbf{W}^{-1} = \begin{bmatrix} c/(ac - b^2) & -b/(ac - b^2) \\ -b/(ac - b^2) & a/(ac - b^2) \end{bmatrix}.$$

The correlation coefficient between \mathbf{X}_p and \mathbf{X}_q equals

$$r_{pq} = \frac{\sum_{i=1}^8 (X_{ip} - \bar{X}_{.p})(X_{iq} - \bar{X}_{.q})}{\left[\sum_{i=1}^8 (X_{ip} - \bar{X}_{.p})^2 \right]^{\frac{1}{2}} \left[\sum_{i=1}^8 (X_{iq} - \bar{X}_{.q})^2 \right]^{\frac{1}{2}}},$$

where $\bar{X}_{.p} = (1/8) \sum_{i=1}^8 X_{ip}$ and $\bar{X}_{.q} = (1/8) \sum_{i=1}^8 X_{iq}$.

In the matrices of the designs 1 and 2 we however have, ignoring column \mathbf{x}_0 , since r_{pq} is not defined for $X_{ip} = x_{0i}$, that $\bar{X}_{.p} = \bar{X}_{.q} = 0$, hence

$$r_{pq} = \frac{\sum_{i=1}^8 X_{ip} X_{iq}}{\left[\sum_{i=1}^8 X_{ip}^2 \sum_{i=1}^8 X_{iq}^2 \right]^{\frac{1}{2}}} = \frac{b}{\sqrt{ac}}.$$

Strictly speaking we should say that r_{pq} is not a correlation coefficient, since \mathbf{X}_p and \mathbf{X}_q are not random. Therefore r_{pq} is a measure of the linear dependence between \mathbf{X}_p and \mathbf{X}_q .

When we have a completely orthogonal design the $\mathbf{X}'\mathbf{X}$ matrix is diagonal and the variance of the estimated regression coefficient $\hat{\beta}_p$ corresponding to column \mathbf{X}_p in the \mathbf{X} matrix equals

$$\sigma_{\hat{\beta}_p}^2 = \sigma^2 / \sum_{i=1}^8 X_{ip}^2 = \sigma^2 / a.$$

The matrices of design 1 and 2 were however not orthogonal and the variance of $\hat{\beta}_p$ equals the diagonal element in $(\mathbf{X}'\mathbf{X})^{-1}$ corresponding to column \mathbf{X}_p of the \mathbf{X} matrix.

In reality we therefore have

$$\sigma_{\hat{\beta}_p}^2 = \sigma^2 c / (ac - b^2).$$

The variance of $\hat{\beta}_p$ has therefore been increased by a factor of

$$\frac{\sigma^2 c / (ac - b^2)}{\sigma^2 / a} = \frac{ac}{(ac - b^2)} = \frac{1}{1 - b^2 / ac} = \frac{1}{1 - r_{pq}^2}.$$

Marquardt (1970) called $1/(1 - r_{pq}^2)$ the *variance inflation factor* (VIF) because it is the factor by which the variance of an estimated regression coefficient is increased due to nonorthogonality.

Hence

$$\text{VIF} = 1/(1 - r_{pq}^2). \quad (4.2)$$

When we write the correlation matrix \mathbf{r} of \mathbf{X}_p and \mathbf{X}_q we have

$$\mathbf{r} = \begin{bmatrix} r_{pp} & r_{pq} \\ r_{pq} & r_{qq} \end{bmatrix} = \begin{bmatrix} 1 & r_{pq} \\ r_{pq} & 1 \end{bmatrix} = \begin{bmatrix} 1 & b/\sqrt{ac} \\ b/\sqrt{ac} & 1 \end{bmatrix}$$

and

$$\mathbf{r}^{-1} = \begin{bmatrix} 1/(1 - r_{pq}^2) & -r_{pq}/(1 - r_{pq}^2) \\ -r_{pq}/(1 - r_{pq}^2) & 1/(1 - r_{pq}^2) \end{bmatrix} = \begin{bmatrix} \text{VIF} & -r_{pq}/(1 - r_{pq}^2) \\ -r_{pq}/(1 - r_{pq}^2) & \text{VIF} \end{bmatrix}.$$

We see that the VIF of $\hat{\beta}_p$ therefore equals the corresponding diagonal element of the inverse of the 2×2 correlation matrix \mathbf{r} .

Brownlee (1965) has shown that

$$\text{VIF} = r_{pp}^{-1} = 1/(1 - r_p^2), \quad (4.3)$$

where r_p is the multiple correlation coefficient of \mathbf{X}_p with all other \mathbf{X} 's and r_{pp}^{-1} is the i^{th} diagonal element of the inverse of the correlation matrix \mathbf{r} .

The expression (4.2) is therefore a special case of (4.3). From (4.3) we see that the VIF approaches infinity when r_p increases to 1 and equals 1 if r_p is zero.

Expression (4.3) clearly shows why the VIF is a measure for orthogonality because it is directly linked to r_p , the multiple correlation coefficient. For this reason its value is independent of the scaling of the \mathbf{X}_p .

Because the VIF equals the factor by which the variance of an estimated regression coefficient increases due to nonorthogonality, it is a useful tool to judge and to compare experimental designs. We shall therefore calculate the VIF's for all designs to be presented later on.

Of course it is desirable that the VIF is as close as possible to its minimum value of $\text{VIF} = 1$.

Some authors prefer VIF's smaller than 5, other allow values up to 10. It is clear that a β is poorly estimated when the VIF is large since the variance of $\hat{\beta}$ will then be large.

In Appendix 7A we shall give a method to examine large VIF's in more detail.

The inverse of the complete correlation matrix of design 2 has been given as \mathbf{r}^{-1} with design 8.1 of the Appendix. For design 1 we have, the groups (p, q) being (2,3), (5,6) and (7,8),

$$r_{pq}^2 = \frac{16^2/5}{8 \times 8} = 0.80 \quad r_{pq} = 0.89$$

and $\text{VIF} = 1/(1 - 0.80) = 5$.

For design 2 we find

$$r_{pq}^2 = \frac{8^2/5}{8 \times 8} = 0.20 \quad r_{pq} = 0.45$$

and $\text{VIF} = 1/(1 - 0.20) = 1.25$ (see also design 8.1).

Design 2 therefore has 6 VIF's which are 4 times smaller than the corresponding VIF's of design 1 and we now also understand why the corresponding variances differed by a factor 4 as stated in the previous section.

It is because the correlation coefficient between \mathbf{X}_p , for $p = 2, 3, 5, 6, 7$ and 8, with all other \mathbf{X} 's is large for design 1 ($r_{pq} = 0.89$) and small ($r_{pq} = 0.45$) for design 2.

4.4. The alias structure of the $4 \times 2 \times 2/8$ design

The model used in Section 4.2 for design 2 can be written in matrix notation as

$$\mathbf{E}[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta},$$

where \mathbf{X} is the matrix of column vectors and

$$\boldsymbol{\beta}' = [\beta_0, \beta_1, \beta_{23}, \beta_{11}, \beta_2, \beta_{13}, \beta_3, \beta_{12}].$$

It might be the case that the model considered is not correct since we did not use terms such as Pc_i (factor P cubic), Pc_iQ_i , Pc_iR_i etc.

Suppose that the true model can be written as, see *Seber* (1977; Chapter 6) and *Draper and Smith* (1981; Chapter 2),

$$\mathbf{E}[\mathbf{Y}] = \mathbf{X}\beta + \mathbf{Z}\gamma ,$$

where

$$\gamma' = [\gamma_{111}, \gamma_{11123}, \gamma_{11112}, \gamma_{11113}, \gamma_{1112}, \gamma_{1113}, \gamma_{1123}, \gamma_{1123}], \quad 1)$$

in which the indices 1, 2 and 3 in γ' refer to the factors P , Q and R while \mathbf{Z} is the matrix of column vectors corresponding to

$$\gamma_{111}, \gamma_{11123}, \dots, \gamma_{1123} .$$

Since $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}$ we have

$$\begin{aligned} \mathbf{E}(\hat{\beta}) &= \mathbf{E}\{(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}\} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{E}(\mathbf{Y}) = \\ &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'(\mathbf{X}\beta + \mathbf{Z}\gamma) = \\ &= (\mathbf{X}'\mathbf{X})^{-1} (\mathbf{X}'\mathbf{X})\beta + (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Z}\gamma \\ &= \beta + (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Z}\gamma . \end{aligned}$$

The expression $(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Z}\gamma$ is called the alias matrix of β .

We shall therefore calculate $(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Z}$.

We first determine \mathbf{Z} . The elements of the column vectors of \mathbf{Z} are

¹One, two or three identical indices refer to a linear, quadratic or cubic effect, respectively.

$$Pc_i = (-A_i + 2B_i)/\sqrt{5}$$

$$Pc_iQ_iR_i = (-A_i + 2B_i) (B_i)/\sqrt{5} = (-A_iB_i + 2)/\sqrt{5}$$

$$Pc_iQ_i = (-A_i + 2B_i) (C_i)/\sqrt{5} = (-A_iC_i + 2B_iC_i)/\sqrt{5}$$

$$Pc_iR_i = (-A_i + 2B_i) (B_iC_i)/\sqrt{5} = (-A_iB_iC_i + 2C_i)/\sqrt{5}$$

$$Pq_iQ_i = A_iB_iC_i$$

$$Pq_iR_i = A_iB_iB_iC_i = A_iC_i$$

$$Pl_iQ_iR_i = (2A_i + B_i) (B_i)/\sqrt{5} = (2A_iB_i + 1)/\sqrt{5}$$

$$Pq_iQ_iR_i = A_iB_iB_i = A_i .$$

We can now, using Table 4.2, construct the Z matrix of column vectors which is given in Table 4.7.

Pc_i	$Pc_iQ_iR_i$	Pc_iQ_i	Pc_iR_i	Pq_iQ_i	Pq_iR_i	$Pl_iQ_iR_i$	$Pq_iQ_iR_i$
$-1/\sqrt{5}$	$1/\sqrt{5}$	$1/\sqrt{5}$	$-1/\sqrt{5}$	-1	1	$3/\sqrt{5}$	-1
$-3/\sqrt{5}$	$3/\sqrt{5}$	$3/\sqrt{5}$	$-3/\sqrt{5}$	1	-1	$-1/\sqrt{5}$	1
$3/\sqrt{5}$	$3/\sqrt{5}$	$-3/\sqrt{5}$	$-3/\sqrt{5}$	1	1	$-1/\sqrt{5}$	-1
$1/\sqrt{5}$	$1/\sqrt{5}$	$-1/\sqrt{5}$	$-1/\sqrt{5}$	-1	-1	$3/\sqrt{5}$	1
$-1/\sqrt{5}$	$1/\sqrt{5}$	$-1/\sqrt{5}$	$1/\sqrt{5}$	1	-1	$3/\sqrt{5}$	-1
$-3/\sqrt{5}$	$3/\sqrt{5}$	$-3/\sqrt{5}$	$3/\sqrt{5}$	-1	1	$-1/\sqrt{5}$	1
$3/\sqrt{5}$	$3/\sqrt{5}$	$3/\sqrt{5}$	$3/\sqrt{5}$	-1	-1	$-1/\sqrt{5}$	-1
$1/\sqrt{5}$	$1/\sqrt{5}$	$1/\sqrt{5}$	$1/\sqrt{5}$	1	1	$3/\sqrt{5}$	1

Table 4.7. Z matrix of column vectors.

Using the expressions of design 2 we obtain

$$x_{0i} = 1$$

$$Pl_i = (2A_i + B_i)/\sqrt{5}$$

$$Q_i R_i = B_i$$

$$Pq_i = A_i B_i$$

$$Q_i = C_i$$

$$Pl_i R_i = (2A_i B_i C_i + C_i)/\sqrt{5}$$

$$R_i = B_i C_i$$

$$Pl_i Q_i = (2A_i C_i + B_i C_i)/\sqrt{5}$$

We find

$$\mathbf{X}'\mathbf{Z} = \begin{bmatrix} 0 & 16/\sqrt{5} & 0 & 0 & 0 & 0 & 8/\sqrt{5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16/\sqrt{5} \\ 16/\sqrt{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -8/\sqrt{5} & 0 & 0 & 0 & 0 & 16/\sqrt{5} & 0 \\ 0 & 0 & 0 & 16/\sqrt{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 16/\sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 16/\sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 16/\sqrt{5} & 0 & 0 \end{bmatrix}$$

and

$$(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Z} = \begin{bmatrix} 0 & 2/\sqrt{5} & 0 & 0 & 0 & 0 & 1/\sqrt{5} & 0 \\ -0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5\sqrt{5} \\ 0.5\sqrt{5} & 0 & 0 & 0 & 0 & 0 & 0 & -0.5 \\ 0 & -1/\sqrt{5} & 0 & 0 & 0 & 0 & 2/\sqrt{5} & 0 \\ 0 & 0 & 0 & 0.5\sqrt{5} & -0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.5 & 0.5\sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 0.5\sqrt{5} & 0 & 0 & -0.5 & 0 & 0 \\ 0 & 0 & -0.5 & 0 & 0 & 0.5\sqrt{5} & 0 & 0 \end{bmatrix}$$

We can write the complete model

$$\mathbf{E}(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}$$

also as

$$\mathbf{E}(\mathbf{Y}) = \begin{bmatrix} x_{0i} \\ Pl_i \\ Q_i R_i \\ Pq_i \\ Q_i \\ Pl_i R_i \\ R_i \\ Pl_i Q_i \end{bmatrix}' \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_{23} \\ \beta_{11} \\ \beta_2 \\ \beta_{13} \\ \beta_3 \\ \beta_{12} \end{bmatrix} + \begin{bmatrix} Pc_i \\ Pc_i Q_i R_i \\ Pc_i Q_i \\ Pc_i R_i \\ Pq_i Q_i \\ Pq_i R_i \\ Pl_i Q_i R_i \\ Pq_i Q_i R_i \end{bmatrix}' \cdot \begin{bmatrix} \gamma_{111} \\ \gamma_{11123} \\ \gamma_{1112} \\ \gamma_{1113} \\ \gamma_{112} \\ \gamma_{113} \\ \gamma_{123} \\ \gamma_{1123} \end{bmatrix}.$$

Using $\mathbf{E}(\hat{\beta}) = \beta + (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Z}\boldsymbol{\gamma}$ we may write the alias matrix as

$$E(\hat{\beta}_0) = \beta_0 + (2/\sqrt{5}) \gamma_{11123} + (1/\sqrt{5}) \gamma_{123}$$

$$E(\hat{\beta}_1) = \beta_1 + (-0.5) \gamma_{111} + (0.5\sqrt{5}) \gamma_{1123}$$

$$E(\hat{\beta}_{23}) = \beta_{23} + (0.5\sqrt{5}) \gamma_{111} - 0.5 \gamma_{1123}$$

$$E(\hat{\beta}_{23}) = \beta_{11} + (-1/\sqrt{5}) \gamma_{11123} + (2/\sqrt{5}) \gamma_{123}$$

$$E(\hat{\beta}_2) = \beta_2 + (0.5\sqrt{5}) \gamma_{1113} - 0.5 \gamma_{112}$$

$$E(\hat{\beta}_{13}) = \beta_{13} + (-0.5) \gamma_{1113} + (0.5\sqrt{5}) \gamma_{112}$$

$$E(\hat{\beta}_3) = \beta_3 + (0.5\sqrt{5}) \gamma_{1112} - 0.5 \gamma_{113}$$

$$E(\hat{\beta}_{12}) = \beta_{12} + (-0.5) \gamma_{1112} + (0.5\sqrt{5}) \gamma_{113}.$$

It is striking that each β is confounded with two γ 's and that each γ occurs twice in each of the expressions above. These expressions can be useful to explain certain ambiguities in the estimates of the β 's.

4.5. The D - and G -efficiency of the $4 \times 2 \times 2/8$ design

4.5.1. The calculation of the D -efficiency

Using formulae (2.14) and (2.15) of Section 2.3 we may write

$$D\text{-efficiency} = 100(\det(\mathbf{M}(\xi))/\max \det(\mathbf{M}(\xi)))^{(1/P)}.$$

Model (3.1) may also be used for the $4 \times 2 \times 2/8$ design. We then have $d = 1$ and $k = 3$ and from Table 3.1 we find that

$$\max \det(\mathbf{M}(\xi)) = 0.0819200. \quad (4.4)$$

We should remember that (4.4) was obtained using model (3.1) and $-1 \leq x_i \leq +1$ for $i = 1, 2, 3$.

We therefore have to calculate $\det(\mathbf{M}(\xi))$ using the scaling $-1 \leq x_i \leq +1$ for the independent variables x_i and model (3.1).

The $\mathbf{X}'\mathbf{X}$ matrix we used for the $4 \times 2 \times 2/8$ design was, see Section 4.2,

$$\mathbf{X}'_1 \mathbf{X}_1 = \begin{bmatrix} x_{0i} & P_i & Q_i R_i & P q_i & Q_i & P_i R_i & R_i & P_i Q_i \\ 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 8/\sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & 8/\sqrt{5} & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 8/\sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 8/\sqrt{5} & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 8/\sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 & 8/\sqrt{5} & 8 \end{bmatrix}$$

and

$$\det(\mathbf{X}'\mathbf{X}) = \det(\mathbf{X}'_1 \mathbf{X}_1) = 8^8 (4/5)^3. \quad (4.6)$$

From Table 4.5b we obtain

$$\mathbf{X}_1 = \begin{matrix} & \begin{matrix} x_{oi} & Pl_i & Q_i R_i & Pq_i & Q_i & Pl_i R_i & R_i & Pl_i Q_i \end{matrix} \\ \begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix} & \begin{bmatrix} -3/\sqrt{5} & -1 & 1 & -1 & -3/\sqrt{5} & 1 & 3/\sqrt{5} \\ 1/\sqrt{5} & -1 & -1 & -1 & 1/\sqrt{5} & 1 & -1/\sqrt{5} \\ -1/\sqrt{5} & 1 & -1 & -1 & 1/\sqrt{5} & -1 & 1/\sqrt{5} \\ 3/\sqrt{5} & 1 & 1 & -1 & -3/\sqrt{5} & -1 & -3/\sqrt{5} \\ -3/\sqrt{5} & -1 & 1 & 1 & 3/\sqrt{5} & -1 & -3/\sqrt{5} \\ 1/\sqrt{5} & -1 & -1 & 1 & -1/\sqrt{5} & -1 & 1/\sqrt{5} \\ -1/\sqrt{5} & 1 & 1 & 1 & -1/\sqrt{5} & 1 & -1/\sqrt{5} \\ 3/\sqrt{5} & 1 & 1 & 1 & 3/\sqrt{5} & 1 & 3/\sqrt{5} \end{bmatrix} \end{matrix} \quad (4.7)$$

If we had used the scaling $-1 \leq x_i \leq +1$ for $i = 1, 2, 3$ and the model (3.1), the \mathbf{X} matrix would have been

$$\mathbf{X}_2 = \begin{matrix} & \begin{matrix} x_{oi} & x_{1i} & x_{2i}x_{3i} & x_{1i}^2 & x_{2i} & x_{1i}x_{3i} & x_{3i} & x_{1i}x_{2i} \end{matrix} \\ \begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix} & \begin{bmatrix} -1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1/3 & -1 & 1/9 & -1 & 1/3 & 1 & -1/3 \\ -1/3 & 1 & 1/9 & -1 & 1/3 & -1 & 1/3 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1/3 & -1 & 1/9 & 1 & -1/3 & -1 & 1/3 \\ -1/3 & 1 & 1/9 & 1 & -1/3 & 1 & -1/3 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \end{matrix} \quad (4.8)$$

From (4.7) and (4.8) it follows that

$$x_{1i} = (Pl_i \sqrt{5})/3, \quad x_{2i}x_{3i} = Q_i R_i, \quad x_{1i}^2 = (4/9) Pq_i + (5/9) \quad (4.9a)$$

$$x_{2i} = Q_i, \quad x_{1i}x_{3i} = (Pl_i R_i \sqrt{5})/3 \quad (4.9b)$$

$$x_{3i} = R_i, \quad x_{1i}x_{2i} = (Pl_i Q_i \sqrt{5})/3. \quad (4.9c)$$

and $\mathbf{X}_2 = \mathbf{X}_1 \mathbf{L}$, where

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 & 5/9 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{5}/3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4/9 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5}/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{5}/3 \end{bmatrix} . \quad (4.9d)$$

Therefore

$$\det(\mathbf{X}'_2 \mathbf{X}_2) = \det(\mathbf{X}'_2 \mathbf{X}_2) = \det((\mathbf{X}_1 \mathbf{L})' \mathbf{X}_1 \mathbf{L})$$

or

$$\det(\mathbf{X}'_2 \mathbf{X}_2) = \det(\mathbf{L}' \mathbf{X}'_1 \mathbf{X}_1 \mathbf{L}) = \det(\mathbf{L}') \det(\mathbf{X}'_1 \mathbf{X}_1) \det(\mathbf{L}) = (\det(\mathbf{L}))^2 \det(\mathbf{X}'_1 \mathbf{X}_1) \quad (4.10)$$

since \mathbf{L} and $\mathbf{X}'_1 \mathbf{X}_1$ are square matrices.

It is easily seen that

$$\det(\mathbf{L}) = 4(\sqrt{5})^3/3^5 \quad \text{and} \quad (\det(\mathbf{L}))^2 = 4^2 \times 5^3/3^{10} . \quad (4.11)$$

From (4.6), (4.10) and (4.11) it follows that

$$\det(\mathbf{X}'_2 \mathbf{X}_2) = 4^2(8^8(4/5)^3) (5^3/3^{10}) = 8^8(4^5/3^{10}) .$$

Since $\det(\mathbf{M}(\xi)) = \det((\mathbf{X}'_2 \mathbf{X}_2)/N) = \det(\mathbf{X}'_2 \mathbf{X}_2)/N^P$ we have, for $N = P = 8$

$$\det(\mathbf{M}(\xi)) = 8^8 \times 4^5/(3^{10} \times 8^8) = 4^5/3^{10}$$

and

$$D\text{-efficiency} = 100((4^5/3^{10})/0.08192)^{(1/8)} = 82.4\% .$$

Formula (4.10) is very usefully since it can be used to calculate the determinant of $\mathbf{X}'_2\mathbf{X}_2$ from $\mathbf{X}'_1\mathbf{X}_1$ if the elements of \mathbf{X}_2 can be written as linear functions of the elements of \mathbf{X}_1 .

Since the D -efficiency found equals 82.4% we can ask ourselves whether an $4 \times 2 \times 2/8$ design can be found with a higher D -efficiency.

We can write the design matrix of the $4 \times 2 \times 2/8$ design, using the variables $-1 \leq x_i \leq 1$, $i = 1, 2, 3$, instead of x_P, x_Q and x_R . We derive this new design matrix from Table 4.5a and find values given in Table 4.8.

Exp.	x_1	x_2	x_3
unit			
1	-1	-1	1
2	1/3	-1	1
3	-1/3	-1	-1
4	1	-1	-1
5	-1	1	-1
6	1/3	1	-1
7	-1/3	1	1
8	1	1	1

Table 4.8. The $4 \times 2 \times 2/8$ design.

The appropriate model for this design is (3.1) for $d = 1$ and $k = 3$.

According to Table 3.1, the D -optimal design for this model contains design points such that 80% of them are of the type $\pm 1, \pm 1, \pm 1$ and 20% of the type $0, \pm 1, \pm 1$. Table 4.8 does not contain values $x_1 = 0$ but only values $x_1 = -1/3$ and $x_1 = +1/3$. We therefore have to compromise in our effort to find a better $4 \times 2 \times 2/8$ design.

We therefore will construct a design with

$0.80 \times 8 \approx 6$ points of the type $\pm 1, \pm 1, \pm 1$ and

$0.20 \times 8 \approx 2$ points of the type $\pm 1/3, \pm 1, \pm 1$.

We find the design given in Table 4.9.

Exp.	x_1	x_2	x_3
unit			
1	-1	-1	1
2	-1	1	1
3	-1	1	-1
4	-1/3	-1	-1
5	1/3	1	1
6	1	-1	1
7	1	-1	-1
8	1	1	-1

Table 4.9. A $4 \times 2 \times 2/8$ design.

When we calculate $\det(\mathbf{X}'\mathbf{X})$ for the above design it appears that this value equals 0 and $(\mathbf{X}'\mathbf{X})$ is singular.

Further efforts were made to find a better $4 \times 2 \times 2/8$ design but none were successful.

4.5.2. The calculation of the G-efficiency

The G-efficiency is defined as

$$G\text{-efficiency} = 100P / (N \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))), \quad (4.12)$$

see (2.27).

For the $4 \times 2 \times 2/8$ design we had

$$\mathbf{f}'(\mathbf{x}) = (x_0, Pl, QR, Pq, Q, PlR, R, PlQ) \quad (4.13)$$

$$(\mathbf{X}'\mathbf{X})^{-1} = (1/8) \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5/4 & -(1/4)\sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & -(1/4)\sqrt{5} & 5/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5/4 & -(1/4)\sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & -(1/4)\sqrt{5} & 5/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5/4 & -(1/4)\sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 & -(1/4)\sqrt{5} & 5/4 \end{bmatrix} \quad (4.14)$$

Using (2.49) we can find that

$$Pq_i = (5/4) (Pl_i^2 - 1) . \quad (4.15)$$

From (4.13), (4.14) and (4.15) we find

$$\begin{aligned} f'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} f(\mathbf{x}) &= (1/8) (1 + (5/4)^2 (Pl^2 - 1)^2 + \\ &+ (5/4) (Pl^2Q^2 + Pl^2R^2 + Q^2R^2 + Pl^2 + Q^2 + R^2) - 1.5\sqrt{5} PlQR) . \end{aligned} \quad (4.16)$$

Since

$$-3/\sqrt{5} \leq Pl_i \leq 3/\sqrt{5} , \quad -1 \leq Q < +1 \quad \text{and} \quad -1 \leq R \leq +1 ,$$

we can easily see that $\max f'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} f(\mathbf{x})$ is reached when using one of the four following design points.

Design point	Pl_i	Q_i	R_i
1	$3/\sqrt{5}$	-1	+1
2	$3/\sqrt{5}$	+1	-1
3	$-3/\sqrt{5}$	-1	-1
4	$-3/\sqrt{5}$	+1	+1

Substituting any of these sets (Pl_i, Q_i, R_i) into (4.16) gives

$$\max (\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})) = 17/8 .$$

Using (4.12) we obtain

$$G\text{-efficiency} = 100 \times 8 / (8 \times 17/8) = 47.1\% .$$

4.6. An application of the $4 \times 2 \times 2/8$ design

To study the light output of a particular type of lamp, it was decided to examine the effect of three factors P , Q and R . These factors and their levels are presented in Table 4.10. The model used is given in (4.1).

Factor	Levels
P	The amount of amalgam 3, 5, 7, 9,
Q	Type of gas in the lamp G1, G2
R	Type of glas used I, II

Table 4.10. Factors and levels of lamp experiment.

Only a small experiment could be carried out because the lamps were expensive and the available time in which to carry out the experiment was limited.

It was therefore decided to carry out a half replicate of a $4 \times 2 \times 2$ design. The results, the light output of one lamp in each "cell", are given in Table 4.11. This design has a structure as given in Table 4.6a and 4.6b.

		Q: Type of gas		G1		G2	
		x_Q		0		1	
P: Amount of amalgam	R: Type of glass		I	II	I	II	
	x_R		0	1	0	1	
		x_P					
3	0			32.9	13.9		
5	1		21.7				5.0
7	2			24.2	14.6		
9	3		24.5				15.9

Table 4.11. Data of the lamp experiment.

We can now, using Table 4.5b, write the X and Y matrix and find

x_{0i}	Pl_i	Q_iR_i	Pq_i	Q_i	Pl_iR_i	R_i	Pl_iQ_i	Y_i
1	$-3/\sqrt{5}$	-1	1	-1	$-3/\sqrt{5}$	1	$3/\sqrt{5}$	32.9
1	$1/\sqrt{5}$	-1	-1	-1	$1/\sqrt{5}$	1	$-1/\sqrt{5}$	24.2
1	$-1/\sqrt{5}$	1	-1	-1	$1/\sqrt{5}$	-1	$1/\sqrt{5}$	21.7
1	$3/\sqrt{5}$	1	1	-1	$-3/\sqrt{5}$	-1	$-3/\sqrt{5}$	24.5
1	$-3/\sqrt{5}$	-1	1	1	$3/\sqrt{5}$	-1	$-3/\sqrt{5}$	13.9
1	$1/\sqrt{5}$	-1	-1	1	$-1/\sqrt{5}$	-1	$1/\sqrt{5}$	14.6
1	$-1/\sqrt{5}$	1	-1	1	$-1/\sqrt{5}$	1	$-1/\sqrt{5}$	5.0
1	$3/\sqrt{5}$	1	1	1	$3/\sqrt{5}$	1	$3/\sqrt{5}$	15.9

Hence

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} 152.7 \\ -7.1/\sqrt{5} \\ -18.5 \\ 21.7 \\ -53.9 \\ -56.5/\sqrt{5} \\ 3.3 \\ 38.3/\sqrt{5} \end{bmatrix}$$

Using $(\mathbf{X}'\mathbf{X})^{-1}$ as calculated in Section 4.2 we find

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y} = \begin{bmatrix} 19.08750 \\ 0.35625\sqrt{5} \\ -2.66875 \\ 2.71250 \\ -6.65625 \\ -0.08125\sqrt{5} \\ -0.68125 \\ 1.09375\sqrt{5} \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_{23} \\ \hat{\beta}_{11} \\ \hat{\beta}_2 \\ \hat{\beta}_{13} \\ \hat{\beta}_3 \\ \hat{\beta}_{12} \end{bmatrix}$$

Using equation (2.6) we have

$$\mathbf{e}'\mathbf{e} = \mathbf{Y}'\mathbf{Y} - \hat{\beta}'\mathbf{X}'\mathbf{Y} . \quad (4.17)$$

Because the number of observations equals the number of β 's we have $\mathbf{e}'\mathbf{e} = 0$ and

$$\mathbf{Y}'\mathbf{Y} = \hat{\beta}'\mathbf{X}'\mathbf{Y} . \quad (4.18)$$

Equation (4.18) provides a check because we can calculate $\mathbf{Y}'\mathbf{Y}$ and $\hat{\beta}'\mathbf{X}'\mathbf{Y}$ separately.

We have

$$\mathbf{Y}'\mathbf{Y} = \sum_{i=1}^8 y_i^2 = 32.9^2 + 24.2^2 + \dots + 15.9^2 = 3423.37$$

$$\begin{aligned}\hat{\beta}'\mathbf{X}'\mathbf{Y} &= 19.08750 \times 152.7 + 0.35625\sqrt{5} \times (-7.1/\sqrt{5}) + \dots + 1.09375\sqrt{5} \times 38.3/\sqrt{5} \\ &= 3423.37 .\end{aligned}$$

From the results of previous experiments we have an estimate of σ^2 , namely $\hat{\sigma}^2 = 16.28$ with 20 degrees of freedom.

We can now obtain the analysis of variance as given in Table 4.12.

Model component	Sum of squares	Degrees of freedom	Mean square	Calculated F -value
β_0	2914.66	1	2914.66	179.03
(β_1, β_{23})	46.84	2	23.42	1.44
β_{11}	58.86	1	58.86	3.61
(β_2, β_{13})	363.36	2	181.68	11.16
(β_3, β_{12})	39.64	2	19.82	1.22
—				
Total	3423.36			
—				

Table 4.12. Analysis of variance for the lamp experiment.

The F -value was calculated using $\hat{\sigma}^2 = 16.28$ in the denominator. Using a significance level of 10% for F we have

$$F_{20,0.90}^1 = 2.97 \quad F_{20,0.90}^2 = 2.59 .$$

We conclude that β_0 , β_{11} and the group (β_2, β_{13}) are significant. In order to examine the estimates of β in more detail we again give these estimates together with their standard deviations and the appropriate t -test.

The estimated standard deviation of $\hat{\beta}$ is obtained by multiplying the corresponding diagonal element of $(\mathbf{X}'\mathbf{X})^{-1}$ by $\hat{\sigma}^2$ and taking the square root. We find

	$\hat{\sigma}_{\hat{\beta}}$	$t = (\hat{\beta})/\hat{\sigma}_{\hat{\beta}}$
$\hat{\beta}_0 = 19.0875$	1.4267	13.38
$\hat{\beta}_1 = 0.3562\sqrt{5}$	1.5951	0.50
$\hat{\beta}_{23} = -2.6688$	1.5951	-1.67
$\hat{\beta}_{11} = 2.7125$	1.4267	1.90
$\hat{\beta}_2 = -6.6562$	1.5951	4.17
$\hat{\beta}_{13} = -0.0812\sqrt{5}$	1.5951	0.11
$\hat{\beta}_3 = 0.6812$	1.5951	0.42
$\hat{\beta}_{12} = 1.0938\sqrt{5}$	1.5951	1.53

The 10%-point for the two sided t -value with 20 degrees of freedom equals 1.725 and we now find that β_0 , β_{11} and β_2 are significant. Although the group (β_2, β_{13}) was significant it is clear from the small t -value for $\hat{\beta}_{13}$ that β_{13} is not relevant. However a significant value of β_{11} implies an effect of factor P . We therefore decide to use the estimate $\hat{\beta}_1$ as well in order to obtain a correct measure of the P -effect.

Our estimated model therefore is

$$\widehat{E}(y_i) = \hat{\beta}_0 x_{0i} + \hat{\beta}'_1 P l_i + \hat{\beta}_{11} P q_i + \hat{\beta}'_2 Q_i . \quad (4.19)$$

The estimates for β_0 and β_{11} do not change because they were not correlated with other $\hat{\beta}$'s.

We found

$$\hat{\beta}_0 = 19.0875$$

$$\hat{\beta}_{11} = 2.7125 .$$

The $X'X$ matrix corresponding to (4.19) is diagonal with elements to be obtained from the original $X'X$ matrix.

Using the appropriate diagonal element of $X'X$ and the corresponding element of $X'Y$ we find new estimates of β_1 and β_2 , namely

$$\hat{\beta}'_1 = -7.1/(8\sqrt{5}) = -0.3969$$

$$\hat{\beta}'_2 = -53.9/8 = -6.7375 .$$

The estimated model therefore is

$$E(\widehat{y}_i) = 19.09 - 0.40PI_i + 2.71Pq_i - 6.74Q_i . \quad (4.20)$$

If we denote the levels of P and Q by $x_P = 0, 1, 2, 3$ and $x_Q = 0, 1$, respectively, we have the following relations between x_{P_i} , PI_i , Pq_i and between x_{Q_i} and Q_i .

$$PI_i = (-3 + 2x_{P_i})/\sqrt{5} \quad (4.21)$$

$$Pq_i = 1 - 3x_{P_i} + x_{P_i}^2 \quad (4.22)$$

and

$$Q_i = -1 + 2x_{Q_i} . \quad (4.23)$$

See also formula (2.49).

Substituting (4.21), (4.22) and (4.23) in (4.20) we find

$$E(\widehat{y}_i) = 29.08 - 8.49x_{P_i} + 2.71x_{P_i}^2 - 13.48x_{Q_i} . \quad (4.24)$$

For the two types of gas G1($x_{Q_i} = 0$) and G2($x_{Q_i} = 1$) we substitute $x_{Q_i} = 0$ and $x_{Q_i} = 1$, respectively, in (4.24) and find

$$G1(x_{Q_i} = 0) : E(\widehat{y}_i) = 29.08 - 8.49x_{P_i} + 2.71x_{P_i}^2 \quad (4.25)$$

$$G2(x_{Q_i} = 1) : E(\widehat{y}_i) = 15.60 - 8.49x_{P_i} + 2.71x_{P_i}^2 . \quad (4.26)$$

These formulae have, together with the original observations, been plotted in Figure 4.1.

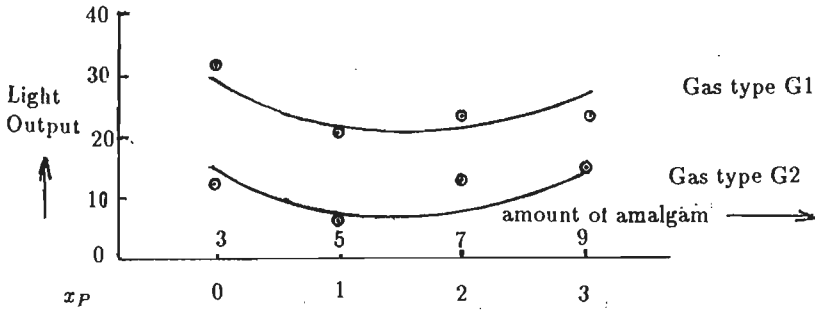


Fig. 4.1. Relation between the amount of amalgam and light output for two types of gas.

Figure 4.1 is very interesting because it shows the large and constant difference between the two types of gas and a minimum value of light output for $x_P = 1.57$, equivalent to an amount of amalgam of 6.14.

The value of $x_P = 1.57$ was obtained by differentiating (4.25) or (4.26) and equating the resulting formula to zero.

The highest light output is obtained for $x_P = 0$ and gas type G1. The corresponding light output is obtained by substituting $x_P = 0$ in (4.25). We find

$$\widehat{E}(y) = 29.08 .$$

4.7. The $3 \times 2 \times 2$ design in 8 experimental units

In order to construct a $3 \times 2 \times 2$ design in 8 experimental units, we again employ the X matrix of column vectors for a 2^3 design as presented in Table 4.13.

Experimental

unit	x_{0i}	A_i	B_i	C_i	$A_i B_i$	$A_i C_i$	$B_i C_i$	$A_i B_i C_i$
1	1	-1	-1	-1	+1	+1	+1	-1
2	1	+1	-1	-1	-1	-1	+1	+1
3	1	-1	+1	-1	-1	+1	-1	+1
4	1	+1	+1	-1	+1	-1	-1	-1
5	1	-1	-1	+1	+1	-1	-1	+1
6	1	+1	-1	+1	-1	+1	-1	-1
7	1	-1	+1	+1	-1	-1	+1	-1
8	1	+1	+1	+1	+1	+1	+1	+1

Table 4.13. The \mathbf{X} matrix of column vectors for the 2^3 design.

The factors to be used are as follows:

P : A quantitative three-level factor with equally spaced levels 0, 1 and 2.

Q : A two-level factor with levels $Q_1 = -1$ and $Q_2 = +1$, or $x_{Q1} = 0$ and $x_{Q2} = 1$.

R : A two-level factor with levels $R_1 = -1$ and $R_2 = +1$, or $x_{R1} = 0$ and $x_{R2} = 1$.

Using again orthogonal polynomials Pl and Pq as defined in Section 2.9, we have the following mathematical model

$$y_i = \beta_0 x_{0i} + \beta_1 Pl_i + \beta_{23} Q_i R_i + \beta_{11} Pq_i + \beta_2 Q_i + \beta_{13} Pl_i R_i + \beta_3 R_i + \beta_{12} Pl_i Q_i + \varepsilon_i \quad (4.27)$$

This model is the same as (4.1) and since it contains 8 parameters β , a design of 8 experimental units should again be sufficient. To find the column vector elements $Pl_i, R_i, \dots, Pl_i Q_i$ we use the \mathbf{X} matrix of Table 4.13.

We shall employ the technique of replacement and collapsing as summarized in Table 2.6 of Section 2.10.

We use the relations according to (2.50) and (2.51), i.e.

$$Pl_i = (A_i - A_i B_i) / \sqrt{2}$$

$$Pq_i = -B_i \ .$$

These equations represent the replacement of the two factors A and B with two levels each

by a three-level factor.

The column vectors \mathbf{Q} and \mathbf{R} can be obtained by choosing two vectors from the set $\mathbf{C}, \mathbf{AC}, \mathbf{BC}, \mathbf{ABC}$, in the matrix of Table 4.13. We can therefore, as in Section 4.2 construct 6 possible designs as presented in Table 4.14.

Nr. of design	Column vector elements		
	Q_i	R_i	$\rightarrow Q_i R_i$
1	C_i	$A_i C_i$	A_i
2	C_i	$B_i C_i$	B_i
3	C_i	$A_i B_i C_i$	$A_i B_i$
4	$A_i C_i$	$B_i C_i$	$A_i B_i$
5	$A_i C_i$	$A_i B_i C_i$	B_i
6	$B_i C_i$	$A_i B_i C_i$	A_i

Table 4.14. Six possible $3 \times 2 \times 2/8$ designs.

Designs 2 and 5 cannot be used since $Q_i R_i = B_i = -Pq_i$, which means that $\hat{\beta}_{23}$ will be confounded with $\hat{\beta}_{11}$.

When we examine the other designs by writing the relevant design matrices as in Section 4.2 and Table 4.4a we find that there are only two different designs as given in Table 4.15a and 4.15b.

$x_P \backslash x_Q$	0		1		
	x_R	0	1	0	1
0		1	5		
1	4	3	7	8	
2	2			6	

Design 1, $Q_i = C_i, R_i = A_i C_i$

Design 6, $Q_i = B_i C_i, R_i = A_i B_i C_i$

Table 4.15a.

$x_P \backslash x_Q$	0		1		
	x_R	0	1	0	1
0	1			5	
1	4	3	7	8	
2		2	6		

Design 3, $Q_i = C_i, R_i = A_i B_i C_i$

Design 4, $Q_i = A_i C_i, R_i = A_i B_i C_i$

Table 4.15b.

When we compare Table 4.15a with Table 4.15b we can easily see that they represent the same design since the only difference between these tables is the interchange of levels 0 and

2 of factor P . We can see this if we assign level 0 to level 2 and level 2 to level 0 of factor P in Table 4.15b. We then obtain the design of Table 4.15a.

We now proceed to examine design 1 in more detail.

Using the same method as in Section 4.2 we may write the elements of the column vectors of the X matrix for design 1. We find, see Table 4.16

$$\begin{array}{ll}
 x_{0i} = 1 & Pl_i = (A_i - A_i B_i)/\sqrt{2} \\
 Q_i R_i = A_i & Pq_i = -B_i \\
 Q_i = C_i & Pl_i R_i = (C_i - B_i C_i)/\sqrt{2} \\
 R_i = A_i C_i & Pl_i Q_i = (A_i C_i - A_i B_i C_i)/\sqrt{2}
 \end{array}$$

Table 4.16. Column vector elements for a $3 \times 2 \times 2/8$ design.

As in Section 4.2 we can use these formulae to calculate $X'X$ directly, the result being

$$X'X = \begin{array}{cccccccc}
 x_{0i} & Pl_i & Q_i R_i & Pq_i & Q_i & Pl_i R_i & R_i & Pl_i Q_i \\
 \left[\begin{array}{cccccccc}
 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 8 & 4/\sqrt{2} & 0 & 0 & 0 & 0 & 0 \\
 0 & 4/\sqrt{2} & 8 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 8 & 4/\sqrt{2} & 0 & 0 \\
 0 & 0 & 0 & 0 & 4/\sqrt{2} & 8 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 8 & 4/\sqrt{2} \\
 0 & 0 & 0 & 0 & 0 & 0 & 4/\sqrt{2} & 8
 \end{array} \right]
 \end{array} \tag{4.28}$$

and

$$(\mathbf{X}'\mathbf{X})^{-1} = \frac{1}{4} \begin{bmatrix} 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1/\sqrt{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/\sqrt{2} & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/\sqrt{2} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1/\sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & -1/\sqrt{2} & 1 \end{bmatrix} \quad (4.29)$$

The $(\mathbf{X}'\mathbf{X})^{-1}$ matrix shows that there are three pairs of $\hat{\beta}$'s correlated namely $(\hat{\beta}_1, \hat{\beta}_{23})$, $(\hat{\beta}_2, \hat{\beta}_{13})$ and $(\hat{\beta}_3, \hat{\beta}_{12})$.

The relevant correlation coefficient equals

$$\rho_{pq} = \frac{\text{cov}(\hat{\beta}_p, \hat{\beta}_q)}{\sqrt{(\text{var}(\hat{\beta}_p) \text{var}(\hat{\beta}_q))}} = \frac{-(1/2)(1/4)\sqrt{2}}{\sqrt{((1/4)(1/4))}} = -0.71.$$

This correlation coefficient is fairly high and we can ask ourselves whether a better design can be found. Design 8.2 of the Appendix gives more detail about design 1 of Table 4.15a such as \mathbf{r}^{-1} . The main diagonal of this matrix contains 6 two's meaning that 6 VIF's equal two which is not excessively large.

We already saw that the designs 2, 3, 4, 5 and 6 listed in Table 4.14 do not give a better design.

The only other possibility is to find out whether a different collapsing procedure produces a better design. To this end we consider the collapsing given in Table 2.7 which is reproduced in Table 4.17.

Four level factor		Three level factor					
x'_{pi}		x_{pi}	A_i	B_i	$A_i B_i$	Pi	Pq_i
0	→	0	-1	-1	+1	$-5/\sqrt{11}$	$+2\sqrt{(2/11)}$
2	→	2	+1	-1	-1	$+3/\sqrt{11}$	$+1\sqrt{(2/11)}$
1	→	1	-1	+1	-1	$-1/\sqrt{11}$	$-4\sqrt{(2/11)}$
3	→	2	+1	+1	+1	$+3/\sqrt{11}$	$+1\sqrt{(2/11)}$

Table 4.17. Collapsing a four-level factor to a three-level factor with relevant column vectors.

The quantities in Table 4.17 are related as follows

$$Pl_i = (3A_i + B_i - A_i B_i) / \sqrt{11}$$

$$Pq_i = \{A_i - 3(B_i - A_i B_i) / 2\} \sqrt{(2/11)}$$

$$Pl_i = (-5 + 4x_{Pi}) / \sqrt{11} \rightarrow x_{Pi} = (Pl_i \sqrt{11} + 5) / 4$$

$$Pq_i = \{+2 - (23/2)x_{Pi} + (11/2)x_{Pi}^2\} \sqrt{(2/11)}.$$

Again we can make 6 possible choices for the pair Q_i and R_i , but a thorough investigation revealed that again two of these produced designs with complete confounding between some β 's while the remaining 4 designs were in fact identical.

We therefore examine only one of these corresponding with

$$Pl_i = (3A_i + B_i - A_i B_i) / \sqrt{11}$$

$$Pq_i = (A_i - 3(B_i - A_i B_i) / 2) \sqrt{2/11}$$

$$Q_i = C_i$$

$$R_i = B_i C_i.$$

(4.30)

We can now calculate $X'X$; $(X'X)^{-1}$ and r^{-1} and obtain the following results

$$X'X = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 2.412 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.412 & 8 & -5.117 & 0 & 0 & 0 & 0 \\ 0 & 0 & -5.117 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 2.412 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.412 & 8 & 0 & -4.364 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 2.412 \\ 0 & 0 & 0 & 0 & 0 & -4.364 & 2.412 & 8 \end{bmatrix}$$

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.148 & -0.075 & -0.048 & 0 & 0 & 0 & 0 \\ 0 & -0.075 & 0.25 & 0.16 & 0 & 0 & 0 & 0 \\ 0 & -0.048 & 0.16 & 0.227 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.145 & -0.065 & 0.012 & -0.039 \\ 0 & 0 & 0 & 0 & -0.065 & 0.215 & -0.039 & 0.129 \\ 0 & 0 & 0 & 0 & 0.012 & -0.039 & 0.145 & -0.065 \\ 0 & 0 & 0 & 0 & -0.039 & 0.129 & -0.065 & 0.215 \end{bmatrix}$$

$$\mathbf{r}^{-1} = \begin{bmatrix} 1.182 & -0.603 & -0.386 & 0 & 0 & 0 & 0 \\ -0.603 & 2 & 1.279 & 0 & 0 & 0 & 0 \\ -0.386 & 1.279 & 1.818 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.156 & -0.518 & 0.094 & -0.311 \\ 0 & 0 & 0 & -0.518 & 1.719 & -0.311 & 1.031 \\ 0 & 0 & 0 & 0.094 & -0.311 & 1.156 & -0.518 \\ 0 & 0 & 0 & -0.311 & 1.031 & -0.518 & 1.719 \end{bmatrix}$$

The correlation matrix corresponding to $(\mathbf{X}'\mathbf{X})^{-1}$ equals

$$\rho_{pq} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 1 & -0.39 & -0.26 & 0 & 0 & 0 & 0 \\ & & 1 & 0.67 & 0 & 0 & 0 & 0 \\ & & & 1 & 0 & 0 & 0 & 0 \\ & & & & 1 & -0.37 & 0.08 & -0.22 \\ \text{Omitted because} & & & & & 1 & -0.22 & 0.60 \\ \text{of symmetry} & & & & & & 1 & -0.37 \\ & & & & & & & 1 \end{bmatrix}$$

The ρ_{pq} matrix shows that we now have 9 non-zero correlation coefficients instead of three. Moreover two of these are fairly high namely 0.67 and 0.60, which is very close to the value of 0.71 found earlier.

On the other hand, the matrix \mathbf{r}^{-1} shows that only one VIF equals 2 whereas the six others are less than 2. See also design 8.3 of the Appendix for other particulars.

The advantages of the design corresponding with (4.30) are however not obvious and we decide to continue with design 1 of Table 4.15a.

4.8. The alias structure of the $3 \times 2 \times 2/8$ design.

It might be the case that the model (4.27) is not complete because 4 components should be added, i.e.

$$\gamma_{112}Pq_iQ_i + \gamma_{113}Pq_iR_i + \gamma_{123}Pl_iQ_iR_i + \gamma_{1123}Pq_iQ_iR_i . \quad (4.31)$$

Using Table 4.16 we can easily calculate

$$\begin{aligned} Pq_iQ_i &= -B_iC_i & Pq_iR_i &= -A_iB_iC_i \\ Pl_iQ_iR_i &= (1 - B_i)/\sqrt{2} & Pq_iQ_iR_i &= -A_iB_i . \end{aligned}$$

Using the same method as in Section 4.4 gives the following results

$$\begin{aligned} E(\hat{\beta}_0) &= \beta_0 + 0.5\gamma_{123}\sqrt{2} & E(\hat{\beta}_2) &= \beta_2 - \gamma_{112} \\ E(\hat{\beta}_1) &= \beta_1 + \gamma_{1123}\sqrt{2} & E(\hat{\beta}_{13}) &= \beta_{13} + \gamma_{112}\sqrt{2} \\ E(\hat{\beta}_{23}) &= \beta_{23} - \gamma_{1123} & E(\hat{\beta}_3) &= \beta_3 - \gamma_{113} \\ E(\hat{\beta}_{11}) &= \beta_{11} + 0.5\gamma_{123}\sqrt{2} & E(\hat{\beta}_{12}) &= \beta_{12} + 0.5\gamma_{113}\sqrt{2} . \end{aligned}$$

4.9. An application of the $3 \times 2 \times 2/8$ design

A certain type of wire is produced with an oxyde layer. The layer thickness is an important quality characteristic and it is determined by means of weighing. The development department wanted to examine the effect of three factors on oxyde layer thickness in a small scale experiment. The factors with their levels are given in Table 4.18.

Factor	Level
P : The amount of gas	1, 3, 5 liters/minute
Q : The amount of air	3.0, 4.5 liters/minute
R : Wire	I, II

Table 4.18. Factors and levels of wire experiment.

Design 1 of Table 4.15a was used and this design together with the data are given in Table 4.19.

		Q: amount of air		4.5	
		3.0		1	
P: amount of gas	x_Q	0		1	
	R: Wire	I	II	I	II
	x_R	0	1	0	1
	x_P				
1	0		7.61	7.23	
3	1	5.02	4.72	6.06	5.76
5	2	3.04			5.40

Table 4.19. Experimental design and data of wire experiment.

From previous experiments we have an estimate of σ^2 , $\hat{\sigma}^2 = 0.1180$ with 17 degrees of freedom. From Table 4.13 and Table 4.16 we obtain Table 4.20 containing the X matrix of column vectors and the vector of observations Y.

Exp. unit	x_{0i}	Pl_i	Q_iR_i	Pq_i	Q_i	Pl_iR_i	R_i	Pl_iQ_i	Y_i
1	1	$-\sqrt{2}$	-1	1	-1	$-\sqrt{2}$	1	$\sqrt{2}$	7.61
2	1	$\sqrt{2}$	1	1	-1	$-\sqrt{2}$	-1	$-\sqrt{2}$	3.04
3	1	0	-1	-1	-1	0	1	0	4.72
4	1	0	1	-1	-1	0	-1	0	5.02
5	1	$-\sqrt{2}$	-1	1	1	$\sqrt{2}$	-1	$-\sqrt{2}$	7.23
6	1	$\sqrt{2}$	1	1	1	$\sqrt{2}$	1	$\sqrt{2}$	5.40
7	1	0	-1	-1	1	0	-1	0	6.06
8	1	0	1	-1	1	0	1	0	5.76

Table 4.20. X matrix and Y vector for the wire experiment.

Hence

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} 44.84 \\ -6.40\sqrt{2} \\ -6.40 \\ 1.72 \\ 4.06 \\ 1.98\sqrt{2} \\ 2.14 \\ 2.74\sqrt{2} \end{bmatrix}$$

Using (4.29) we obtain

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y} = \begin{bmatrix} 5.605 \\ -0.800\sqrt{2} \\ 0.000 \\ 0.215 \\ 0.520 \\ -0.0125\sqrt{2} \\ -0.150 \\ 0.4175\sqrt{2} \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_{23} \\ \hat{\beta}_{11} \\ \hat{\beta}_2 \\ \hat{\beta}_{13} \\ \hat{\beta}_3 \\ \hat{\beta}_{12} \end{bmatrix}$$

Carrying out similar calculations as in Section 4.6 we find

$$\mathbf{Y}'\mathbf{Y} = \sum_{i=1}^8 y_i^2 = 7.61^2 + 3.04^2 + \dots + 5.76^2 = 265.9666$$

$$\hat{\beta}\mathbf{X}'\mathbf{Y} = 5.605 \times 44.84 + 2 \times (-0.800) \times (-6.40) + \dots + (0.4175\sqrt{2}) \times (2.74\sqrt{2})$$

$$\hat{\beta}\mathbf{X}'\mathbf{Y} = 265.9666 .$$

Model component	Sum of squares	Degrees of freedom	Mean square	Calculated F -value
β_0	251.3282	1	251.3282	2129.90
β_1, β_{23}	10.2400	2	5.12	43.39
β_{11}	0.3698	1	0.3698	3.13
β_2, β_{13}	2.0617	2	1.0308	8.74
β_3, β_{12}	1.9669	2	0.9834	8.33

Table 4.21. Analysis of variance for wire experiment.

For a significance level of 0.05 we have the critical F -values

$$F_{17,0.95}^1 = 4.45 \quad \text{and} \quad F_{17,0.95}^2 = 3.59 .$$

We conclude that β_0 and the sets $(\beta_1, \beta_{23}), (\beta_2, \beta_{13}), (\beta_3, \beta_{12})$ are significant.

To examine the estimates of the β 's in more detail we, as in Section 4.6, calculate $\hat{\sigma}_{\hat{\beta}}$ and the appropriate t -test. We obtain

	$\hat{\sigma}_{\hat{\beta}}$	$t = \hat{\beta}/\hat{\sigma}_{\hat{\beta}}$
$\hat{\beta}_0 = 5.605$	0.1215	46.13
$\hat{\beta}_1 = -0.800\sqrt{2}$	0.1718	-6.59
$\hat{\beta}_{23} = 0.000$	0.1718	0.00
$\hat{\beta}_{11} = 0.215$	0.1215	1.77
$\hat{\beta}_2 = 0.520$	0.1718	3.03
$\hat{\beta}_{13} = -0.0125\sqrt{2}$	0.1718	-0.10
$\hat{\beta}_3 = -0.150$	0.1718	-0.87
$\hat{\beta}_{12} = 0.4175\sqrt{2}$	0.1718	3.44 .

The 5%-point for the two sided t -value with 17 degrees of freedom equals 2.11.

We conclude that β_0 , β_1 , β_2 and β_{12} are significant, which means that we have no effect of the factor $R(\text{wire})$.

However, a significant β_1 means that the factor P has an effect. In order to have a better estimate of the P -effect we shall also use $\hat{\beta}_{11} = 0.215$, the more so since the corresponding t -value is fairly large.

Since however the sets of estimates $(\hat{\beta}_1, \hat{\beta}_{23})$, $(\hat{\beta}_2, \hat{\beta}_{13})$ and $(\hat{\beta}_3, \hat{\beta}_{12})$ are correlated, we have to find new estimates for β_1 , β_2 and β_{12} corresponding to the model

$$E(y_i) = \beta_0 x_{0i} + \beta_1 P_i + \beta_{11} P_i + \beta_2 Q_i + \beta_{12} P_i Q_i . \quad (4.32)$$

The $\mathbf{X}'\mathbf{X}$ matrix corresponding to (4.32) is diagonal with elements to be obtained from Table 4.20 and which are all equal to 8.

Since $\mathbf{X}'\mathbf{X}\hat{\beta} = \mathbf{X}'\mathbf{Y}$ we have new estimates for β_1 , β_2 and β_{12} , namely

$$\hat{\beta}'_1 = (-6.40\sqrt{2})/8 = -1.1314$$

$$\hat{\beta}'_2 = 4.06/8 = 0.508$$

$$\hat{\beta}'_{12} = (2.74\sqrt{2})/8 = 0.4844 .$$

The estimate $\hat{\beta}'_1$ has the same value as $\hat{\beta}_1$ and the values of $\hat{\beta}'_2$ and $\hat{\beta}'_{12}$ are only slightly different from $\hat{\beta}_2$ and $\hat{\beta}_{12}$ respectively. We now have

$$\widehat{E}(y_i) = 5.605 - 1.1314Pl_i + 0.215Pq_i + 0.508Q_i + 0.4844Pl_iQ_i . \quad (4.33)$$

Since

$$Pl_i = (-1 + x_{Pi})\sqrt{2}$$

$$Pq_i = 1 - 4x_{Pi} + 2x_{Pi}^2$$

$$Q_i = -1 + 2x_{Qi} ,$$

see also formulae (2.50), (2.51) and (4.23),

we obtain, after substituting these expressions in (4.33),

$$\widehat{E}(y_i) = 7.597 - 3.145x_{Pi} + 0.430x_{Pi}^2 - 0.354x_{Qi} + 1.370x_{Pi}x_{Qi} . \quad (4.34)$$

Equation (4.34) has been presented graphically in Figure 4.2, together with the original observations.

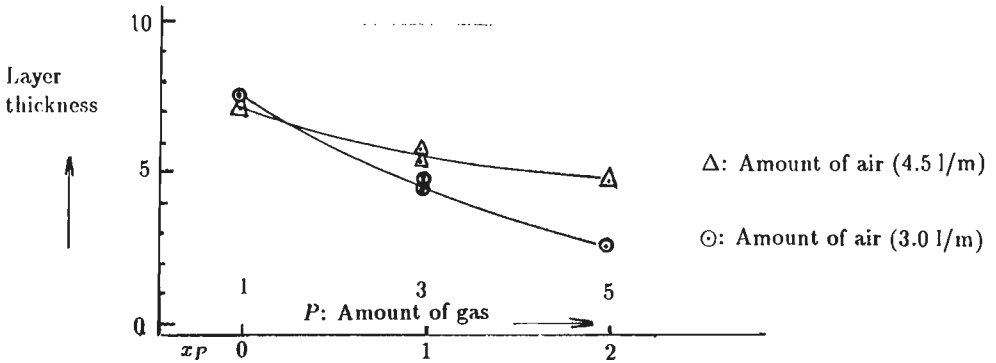


Fig. 4.2. Relation between amount of gas and layer thickness.

4.10. Summary of designs with 8 experimental units

The designs with 8 experimental units which have been discussed so far, have been numbered and listed in Table 4.22.

Design number	Group number	Design	Fraction	Largest $ \rho $	Remarks
8.1	I	$4 \times 2 \times 2/8$	$1/2$	0.45	Clumpwise orthogonality (See Table 4.6a)
8.2	I	$3 \times 2 \times 2/8$	$2/3$	0.71	Clumpwise orthogonality (See Table 4.15a)
8.3	I	$3 \times 2 \times 2/8$	$2/3$	0.67	Clumpwise orthogonality (See Table 4.17)
8.4	I	$3 \times 2 \times 2/8$	$2/3$	0.71	Clumpwise orthogonality (Identical with design 8.2)

Table 4.22. A number of fractional factorial experimental designs for quantitative factors with 8 experimental units.

The designs listed in Table 4.22 form a group since their source is the first design 8.1. The other designs are derived from 8.1 through collapsing.

Design 8.4 was derived from design 8.1 using a collapsing procedure to be given in Section 5.3.

Design 8.2 was also derived from design 8.1 using the collapsing procedure of Table 2.6. These two different collapsing techniques resulted in two sets of design generators, a definition of which will be given in Section 5.2, but the resulting designs turned out to be identical.

The D - and G -efficiencies of designs 8.2 and 8.3 were also calculated using the same method as in Section 4.5. We found

Design	D -efficiency	G -efficiency
8.2	68.4	25.0
8.3	81.3	25.0

Designs 8.1 up to and including 8.4 have been fully presented in the Appendix and will be discussed in more detail in Chapter 7.

CHAPTER 5

Designs using 16 and 32 experimental units

5.1. The 2^4 design

The 2^4 design shall now be used to construct a variety of designs with three or four factors, each of which has two, three or four levels.

As before we stipulate that the three- and four-level factors are quantitative and have equally spaced levels.

We shall, as already announced in Chapter 1, use two construction methods.

The first one uses methods similar to those used in Chapter 4 and will be dealt with in the Sections 5.2, 5.3 and 5.4.

The second method uses the properties of the D -optimal designs as discussed in Chapter 3. Designs derived from D -optimal designs will be treated in Section 5.7.

In Chapter 4 we found that only 3 designs with factors having more than two levels could be derived from the 2^3 design.

We shall see that the number of designs which can be derived from the 2^4 design is far greater. Because we shall frequently make use of the X matrix of column vectors of the 2^4 design we give this matrix in Table 5.1.

Nr. exp.	x_0	A	B	C	D	AB	AC	AD	BC	BD	CD	ABC	ABD	ACD	BCD	ABCD
1	1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	-1	-1	1
2	1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1
3	1	-1	1	-1	-1	-1	1	1	-1	-1	1	1	1	-1	1	-1
4	1	1	1	-1	-1	1	-1	-1	-1	-1	1	-1	-1	1	1	1
5	1	-1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1
6	1	1	-1	1	-1	-1	1	-1	-1	1	-1	-1	1	-1	1	1
7	1	-1	1	1	-1	-1	-1	1	1	-1	-1	-1	1	1	-1	1
8	1	1	1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	-1	-1
9	1	-1	-1	-1	1	1	1	-1	1	-1	-1	-1	1	1	1	-1
10	1	1	-1	-1	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1
11	1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1
12	1	1	1	-1	1	1	-1	1	-1	1	-1	-1	1	-1	-1	-1
13	1	-1	-1	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1
14	1	1	-1	1	1	-1	1	1	-1	-1	1	-1	-1	1	-1	-1
15	1	-1	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1	1	-1
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table 5.1. The X matrix of column vectors for the 2^4 design.

The \mathbf{X} matrix of Table 5.1 has similar properties as the \mathbf{X} matrix of the 2^3 design as discussed in Section 4.1 and 4.2.

It is well known from the literature that the 2^4 design can be used to estimate effects of 4, 5, ..., 15 two-level factors. For 4 and 5 factors it is possible to estimate all main effects and two-factor interactions.

If more than 5 factors are used, only the main effects and under certain conditions some two-factor interactions can be estimated.

In the next sections we shall construct designs, using the 2^4 design, with factors having more than two levels. We shall however ignore the $4 \times 2 \times 2/16$ design since it contains 16 experimental units. Its construction and analysis is therefore straightforward.

We shall instead try to construct a half replicate of the $4 \times 4 \times 2$ design from the \mathbf{X} matrix of Table 5.1.

5.2. The $4 \times 4 \times 2$ orthogonal design with 16 experimental units

The factors to be used are the following:

P, Q : Two quantitative factors with 4 equally spaced levels $x_P = 0, 1, 2, 3$ and $x_Q = 0, 1, 2, 3$

R : A two-level factor with levels $R_1 = -1$ and $R_2 = +1$ or $x_{R1} = 0$ and $x_{R2} = 1$.

Using the restrictions as given in Section 1.6 we have the mathematical model of the observations y_i as given in (5.1).

$$y_i = \beta_0 x_{oi} + \beta_1 P l_i + \beta_{11} P q_i + \beta_2 Q l_i + \beta_{22} Q q_i + \beta_3 R_i + \beta_{12} P l_i Q l_i + \beta_{13} P l_i R_i + \beta_{23} Q l_i R_i + \varepsilon_i, \quad i = 1, 2, \dots, 16, \quad (5.1)$$

where $E(\varepsilon) = \mathbf{0}$ and $E(\varepsilon' \varepsilon) = \sigma^2 \mathbf{I}$; \mathbf{I} is the identity matrix.

Since (5.1) contains 9 parameters β , the number of 16 experimental units is sufficient and allows an estimate of σ^2 with $16 - 9 = 7$ degree of freedom.

To construct the matrix of column vectors for (5.1) we employ a procedure similar to the one used in Section 4.2.

We find, using the column vectors $\mathbf{A}, \mathbf{B}, \dots, \mathbf{ABCD}$ of Table 5.1, the expressions given in Table 5.2.

$x_{0i} = 1$ $Pl_i = (2A_i + B_i)/\sqrt{5}$ $Pq_i = A_i B_i$ $Ql_i = (2C_i + D_i)/\sqrt{5}$ $Qq_i = C_i D_i$ $R_i = A_i B_i C_i D_i$ $Pl_i Ql_i = (4A_i C_i + 2A_i D_i + 2B_i C_i + B_i D_i)/5$ $Pl_i R_i = (2B_i C_i D_i + A_i C_i D_i)/\sqrt{5}$ $Ql_i R_i = (2A_i B_i D_i + A_i B_i C_i)/\sqrt{5} .$

Table 5.2. Column vector elements for the $4 \times 4 \times 2/16$ design.

The manner in which the expressions of Table 5.2 were found will now be explained.

The expressions for Pl_i , Pq_i , Ql_i and Qq_i imply that we have used the technique of replacement twice, since we assigned the column vectors \mathbf{A} , \mathbf{B} and \mathbf{AB} to \mathbf{Pl} and \mathbf{Pq} while those for \mathbf{C}, \mathbf{D} and \mathbf{CD} were assigned to \mathbf{Ql} and \mathbf{Qq} .

We therefore replaced the factors A and B by the four-level factor P and the factors C and D by the four-level factor Q . See also Section 2.9.

We therefore used 6 columns of Table 5.1 to calculate the 4 column vectors for the factors P and Q .

We have to select one more column vector in Table 5.1 for the remaining two-level factor R . We have in principle the choice from nine vectors, but it will appear that only one of these is suitable.

First of all it is evident that from the choice

$Pl_i = (2A_i + B_i)/\sqrt{5}$ and $Ql_i = (2C_i + D_i)/\sqrt{5}$, it follows that

$$Pl_i Ql_i = (4A_i C_i + 2A_i D_i + 2B_i C_i + B_i D_i)/5. \quad (5.2)$$

Formula (5.2) shows that the column vector for **PlQl** is calculated from 4 “interaction columns” of Table 5.1.

If we use one of these columns for the factor R , we immediately introduce a non zero off-diagonal element in $X'X$ and hence correlation between $\hat{\beta}$'s.

To avoid this we have to choose from the remaining column vectors **ABC**, **ABD**, **ACD**, **BCD** and **ABCD**.

Suppose we choose $R_i = A_i B_i C_i$. We then have $Pl_i R_i = (2B_i C_i + A_i C_i)/\sqrt{5}$ which are terms already in (5.2) and we again introduce non zero off-diagonal elements in $X'X$.

It appears that the only way to avoid this phenomenon is to choose $R_i = A_i B_i C_i D_i$ as was done in Table 5.2.

When we examine the expressions in Table 5.2 more closely we see that all column vectors of Table 5.1 appear only once.

It follows that all inner products of the vectors in Table 5.2 such as (x_0, Pl) , (Pl, Pq) , (Pl, Ql) , ..., (PIR, QIR) are equal to zero and that means that $X'X$ corresponding to model (5.1) is diagonal and we therefore have an orthogonal design.

The vector elements $Pl_i Ql_i$, $Pl_i R_i$ and $Ql_i R_i$ in Table 5.2 are calculated from other vector elements belonging to a group, which we shall call the *design generators*.

These are for our particular example given in Table 5.3.

$Pl_i = (2A_i + B_i)/\sqrt{5}$	$Pq_i = A_i B_i$
$Ql_i = (2C_i + D_i)/\sqrt{5}$	$Qq_i = C_i D_i$
$R_i = A_i B_i C_i D_i$	

Table 5.3. Design generators for the $4 \times 4 \times 2/16$ design.

It is extremely important to choose these generators very carefully since they determine the structure of the $X'X$ and therefore of the $(X'X)^{-1}$ matrix.

It is also stressed that the design generators not only yield some of the expressions in Table 5.2 but also enable us to calculate $X'X$ analytically using Table 5.2.

We find

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix}
 x_0 & Pl & Pq & Ql & Qq & R & PlQl & PlR & QlR \\
 16 & & & & & & & & \\
 & 16 & & & & & & & \\
 & & 16 & & & & & & \\
 & & & 16 & & & & & \\
 & & & & 16 & & & & \\
 & & & & & 16 & & & \\
 & & & & & & 16 & & \\
 & & & & & & & 16 & \\
 & & & & & & & & 16
 \end{bmatrix} \quad (5.3)$$

and

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix}
 1/16 & & & & & & & & \\
 & 1/16 & & & & & & & \\
 & & 1/16 & & & & & & \\
 & & & 1/16 & & & & & \\
 & & & & 1/16 & & & & \\
 & & & & & 1/16 & & & \\
 & & & & & & 1/16 & & \\
 & & & & & & & 1/16 & \\
 & & & & & & & & 1/16
 \end{bmatrix} \quad (5.4)$$

It appears that $\mathbf{X}'\mathbf{X}$ and $(\mathbf{X}'\mathbf{X})^{-1}$ are not only diagonal, but also have as diagonal elements the numbers 16 and $(1/16)$, respectively.

This was achieved by choosing the orthogonal polynomial values as given in Table 2.5. The matrices $\mathbf{X}'\mathbf{X}$ and $(\mathbf{X}'\mathbf{X})^{-1}$ are therefore equal to the $\mathbf{X}'\mathbf{X}$ and $(\mathbf{X}'\mathbf{X})^{-1}$ of the 2^4 design.

Having the number 16 as diagonal elements in $\mathbf{X}'\mathbf{X}$ is especially important since it facilitates the comparison with other designs. To find the design matrix we use the equations (4.21) and (4.23) and we write

$$Pl_i = (-3 + 2x_{Pi})/\sqrt{5} \quad (5.5)$$

$$Ql_i = (-3 + 2x_{Q_i})/\sqrt{5} \quad (5.6)$$

$$R_i = -1 + 2x_{R_i} . \quad (5.7)$$

Equations (5.5) and (5.6) are relations for four-level factors, equation (5.7) is valid for a two-level factor.

Using Table 5.2, (5.5), (5.6) and (5.7) we find

$$x_{P_i} = (3 + Pl_i \sqrt{5})/2 = (3 + 2A_i + B_i)/2 \quad (5.8a)$$

$$x_{Q_i} = (3 + Ql_i \sqrt{5})/2 = (3 + 2C_i + D_i)/2 \quad (5.8b)$$

$$x_{R_i} = (1 + R_i)/2 = (1 + A_i B_i C_i D_i)/2 . \quad (5.8c)$$

Substituting the values of Pl_i , Ql_i and R_i of Table 5.2 or A_i , B_i , C_i , D_i and $A_i B_i C_i D_i$ of Table 5.1 into the equations (5.8) results in the design matrix for the $4 \times 4 \times 2/16$ design, which is given in Table 5.4.

	x_P	x_Q	x_R
	0	0	1
	2	0	0
	1	0	0
	3	0	1
	0	2	0
	2	2	1
	1	2	1
	3	2	0
	0	1	0
	2	1	1
	1	1	1
	3	1	0
	0	3	1
	2	3	0
	1	3	0
	3	3	1

Table 5.4. Design matrix for the orthogonal $4 \times 4 \times 2/16$ design.

The whole procedure described in this section is summarized in Design 8.5 of the Appendix.

5.3. The $4 \times 3 \times 2$ design with 16 experimental units

In order to construct the $4 \times 3 \times 2$ design, we shall collapse the four-level factor Q used in the previous section to a three-level factor Q .

We shall however use a modified collapsing procedure, which will shortly be explained.

The collapsing procedure used so far, is reproduced in Table 5.5 which is identical to Table 2.6 of Section 2.10.

Four level		Three level					
factor		factor					
x'_{Pi}		x_{Pi}	A_i	B_i	$A_i B_i$	Pl_i	Pq_i
0	→	0	-1	-1	+1	$-\sqrt{2}$	+1
2	→	2	+1	-1	-1	$+\sqrt{2}$	+1
1	→	1	-1	+1	-1	0	-1
3	→	1	+1	+1	+1	0	-1

Table 5.5. Collapsing a four-level factor to a three-level factor with relevant column vectors.

The quantities in Table 5.5 are related as follows

$$Pl_i = (A_i - A_i B_i) / \sqrt{2}$$

$$Pq_i = -B_i$$

$$Pl_i = (-1 + x_{Pi}) \sqrt{2} \longrightarrow x_{Pi} = 1 + Pl_i / \sqrt{2}$$

$$Pq_i = 1 - 4x_{Pi} + 2x_{Pi}^2 .$$

When we consider the column vectors \mathbf{A} , \mathbf{B} and \mathbf{AB} we can easily see that they are equivalent in a 2^n design, since each of them contains an equal number of -1 's and $+1$'s and their inner products are all zero.

We now ask ourselves whether we can make use of this property since the collapsing procedure of Table 5.5 has the unsatisfactory aspect that the orthogonal polynomial values Pl_i

and Pq_i were derived from columns which are different from those used in the case when we had a four-level factor. We then had

$$Pl_i = (2A_i + B_i)/\sqrt{5} \quad (5.9)$$

$$Pq_i = A_i B_i . \quad (5.10)$$

After collapsing we have, see Table 5.5,

$$Pl_i = (A_i - A_i B_i)/\sqrt{2} \quad (5.11)$$

$$Pq_i = -B_i . \quad (5.12)$$

Note that expressions (5.10) and (5.12) can be obtained by multiplying the letter groups of (5.9) and (5.11), respectively. Recall that $A_i^2 = 1$.

The comparison of equation (5.9) with equation (5.11) shows that Pl is a function of A and B in (5.9) and a function of A and AB in (5.11), the consequence being that collapsing a four-level factor to a three-level factor will completely change the $X'X$ matrix.

If we could find a collapsing procedure where Pl remains a linear function of A and B and Pq remains a linear function AB , we will have a desirable situation since zero elements of $X'X$ will remain zero.

This property is very desirable, because once we have a satisfactory design with a four-level factor we can quickly change to a design with that particular factor collapsed to a three-level factor since zero elements in $X'X$ will remain zero.

An orthogonal design with a four-level factor can therefore quickly be changed into an orthogonal design with a three-level factor.

It appears that a number of possibilities exist to reach this goal. One of these is given in Table 5.6, where $Pl_i = (A_i + B_i)/\sqrt{2}$.

A second possibility would have been $Pl_i = (A_i - B_i)/\sqrt{2}$.

Four-level factor		Three-level factor					
x'_{P_i}		x_{P_i}	A_i	B_i	$A_i B_i$	Pl_i	Pq_i
0	→	0	-1	-1	+1	$-\sqrt{2}$	+1
2	→	1	+1	-1	-1	0	-1
1	→	1	-1	+1	-1	0	-1
3	→	2	+1	+1	+1	$+\sqrt{2}$	+1

Table 5.6. Collapsing a four-level factor to a three-level factor with relevant column vectors.

The quantities in Table 5.6 are related as follows

$$Pl_i = (A_i + B_i)/\sqrt{2} = (-1 + x_{P_i})\sqrt{2} \rightarrow x_{P_i} = 1 + Pl_i/\sqrt{2}$$

$$Pq_i = A_i B_i = 1 - 4x_{P_i} + 2x_{P_i}^2 .$$

The formulae for the orthogonal polynomial values now are

$$Pl_i = (A_i + B_i)/\sqrt{2} \tag{5.13}$$

$$Pq_i = A_i B_i \tag{5.14}$$

and

$$\sum_{i=1}^4 Pl_i^2 = \sum_{i=1}^4 Pq_i^2 = 4 .$$

Formulae (5.13) and (5.14) now have the same structure as (5.9) and (5.10), since Pl is again a function of A and B , whereas Pq has not even changed at all.

It is interesting to note the difference in collapsing procedure.

In Table 5.5 we only collapsed level 3 of x'_P to a level 1 of x_P . In Table 5.6 we collapsed two levels namely levels 2 and 3 of x'_P to the levels 1 and 2 of x_P , respectively.

It has now become very easy to change the $4 \times 4 \times 2$ design into a $4 \times 3 \times 2$ design.

We use the design generators of Table 5.3 and only change the expression for Ql_i into

$$QI_i = (C_i + D_i)/\sqrt{2}.$$

The column vector elements for the $4 \times 3 \times 2$ design are now given in Table 5.7.

$x_{0i} = 1$
$PI_i = (2A_i + B_i)/\sqrt{5}$
$Pq_i = A_i B_i$
$QI_i = (C_i + D_i)/\sqrt{2}$
$Qq_i = C_i D_i$
$R_i = A_i B_i C_i D_i$
$PI_i QI_i = (2A_i C_i + 2A_i D_i + B_i C_i + B_i D_i)/\sqrt{10}$
$PI_i R_i = (2B_i C_i D_i + A_i C_i D_i)/\sqrt{5}$
$QI_i R_i = (A_i B_i D_i + A_i B_i C_i)/\sqrt{2}$

Table 5.7. Column vector elements for the $4 \times 3 \times 2/16$ design.

For further information as regards this design we refer to the Appendix where the details of the $4 \times 3 \times 2/16$ design are given in Design 8.6.

The collapsing technique given in Table 5.6 was also applied to the $4 \times 2 \times 2/8$ design of Table 4.6a. The results are presented as Design 8.4 in the Appendix. It however appears that the design matrices of design 8.4 and 8.2 are identical although their design generators are different.

5.4. Other designs with 16 experimental units

Using methods described in the preceding section we derived a total of 7 designs with 16 experimental units namely designs 8.5, 8.6, 8.11, 8.12, 8.13a, 8.14a and 8.15a.

Initially we constructed a total of 20 designs with 16 experimental units, but 13 of these had

undesirable properties, such as low D - and G -efficiencies and we modified these designs using properties of the D -optimal designs given in Chapter 3.

These modified designs are discussed in Section 5.7.

The designs 8.11, a $4 \times 2 \times 2 \times 2/16$ design, and 8.12, a $3 \times 2 \times 2 \times 2/16$ design also turned out to be orthogonal. The designs 8.13a, 8.14a and 8.15a are clumpwise orthogonal.

To examine each design we had to do some time consuming calculations such as the computation of $\mathbf{X}'\mathbf{X}$ and $(\mathbf{X}'\mathbf{X})^{-1}$. We therefore made use of an extremely versatile personal computer program called "MATH CAD"¹. It is a program for working with formulas, numbers, text and graphs. It can be used to solve many mathematical problems symbolically or numerically. We used it for the construction of the designs and for the calculation of the design characteristics. These designs are presented in the Appendix and listed in Table 4.22 and Table 5.12.

5.5. The input and output of Math Cad for designs 8.1–8.6 and 8.11–8.15a

The input of Math Cad consists of the \mathbf{X} matrix of column vectors for the 2^3 or 2^4 design. See Table 4.2 and Table 5.1. The input for designs other than those given above is the design matrix. See for instance design 8.7.

The output of Math Cad contains information as described under the headings a) to h) below. This information is given with each of the designs above and is presented in the Appendix.

- a) The design generators. See for instance Table 5.3.
- b) The design matrix elements $DM_{i,j}$.
- c) The design matrix given by \mathbf{DM}^T .

In this matrix the first row refers to the first factor P .
The second row refers to the second factor Q , etc.

The factors corresponding to the rows of the design matrix have 4, 3 or 2 levels, indicated by the sets $(0, 1, 2, 3)$, $(0, 1, 2)$ and $(0, 1)$, respectively.

¹Math Cad can be obtained from "Math Soft Inc.". 201 Broadway, Cambridge, Massachusetts, 02139 USA.

The elements of the design matrix $DM_{i,j}$ were derived using the following formulae:

For a *four*-level factor P with levels $x_{Pi} = 0, 1, 2, 3$ we have vector elements x_{Pi} and

$$x_{Pi} = (3 + Pi\sqrt{5})/2.$$

See also (2.49).

For a *three*-level factor Q obtained through collapsing a four-level factor, with the levels of Q being $x_{Qi} = 0, 1, 2$, we have vector elements x_{Qi} and $x_{Qi} = 1 + Qi/\sqrt{2}$. See also (2.52).

For a *two*-level factor R with levels $x_{Ri} = 0, 1$, we have $x_{Ri} = 0, 1$ and vector elements $x_{Ri} = (1 + Ri)/2$.

Of course the factors P , Q and R may also have a number of levels other than given above, as long as we use the formula corresponding to the correct number of levels.

d) The algebraic expressions for the X matrix of column vectors are given. The numerical values of the elements of these vectors are omitted for reasons of space, but can be generated by Math Cad if so desired.

e) $X'X$ and $\det(X'X)$ are given and written as XTX and $|XTX|$ respectively.

XTX is presented because it is important to have $X'X$ matrices with as many zero's as possible, in order to have orthogonal or nearly orthogonal designs.

$\det(X'X)$ is a measure of the hyper volume of the joint confidence region for the β 's.

The larger $\det(X'X)$ the smaller this region and the smaller the variances of the β 's. The value of $\det(X'X)$ is also used to calculate the D -efficiency of a design. We shall return to this measure in Chapter 7, where we compare the various designs.

f) $(X'X)^{-1}$ is presented as $XTXI$.

$(X'X)^{-1}$ is an important matrix since the diagonal elements are equal to $\sigma_{\hat{\beta}_p}^2/\sigma^2$ and thus are a measure of the variance of the $\hat{\beta}$'s.

The sum of the diagonal elements of a matrix is known as the trace of a matrix. The trace of $(X'X)^{-1}$ is given as $\text{tr}(XTXI)$.

When we divide this value by the number of terms in the model, we then obtain the average value of $\sigma_{\hat{\beta}_p}^2/\sigma^2$.

Further discussion of $\text{tr}(XTXI)$ will be done in Chapter 7.

- g) The matrices \mathbf{r} and \mathbf{r}^{-1} , see Section 4.3, together with $\det(\mathbf{r})$ which is written as $|\mathbf{r}|$ and trace \mathbf{r}^{-1} , given as $\text{tr}[\mathbf{r}^{-1}]$.

The designs 8.1, 8.2, 8.3, 8.4, 8.5, 8.6, 8.11, 8.12, 8.13a, 8.14a, 8.15a have the property that

$$\mathbf{X}'\mathbf{X} = N \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \hline 0 & & & & \\ 0 & \text{matrix } \mathbf{r} & & & \\ \vdots & & & & \\ 0 & & & & \end{bmatrix} \quad (5.15)$$

and

$$(\mathbf{X}'\mathbf{X})^{-1} = \frac{1}{N} \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \hline 0 & & & & \\ 0 & \text{matrix } \mathbf{r}^{-1} & & & \\ \vdots & & & & \\ 0 & & & & \end{bmatrix}, \quad (5.16)$$

due to the choice of scaling the columns of the \mathbf{X} matrix.

From (5.15) it follows that

$$\det(\mathbf{X}'\mathbf{X})/N^P = \det(\mathbf{r}). \quad (5.17)$$

We shall use (5.17) to calculate the D -efficiency of some designs. Complete orthogonality of designs occurs if all correlation coefficients in \mathbf{r} equal zero. In that case \mathbf{r} is the identity matrix \mathbf{I} , $\det(\mathbf{r}) = |\mathbf{r}| = 1$ and $\text{trace}(\mathbf{r}^{-1}) = \text{tr}[\mathbf{r}^{-1}]$ equals the number of parameters in the assumed model, excluding the intercept β_0 . For a non orthogonal design $\det(\mathbf{r}) = |\mathbf{r}|$ is less than one and $\text{trace}(\mathbf{r}^{-1})$ exceeds the number of parameters in the assumed model.

Thus $\det(\mathbf{r})$ and $\text{trace}(\mathbf{r}^{-1})$ are the second and third measure of non-orthogonality, the diagonal elements of \mathbf{r}^{-1} , the variance inflation factors, being the first.

- h) If we assign the symbol c_{pq} to the elements of $(\mathbf{X}'\mathbf{X})^{-1}$, we can define

$$\rho_{pq} = c_{pq} / \sqrt{(c_{pp} \cdot c_{qq})}$$

ρ being the matrix of correlation coefficients between the estimates of the β 's, the parameters in the regression model such as given in for instance equation (5.1).

The elements ρ_{pq} are also given by Math Cad.

The D - and G -efficiency of each design was also computed but these design characteristics will be discussed in Chapter 7.

5.6. The improvement of D - and G -efficiency by using additional design points

It appeared to be possible to construct a $4 \times 4 \times 4/16$ design using the design generators

$$Pl_i = (2A_i + B_i)/\sqrt{5} \quad Pq_i = A_i B_i$$

$$Ql_i = (2C_i + D_i)/\sqrt{5} \quad Qq_i = C_i D_i$$

$$Rl_i = (2A_i B_i D_i + A_i C_i D_i)/\sqrt{5} \quad Rq_i = B_i C_i .$$

The resulting design however turned out to have a low D - and G -efficiency namely

$$D\text{-efficiency} = 69.7\% , \quad G\text{-efficiency} = 35.6\% .$$

The G -efficiency has not been calculated according to the method used in Section 4.5.2, because the calculation of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ yielded a complicated fourth degree polynomial in the variables Pl , Ql and Rl , the maximum of which was not easily found.

We calculated instead the value of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ for each of the $4 \times 4 \times 4 = 64$ candidate points.

A maximum value of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}) = 1.757$ was found for each of the following six points

x_P	x_Q	x_R
0	0	3
0	3	0
3	0	0
0	3	3
3	0	3
3	3	0

and the G -efficiency was calculated assuming that 1.757 was indeed the maximum of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ for the whole experimental region, a cube with vertices having as coordinates the 8 combinations from the set $(\pm 1, \pm 1, \pm 1)$.

Because the maximum may be slightly higher than 1.757 it is possible that the G -efficiency is slightly overestimated.

None of the 6 points above were design points but if we add these to the 16 design points we increase the D -efficiency to 87.8% and the G -efficiency to 60.2%.

It is, generally speaking, an effective method to increase D - and G -efficiency by adding design points where $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ is high; see *Evans (1979)*. A disadvantage of this approach is the increase in the number of design points.

5.7. The construction of designs with 16 experimental units using D -optimal designs

The strategy outlined in the previous section is not satisfactory, because we had to increase the size of the experimental design. We shall therefore try to find a better $4 \times 4 \times 4/16$ design using a different approach. The appropriate model to be used for the $4 \times 4 \times 4/16$ design is (3.1) for $k = d = 3$.

Using Table 3.1 we find that for $k = d = 3$ the D -optimal design consists of design points as given in Table 5.8.

- 57.6% of the points are of the type $\pm 1, \pm 1, \pm 1$
- 22.7% of the points are of the type $0, \pm 1, \pm 1$
- 19.7% of the points are of the type $0, 0, \pm 1$

Table 5.8. Design points of the D -optimal $3 \times 3 \times 3$ design.

Since we only use 16 design points we can never realize the percentages of Table 5.8 in practice and we therefore have to use approximate values.

Moreover, since we employ 4 levels, we do not have the level 0, but have to use $\pm(1/3)$ instead, remembering that levels $\pm(1/3)$ will become a level 0 after collapsing.

We then set up the design of Table 5.9.

Exp. unit	x_{1i}	x_{2i}	x_{3i}
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	-1/3	-1/3	-1/3
10	1	-1	-1/3
11	-1/3	1	-1
12	1	1/3	-1
13	-1	-1/3	1
14	1/3	-1	1
15	-1	1	1/3
16	1/3	1/3	1/3

Table 5.9. A $4 \times 4 \times 4/16$ design.

Examining Table 5.9 we see that

8 points = 50% are of the type $\pm 1 \pm 1 \pm 1$,

these points form a 2^3 design,

6 points = 37.5% are of the type $\pm 1/3 \pm 1 \pm 1$

2 points = 12.5% are of the type $\pm 1/3 \pm 1/3 \pm 1/3$.

When we compare these percentages with those in Table 5.8 we see some discrepancies as regards the groups $(\pm 1, \pm 1, \pm 1)$ and $(0, \pm 1, \pm 1)$.

Moreover, we used two points of the type $\pm 1/3 \pm 1/3 \pm 1/3$ which do not occur at all in Table 5.8, but we used these, to have two “center points” when the three four-level factors are collapsed to three-level factors.

These center points are however not desirable from the D -efficiency point of view because they do not occur at all in the D -optimal design of Table 5.8. It is, on the other hand, very often desirable to include these points in an experiment, because they represent “normal” or “standard” operating conditions.

We nevertheless calculated the D - and G -efficiency of the design in Table 5.9.

The G -efficiency was calculated using the maximum value of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ in $4 \times 4 \times 4 = 64$ candidate points. We found a value of 1.084 and the G -efficiency is, using (2.26)

$$G\text{-efficiency} = 100 \times 10 / (16 \times 1.084) = 57.7\% .$$

From design 8.7 in the Appendix we obtain

$$\det \left(\frac{\mathbf{X}'\mathbf{X}}{16} \right) = 1.566 \times 10^{-4} .$$

From Table 3.1 we obtain, for $k = d = 3$

$$\max \det(\mathbf{M}(\xi)) = 0.000578313 .$$

Using (2.15) we find

$$D\text{-efficiency} = 100(1.566 \times 10^{-4} / 0.000578313)^{(1/10)} = 87.8\% .$$

Since both D - and G -efficiency have satisfactory values we accept the design of Table 5.9. The levels of the three factors P , Q and R are given as 0, 1, 2 and 3.

The relation between these levels and the values of x_1 , x_2 and x_3 are given with the design matrix of design (8.7).

Other features of this design, computed by Math Cad, are also given in the Appendix such as

$$\mathbf{X}'\mathbf{X}, (\mathbf{X}'\mathbf{X})^{-1}, \mathbf{r}^{-1}, \det(\mathbf{r}), \text{trace}((\mathbf{X}'\mathbf{X})^{-1}), \text{trace}(\mathbf{r}^{-1}) \text{ and } \rho .$$

Many of these values seem satisfactory, such as large $\det(\mathbf{r})$ and small VIF's. They will be discussed in more detail in Chapter 7.

The matrix \mathbf{r} is omitted with design (8.7) for reasons of space.

Three other designs were derived from design (8.7) by collapsing 1, 2 and 3 four-level factors into three-level factors.

The collapsing is achieved as indicated in Table 5.10.

Four-level factor		Three-level factor	
x'_P or x'_Q or x'_R	x'_1 or x'_2 or x'_3	x_P or x_Q or x_R	x_1 or x_2 or x_3
	0	-1	0
	1	-1/3	1
	2	1/3	1
	3	1	2

Table 5.10. Collapsing a four-level factor into a three-level factor.

The collapsing procedure of Table 5.10 is identical to the method used in Table 5.6.

The designs obtained through collapsing are given as design (8.8), (8.9) and (8.10) in the Appendix.

Three other groups of designs were constructed namely

- **Group Vb.** A $4 \times 4 \times 2 \times 2/16$ design and two additional designs derived through collapsing one and two four-level factors.
- **Group VI.** A $4 \times 4 \times 4 \times 2/16$ design and three other designs obtained by collapsing.
- **Group VII.** A $4 \times 4 \times 4 \times 4/16$ design and four other designs also constructed by collapsing one, two, three and four factors.

The model appropriate to the $4 \times 4 \times 2 \times 2/16$ design is (3.1) for $d = 2$ and $k = 4$.

The D -optimal design for this model is obtained from Table 3.1 and is given in Table 5.11.

- 70.5% design points of the type $\pm 1 \pm 1 \pm 1 \pm 1$
- 25.2% design points of the type $0 \pm 1 \pm 1 \pm 1$
- 4.2% design points of the type $0 0 \pm 1 \pm 1$.

Table 5.11. Design points of the D -optimal $3 \times 3 \times 2 \times 2$ design.

The $4 \times 4 \times 2 \times 2/16$ design we eventually found is presented as design (8.13b) in the Appendix. The 8 design points of the type $\pm 1, \pm 1, \pm 1, \pm 1$ comprise 50% of the total and form a half replicate of a 2^4 design with defining contrast $ABCD$, which means that the half replicate contains only those treatment combinations which have the + sign in the calculation of the four-factor interaction $ABCD$. The remaining points are of the type $\pm 1/3, \pm 1, \pm 1, \pm 1$. Although we tried several designs with a better fit to the D -optimal design, we were not successful and design (8.13b) was the best we could find with D -efficiency = 84.6% and G -efficiency = 57.6%.

Design (8.13b) and the two designs (8.14b) and (8.15b) derived from it through collapsing, are of the same group as the set (8.13a), (8.14a) and (8.15a), which were constructed using design generators.

These two groups will be compared in more detail in Chapter 7.

When we tried to find suitable $4 \times 4 \times 4 \times 2/16$ and $4 \times 4 \times 4 \times 4/16$ designs using a similar approach as in the case of the $4 \times 4 \times 2 \times 2/16$ design we found designs which were not satisfactory. Although they had a fairly high D -efficiency they had a small G -efficiency.

We for instance found a $4 \times 4 \times 4 \times 2/16$ and a $4 \times 4 \times 4 \times 4/16$ design with D - and G -efficiencies of 83.0%, 30.3% for the $4 \times 4 \times 4 \times 2/16$ and 89.9%, 28.8% for the $4 \times 4 \times 4 \times 4/16$ design, respectively. These designs were also unsatisfactory because some $\hat{\beta}$'s corresponding to quadratic terms had high variances.

We then used a routine from the computer package SAS which uses the *Mitchell* (1974a) algorithm. This algorithm selects a subset of 16 points with the maximum value of $\det(\mathbf{X}'\mathbf{X})$ from the $4 \times 4 \times 4 \times 4 = 256$ candidate points. We found a $4 \times 4 \times 4 \times 4/16$ design (8.20) with a slightly better D -efficiency of 84.9%, a much better G -efficiency of 38.3% and smaller variances for the $\hat{\beta}$'s of the quadratic terms.

When we consider the design matrix of design (8.20) in the Appendix, we see that the levels of the fourth factor S occur

- 7 times for the level 0 or -1
- 3 times for the level 1 or $-1/3$
- 0 times for the level 2 or $1/3$
- 6 times for the level 3 or 1.

We can therefore easily change this factor into a two-level factor with 8 times the level -1 and 8 times the level $+1$ and thus obtain a $4 \times 4 \times 4 \times 2/16$ design.

Since we already have the level -1 seven times, we have to change one of the 3 levels with value $-1/3$ into a level -1 and the remaining levels $-1/3$ into $+1$. We therefore have 3 possibilities to achieve this. We tried all three and chose the one which produced the highest D -efficiency which had a value of 87.5%. The G -efficiency is 47.0%. This design is presented as design (8.16) of the Appendix.

In this chapter we also find the designs (8.17), (8.18) and (8.19) derived from design (8.16) using collapsing.

The designs (8.21), (8.22), (8.23) and (8.24) were likewise derived from design (8.20).

5.8. General remarks about designs with 16 experimental units

Since "good" designs have small or even zero values for ρ_{pq} , we indicated the largest $|\rho_{pq}|$ for each design in Table 5.12. When choosing the largest $|\rho_{pq}|$ we ignored correlation coefficients of $\hat{\beta}_0$ with the other $\hat{\beta}$'s because such a coefficient can easily be made zero if we subtract the average value of the elements of a column in \mathbf{X} from each element in that column. The diagonal elements of $(\mathbf{X}'\mathbf{X})^{-1}$ are also interesting since they are proportional to $\sigma_{\hat{\beta}}^2$. They, and other design characteristics, will be discussed further in Chapter 7 where several designs will be compared.

The designs of Table 5.12 have been divided into six groups. The first group is the simplest one since it has only three factors, two of these factors having only two levels. Proceeding from group II to group VII shows designs of increasing complexity, since the number of factors and the number of levels increases to the extent that a $4 \times 4 \times 4 \times 4/16$ design was constructed, being a $(1/16)$ th replicate of a 4^4 design.

From the first design in each group we derived a set of designs by collapsing one, two, three or four four-level factors to three-level factors.

We can see that by looking at the largest ρ for each design that collapsing sometimes increases this value, which is of course undesirable. Collapsing has hardly an effect within groups III, VI and VII. We can ask ourselves whether it is necessary to collapse at all since both the four- and the three-level factors are quantitative. Why choose three quantitative levels and not four because the number of experimental units remains 16 anyway?

Design number	Group number	DESIGN	Fraction	Largest $ \rho $	Remarks
8.5	II	$4 \times 4 \times 2/16$	1/2	0	Orthogonal design
8.6		$4 \times 3 \times 2/16$	2/3	0	Orthogonal design
8.7	III	$4 \times 4 \times 4/16$	1/4	0.339	Linear effects orthogonal
8.8		$4 \times 4 \times 3/16$	1/3	0.394	Linear effects orthogonal
8.9		$4 \times 3 \times 3/16$	4/9	0.404	Linear effects orthogonal
8.10		$3 \times 3 \times 3/16$	16/27	0.362	Linear effects orthogonal
8.11	IV	$4 \times 2 \times 2 \times 2/16$	1/2	0	Orthogonal design
8.12		$3 \times 2 \times 2 \times 2/16$	2/3	0	Orthogonal design
8.13a	Va	$4 \times 4 \times 2 \times 2/16$	1/4	0.436	Clumpwise orthogonality
8.14a		$4 \times 3 \times 2 \times 2/16$	1/3	0.667	Clumpwise orthogonality
8.15a		$3 \times 3 \times 2 \times 2/16$	4/9	0.577	Clumpwise orthogonality
8.13b	Vb	$4 \times 4 \times 2 \times 2/16$	1/4	0.500	Clumpwise orthogonality
8.14b		$4 \times 3 \times 2 \times 2/16$	1/3	0.621	Clumpwise orthogonality
8.15b		$3 \times 3 \times 3 \times 2/16$	8/27	0.707	Clumpwise orthogonality
8.16	VI	$4 \times 4 \times 4 \times 2/16$	1/8	0.445	
8.17		$4 \times 4 \times 3 \times 2/16$	1/6	0.412	
8.18		$4 \times 3 \times 3 \times 2/16$	2/9	0.405	
8.19		$3 \times 3 \times 3 \times 2/16$	8/27	0.402	
8.20	VII	$4 \times 4 \times 4 \times 4/16$	1/16	0.385	
8.21		$4 \times 4 \times 4 \times 3/16$	1/12	0.395	
8.22		$4 \times 4 \times 3 \times 3/16$	1/9	0.302	
8.23		$4 \times 3 \times 3 \times 3/16$	4/27	0.309	
8.24		$3 \times 3 \times 3 \times 3/16$	16/81	0.372	

Table 5.12. A number of 23 different fractional factorial experimental designs for quantitative factors with 16 experimental units.

There are of course quantitative factors which can be set at any desired number of levels such as temperature, pressure, etc., but there are situations that only three quantitative levels can be obtained, for instance when only three equally spaced levels of wire diameter are available.

In such a situation one may wish to employ a design with one or more factors at three levels, obtained through collapsing four-level factors.

However, we shall encounter designs in Chapter 6 with three-level factors which were not obtained through collapsing.

In Chapter 7 we shall compare some designs of Chapter 5 with those in Chapter 6 and shall formulate recommendations as to their use.

It was stated before that if the method of design generators is used, their choice determines an experimental design. Unfortunately, efforts to find straightforward rules as to the choice of a suitable set of design generators, have so far not been successful.

A strategy consisting of trial and error in combination with Math Cad has been used. It took for instance 5 trials to find a suitable $4 \times 4 \times 2 \times 2/16$ design. The first four invariably resulted in a singular $X'X$ matrix.

A number of 10 designs in Table 5.12 have clumpwise orthogonality and 4 designs are orthogonal.

We do not pretend that the designs listed in Table 5.12 are the best, but they will certainly be of practical value for all those who want to derive much information from a limited number of 16 experimental units.

5.9. Designs with 32 experimental units

The methods developed in the preceding sections have made clear how designs for quantitative factors with 2, 3 and 4 levels can be constructed from 2^3 and 2^4 designs.

It is therefore logical to try and construct designs derived from the 2^5 factorial.

However, since we already constructed 23 different designs using 16 experimental units, it is obvious that the number of designs which can be made from the 2^5 design will be much larger than 23.

We shall therefore restrict the number of designs to be made. We first of all will try to construct a $4 \times 4 \times 4 \times 4 \times 4$ design using 2^5 experimental units. If we succeed we shall derive 5 others by successively collapsing one, two, three, four and five factors into factors with three levels.

We shall use the 32 column vectors of the 2^5 design. These vectors are not reproduced here, but they are a logical extension of those in Table 5.1.

The 5 four-level factors to be used are labelled P , Q , R , S and T and we try a balanced set of design generators as given in Table 5.13.

$Pl_i = (2A_i + A_iB_iC_iD_i)/\sqrt{5}$	$Pq_i = B_iC_iD_i$
$Ql_i = (2B_i + B_iC_iD_iE_i)/\sqrt{5}$	$Qq_i = C_iD_iE_i$
$Rl_i = (2C_i + A_iC_iD_iE_i)/\sqrt{5}$	$Rq_i = A_iD_iE_i$
$Sl_i = (2D_i + A_iB_iD_iE_i)/\sqrt{5}$	$Sq_i = A_iB_iE_i$
$Tl_i = (2E_i + A_iB_iC_iE_i)/\sqrt{5}$	$Tq_i = A_iB_iC_i$

Table 5.13. Design generators for the $4 \times 4 \times 4 \times 4 \times 4/32$ design.

The generators of Table 5.13 were further “processed” as described in Section 5.5, using Math Cad.

The resulting design had clumpwise orthogonality meaning that each linear effect was not correlated with other $\hat{\beta}$'s.

However the design is not used since the D -efficiency had a low value of 61.0%.

We therefore used the approach described in Section 5.7.

The model to be used for the $4 \times 4 \times 4 \times 4 \times 4/32$ design is (3.1) for $k = d = 5$.

From Table 3.1 we derive that the D -optimal design for $k = d = 5$ has design points as given in Table 5.14.

61.6% of the points are of the type $\pm 1, \pm 1, \pm 1, \pm 1, \pm 1$

2.6% of the points are of the type $0, \pm 1, \pm 1, \pm 1, \pm 1$

35.8% of the points are of the type $0, 0, \pm 1, \pm 1, \pm 1$

Table 5.14. Design points of the D -optimal $3 \times 3 \times 3 \times 3 \times 3$ design.

The design we realized had

16 or 50% of the points of the type $\pm 1, \pm 1, \pm 1, \pm 1, \pm 1$.

These 16 points were a half replicate of the 2^5 design with defining contrast $ABCDE$.

We further had

5 or 15.6% of the points of the type $\pm 1/3, \pm 1, \pm 1, \pm 1, \pm 1$,

10 or 31.3% of the points of the type $\pm 1/3, \pm 1/3, \pm 1, \pm 1, \pm 1$

and

one or 3.1% of the points of the type $\pm 1/3, \pm 1/3, \pm 1/3, \pm 1/3, \pm 1/3$.

The choice of these points does not fit too closely with the design of Table 5.14 but the point of the type $\pm 1/3, \pm 1/3, \pm 1/3, \pm 1/3, \pm 1/3$ was deliberately chosen because it represents standard operating conditions when all factors have been collapsed to a three-level factor.

The D - and G -efficiency of this design have values of 87.8% and 55.7%, respectively, which is quite satisfactory. Five other designs were derived from design (8.25) by collapsing. They are given as (8.26), (8.27), (8.28), (8.29) and (8.30) in the Appendix. To save space we only gave the design matrix and the column vectors of the X matrix in the Appendix. More details of these designs will be given in Chapter 7. Some particulars of these designs are given in Table 5.16.

Design number	Group number	Design	Fraction	Largest $ \rho $
8.25	VIII	$4 \times 4 \times 4 \times 4 \times 4/32$	1/32	0.351
8.26		$4 \times 4 \times 4 \times 4 \times 3/32$	1/24	0.353
8.27		$4 \times 4 \times 4 \times 3 \times 3/32$	1/18	0.346
8.28		$4 \times 4 \times 3 \times 3 \times 3/32$	2/27	0.326
8.29		$4 \times 3 \times 3 \times 3 \times 3/32$	8/81	0.319
8.30		$3 \times 3 \times 3 \times 3 \times 3/32$	32/243	0.316

Table 5.16. A number of 6 fractional factorial designs for quantitative factors with 32 experimental units.

5.10. An application of the $3 \times 3 \times 3 \times 3 \times 3/32$ design

5.10.1. Introduction and problem definition

A machine is being used to produce a material of which a certain quality characteristic y has to meet a target value of 500 units.

It was thought that the value of this characteristic could be changed by adjusting the settings on 5 machine dials.

We indicate the settings on these dials by the variables x_1, x_2, x_3, x_4 and x_5 .

Because the effect of the changes in the values of the x_i on y was not exactly known and since it was thought that interactions between the 5 variables might be possible, management decided to carry out an experiment in order to examine the effect of the x_i on y in more detail.

A working group was then formed and after a thorough discussion the participants of

this group decided to design an experiment in such a way that

- each variable could be examined at three levels in order to be able to estimate linear and quadratic effects,
- linear by linear interactions could be estimated,
- a measure of experimental error could be obtained from the experimental data.

Design (8.30), a $3 \times 3 \times 3 \times 3 \times 3/32$ design meets the requirements mentioned above and the working group decided to use this plan.

5.10.2. Analysis of the experimental data

The three levels of each of the 5 variables are coded and are indicated by $-1, 0$ and $+1$. The 32 treatment combinations are given in Table 5.17 in a random order together with the observations y_i , the predicted values \hat{y}_i and the residuals $r_i = y_i - \hat{y}_i$. The values \hat{y}_i and r_i will be discussed later.

The data were analyzed using the software package "STATA". The results are given in Table 5.18, which contains the analysis of variance and the 21 estimated regression coefficients of the second degree polynomial model, together with the relevant t -test for each regression coefficient.

We define:

RSS_P : the residual sum of squares.

$CTSS = \sum_{i=1}^N (y_i - \bar{y})^2 = \mathbf{Y}'\mathbf{Y} - n\bar{y}^2$: The corrected total sum of squares.

$R^2 = 1 - \frac{RSS_P}{CTSS}$: The square of the multiple correlation coefficient or the proportion of total variation explained by regression.

$R_a^2 = 1 - \frac{RSS_P/(N - P)}{CTSS/(N - 1)}$: Adjusted R^2 .

Both R^2 and R_a^2 are discussed in Chapter 2 of *Draper and Smith* (1981).

From the analysis of variance we obtain:

Exp. unit	x_1	x_2	x_3	x_4	x_5	y_i	\hat{y}_i	$r_i = y_i - \hat{y}_i$
1	-1	-1	-1	1	1	395.69	398.40	-2.71
2	1	-1	0	1	1	441.48	436.72	4.76
3	-1	0	-1	0	1	450.09	440.72	9.37
4	-1	-1	0	-1	0	451.19	464.09	-12.90
5	-1	1	1	-1	-1	612.29	607.76	4.53
6	1	-1	1	-1	-1	540.28	540.51	-.23
7	-1	-1	-1	-1	-1	448.89	442.43	6.46
8	0	1	1	1	0	587.70	575.02	12.68
9	0	0	0	0	0	502.19	506.41	-4.22
10	1	0	-1	-1	1	434.68	440.72	-6.04
11	0	1	0	-1	-1	550.50	558.71	-8.21
12	-1	-1	1	1	-1	532.05	540.51	-8.46
13	1	-1	-1	-1	1	408.94	398.40	10.54
14	1	0	-1	-1	0	464.54	462.73	1.81
15	0	0	1	-1	-1	576.65	582.83	-6.18
16	1	1	-1	1	1	465.32	465.65	-.33
17	1	1	-1	-1	-1	494.17	509.67	-15.50
18	1	-1	-1	1	-1	453.36	442.43	10.93
19	-1	1	1	0	1	521.69	542.27	-20.58
20	1	-1	1	1	1	482.85	475.03	7.82
21	-1	-1	1	-1	1	466.10	475.02	-8.92
22	1	1	1	1	-1	610.07	607.76	2.31
23	0	-1	1	1	1	469.86	475.02	-5.16
24	1	1	1	-1	1	545.16	542.28	2.88
25	-1	1	-1	1	-1	505.67	509.67	-4.00
26	-1	1	-1	-1	1	458.01	465.65	-7.64
27	-1	-1	-1	0	0	416.06	420.41	-4.35
28	-1	1	1	1	1	555.48	542.28	13.20
29	-1	1	1	1	0	587.69	575.02	12.67
30	0	1	-1	0	-1	517.68	509.67	8.01
31	1	-1	0	0	-1	493.72	491.47	2.25
32	1	0	0	1	-1	539.06	533.79	5.27

Table 5.17. Experimental design, observations y_i , predicted values \hat{y}_i and residuals r_i .

```
. regress y x1-x5 x1x2-x5x5
(obs=32)
```

Source	SS	df	MS	Number of obs = 32	
Model	107775.277	20	5388.76384	F(20, 11) =	55.21
Residual	1073.75021	11	97.6136557	Prob > F =	0.0000
Total	108849.027	31	3511.25893	R-square =	0.9901
				Adj R-square =	0.9722
				Root MSE =	9.88

Variable	Coefficient	Std. Error	t	Prob > t	Mean
y					499.3472
x1	2.245109	2.158131	1.040	0.321	0
x2	32.89701	2.087531	15.759	0.000	0
x3	42.53926	2.16485	19.650	0.000	0
x4	3.053995	2.035407	1.500	0.162	0
x5	-28.00202	2.062251	-13.578	0.000	0
x1x2	-3.550977	2.246666	-1.581	0.142	-.0625
x1x3	1.530184	2.234878	0.685	0.508	-.0625
x1x4	1.142438	2.298276	0.497	0.629	0
x1x5	1.451156	2.254356	0.644	0.533	-.0625
x2x3	4.016595	2.2827	1.760	0.106	.0625
x2x4	2.302004	2.298583	1.001	0.338	0
x2x5	.0851292	2.295846	0.037	0.971	-.0625
x3x4	.7039211	2.275196	0.309	0.763	.125
x3x5	-5.091533	2.282576	-2.231	0.047	0
x4x5	.5098388	2.273378	0.224	0.827	.0625
x1x1	-2.022752	5.639479	-0.359	0.727	.8125
x2x2	-10.87922	5.347241	-2.035	0.067	.8125
x3x3	4.81365	5.333714	0.902	0.386	.8125
x4x4	1.94592	5.335147	0.365	0.722	.8125
x5x5	.0070587	5.55815	0.001	0.999	.8125
_cons	503.931	6.650707	75.771	0.000	1

Table 5.18. Regression analysis and analysis of variance using the complete model.

```
. regress y x2 x3 x5 x2x2 x3x5
(obs=32)
```

Source	SS	df	MS	Number of obs = 32	
Model	106505.268	5	21301.0537	F(5, 26) =	236.30
Residual	2343.75863	26	90.1445628	Prob > F =	0.0000
				R-square =	0.9785
				Adj R-square =	0.9743
Total	108849.027	31	3511.25893	Root MSE =	9.4944

Variable	Coefficient	Std. Error	t	Prob > t	Mean
y					499.3472
x2	33.62368	1.874913	17.933	0.000	0
x3	43.67861	1.898855	23.003	0.000	0
x5	-27.37664	1.867592	-14.659	0.000	0
x2x2	-8.694429	4.553478	-1.909	0.067	.8125
x3x5	-5.366259	2.117945	-2.534	0.018	0
_cons	506.4114	4.062611	124.652	0.000	1

Table 5.19. Regression analysis and analysis of variance using 6 terms in the model.

$$R^2 = 1 - (1073.75021) / (108849.027) = 0.9901$$

$$R_a^2 = 1 - \frac{1073.75021 / (32 - 21)}{108849.027 / (32 - 1)} = 0.9722 .$$

The values of R^2 and R_a^2 are also given in Table 5.18. Since both R^2 and R_a^2 are close to unity, we find a strong relationship between y and the variables x_1, x_2, \dots, x_5 .

The estimate of the standard deviation of the experimental error is given as

$$\text{Root MSE} = 9.88.$$

When we examine the t -tests of the regression coefficients in Table 5.18 we see that only 6 of these are significant at the 5% level namely

$$\beta_0, \beta_2, \beta_3, \beta_5, \beta_{35} \text{ and } \beta_{22}$$

(the t -test for β_{22} nearly reaches the 5% level).

A second regression analysis was therefore carried out using only the 6 parameters, mentioned above, in the model.

The results are given in Table 5.19.

When we compare the results in Table 5.18 with those in Table 5.19, it is striking that the estimates of the β 's have hardly changed. The reason for it is that design 8.30 has excellent characteristics such as a large measure of orthogonality and small coefficients of correlation between the estimates of the β 's.

See Table 7.3g in Chapter 7.

We moreover find small changes in R^2 , R_a^2 and Root MSE.

The final regression equation is obtained from Table 5.19; we find

$$\hat{y} = 506.41 + 33.62x_2 + 43.68x_3 - 27.38x_5 - 8.19x_2^2 - 5.37x_3x_5 . \quad (5.17)$$

It appears from (5.17) that no effects of x_1 and x_4 were found.

There are many possibilities to obtain a value of \hat{y} which is close to 500. One of these is to choose $x_2 = +1$, $x_3 = 0$, $x_5 = +1$.

Substituting these values in (5.17) yields: $\hat{y} = 503.96$. Formula (5.17) is used to calculate \hat{y} for all the 32 design points. We then calculated the residuals $r_i = y_i - \hat{y}_i$.

See Table 5.17. These residuals were plotted against \hat{y}_i in Figure 5.1. Since no particular patterns occur in the r_i , we may conclude that the estimated model is quite adequate.

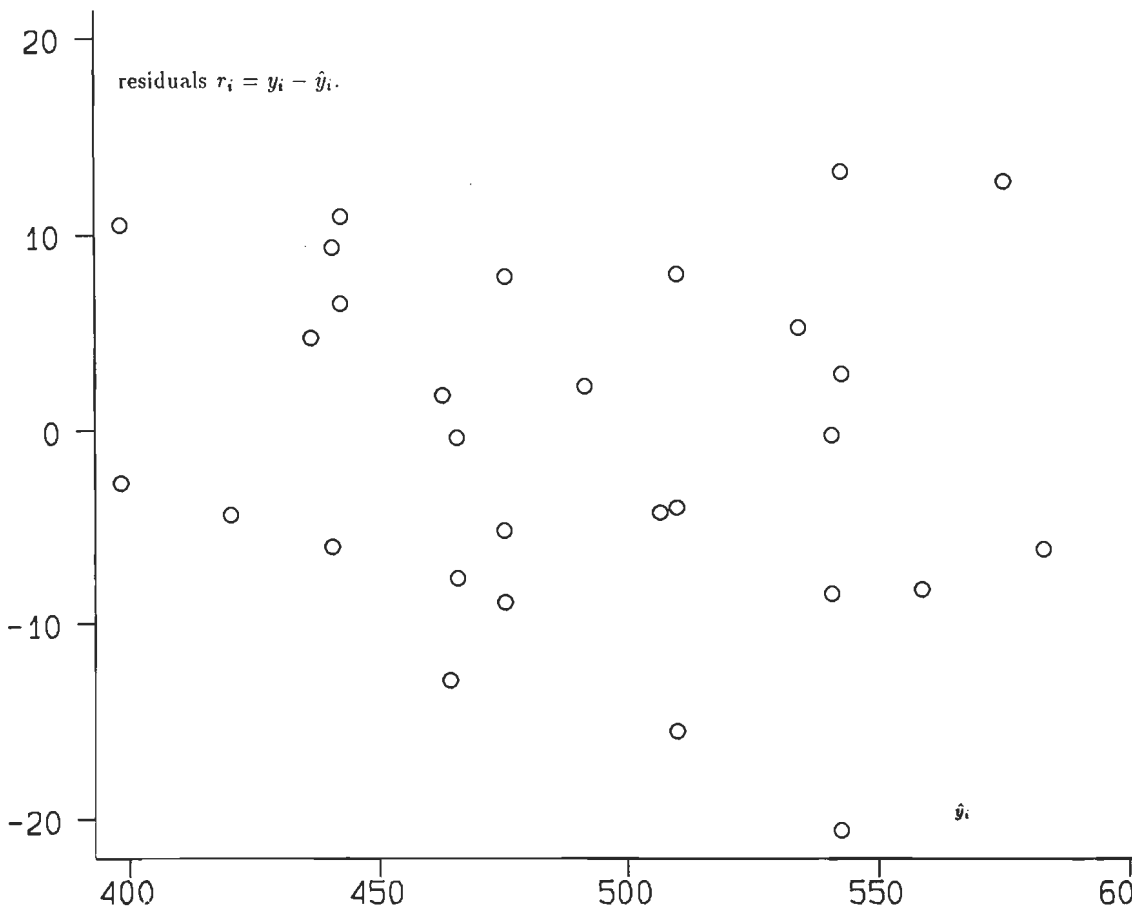


Figure 5.1. residuals against \hat{y}_i

CHAPTER 6

Designs with two and three levels

6.1. The 2×3^7 main-effect design

During the past 30 years many so called main-effect plans were published. See *Addelman* (1962a,1962b) and *Taguchi* (1987).

We shall show that some of these plans can also be used to estimate linear by linear interactions as well, while maintaining a large measure of orthogonality.

To illustrate our point we shall make use of the 2×3^7 orthogonal main-effect plan, of which the design matrix is given in Table 6.1.

x_{W_i}	x_{P_i}	x_{Q_i}	x_{R_i}	x_{S_i}	x_{T_i}	x_{U_i}	x_{V_i}
0	0	0	0	0	0	0	0
0	0	1	1	1	1	1	1
0	0	2	2	2	2	2	2
0	1	0	0	1	1	2	2
0	1	1	1	2	2	0	0
0	1	2	2	0	0	1	1
0	2	0	1	0	2	1	2
0	2	1	2	1	0	2	0
0	2	2	0	2	1	0	1
1	0	0	2	2	1	1	0
1	0	1	0	0	2	2	1
1	0	2	1	1	0	0	2
1	1	0	1	2	0	2	1
1	1	1	2	0	1	0	2
1	1	2	0	1	2	1	0
1	2	0	2	1	2	0	1
1	2	1	0	2	0	1	2
1	2	2	1	0	1	2	0

Table 6.1. An orthogonal 2×3^7 main-effect design.

The name “main-effect plan” is given because the matrix $X'X$ corresponding to the main effects is diagonal, which means orthogonal estimates of the main effects.

In the next Section we shall make use of Table 6.1 to construct a $3 \times 3 \times 3 \times 2$ design using 18 experimental units, which means that we shall construct a $1/3$ replicate of a $3^3 \times 2$ design.

6.2. The $3 \times 3 \times 3 \times 2$ design in 18 experimental units

We assign the letters P , Q and U to the three quantitative factors with equally spaced levels

$$x_P = 0, 1, 2, \quad x_Q = 0, 1, 2 \quad \text{and} \quad x_U = 0, 1, 2 .$$

The letter W is used for the two-level factor with levels $x_W = 0, 1$ or with levels $W_1 = -1$ and $W_2 = +1$.

Using the restrictions as mentioned in Section 1.6 we have the following mathematical model of the observations y_i

$$\begin{aligned} E(y_i) = & \beta_0 x_{0i} + \beta_1 W_i + \beta_2 P_i + \beta_{22} P_i^2 + \beta_3 Q_i + \beta_{33} Q_i^2 + \beta_4 U_i + \beta_{44} U_i^2 + \\ & + \beta_{12} W_i P_i + \beta_{13} W_i Q_i + \beta_{14} W_i U_i + \beta_{23} P_i Q_i + \beta_{24} P_i U_i + \\ & + \beta_{34} Q_i U_i , \end{aligned} \tag{6.1}$$

with $\text{var}(y_i) = \sigma^2$.

Formula (6.1) can be written as

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} .$$

The elements of the column vectors of \mathbf{X} are generated as follows, using the notation of "Math CAD", " $X_{i,p}$ ", instead of " X_{ip} ". The first column is given by

$$X_{i,1} = x_{0i} = 1 .$$

We now proceed to derive the other columns of \mathbf{X} .

To ensure orthogonality of the estimates of the β 's as much as possible, we again use orthogonal polynomials to represent the effect of W , P , Q and U . The first degree polynomial of a two-level factor W is

$$W = 2x_W - 1 . \tag{6.2}$$

Its values are tabulated in Table 6.2.

x_{W_i}	W_i
0	-1
1	+1

Table 6.2. Values of x_{W_i} and W_i .

Again we have $\sum_{i=1}^{18} W_i^2 = 18 = N =$ the number of experimental units of the design.

The first and second degree orthogonal polynomial values of an equally spaced three-level factor P are

$$Pl_i = (1/2) (x_{P_i} - 1) \sqrt{6} \tag{6.3}$$

and

$$Pq_i = ((3/2) (x_{P_i} - 1)^2 - 1) \sqrt{2} = (Pl_i^2 - 1) \sqrt{2} , \tag{6.4}$$

respectively.

It follows from (6.3) that $x_{P_i} = 1 + (1/3) Pl_i \sqrt{6}$.

Substituting the values $x_{P_i} = 0, 1$ and 2 in (6.3) and (6.4) we obtain orthogonal polynomial values for a three-level factor. See Table 6.3.

x_{P_i}	Pl_i	Pq_i
0	$-(1/2) \sqrt{6}$	$(1/2) \sqrt{2}$
1	0	$-\sqrt{2}$
2	$+(1/2) \sqrt{6}$	$(1/2) \sqrt{2}$

Table 6.3. Orthogonal polynomial values for a three-level factor.

We can easily verify that $\sum_{i=1}^{18} Pl_i^2 = \sum_{i=1}^{18} Pq_i^2 = N = 18$.

Values of Ql_i, Qq_i, Ul_i and Uq_i can similarly be obtained. Using Table 6.1 and the expressions

(6.2), (6.3) and (6.4) we can compute the column vector elements of the \mathbf{X} matrix as given below in Table 6.4.

$X_{i,1} = x_{0i}$	$= 1$	$X_{i,2} = W_i$	$= 2x_{W_i} - 1$
$X_{i,3} = Pl_i$	$= (x_{P_i} - 1)\sqrt{6}/2$	$X_{i,4} = Pq_i$	$= (X_{i,3}^2 - 1)\sqrt{2}$
$X_{i,5} = Ql_i$	$= (x_{Q_i} - 1)\sqrt{6}/2$	$X_{i,6} = Qq_i$	$= (X_{i,5}^2 - 1)\sqrt{2}$
$X_{i,7} = Ul_i$	$= (x_{U_i} - 1)\sqrt{6}/2$	$X_{i,8} = Uq_i$	$= (X_{i,7}^2 - 1)\sqrt{2}$
$X_{i,9} = W_i Pl_i$	$= X_{i,2} X_{i,3}$	$X_{i,10} = W_i Ql_i$	$= X_{i,2} X_{i,5}$
$X_{i,11} = W_i Ul_i$	$= X_{i,2} X_{i,7}$	$X_{i,12} = Pl_i Ql_i$	$= X_{i,3} X_{i,5}$
$X_{i,13} = Pl_i Ul_i$	$= X_{i,3} X_{i,7}$	$X_{i,14} = Ql_i Ul_i$	$= X_{i,5} X_{i,7}$

Table 6.4. Column vector elements of the $3 \times 3 \times 3 \times 2/18$ design.

The D - and G -efficiency of the $3 \times 3 \times 3 \times 2/18$ design are 80.1% and 26.9%, respectively. Further details are given in design 8.31 of the Appendix, such as

- The design matrix obtained from the columns \mathbf{x}_W , \mathbf{x}_P , \mathbf{x}_Q and \mathbf{x}_U of Table 6.1.
- The $X_{i,j}$ -values as given in Table 6.4, $i = 1, 2, \dots, 18$, $j = 1, 2, \dots, 14$.
- The $\mathbf{X}'\mathbf{X}$ - and the $(\mathbf{X}'\mathbf{X})^{-1}$ -matrix.
The matrices \mathbf{r} and \mathbf{r}^{-1} .
- The matrix $\boldsymbol{\rho}$, the elements of which are the correlations between the β -estimates.

$\mathbf{X}'\mathbf{X}$, $(\mathbf{X}'\mathbf{X})^{-1}$, \mathbf{r} , \mathbf{r}^{-1} and $\boldsymbol{\rho}$ were calculated with the aid of Math Cad. This program was also used to evaluate the use of the column vectors \mathbf{x}_R , \mathbf{x}_S , \mathbf{x}_T and \mathbf{x}_V of Table 6.1, instead of \mathbf{x}_U .

However, using \mathbf{x}_U proved to be the best choice since it produced a $\boldsymbol{\rho}$ -matrix with many zero's and relatively small non zero ρ_{pq} -values.

6.3. The $3 \times 3 \times 2 \times 2$ design in 18 experimental units

The design to be constructed will be derived by collapsing the third three-level factor in the $3 \times 3 \times 3 \times 2/18$ design to a two-level factor. The factors are labelled P , Q , U and W .

We label the factor to be collapsed with U and we can now present the collapsing procedure as in Table 6.5.

Levels of the three-level factor		Levels of the two-level factor
x'_U		x_U
0		0
1	→	1
2		0

Table 6.5. Collapsing a three-level factor into a two-level factor.

Since U now only has two levels we only have to find the first degree polynomial U as a function of x_U .

Using the method given in *Addelman* (1962a) and Appendix 6A, we have

$$U = (3x_U - 1)/\sqrt{2} \quad \text{and} \quad \sum_{i=1}^{18} U_i^2 = N = 18. \quad (6.5)$$

Substituting $x_U = 0$ and $x_U = 1$ into (6.5) gives the orthogonal polynomial values U_i for the two-level collapsed factor.

These values have, together with the orthogonal polynomial values U'_i and Uq'_i for a three-level factor, see also Table 6.3, been presented in Table 6.6.

x'_{U_i}	U'_i	Uq'_i	x_{U_i}	U_i
0	$-(1/2)\sqrt{6}$	$(1/2)\sqrt{2}$	0	$-(1/2)\sqrt{2}$
1	0	$-\sqrt{2}$	1	$\sqrt{2}$
2	$(1/2)\sqrt{6}$	$(1/2)\sqrt{2}$	0	$-(1/2)\sqrt{2}$

Table 6.6. Orthogonal polynomial values for a three-level factor and a two-level collapsed factor.

It is interesting to note that $U_i = -Uq'_i$.

A simple calculation gives the relation between x_{U_i} and x'_{U_i} . We find

$$x_{U_i} = 2x'_{U_i} - (x'_{U_i})^2 . \quad (6.6)$$

Equation (6.6) enables us to generate the design matrix for the $3 \times 3 \times 2 \times 2/18$ design from the $3 \times 3 \times 3 \times 2/18$ design, using Math Cad.

The collapsing procedure procedure also requires a new matrix \mathbf{X} of column vectors. This entails a small modification of Table 6.4 through the use of (6.5) and (6.6).

The column vector elements for the $3 \times 3 \times 2 \times 2/18$ design can now be calculated and are given in Table 6.7.

$X_{i,1} = X_{0i}$	$= 1$	$X_{i,2} = W_i$	$= 2x_{W_i} - 1$
$X_{i,3} = Pl_i$	$= ((x_{P_i} - 1)\sqrt{6})/2$	$X_{i,4} = Pq_i$	$= (X_{i,3}^2 - 1)\sqrt{2}$
$X_{i,5} = Ql_i$	$= ((x_{Q_i} - 1)\sqrt{6})/2$	$X_{i,6} = Qq_i$	$= (X_{i,5}^2 - 1)\sqrt{2}$
$X_{i,7} = U_i$	$= (3x_{U_i} - 1)/\sqrt{2}$		
$X_{i,8} = W_i Pl_i$	$= X_{i,2} X_{i,3}$	$X_{i,9} = W_i Ql_i$	$= X_{i,2} X_{i,5}$
$X_{i,10} = W_i U_i$	$= X_{i,2} X_{i,7}$	$X_{i,11} = Pl_i Ql_i$	$= X_{i,3} X_{i,5}$
$X_{i,12} = Pl_i U_i$	$= X_{i,3} X_{i,7}$	$X_{i,13} = Ql_i U_i$	$= X_{i,5} X_{i,7}$

Table 6.7. Column vector elements of the $3 \times 3 \times 2 \times 2/18$ design.

Math Cad was used to generate the other details of the $3 \times 3 \times 2 \times 2/18$ design and the results are given in design 8.32 of the Appendix.

This design has the desirable property that the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix contains many zero's and that the few non zero ρ -values are, on the whole, rather small.

6.4. Other designs with 18 and 27 experimental units

Collapsing the second factor of the $3 \times 3 \times 2 \times 2/18$ design using the method described in Section 6.3 gives the $3 \times 2 \times 2 \times 2/18$ design as given in the Appendix under number 8.33.

Three designs with 27 experimental units are constructed. They are numbered 8.34, 8.35 and 8.36.

The $3 \times 3 \times 3 \times 3/27$ design was generated using 4 of the 13 orthogonal columns of the 3^{13} main-effect design with 27 experimental units.

Design number	Group number	Design	Fraction	Largest $ \rho $	Remarks
8.31	IX	$3 \times 3 \times 3 \times 2/18$	1/3	0.655	Clumpwise orthogonality
8.32	IX	$3 \times 3 \times 2 \times 2/18$	1/2	0.655	Clumpwise orthogonality
8.33	IX	$3 \times 2 \times 2 \times 2/18$	3/4	0.655	Clumpwise orthogonality
8.34	X	$3 \times 3 \times 3 \times 3/27$	1/3	0.250	Clumpwise orthogonality
8.35	X	$3 \times 3 \times 3 \times 2/27$	1/2	0.433	Clumpwise orthogonality
8.36	X	$3 \times 3 \times 2 \times 2/27$	3/4	0.250	Clumpwise orthogonality

Table 6.8. Six fractional factorial designs for quantitative factors with 18 and 27 experimental units.

This design was constructed using Galois fields. See *Kempthorne (1979)* and *Addelman (1962a)*.

The designs 8.35 and 8.36 were again obtained through collapsing. The 3 designs with 27 experimental units are of an excellent quality since their $(\mathbf{X}'\mathbf{X})^{-1}$ matrices contain very few non zero off-diagonal elements. These designs are therefore nearly orthogonal. A few details of the designs just discussed are given in Table 6.8. Efforts were made using Math Cad, to obtain a suitable $3 \times 3 \times 3 \times 3 \times 3/27$ design from 5 orthogonal columns of the 3^{13} main-effect design, but these have not been successful since all the matrices $\mathbf{X}'\mathbf{X}$ were singular. However, we found a $3 \times 3 \times 3 \times 3 \times 3/27$ design in *Mitchell and Bayne (1978)* with a *D*-efficiency of 95.2% and a *G*-efficiency of 65.9%. See design 8.42 in the Appendix.

6.5. Miscellaneous designs

In order to judge and compare the designs thus far developed, we took a few designs from the literature and calculated the usual details of each with Math Cad. These designs are listed

in Table 6.9.

Design number	Group number	DESIGN	Fraction	Largest $ \rho $	Remarks
8.37	XI	$3 \times 3 \times 3/15$	$5/9$	0.077	A Box Behnken design, clumpwise orthogonality
8.38	XI	$3 \times 3 \times 3 \times 3/27$	$1/3$	0.333	A Box Behnken design, clumpwise orthogonality
8.39	XI	$3 \times 3 \times 3 \times 3/15$	$5/27$	0.350	A Rechtschaffner design, a saturated fraction
8.40	XI	$3 \times 3 \times 3 \times 3 \times 3/21$	$7/81$	0.225	A Rechtschaffner design, a saturated fraction with clumpwise orthogonality
8.41	XI	$3 \times 3 \times 3 \times 2/18$	$1/3$	0.334	A Webb design
8.42	XI	$3 \times 3 \times 3 \times 3 \times 3/27$	$1/9$	0.281	A Mitchell and Bayne design

Table 6.9. Six miscellaneous designs for quantitative factors with 15, 18, 21 and 27 experimental units.

The designs 8.37–8.40 all have factors with three equally spaced levels.

However, since these levels occur with unequal frequency we had to calculate special orthogonal polynomials for each of them in such a way that the relations

$$\sum P l_i^2 = \sum P q_i^2 = \sum Q l_i^2 = \dots = N ,$$

were satisfied as well, N being the number of experimental units of a design.

All these orthogonal polynomial values are given in Section 6.6 and an example of the calculation of a set of orthogonal polynomials is given in Appendix 6A.

Designs 8.37 and 8.38 are taken from *Box and Behnken* (1960), the designs 8.39 and 8.40

were constructed with the generators described in *Rechtschaffner* (1967).

Design 8.41 is given in *Webb* (1971).

Design 8.42 is obtained from *Mitchell and Bayne* (1978).

None of the designs 8.37 to 8.42 inclusive are orthogonal but all have small ρ -values.

For further details of the designs we refer to Chapter 7, where the designs are compared and to the Appendix, where the details of each design are given.

6.6. Orthogonal polynomial values for designs 8.37–8.40

In each of the Tables 6.10–6.13 we present the relevant orthogonal polynomial values and also the frequency with which each of the levels 0, 1 and 2 occurs. These frequencies were obtained from the designs 8.37–8.40 of the Appendix.

x_{P_i}	frequency	Pl_i	Pq_i
0	4	$-(1/2)\sqrt{7.5}$	0.9354
1	7	0	-1.0690
2	4	$+(1/2)\sqrt{7.5}$	0.9354
Relations: $Pl_i = 0.5(x_{P_i} - 1)\sqrt{7.5}$			
$Pq_i = (7 - 30x_{P_i} + 15x_{P_i}^2)/\sqrt{56}$			
$\sum_{i=1}^{15} Pl_i^2 = \sum_{i=1}^{15} Pq_i^2 = 15 = N.$			

Table 6.10. Orthogonal polynomial values for the $3 \times 3 \times 3/15$ Box Behnken design.

x_{P_i}	frequency	Pl_i	Pq_i
0	6	-1.5	1.1180
1	15	0	-0.8944
2	6	+1.5	1.1180
Relations: $Pl_i = 1.5(x_{P_i} - 1)$			
$Pq_i = (5 - 18x_{P_i} + 9x_{P_i}^2)/\sqrt{20}$			
$\sum_{i=1}^{27} Pl_i^2 = \sum_{i=1}^{27} Pq_i^2 = 27 = N.$			

Table 6.11. Orthogonal polynomial values for the $3 \times 3 \times 3 \times 3/27$ Box Behnken design.

x_{P_i}	frequency	Pl_i	Pq_i
0	5	-1.2814	0.5983
1	3	-0.1508	-1.9943
2	7	0.9799	0.4274
Relations: $Pl_i = (-17 + 15x_{P_i})/\sqrt{176}$			
$Pq_i = (21 - 179x_{P_i} + 88x_{P_i}^2)/\sqrt{1232}$			
$\sum_{i=1}^{15} Pl_i^2 = \sum_{i=1}^{15} Pq_i^2 = 15 = N.$			

Table 6.12. Orthogonal polynomial values for the $3 \times 3 \times 3 \times 3/15$ Rechtschaffner design.

x_{P_i}	frequency	Pl_i	Pq_i
0	8	-1.1660	0.5152
1	4	-0.0530	-2.0609
2	9	1.0600	0.4580
Relations: $Pl_i = (-22 + 21x_{P_i})/\sqrt{356}$			
$Pq_i = (18 - 179x_{P_i} + 89x_{P_i}^2)\sqrt{(7/8544)}$			
$\sum_{i=1}^{21} Pl_i^2 = \sum_{i=1}^{21} Pq_i^2 = 21 = N.$			

Table 6.13. Orthogonal polynomial values for the $3 \times 3 \times 3 \times 3 \times 3/21$ Rechtschaffner design.

Appendix 6A. The calculation of orthogonal polynomials

The general formulae for the first and second degree orthogonal polynomials are

$$Pl = \lambda_1(\alpha + \beta x_P) \quad , \quad \lambda_1 \neq 0 \quad (6.7)$$

and

$$Pq = \lambda_2(\gamma + \delta x_P + \varepsilon x_P^2) \quad , \quad \lambda_2 \neq 0 \quad , \quad (6.8)$$

respectively.

The following conditions have to be met

$$\sum_{i=1}^N Pl_i = \sum_{i=1}^N Pq_i = \sum_{i=1}^N Pl_i Pq_i = 0 \quad , \quad (6.9)$$

and

$$\sum_{i=1}^N Pl_i^2 = \sum_{i=1}^N Pq_i^2 = N \quad , \quad (6.10)$$

where N is the number of experimental units of the design.

Condition (6.10) has to be met in order to have as many N 's as possible in the diagonal of the $X'X$ matrix. This condition enables us to compare designs with an equal or nearly equal number of experimental units, but with a varying number of factors and levels per factor, more easily. We shall discuss this point in more detail in Chapter 7.

We now proceed to calculate the parameters $\alpha, \beta, \gamma, \delta, \varepsilon, \lambda_1$ and λ_2 . Conditions (6.9) can be written as

$$\sum_{i=1}^N (\alpha + \beta x_{Pi}) = 0 \quad (6.11)$$

$$\sum_{i=1}^N (\gamma + \delta x_{Pi} + \varepsilon x_{Pi}^2) = 0 \quad (6.12)$$

$$\sum_{i=1}^N (\alpha + \beta x_{Pi}) (\gamma + \delta x_{Pi} + \varepsilon x_{Pi}^2) = 0 \quad . \quad (6.13)$$

Condition (6.10) can be written as

$$\lambda_1^2 \cdot \sum_{i=1}^N (\alpha + \beta x_{Pi})^2 = N \quad , \quad (6.14)$$

and

$$\lambda_2^2 \cdot \sum_{i=1}^N (\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2)^2 = N, \quad (6.15)$$

respectively.

As an example we shall calculate the orthogonal polynomial values of Table 6.12. We then have $N = 15$.

Hence

x_{P_i}	frequency	$\alpha + \beta x_{P_i}$
0	5	α
1	3	$\alpha + \beta$
2	7	$\alpha + 2\beta$.

We first try to meet condition (6.11); therefore,

$$\sum_{i=1}^{15} (\alpha + \beta x_{P_i}) = 5\alpha + 3(\alpha + \beta) + 7(\alpha + 2\beta) = 15\alpha + 17\beta = 0.$$

There are an infinite number of sets (α, β) which satisfy $15\alpha + 17\beta = 0$, but for simplicity's sake we prefer the smallest integer set (α, β) .

We therefore have $\alpha = -17, \beta = +15$.

We can now present the numerical values of $\alpha + \beta x_{P_i}$ and $(\alpha + \beta x_{P_i})^2$ in Table 6.14.

x_{P_i}	frequency	$\alpha + \beta x_{P_i}$	$(\alpha + \beta x_{P_i})^2$
0	5	-17	289
1	3	-2	4
2	7	13	169

Table 6.14. Values of $\alpha + \beta x_{P_i}$ and $(\alpha + \beta x_{P_i})^2$.

According to (6.14) we have

$$\lambda_1^2 \sum_{i=1}^{15} (\alpha + \beta x_{P_i}^2) = 15.$$

Hence

$$\lambda_1^2(5 \times 289 + 3 \times 4 + 7 \times 169) = 15 ,$$

thus

$$\lambda_1 = 1/\sqrt{176} .$$

Formula (6.7) can now be written as

$$Pl = (-17 + 15x_P)/\sqrt{176} . \tag{6.16}$$

Equation (6.16) has also been given in Table 6.12.

Substituting $x_P = 0, 1$ and 2 in (6.16) we find the three values of Pl_i given in Table 6.12.

We now proceed to calculate $\gamma, \delta, \varepsilon$ and λ_2 . Using (6.12) we find,

x_{P_i}	frequency	$\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2$
0	5	γ
1	3	$\gamma + \delta + \varepsilon$
2	7	$\gamma + 2\delta + 4\varepsilon$.

According to (6.12) we have

$$\sum_{i=1}^{15} (\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2) = 5\gamma + 3(\gamma + \delta + \varepsilon) + 7(\gamma + 2\delta + 4\varepsilon) = 0 ,$$

or

$$15\gamma + 17\delta + 31\varepsilon = 0 . \tag{6.17}$$

According to (6.13) we have

$$\sum_{i=1}^{15} (\alpha + \beta x_{P_i}) (\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2) = 0 .$$

Using the values $\alpha + \beta x_{P_i}$ and their frequencies from Table 6.14, we may write

$$5 \times (-17)\gamma + 3 \times (-2)(\gamma + \delta + \varepsilon) + 7 \times (13)(\gamma + 2\delta + 4\varepsilon) = 0$$

or

$$176\delta + 358\varepsilon = 0. \tag{6.18}$$

Expressions (6.17) and (6.18) form a set of two equations in three unknowns γ , δ and ε and we therefore have an infinite number of solutions.

However, the set with the smallest integer values, which satisfies these equations, is

$$\gamma = 21, \quad \delta = -179 \quad \text{and} \quad \varepsilon = 88.$$

The numerical values of $\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2$ and $(\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2)^2$ can now be calculated and are given in Table 6.15.

x_{P_i}	frequency	$\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2$	$(\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2)^2$
0	5	21	441
1	3	-70	4900
2	7	15	225

Table 6.15. Values of $\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2$ and $(\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2)^2$.

According to (6.15) we have,

$$\lambda_2^2 \sum_{i=1}^{15} (\gamma + \delta x_{P_i} + \varepsilon x_{P_i}^2)^2 = 15,$$

hence

$$\lambda_2^2(5 \times 441 + 3 \times 4900 + 7 \times 225) = 15,$$

thus $\lambda_2 = 1/\sqrt{1232}$.

Equation (6.8) can now be written as

$$Pq = (21 - 179x_P + 88x_P^2)/\sqrt{1232}, \tag{6.19}$$

and this formula is given in Table 6.12.

Substituting $x_P = 0, 1$ and 2 in (6.19) gives the three values for Pq as presented in Table 6.12.

It is pointed out that the orthogonal polynomials (6.16) and (6.19) basically contain 5 and not 7 parameters. These 5 parameters have to satisfy the 5 equations (6.11), ..., (6.15).

We can write (6.7) and (6.8) namely as follows

$$Pl = \alpha' + \beta' x_P, \quad (6.20)$$

$$Pq = \gamma' + \delta' x_P + \varepsilon' x_P^2, \quad (6.21)$$

in which

$$\alpha' = \lambda_1 \alpha, \quad \beta' = \lambda_1 \beta,$$

$$\gamma' = \lambda_2 \gamma, \quad \delta' = \lambda_2 \delta, \quad \varepsilon' = \lambda_2 \varepsilon.$$

The parameters λ_1 and λ_2 were only introduced for ease of calculation and presentation, since we could now calculate $\alpha, \beta, \gamma, \delta$ and ε first and λ_1 and λ_2 later on.

The introduction of λ_1 and λ_2 also enabled us to write the polynomial coefficients with integer numbers.

Although the choice of $\alpha, \beta, \gamma, \delta$ and ε was rather arbitrary, the *absolute* values of $\alpha', \beta', \gamma', \delta'$ and ε' are unique.

It is namely easily seen that the sets

$$(-\alpha', -\beta', \gamma', \delta', \varepsilon'), \quad (-\alpha', -\beta', -\gamma', -\delta', -\varepsilon')$$

and

$$(\alpha', \beta', -\gamma', -\delta', -\varepsilon')$$

also satisfy (6.7) and (6.8).

CHAPTER 7

Evaluation and comparison of the designs

7.1. Introduction

To evaluate and compare the designs, we made use of the articles written by *Hahn, Meeker and Feder* (1976), *Lucas* (1976), *Marquardt* (1970) and *Snee* (1973a,1985).

We also refer to Section 5.5 where the output of Math Cad was explained. It is given for each design in the Appendix. It has been summarized for each design in Tables 7.3a, 7.3b, ..., 7.3j.

The variance of an estimated regression coefficient is according to *Snee* (1973a)

$$\sigma_{\hat{\beta}_p}^2 = \sigma^2 / \left[\sum_{i=1}^N (X_{ip} - \bar{X}_{.p})^2 (1 - r_p^2) \right], \quad (7.1)$$

where r_p is the multiple correlation coefficient of X_p with all other X 's.

Equation (7.1) may according to (4.3) be written as

$$\sigma_{\hat{\beta}_p}^2 = \sigma^2(\text{VIF}) / \sum_{i=1}^N (X_{ip} - \bar{X}_{.p})^2,$$

where

$$\bar{X}_{.p} = (1/N) \sum_{i=1}^N X_{ip}.$$

However, in the designs 8.1, ..., 8.6, 8.11, 8.12, 8.13a, 8.14a, 8.15a, 8.31, ..., 8.36 we have $\bar{X}_{.p} = 0$, hence for those designs

$$\sigma_{\hat{\beta}_p}^2 = \sigma^2(\text{VIF}) / \sum_{i=1}^N X_{ip}^2. \quad (7.2)$$

Because the VIF is a function of the multiple correlation coefficient of X_p with all other vectors X , it is independent of the scaling of X_p .

However, $\sigma_{\hat{\beta}_p}^2$ depends on $\sum_{i=1}^N X_{ip}^2$, the diagonal elements of $X'X$ and therefore depends on the scaling of X_{ip} .

This fact makes it difficult to compare σ_{β}^2 's of designs with a varying number of factors and levels per factor, even if the number of experimental units is fixed.

We have avoided this difficulty by choosing the orthogonal polynomials for each of the designs 8.1, ..., 8.6, 8.11, 8.12, 8.13a, 8.14a, 8.15a, 8.31, ..., 8.36 in such a way that

$$\sum_{i=1}^N P l_i^2 = \sum_{i=1}^N Q l_i^2 = \dots = N, \quad (7.3)$$

$$\sum_{i=1}^N P q_i^2 = \sum_{i=1}^N Q q_i^2 = \dots = N. \quad (7.4)$$

It then however appeared that all diagonal elements of $\mathbf{X}'\mathbf{X}$ were equal to N for each of these designs. We shall therefore call such designs N -designs from now on. This fact will make the comparison of σ_{β}^2 's of these designs easier, because changes in σ_{β}^2 within groups I, II, IV, Va, IX and X as given in Tables 4.22, 5.12 and 6.8, will only be caused by changes in the VIF. The reason that $\sum_{i=1}^N X_{ip}^2 = N$ for the N -designs is caused by the fact that all these designs have been constructed from orthogonal main-effect designs, (7.3) and (7.4) apply and

$$\sum_{i=1}^N X_{ip}^2 = N, \quad \text{for all } 2^n \text{ designs.}$$

The fact that we interfere with the scaling of the X_{ip} is less arbitrary than it appears at first sight.

When for instance the factor temperature is set at the levels 230, 250 and 270 degrees centigrade, it is customary to "code" these levels by using $-1, 0$ and $+1$.

It is obvious that we could have used the coded levels $-5, 0$ and $+5$ as well, since they are also equally spaced.

We used the coded levels

$$-(1/2)\sqrt{6} \quad 0 \quad +(1/2)\sqrt{6} \quad \text{for a three-level factor}$$

and

$$-\sqrt{2} \quad 0 \quad +\sqrt{2} \quad \text{for a collapsed three-level factor derived from a four-level factor.}$$

Since these are also equally spaced there is no objection as to their use.

We shall prove that $\sum_{i=1}^N X_{ip}^2 = N$ for two N -designs in the next section.

7.2. The value of $\sum_{i=1}^N X_{ip}^2$ for the N -designs

THEOREM 7.2.1.

The designs 8.1, ..., 8.6, 8.11, 8.12, 8.13a, 8.14a, 8.15a, 8.31, ..., 8.36 are N -designs.

Proof. We shall prove the theorem for two designs.

We first consider design 8.14a ($4 \times 3 \times 2 \times 2/16$) from the Appendix.

The column vectors elements of \mathbf{X} are obtained from design 8.14a and are given below:

$$\begin{aligned} X_{i,1} &= x_{0i} = 1 & X_{i,2} &= Pq_i \\ X_{i,3} &= Qq_i & X_{i,4} &= R_i \\ X_{i,5} &= Pl_i & X_{i,6} &= Pl_i R_i \\ X_{i,7} &= Ql_i S_i & X_{i,8} &= Ql_i \\ X_{i,9} &= Ql_i R_i & X_{i,10} &= Pl_i S_i \\ X_{i,11} &= Pl_i Ql_i & X_{i,12} &= S_i & X_{i,13} &= R_i S_i . \end{aligned}$$

We use the notation of Math Cad, " $X_{i,p}$ " instead of " X_{ip} ".

There are $N = 16$ values $x_{0i} = 1$ and therefore $\sum_{i=1}^N x_{0i}^2 = N = 16$.

For $X_{i,2}$, $X_{i,3}$, $X_{i,4}$, $X_{i,5}$, $X_{i,8}$ and $X_{i,12}$ we have $\sum_{i=1}^N X_{i,p}^2 = N$ since the orthogonal polynomials were so scaled and because (7.3) and (7.4) apply.

We now consider the next diagonal element of $\mathbf{X}'\mathbf{X}$,

$$\sum_{i=1}^N (X_{i,6})^2 = (\mathbf{PIR}, \mathbf{PIR}) . \tag{7.5}$$

From design (8.14a) we obtain

$$Pl_i R_i = (2A_i + B_i) (A_i B_i C_i D_i) / \sqrt{5} = (2B_i C_i D_i + A_i C_i D_i) / \sqrt{5} .$$

Substituting \mathbf{PIR} in (7.5) and using the vector notation of Section 4.2, we find

$$\begin{aligned}\sum_{i=1}^N (X_{i,6})^2 &= (2\mathbf{BCD} + \mathbf{ACD}, 2\mathbf{BCD} + \mathbf{ACD}) / 5 \\ &= (4(\mathbf{BCD}, \mathbf{BCD}) + (\mathbf{ACD}, \mathbf{ACD})) / 5 ,\end{aligned}$$

since all inner products such as $(\mathbf{BCD}, \mathbf{ACD})$ vanish because the 2^n design is orthogonal.

Hence

$$\sum_{i=1}^N (X_{i,6})^2 = (4N + N) / 5 = N .$$

To calculate the next diagonal element of $\mathbf{X}'\mathbf{X}$ we consider

$$Q_i S_i = (C_i + D_i) (B_i C_i) / \sqrt{2} = (B_i + B_i C_i D_i) / \sqrt{2}$$

and

$$\begin{aligned}\sum_{i=1}^N (X_{i,7})^2 &= (\mathbf{QIS}, \mathbf{QIS}) = (\mathbf{B} + \mathbf{BCD}, \mathbf{B} + \mathbf{BCD}) / 2 \\ &= ((\mathbf{B}, \mathbf{B}) + (\mathbf{BCD}, \mathbf{BCD})) / 2 = (N + N) / 2 = N .\end{aligned}$$

We can similarly prove that

$$\sum_{i=1}^N (X_{i,9})^2 = \sum_{i=1}^N (X_{i,10})^2 = \sum_{i=1}^N (X_{i,11})^2 = \sum_{i=1}^N (X_{i,13})^2 = N .$$

We have now proved Theorem 7.2.1 for design 8.14a.

Secondly we consider design 8.32 ($3 \times 3 \times 2 \times 2 / 18$) from the Appendix.

The column vector elements of \mathbf{X} are, see also Table 6.7,

$$X_{i,1} = 1 \qquad X_{i,2} = 2x_{W_i} - 1$$

$$X_{i,3} = (1/2) (x_{P_i} - 1) \sqrt{6} \quad X_{i,4} = (X_{i,3}^2 - 1) \sqrt{2}$$

$$X_{i,5} = (1/2) (x_{Q_i} - 1) \sqrt{6} \quad X_{i,6} = (X_{i,5}^2 - 1) \sqrt{2}$$

$$X_{i,7} = (3x_{U_i} - 1) / \sqrt{2}$$

$$X_{i,8} = X_{i,2} X_{i,3} \qquad X_{i,9} = X_{i,2} X_{i,5} \qquad X_{i,10} = X_{i,2} X_{i,7}$$

$$X_{i,11} = X_{i,3} X_{i,5} \qquad X_{i,12} = X_{i,3} X_{i,7} \qquad X_{i,13} = X_{i,5} X_{i,7} .$$

Again we have $\sum_{i=1}^N X_{i,1}^2 = N = 18$ and $\sum_{i=1}^N X_{i,p}^2 = N$ for $p = 2, 3, \dots, 7$, because the orthogonal polynomials were scaled accordingly.

$$\sum_{i=1}^N X_{i,8}^2 = \sum_{i=1}^N X_{i,2}^2 X_{i,3}^2 = \sum_{i=1}^N X_{i,3}^2 = N \text{ since } X_{i,2}^2 = 1.$$

Similarly we have $\sum_{i=1}^N X_{i,9}^2 = \sum_{i=1}^N X_{i,10}^2 = N$.

$$\sum_{i=1}^N X_{i,11}^2 = \sum_{i=1}^N X_{i,3}^2 X_{i,5}^2. \quad (7.6)$$

Because the original 2×3^7 main-effect design as given in Table 6.1 is orthogonal we have

$$\sum_{i=1}^N X_{i,4} X_{i,6} = 0,$$

or

$$\sum_{i=1}^N (X_{i,3}^2 - 1) \sqrt{2} (X_{i,5}^2 - 1) \sqrt{2} = 0,$$

or

$$\sum_{i=1}^N (X_{i,3}^2 X_{i,5}^2 - X_{i,3}^2 - X_{i,5}^2 + 1) = 0,$$

or

$$\sum_{i=1}^N (X_{i,3}^2 X_{i,5}^2) - N - N + N = 0,$$

or

$$\sum_{i=1}^N (X_{i,3}^2 X_{i,5}^2) = N$$

and therefore using (7.6)

$$\sum_{i=1}^N X_{i,11}^2 = N. \quad (7.7)$$

We could have proved (7.7) in a different way.

Because design 8.32 is derived from Table 6.1, an orthogonal design, the level combinations

of each group of two factors occur with equal frequency.

Since the factors P and Q have three levels each, there are 9 combinations of levels. Since there are $N = 18$ experimental units, there are $N/9 = 18/9 = 2$ experimental units for each level combination. Table 7.1 gives the 9 level combinations and the corresponding values of $X_{i,3}^2 X_{i,5}^2$. Table 7.1 was constructed using Table 6.1 and equation (6.3).

$X_{i,5} =$ $(\frac{1}{2})(x_{Qi} - 1)\sqrt{6}$	$X_{i,3} =$ $(\frac{1}{2})(x_{Pi} - 1)\sqrt{6}$	$-\frac{1}{2}\sqrt{6}$	0	$+\frac{1}{2}\sqrt{6}$
	x_P	0	1	2
	x_Q			
$-\frac{1}{2}\sqrt{6}$	0	$(N/9)(36/16)$	$(N/9) \times 0$	$(N/9)(36/16)$
0	1	$(N/9) \times 0$	$(N/9) \times 0$	$(N/9) \times 0$
$+\frac{1}{2}\sqrt{6}$	2	$(N/9)(36/16)$	$(N/9) \times 0$	$(N/9)(36/16)$

Table 7.1. Values of $X_{i,3}^2 X_{i,5}^2$ for the $3 \times 3 \times 2 \times 2/18$ design.

Using Table 7.1 we calculate

$$\sum_{i=1}^N X_{i,11}^2 = \sum_{i=1}^N X_{i,3}^2 X_{i,5}^2 = 4 \times (N/9)(36/16) = N, \text{ q.e.d.}$$

To calculate the value of $\sum_{i=1}^N X_{i,12}^2 = \sum_{i=1}^N X_{i,3}^2 X_{i,7}^2$ we use the method of Table 7.1 and construct Table 7.2, making use of Tables 6.1, 6.3 and 6.6. We use Table 6.6 since $X_{i,7}$ refers to a factor with two levels derived by collapsing a three-level factor.

$X_{i,7} =$ $(3x_{U_i} - 1)\sqrt{2}$	$X_{i,3} =$ $(\frac{1}{2})(x_{P_i} - 1)\sqrt{6}$	$-(\frac{1}{2})\sqrt{6}$	0	$+(\frac{1}{2})\sqrt{6}$
	x_P	0	1	2
	x_U			
$-(\frac{1}{2})\sqrt{2}$	0	$(N/9)(12/16)$	$(N/9) \times 0$	$(N/9)(12/16)$
$\sqrt{2}$	1	$(N/9) \times 3$	$(N/9) \times 0$	$(N/9) \times 3$
$-(\frac{1}{2})\sqrt{2}$	0	$(N/9)(12/16)$	$(N/9) \times 0$	$(N/9)(12/16)$

Table 7.2. Values of $X_{i,3}^2 X_{i,7}^2$ for the $3 \times 3 \times 2 \times 2/18$ design.

From Table 7.2 we obtain

$$\sum_{i=1}^N X_{i,12}^2 = \sum_{i=1}^N X_{i,3}^2 X_{i,7}^2 = 4 \times (N/9)(12/16) + 2 \times (N/9) \times 3 = N .$$

In a similar way we can prove that

$$\sum_{i=1}^N X_{i,13}^2 = N .$$

Theorem 7.2.1 therefore applies to design 8.32.

Theorem 7.2.1 can likewise be proved for the other N -designs.

7.3. Design characteristics

It was already stated in Section 7.1 that the designs 8.1, 8.2, ..., 8.42 are summarized in Tables 7.3a, 7.3b, ..., 7.3j, in which a number of design characteristics have been given.

We again refer to Section 5.5 where many of these characteristics were explained.

The first characteristic of each design in Table 7.3 is the D -efficiency, which was fully explained in Chapter 2.

The second symbol in Table 7.3 is P , the number of parameters β in the regression model.

Important characteristics of a design are the σ_β^2 's, the variances of the β -estimates.

These variances are however dependent on the scale used for the independent variables, which makes it difficult to compare the σ_β^2 's of the various designs. We solved this problem partly by arranging the scaling for the N -designs in such a way that

$$\sum_{i=1}^N X_{ip}^2 = N . \quad (7.8)$$

We then have that if values σ_{β}^2 change within a group of N -designs, for instance within group I consisting of design 8.1, 8.2, 8.3 and 8.4, such a change must be due to a change in the VIF due to collapsing.

The condition given in (7.8) has the additional advantage that the variances of the $\hat{\beta}$'s are equal within an orthogonal design and nearly equal within a design if it is nearly orthogonal. To compare the σ_{β}^2 's in a different way we calculated these values for all the 45 designs of the Appendix using the same scaling for \mathbf{x} as in Chapter 3 for the D -optimal designs that is

$$-1 \leq x_m \leq +1 , \quad m = 1, 2, \dots, k .$$

These σ_{β}^2 -values have, without loss of generality for $\sigma^2 = 1$, been given in Tables 7.4a, 7.4b, ..., 7.4k. However, in the Tables 7.3a, 7.3b, ..., 7.3j we gave for reasons of space only the maximum values of

$$(\sigma_{\hat{\beta}_p}^2/\sigma^2), (\sigma_{\hat{\beta}_{pq}}^2/\sigma^2) \text{ and } (\sigma_{\hat{\beta}_{pp}}^2/\sigma^2) .$$

For the N -designs and the designs 8.37, 8.38, ..., 8.41 we gave two maximum values in the Tables 7.3a...j for each of the three variances mentioned above.

The first value refers to the maximum value of $(\sigma_{\beta}^2/\sigma^2)$ based on the scale $-1 \leq x_m \leq +1$, for $m = 1, 2, \dots, k$.

The second value refers to the maximum value of $(\sigma_{\beta}^2/\sigma^2)$ for the N -designs for which

$$\sum_{i=1}^N X_{ip}^2 = N .$$

The designs 8.37, 8.38, 8.39, 8.40 and 8.41 also have a second maximum value for $(\sigma_{\beta}^2/\sigma^2)$.

For these designs we have

$$\sum_{i=1}^N P l_i^2 = \sum_{i=1}^N Q l_i^2 = \dots = N$$

$$\sum_{i=1}^N P q_i^2 = \sum_{i=1}^N Q q_i^2 = \dots = N .$$

For the designs 8.7, 8.8, 8.9, 8.10, 8.13b, 8.14b, 8.15b, 8.16, 8.17, ..., 8.30 and 8.42 we did not use orthogonal polynomials and the $\max(\sigma_{\beta}^2/\sigma^2)$'s given are based on the scale

$$-1 \leq x_m \leq +1, \quad m = 1, 2, \dots, k.$$

In each of the designs 8.1, 8.2, ..., 8.42 it is obvious whether orthogonal polynomial variables or the variables x_m are used.

The design characteristics given together with each design of the Appendix are calculated from the type of variable used for that particular design and the values given in Table 7.3 are obtained from the design details in the Appendix unless otherwise stated.

For reasons of space we only gave the design matrix and the column vectors of the \mathbf{X} matrix for designs 8.25, ..., 8.30 and 8.42. For the same reason we omitted the matrix \mathbf{r} in the Appendix for a number of designs. Many details of these designs can however be found in Table 7.3g and Table 7.3j.

The value of $(\text{Trace } (\mathbf{X}'\mathbf{X})^{-1})/P$ is equal to the average value of $(\sigma_{\hat{\beta}}^2/\sigma^2)$. For each design in Table 7.3, in which we gave two values of $\max(\sigma_{\hat{\beta}}^2/\sigma^2)$, we also gave two corresponding values of $(\text{trace } (\mathbf{X}'\mathbf{X})^{-1})/P$.

The determinant $|\mathbf{r}|$ and trace (\mathbf{r}^{-1}) have already been explained in Section 5.5.

All VIF's can be found as diagonal elements of \mathbf{r}^{-1} . We only listed the largest in Tables 7.3a, ..., 7.3j. Some designs have replicate observations.

Whenever this is the case we gave the number of degrees of freedom V associated with these replicates, which provides an estimate of σ^2 and enables us to test for lack of fit in a few cases. The expression $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ has been explained in Section 2.4.

The value d which is given for each design is the maximum value of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ in the candidate points of the complete factorial design. See also Sections 5.6 and 5.7.

The largest coefficient of $\hat{\beta}$ of correlation in absolute value between pairs of $\hat{\beta}$'s is given as $|\rho|$.

The next line in Table 7.3 gives the number of experimental units of the design. It is followed by the value of the G -efficiency of the design. We shall come back to this measure in the next section.

The last line in the Tables 7.3a, 7.3b, ..., 7.3j is reserved for remarks. We shall discuss these when we deal with each group of designs.

Table 7.5 gives a complete list of the D - and G -efficiencies of the 45 designs considered. The designs for which the G -efficiency is exact are marked by an asterisk. An exact G -efficiency is found if the exact maximum value of $\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x})$ in the k -dimensional experimental region R is used to compute the G -efficiency. See also Section 4.5.2.

Design number	8.1	8.2	8.3	8.4
Group	I	I	I	I
Design	$4 \times 2 \times 2/8$	$3 \times 2 \times 2/8$	$3 \times 2 \times 2/8$	$3 \times 2 \times 2/8$
<i>D</i> -efficiency	82.4	68.4	81.3	identical with design (8.2)
<i>P</i> : number of parameters in model	8	8	8	
$\max(\sigma_{\beta_p}^2/\sigma^2)$	{ 0.281 0.156	{ 0.500 0.250	{ 0.500 0.148	
$\max(\sigma_{\beta_{pq}}^2/\sigma^2)$	{ 0.281 0.156	{ 0.500 0.250	{ 0.500 0.250	
$\max(\sigma_{\beta_{pp}}^2/\sigma^2)$	{ 0.633 0.125	{ 0.500 0.125	{ 1.250 0.227	
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.283 0.149	{ 0.375 0.219	{ 0.438 0.184	
$ \mathbf{r} $	0.512	0.125	0.264	
trace (\mathbf{r}^{-1})	8.5	13.0	10.75	
largest VIF	1.25	2.0	2.0	
<i>V</i> : degrees of freedom for replication	-	-	-	
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	2.12	4.00	4.00	
largest (ρ)	0.447	0.707	0.671	
<i>N</i> : number of experimental units	8	8	8	
<i>G</i> -efficiency = $100 P/Nd$	47.2	25.0	25.0	
remarks	clumpwise orth.	clumpwise orth.	clumpwise orth.	

Table 7.3a. Design characteristics.

Design number	8.5	8.6	8.7	8.8	8.9	8.10
Group	II	II	III	III	III	III
Design	$4 \times 4 \times 2/16$	$4 \times 3 \times 2/16$	$4 \times 4 \times 4/16$	$4 \times 4 \times 3/16$	$4 \times 3 \times 3/16$	$3 \times 3 \times 3/16$
<i>D</i> -efficiency	82.0	81.3	87.8	89.2	90.9	92.6
<i>P</i> : number of parameters in model	9	9	10	10	10	10
$\max(\sigma_{\beta_p}^2/\sigma^2)$	{ 0.113 0.063	{ 0.125 0.063	0.084	0.089	0.091	0.089
$\max(\sigma_{\beta_{pq}}^2/\sigma^2)$	{ 0.203 0.063	{ 0.225 0.063	0.118	0.123	0.123	0.120
$\max(\sigma_{\beta_{pp}}^2/\sigma^2)$	{ 0.316 0.063	{ 0.316 0.063	0.647	0.678	0.629	0.484
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.178 0.063	{ 0.172 0.063	0.308	0.288	0.268	0.249
$ \mathbf{r} $	1.000	1.000	0.387	0.400	0.413	0.427
trace (\mathbf{r}^{-1})	8.00	8.00	11.40	11.27	11.16	11.06
largest VIF	1.00	1.00	1.53	1.61	1.53	1.45
<i>V</i> : degrees of freedom for replication	-	4	-	-	-	1
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	0.902	0.953	1.084	1.131	1.091	1.021
largest (ρ)	0	0	0.339	0.394	0.404	0.362
<i>N</i> : number of experimental units	16	16	16	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	62.3	59.0	57.7	55.3	57.3	61.2
remarks	orth. design	orth. design	clumpw. orth.	clumpw. orth.	clumpw. orth.	clumpw. orth.

Table 7.3b. Design characteristics.

Design number	8.11	8.12
Group	IV	IV
Design	$4 \times 2 \times 2 \times 2/16$	$3 \times 2 \times 2 \times 2/16$
<i>D</i> -efficiency	90.1	88.6
<i>P</i> : number of parameters in model	12	12
$\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$	{ 0.113 0.063	{ 0.125 0.063
$\max(\sigma_{\hat{\beta}_{rs}}^2/\sigma^2)$	{ 0.113 0.063	{ 0.125 0.063
$\max(\sigma_{\hat{\beta}_{rr}}^2/\sigma^2)$	{ 0.316 0.063	{ 0.250 0.063
$(\text{trace } (\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.108 0.063	{ 0.104 0.063
$ \mathbf{r} $	1.000	1.000
$\text{trace } (\mathbf{r}^{-1})$	11.00	11.00
largest VIF	1.00	1.00
<i>V</i> : degrees of freedom for replication	-	4
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	0.950	1.000
largest (ρ)	0	0
<i>N</i> : number of experimental units	16	16
<i>G</i> -efficiency = $100 P/Nd$	78.9	75.0
remarks	orth. design	orth. design

Table 7.3c. Design characteristics.

Design number	8.13a	8.14a	8.15a
Group	V	V	V
Design	$4 \times 4 \times 2 \times 2/16$	$4 \times 3 \times 2 \times 2/16$	$3 \times 3 \times 2 \times 2/16$
<i>D</i> -efficiency	75.2	69.0	68.1
<i>P</i> : number of parameters in model	13	13	13
$\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$	{ 0.139 0.077	{ 0.150 0.075	{ 0.188 0.094
$\max(\sigma_{\hat{\beta}_{rs}}^2/\sigma^2)$	{ 0.298 0.092	{ 0.450 0.125	{ 0.500 0.125
$\max(\sigma_{\hat{\beta}_{rr}}^2/\sigma^2)$	{ 0.316 0.063	{ 0.316 0.063	{ 0.250 0.063
$(\text{trace } (\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.176 0.076	{ 0.206 0.091	{ 0.207 0.091
$ \mathbf{r} $	0.314	0.125	0.125
$\text{trace } (\mathbf{r}^{-1})$	14.82	18.00	18
largest VIF	1.47	2.00	2.00
<i>V</i> : degrees of freedom for replication	-	-	2
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	2.527	3.674	3.998
largest (ρ)	0.436	0.667	0.577
<i>N</i> : number of experimental units	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	32.2	22.1	20.3
remarks	clumpw. orth.	clumpw. orth.	clumpw. orth.

Table 7.3d. (part 1) Design characteristics.

Design number	8.13b	8.14b	8.15b
Group	V	V	V
Design	$4 \times 4 \times 2 \times 2/16$	$4 \times 3 \times 2 \times 2/16$	$3 \times 3 \times 2 \times 2/16$
<i>D</i> -efficiency	84.6	81.1	76.4
<i>P</i> : number of parameters in model	13	13	13
$\max(\sigma_{\beta_p}^2/\sigma^2)$	0.125	0.125	0.125
$\max(\sigma_{\beta_{pq}}^2/\sigma^2)$	0.141	0.180	0.250
$\max(\sigma_{\beta_{pp}}^2/\sigma^2)$	0.633	0.633	0.500
$(\text{trace } (\mathbf{X}'\mathbf{X})^{-1})/P$	0.238	0.234	0.239
$ \mathbf{r} $	0.192	0.101	0.044
trace (\mathbf{r}^{-1})	15.95	17.88	21
largest VIF	2.00	2.00	2.25
<i>V</i> : degrees of freedom for replication	-	-	-
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	1.411	1.953	2.357
largest (ρ)	0.500	0.621	0.707
<i>N</i> : number of experimental units	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	57.6	41.6	34.5
remarks	clumpw. orth.	clumpw. orth.	clumpw. orth.

Table 7.3d. (part 2) Design characteristics.

Design number	8.16	8.17	8.18	8.19
Group	VI	VI	VI	VI
Design	$4 \times 4 \times 4 \times 2/16$	$4 \times 4 \times 3 \times 2/16$	$4 \times 3 \times 3 \times 2/16$	$3 \times 3 \times 3 \times 2/16$
<i>D</i> -efficiency	87.5	87.2	86.8	87.2
<i>P</i> : number of parameters in model	14	14	14	14
$\max(\sigma_{\beta_p}^2/\sigma^2)$	0.110	0.109	0.109	0.108
$\max(\sigma_{\beta_{pq}}^2/\sigma^2)$	0.124	0.132	0.146	0.149
$\max(\sigma_{\beta_{pp}}^2/\sigma^2)$	0.738	0.746	0.554	0.525
$(\text{trace } (\mathbf{X}'\mathbf{X})^{-1})/P$	0.266	0.254	0.240	0.228
$ \mathbf{r} $	0.301	0.272	0.230	0.219
trace (\mathbf{r}^{-1})	15.77	16.07	16.56	16.75
largest VIF	1.42	1.44	1.45	1.43
<i>V</i> : degrees of freedom for replication	-	-	-	-
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	1.862	1.948	2.272	2.228
largest (ρ)	0.445	0.412	0.405	0.402
<i>N</i> : number of experimental units	16	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	47.0	44.9	38.5	39.3
remarks				

Table 7.3e. Design characteristics.

Design number	8.20	8.21	8.22	8.23	8.24
Group	VII	VII	VII	VII	VII
Design	$4 \times 4 \times 4 \times 4/16$	$4 \times 4 \times 3 \times 3/16$	$4 \times 4 \times 3 \times 3/16$	$4 \times 3 \times 3 \times 3/16$	$3 \times 3 \times 3 \times 3/16$
<i>D</i> -efficiency	84.9	86.2	86.0	85.0	85.8
<i>P</i> : number of parameters in model	15	15	15	15	15
$\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$	0.144	0.136	0.136	0.142	0.140
$\max(\sigma_{\hat{\beta}_{pq}}^2/\sigma^2)$	0.127	0.132	0.138	0.143	0.160
$\max(\sigma_{\hat{\beta}_{pp}}^2/\sigma^2)$	0.836	0.714	0.714	0.634	0.661
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.355	0.334	0.320	0.308	0.304
$ \mathbf{r} $	0.193	0.208	0.191	0.161	0.145
$\text{trace}(\mathbf{r}^{-1})$	18.13	17.81	18.01	18.57	18.85
largest VIF	1.76	1.66	1.66	1.73	1.64
<i>V</i> : degrees of freedom for replication	-	-	-	-	-
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	2.451	2.193	2.046	2.047	2.229
largest (ρ)	0.385	0.395	0.362	0.369	0.372
<i>N</i> : number of experimental units	16	16	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	38.3	42.7	45.8	45.8	42.1
remarks					

Table 7.3f. Design characteristics.

Design number	8.25	8.26	8.27
Group	VIII	VIII	VIII
Design	$4 \times 4 \times 4 \times 4 \times 4/32$	$4 \times 4 \times 4 \times 4 \times 3/32$	$4 \times 4 \times 4 \times 3 \times 3/32$
<i>D</i> -efficiency	87.8	88.1	88.8
<i>P</i> : number of parameters in model	21	21	21
$\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$	0.047	0.047	0.047
$\max(\sigma_{\hat{\beta}_{pq}}^2/\sigma^2)$	0.054	0.054	0.054
$\max(\sigma_{\hat{\beta}_{pp}}^2/\sigma^2)$	0.430	0.428	0.419
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.158	0.153	0.147
$ \mathbf{r} $	0.119	0.113	0.117
$\text{trace}(\mathbf{r}^{-1})$	25.15	25.20	25.06
largest VIF	1.66	1.65	1.64
<i>V</i> : degrees of freedom for replication	-	-	-
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	1.178	1.197	1.175
largest (ρ)	0.351	0.353	0.346
<i>N</i> : number of experimental units	32	32	32
<i>G</i> -efficiency = $100 P/Nd$	55.7	54.8	55.8
remarks			

Table 7.3g. (part 1) Design characteristics.

Design number	8.28	8.29	8.30
Group	VIII	VIII	VIII
Design	$4 \times 4 \times 3 \times 3 \times 3/32$	$4 \times 3 \times 3 \times 3 \times 3/32$	$3 \times 3 \times 3 \times 3 \times 3/32$
<i>D</i> -efficiency	89.4	90.1	90.4
<i>P</i> : number of parameters in model	21	21	21
$\max(\sigma_{\beta_p}^2/\sigma^2)$	0.048	0.048	0.048
$\max(\sigma_{\beta_{pq}}^2/\sigma^2)$	0.054	0.054	0.054
$\max(\sigma_{\beta_{pp}}^2/\sigma^2)$	0.409	0.416	0.326
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.141	0.135	0.130
$ \mathbf{r} $	0.120	0.124	0.119
$\text{trace}(\mathbf{r}^{-1})$	24.96	24.82	24.88
largest VIF	1.58	1.60	1.59
<i>V</i> : degrees of freedom for replication	—	—	—
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	1.183	1.164	1.116
largest (ρ)	0.326	0.319	0.316
<i>N</i> : number of experimental units	32	32	32
<i>G</i> -efficiency = $100 P/Nd$	55.5	56.4	58.8
remarks			

Table 7.3g. (part 2) Design characteristics.

Design number	8.31	8.32	8.33
Group	IX	IX	IX
Design	$3 \times 3 \times 3 \times 2/18$	$3 \times 3 \times 2 \times 2/18$	$3 \times 2 \times 2 \times 2/18$
<i>D</i> -efficiency	80.1	82.1	76.8
<i>P</i> : number of parameters in model	14	13	12
$\max(\sigma_{\beta_p}^2/\sigma^2)$	{ 0.083 0.056	{ 0.104 0.056	{ 0.107 0.056
$\max(\sigma_{\beta_{pq}}^2/\sigma^2)$	{ 0.250 0.111	{ 0.189 0.111	{ 0.179 0.111
$\max(\sigma_{\beta_{pp}}^2/\sigma^2)$	{ 0.313 0.069	{ 0.437 0.097	{ 0.313 0.069
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.192 0.076	{ 0.168 0.070	{ 0.144 0.080
$ \mathbf{r} $	0.164	0.289	0.164
$\text{trace}(\mathbf{r}^{-1})$	18.24	15.40	16.24
largest VIF	2.00	2.00	2.00
<i>V</i> : degrees of freedom for replication	—	—	1
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	2.892	2.571	2.310
largest (ρ)	0.655	0.655	0.655
<i>N</i> : number of experimental units	18	18	18
<i>G</i> -efficiency = $100 P/Nd$	26.9	28.1	28.9
remarks	lin. effects orthogonal	lin. effects orthogonal	lin. effects orthogonal

Table 7.3h. Design characteristics.

Design number	8.34	8.35	8.36
Group	X	X	X
Design	$3 \times 3 \times 3 \times 3/27$	$3 \times 3 \times 3 \times 2/27$	$3 \times 3 \times 2 \times 2/27$
<i>D</i> -efficiency	87.8	84.3	85.8
<i>P</i> : number of parameters in model	15	14	13
$\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$	{ 0.056	{ 0.064	{ 0.070
	{ 0.037	{ 0.037	{ 0.037
$\max(\sigma_{\hat{\beta}_{pp}}^2/\sigma^2)$	{ 0.089	{ 0.103	{ 0.089
	{ 0.040	{ 0.046	{ 0.040
$\max(\sigma_{\hat{\beta}_{pp'}}^2/\sigma^2)$	{ 0.167	{ 0.167	{ 0.167
	{ 0.037	{ 0.037	{ 0.037
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.117	{ 0.110	{ 0.090
	{ 0.038	{ 0.041	{ 0.038
$ \mathbf{r} $	0.824	0.536	0.824
$\text{trace}(\mathbf{r}^{-1})$	14.40	14.38	12.40
largest VIF	1.07	1.23	1.07
<i>V</i> : degrees of freedom for replication	-	-	3
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	1.000	1.322	1.075
largest (ρ)	0.250	0.433	0.250
<i>N</i> : number of experimental units	27	27	27
<i>G</i> -efficiency = $100 P/Nd$	55.6	39.2	44.8
remarks	lin. and quadr. effects orthogonal	lin. and quadr. effects orthogonal	lin. and quadr. effects orthogonal

Table 7.3i. Design characteristics.

Design number	8.37	8.38	8.39
Group	XI	XI	XI
Design	$3 \times 3 \times 3/15$ Box Behnken	$3 \times 3 \times 3 \times 3/27$ Box Behnken	$3 \times 3 \times 3 \times 3/15$ Rechtschaffner
<i>D</i> -efficiency	68.1	51.6	80.2
<i>P</i> : number of parameters in model	10	17	15
$\max(\sigma_{\hat{\beta}_p}^2 / \sigma^2)$	{ 0.125 0.067	{ 0.083 0.037	{ 0.139 0.104
$\max(\sigma_{\hat{\beta}_{pq}}^2 / \sigma^2)$	{ 0.250 0.071	{ 0.250 0.049	{ 0.139 0.085
$\max(\sigma_{\hat{\beta}_{pp}}^2 / \sigma^2)$	{ 0.271 0.067	{ 0.187 0.046	{ 0.886 0.141
$(\text{trace } (\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.227 0.068	{ 0.189 0.044	{ 0.364 0.104
$ \mathbf{r} $	0.984	0.691	0.025
trace (\mathbf{r}^{-1})	9.03	17.00	23.63
largest VIF	1.01	1.25	2.11
<i>V</i> : degrees of freedom for replication	2	-	-
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	1.394	2.410	2.552
largest (ρ)	0.077	0.333	0.350
<i>N</i> : number of experimental units	15	27	15
<i>G</i> -efficiency = $100 P/Nd$	47.8	26.1	39.2
remarks	lin. and int. terms orthogonal	lin. and int. terms orthogonal	-

Table 7.3j. (part 1) Design characteristics.

Design number	8.40	8.41	8.42
Group	XI	XI	XI
Design	$3 \times 3 \times 3 \times 3 \times 3/21$ Rechtschaffner	$3 \times 3 \times 3 \times 2/18$ A Webb design	$3 \times 3 \times 3 \times 3 \times 3/27$ Mitchell and Bayne
<i>D</i> -efficiency	88.6	86.0	95.2
<i>P</i> : number of parameters in model	21	14	21
$\max(\sigma_{\hat{\beta}_p}^2 / \sigma^2)$	{ 0.063 0.050	{ 0.094 0.063	0.051
$\max(\sigma_{\hat{\beta}_{pq}}^2 / \sigma^2)$	{ 0.063 0.041	{ 0.167 0.074	0.061
$\max(\sigma_{\hat{\beta}_{pp}}^2 / \sigma^2)$	{ 0.867 0.134	{ 0.260 0.058	0.348
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	{ 0.267 0.065	{ 0.164 0.063	0.153
$ \mathbf{r} $	0.025	0.444	0.358
trace (\mathbf{r}^{-1})	29.34	14.90	22.22
largest VIF	2.81	1.34	1.25
<i>V</i> : degrees of freedom for replication	-	-	-
$d = \max(\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}))$	1.906	1.964	1.18
largest (ρ)	0.225	0.334	0.281
<i>N</i> : number of experimental units	21	18	27
<i>G</i> -efficiency = $100 P/Nd$	52.5	39.6	65.9
remarks	clumpwise orthogonal	clumpwise orthogonal	

Table 7.3j. (part 2) Design characteristics.

Design number	8.1	8.2	8.3
Group	I	I	I
Design	$4 \times 2 \times 2/8$	$3 \times 2 \times 2/8$	$3 \times 2 \times 2/8$
$\sigma_{\hat{\beta}_0}^2$	0.320	0.250	0.750
$\sigma_{\hat{\beta}_1}^2$	0.281	0.500	0.250
$\sigma_{\hat{\beta}_2}^2$	0.156	0.250	0.188
$\sigma_{\hat{\beta}_3}^2$	0.156	0.250	0.188
$\sigma_{\hat{\beta}_{12}}^2$	0.281	0.500	0.313
$\sigma_{\hat{\beta}_{13}}^2$	0.281	0.500	0.313
$\sigma_{\hat{\beta}_{23}}^2$	0.156	0.250	0.250
$\sigma_{\hat{\beta}_{11}}^2$	0.633	0.500	1.250
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.283	0.375	0.438

Table 7.4a. Values of $\sigma_{\hat{\beta}}^2$ for $\sigma^2 = 1$.

Design number	8.5	8.6
Group	II	II
Design	$4 \times 4 \times 2/16$	$4 \times 3 \times 2/16$
$\sigma_{\beta_0}^2$	0.258	0.223
$\sigma_{\beta_1}^2$	0.113	0.113
$\sigma_{\beta_2}^2$	0.113	0.125
$\sigma_{\beta_3}^2$	0.063	0.063
$\sigma_{\beta_{12}}^2$	0.203	0.225
$\sigma_{\beta_{13}}^2$	0.113	0.113
$\sigma_{\beta_{23}}^2$	0.113	0.125
$\sigma_{\beta_{11}}^2$	0.316	0.316
$\sigma_{\beta_{22}}^2$	0.316	0.250
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.178	0.172

Table 7.4b. Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number	8.7	8.8	8.9	8.10
Group	III	III	III	III
Design	$4 \times 4 \times 4/16$	$4 \times 4 \times 3/16$	$4 \times 3 \times 3/16$	$3 \times 3 \times 3/16$
$\sigma_{\beta_0}^2$	0.526	0.500	0.461	0.413
$\sigma_{\beta_1}^2$	0.084	0.084	0.086	0.089
$\sigma_{\beta_2}^2$	0.084	0.087	0.091	0.089
$\sigma_{\beta_3}^2$	0.084	0.089	0.088	0.089
$\sigma_{\beta_{12}}^2$	0.118	0.118	0.115	0.120
$\sigma_{\beta_{13}}^2$	0.118	0.123	0.123	0.120
$\sigma_{\beta_{23}}^2$	0.118	0.116	0.120	0.120
$\sigma_{\beta_{11}}^2$	0.647	0.607	0.629	0.484
$\sigma_{\beta_{22}}^2$	0.647	0.678	0.511	0.484
$\sigma_{\beta_{33}}^2$	0.647	0.481	0.461	0.484
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.308	0.288	0.268	0.249

Table 7.4c. Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number Group Design	8.11 IV $4 \times 2 \times 2 \times 2/16$	8.12 IV $3 \times 2 \times 2 \times 2/16$
$\sigma^2_{\beta_0}$	0.160	0.125
$\sigma^2_{\beta_1}$	0.113	0.125
$\sigma^2_{\beta_2}$	0.063	0.063
$\sigma^2_{\beta_3}$	0.063	0.063
$\sigma^2_{\beta_4}$	0.063	0.063
$\sigma^2_{\beta_{12}}$	0.113	0.125
$\sigma^2_{\beta_{13}}$	0.113	0.125
$\sigma^2_{\beta_{14}}$	0.113	0.125
$\sigma^2_{\beta_{23}}$	0.063	0.063
$\sigma^2_{\beta_{24}}$	0.063	0.063
$\sigma^2_{\beta_{34}}$	0.063	0.063
$\sigma^2_{\beta_{11}}$	0.316	0.250
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.108	0.104

Table 7.4d. Values of σ^2_{β} for $\sigma^2 = 1$.

Design number Group Design	8.13a V $4 \times 4 \times 2 \times 2/16$	8.14a V $4 \times 3 \times 2 \times 2/16$	8.15a V $3 \times 3 \times 2 \times 2/16$	8.13b V $4 \times 4 \times 2 \times 2/16$	8.14b V $4 \times 3 \times 2 \times 2/16$	8.15b V $3 \times 3 \times 2 \times 2/16$
$\sigma^2_{\beta_0}$	0.258	0.223	0.188	0.828	0.727	0.625
$\sigma^2_{\beta_1}$	0.139	0.135	0.188	0.089	0.088	0.104
$\sigma^2_{\beta_2}$	0.139	0.150	0.188	0.089	0.108	0.104
$\sigma^2_{\beta_3}$	0.063	0.063	0.063	0.063	0.064	0.063
$\sigma^2_{\beta_4}$	0.077	0.075	0.094	0.125	0.125	0.125
$\sigma^2_{\beta_{12}}$	0.298	0.450	0.500	0.141	0.180	0.250
$\sigma^2_{\beta_{13}}$	0.139	0.203	0.188	0.100	0.132	0.167
$\sigma^2_{\beta_{14}}$	0.165	0.225	0.250	0.109	0.124	0.188
$\sigma^2_{\beta_{23}}$	0.139	0.225	0.188	0.100	0.119	0.167
$\sigma^2_{\beta_{24}}$	0.165	0.250	0.250	0.109	0.153	0.188
$\sigma^2_{\beta_{34}}$	0.077	0.113	0.094	0.078	0.094	0.125
$\sigma^2_{\beta_{11}}$	0.316	0.316	0.250	0.633	0.633	0.500
$\sigma^2_{\beta_{22}}$	0.316	0.250	0.250	0.633	0.500	0.500
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.176	0.206	0.207	0.238	0.234	0.239

Table 7.4e. Values of σ^2_{β} for $\sigma^2 = 1$.

Design number	8.16	8.17	8.18	8.19
Group	VI	VI	VI	VI
Design	$4 \times 4 \times 4 \times 2/16$	$4 \times 4 \times 3 \times 2/16$	$4 \times 3 \times 3 \times 2/16$	$3 \times 3 \times 3 \times 2/16$
$\sigma_{\beta_0}^2$	0.986	0.881	0.790	0.724
$\sigma_{\beta_1}^2$	0.110	0.109	0.109	0.108
$\sigma_{\beta_2}^2$	0.081	0.083	0.092	0.092
$\sigma_{\beta_3}^2$	0.089	0.102	0.106	0.110
$\sigma_{\beta_4}^2$	0.076	0.080	0.083	0.086
$\sigma_{\beta_{12}}^2$	0.110	0.108	0.109	0.108
$\sigma_{\beta_{13}}^2$	0.124	0.131	0.132	0.149
$\sigma_{\beta_{14}}^2$	0.097	0.101	0.102	0.113
$\sigma_{\beta_{23}}^2$	0.120	0.132	0.146	0.144
$\sigma_{\beta_{24}}^2$	0.094	0.097	0.112	0.110
$\sigma_{\beta_{34}}^2$	0.103	0.106	0.114	0.120
$\sigma_{\beta_{11}}^2$	0.493	0.514	0.523	0.410
$\sigma_{\beta_{22}}^2$	0.738	0.746	0.554	0.525
$\sigma_{\beta_{33}}^2$	0.500	0.368	0.386	0.397
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.266	0.254	0.240	0.228

Table 7.4f. Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number	8.20	8.21	8.22	8.23	8.24
Group	VII	VII	VII	VII	VII
Design	$4 \times 4 \times 4 \times 4/16$	$4 \times 4 \times 4 \times 3/16$	$4 \times 4 \times 3 \times 3/16$	$4 \times 3 \times 3 \times 3/16$	$3 \times 3 \times 3 \times 3/16$
$\sigma_{\beta_0}^2$	1.586	1.465	1.338	1.249	1.257
$\sigma_{\beta_1}^2$	0.144	0.136	0.136	0.142	0.140
$\sigma_{\beta_2}^2$	0.087	0.085	0.088	0.097	0.094
$\sigma_{\beta_3}^2$	0.095	0.092	0.101	0.103	0.109
$\sigma_{\beta_4}^2$	0.092	0.091	0.095	0.100	0.105
$\sigma_{\beta_{12}}^2$	0.113	0.110	0.109	0.112	0.110
$\sigma_{\beta_{13}}^2$	0.127	0.127	0.133	0.133	0.160
$\sigma_{\beta_{14}}^2$	0.120	0.116	0.118	0.123	0.133
$\sigma_{\beta_{23}}^2$	0.112	0.113	0.122	0.132	0.131
$\sigma_{\beta_{24}}^2$	0.108	0.106	0.109	0.124	0.118
$\sigma_{\beta_{34}}^2$	0.126	0.132	0.138	0.143	0.158
$\sigma_{\beta_{11}}^2$	0.545	0.548	0.575	0.588	0.461
$\sigma_{\beta_{22}}^2$	0.708	0.714	0.714	0.532	0.507
$\sigma_{\beta_{33}}^2$	0.526	0.522	0.395	0.413	0.422
$\sigma_{\beta_{44}}^2$	0.836	0.652	0.634	0.634	0.661
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.355	0.334	0.320	0.308	0.304

Table 7.4g. Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number	8.25	8.26	8.27
Group	VIII	VIII	VIII
Design	$4 \times 4 \times 4 \times 4 \times 4/32$	$4 \times 4 \times 4 \times 4 \times 3/32$	$4 \times 4 \times 4 \times 3 \times 3/32$
$\sigma_{\beta_0}^2$	0.579	0.564	0.541
$\sigma_{\beta_1}^2$	0.046	0.046	0.046
$\sigma_{\beta_2}^2$	0.042	0.042	0.042
$\sigma_{\beta_3}^2$	0.047	0.047	0.047
$\sigma_{\beta_4}^2$	0.040	0.040	0.042
$\sigma_{\beta_5}^2$	0.040	0.043	0.043
$\sigma_{\beta_{12}}^2$	0.049	0.049	0.049
$\sigma_{\beta_{13}}^2$	0.050	0.051	0.051
$\sigma_{\beta_{14}}^2$	0.051	0.051	0.051
$\sigma_{\beta_{15}}^2$	0.048	0.050	0.050
$\sigma_{\beta_{23}}^2$	0.054	0.054	0.054
$\sigma_{\beta_{24}}^2$	0.054	0.054	0.054
$\sigma_{\beta_{25}}^2$	0.052	0.053	0.053
$\sigma_{\beta_{34}}^2$	0.051	0.051	0.053
$\sigma_{\beta_{35}}^2$	0.050	0.050	0.051
$\sigma_{\beta_{45}}^2$	0.052	0.053	0.053
$\sigma_{\beta_{11}}^2$	0.428	0.428	0.419
$\sigma_{\beta_{22}}^2$	0.372	0.377	0.373
$\sigma_{\beta_{33}}^2$	0.386	0.377	0.372
$\sigma_{\beta_{44}}^2$	0.389	0.388	0.297
$\sigma_{\beta_{55}}^2$	0.430	0.337	0.336
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.158	0.153	0.147

Table 7.4h. (part 1) Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number	8.28	8.29	8.30
Group	VIII	VIII	VIII
Design	$4 \times 4 \times 3 \times 3 \times 3/32$	$4 \times 3 \times 3 \times 3 \times 3/32$	$3 \times 3 \times 3 \times 3 \times 3/32$
$\sigma^2_{\beta_0}$	0.511	0.484	0.453
$\sigma^2_{\beta_1}$	0.046	0.046	0.048
$\sigma^2_{\beta_2}$	0.042	0.044	0.045
$\sigma^2_{\beta_3}$	0.048	0.048	0.048
$\sigma^2_{\beta_4}$	0.043	0.042	0.042
$\sigma^2_{\beta_5}$	0.043	0.043	0.044
$\sigma^2_{\beta_{12}}$	0.049	0.051	0.052
$\sigma^2_{\beta_{13}}$	0.050	0.051	0.051
$\sigma^2_{\beta_{14}}$	0.051	0.051	0.054
$\sigma^2_{\beta_{15}}$	0.050	0.051	0.052
$\sigma^2_{\beta_{23}}$	0.054	0.050	0.053
$\sigma^2_{\beta_{24}}$	0.054	0.053	0.054
$\sigma^2_{\beta_{25}}$	0.053	0.054	0.054
$\sigma^2_{\beta_{34}}$	0.053	0.054	0.053
$\sigma^2_{\beta_{35}}$	0.053	0.053	0.053
$\sigma^2_{\beta_{45}}$	0.053	0.053	0.053
$\sigma^2_{\beta_{11}}$	0.419	0.416	0.326
$\sigma^2_{\beta_{22}}$	0.374	0.291	0.293
$\sigma^2_{\beta_{33}}$	0.291	0.293	0.291
$\sigma^2_{\beta_{44}}$	0.304	0.297	0.292
$\sigma^2_{\beta_{55}}$	0.324	0.310	0.316
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.141	0.135	0.130

Table 7.4h. (part 2) Values of σ^2_{β} for $\sigma^2 = 1$.

Design number	8.31	8.32	8.33
Group	IX	IX	IX
Design	$3 \times 3 \times 3 \times 2/18$	$3 \times 3 \times 2 \times 2/18$	$3 \times 2 \times 2 \times 2/18$
$\sigma_{\beta_0}^2$	0.417	0.368	0.224
$\sigma_{\beta_1}^2$	0.083	0.099	0.107
$\sigma_{\beta_2}^2$	0.083	0.104	0.078
$\sigma_{\beta_3}^2$	0.083	0.063	0.078
$\sigma_{\beta_4}^2$	0.056	0.064	0.075
$\sigma_{\beta_{12}}^2$	0.238	0.189	0.179
$\sigma_{\beta_{13}}^2$	0.238	0.142	0.179
$\sigma_{\beta_{14}}^2$	0.146	0.104	0.146
$\sigma_{\beta_{23}}^2$	0.250	0.188	0.141
$\sigma_{\beta_{24}}^2$	0.143	0.099	0.107
$\sigma_{\beta_{34}}^2$	0.143	0.074	0.107
$\sigma_{\beta_{11}}^2$	0.313	0.437	0.313
$\sigma_{\beta_{22}}^2$	0.250	0.250	
$\sigma_{\beta_{33}}^2$	0.250		
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.192	0.168	0.144

Table 7.4i. Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number	8.34	8.35	8.36
Group	X	X	X
Design	$3 \times 3 \times 3 \times 3/27$	$3 \times 3 \times 3 \times 2/27$	$3 \times 3 \times 2 \times 2/27$
$\sigma_{\beta_0}^2$	0.333	0.264	0.195
$\sigma_{\beta_1}^2$	0.056	0.064	0.070
$\sigma_{\beta_2}^2$	0.056	0.064	0.070
$\sigma_{\beta_3}^2$	0.056	0.064	0.047
$\sigma_{\beta_4}^2$	0.056	0.042	0.047
$\sigma_{\beta_{12}}^2$	0.089	0.103	0.089
$\sigma_{\beta_{13}}^2$	0.089	0.103	0.067
$\sigma_{\beta_{14}}^2$	0.089	0.077	0.067
$\sigma_{\beta_{23}}^2$	0.089	0.103	0.067
$\sigma_{\beta_{24}}^2$	0.089	0.077	0.067
$\sigma_{\beta_{34}}^2$	0.089	0.077	0.050
$\sigma_{\beta_{11}}^2$	0.167	0.167	0.167
$\sigma_{\beta_{22}}^2$	0.167	0.167	0.167
$\sigma_{\beta_{33}}^2$	0.167	0.167	
$\sigma_{\beta_{44}}^2$	0.167		
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.117	0.110	0.090

Table 7.4j. Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number Group Design	8.37 XI $3 \times 3 \times 3/15$ Box Behnken	8.38 XI $3 \times 3 \times 3 \times 3/27$ Box Behnken	8.39 XI $3 \times 3 \times 3 \times 3/15$ Rechtschaffner
$\sigma_{\beta_0}^2$	0.333	0.407	0.529
$\sigma_{\beta_1}^2$	0.125	0.083	0.139
$\sigma_{\beta_2}^2$	0.125	0.083	0.139
$\sigma_{\beta_3}^2$	0.125	0.083	0.139
$\sigma_{\beta_4}^2$		0.083	0.139
$\sigma_{\beta_5}^2$			
$\sigma_{\beta_{12}}^2$	0.250	0.250	0.139
$\sigma_{\beta_{13}}^2$	0.250	0.250	0.139
$\sigma_{\beta_{14}}^2$		0.250	0.139
$\sigma_{\beta_{15}}^2$			
$\sigma_{\beta_{23}}^2$	0.250	0.250	0.139
$\sigma_{\beta_{24}}^2$		0.250	0.139
$\sigma_{\beta_{25}}^2$			
$\sigma_{\beta_{34}}^2$		0.250	0.139
$\sigma_{\beta_{35}}^2$			
$\sigma_{\beta_{45}}^2$			
$\sigma_{\beta_{11}}^2$	0.271	0.187	0.886
$\sigma_{\beta_{22}}^2$	0.271	0.187	0.886
$\sigma_{\beta_{33}}^2$	0.271	0.188	0.886
$\sigma_{\beta_{44}}^2$		0.187	0.886
$\sigma_{\beta_{55}}^2$			
$(\text{tr}(X'X)^{-1})/P$	0.227	0.189	0.364

Table 7.4k. (part 1) Values of σ_{β}^2 for $\sigma^2 = 1$.

Design number Group Design	8.40 XI $3 \times 3 \times 3 \times 3 \times 3/21$ Rechtschaffner	8.41 XI $3 \times 3 \times 3 \times 2/18$ A Webb design	8.42 XI $3 \times 3 \times 3 \times 3 \times 3/27$ Mitchell and Bayne
$\sigma^2_{\beta_0}$	0.336	0.399	0.788
$\sigma^2_{\beta_1}$	0.063	0.094	0.048
$\sigma^2_{\beta_2}$	0.062	0.094	0.049
$\sigma^2_{\beta_3}$	0.063	0.094	0.048
$\sigma^2_{\beta_4}$	0.062	0.056	0.050
$\sigma^2_{\beta_5}$	0.063		0.051
$\sigma^2_{\beta_{12}}$	0.063	0.167	0.055
$\sigma^2_{\beta_{13}}$	0.063	0.167	0.054
$\sigma^2_{\beta_{14}}$	0.063	0.094	0.058
$\sigma^2_{\beta_{15}}$	0.063		0.058
$\sigma^2_{\beta_{23}}$	0.063	0.167	0.055
$\sigma^2_{\beta_{24}}$	0.063	0.094	0.055
$\sigma^2_{\beta_{26}}$	0.063		0.055
$\sigma^2_{\beta_{34}}$	0.063	0.094	0.061
$\sigma^2_{\beta_{35}}$	0.063		0.055
$\sigma^2_{\beta_{45}}$	0.063		0.055
$\sigma^2_{\beta_{11}}$	0.867	0.260	0.348
$\sigma^2_{\beta_{22}}$	0.867	0.260	0.307
$\sigma^2_{\beta_{33}}$	0.867	0.260	0.339
$\sigma^2_{\beta_{44}}$	0.867		0.282
$\sigma^2_{\beta_{55}}$	0.867		0.340
$(\text{tr}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.267	0.164	0.153

Table 7.4k. (part 2) Values of σ^2_{β} for $\sigma^2 = 1$.

Design nr.	Design	<i>G</i> -eff.	<i>D</i> -eff.	Remarks
8.1	$4 \times 2 \times 2/8$	47.1*	82.4	clumpw. orth.
8.2	$3 \times 2 \times 2/8$	25.0*	68.4	clumpw. orth.
8.3	$3 \times 2 \times 2/8$	25.0*	81.3	clumpw. orth.
8.4	$3 \times 2 \times 2/8$			identical with 8.2
8.5	$4 \times 4 \times 2/16$	62.3*	82.0	orth. design
8.6	$4 \times 3 \times 2/16$	59.0*	81.3	orth. design
8.7	$4 \times 4 \times 4/16$	57.7	87.8	clumpw. orth.
8.8	$4 \times 4 \times 3/16$	55.3	89.2	clumpw. orth.
8.9	$4 \times 3 \times 3/16$	57.3	90.9	clumpw. orth.
8.10	$3 \times 3 \times 3/16$	61.2	92.6	clumpw. orth.
8.11	$4 \times 2 \times 2 \times 2/16$	78.9*	90.1	orth. design
8.12	$3 \times 2 \times 2 \times 2/16$	75.0*	88.6	orth. design
8.13a	$4 \times 4 \times 2 \times 2/16$	32.2	75.2	clumpw. orth.
8.14a	$4 \times 3 \times 2 \times 2/16$	22.1	69.0	clumpw. orth.
8.15a	$3 \times 3 \times 2 \times 2/16$	20.3	68.1	clumpw. orth.
8.13b	$4 \times 4 \times 2 \times 2/16$	57.6	84.6	clumpw. orth.
8.14b	$4 \times 3 \times 2 \times 2/16$	41.6	81.1	clumpw. orth.
8.15b	$3 \times 3 \times 2 \times 2/16$	34.5	76.4	clumpw. orth.
8.16	$4 \times 4 \times 4 \times 2/16$	47.0	87.5	
8.17	$4 \times 4 \times 3 \times 2/16$	44.9	87.2	
8.18	$4 \times 3 \times 3 \times 2/16$	38.5	86.8	
8.19	$3 \times 3 \times 3 \times 2/16$	39.3	87.2	
8.20	$4 \times 4 \times 4 \times 4/16$	38.3	84.9	
8.21	$4 \times 4 \times 4 \times 3/16$	42.7	86.2	
8.22	$4 \times 4 \times 3 \times 3/16$	45.8	86.0	
8.23	$4 \times 3 \times 3 \times 3/16$	45.8	85.8	
8.24	$3 \times 3 \times 3 \times 3/16$	42.1	85.8	
8.25	$4 \times 4 \times 4 \times 4/32$	55.7	87.8	

Table 7.5. (part 1) *D*- and *G*-efficiencies of 45 designs.

*) Exact value of the *G*-efficiency.

Design nr.	Design	<i>G</i> -eff.	<i>D</i> -eff.	Remarks
8.26	$4 \times 4 \times 4 \times 4 \times 3/32$	54.8	88.1	
8.27	$4 \times 4 \times 4 \times 3 \times 3/32$	55.8	88.8	
8.28	$4 \times 4 \times 3 \times 3 \times 3/32$	55.5	89.4	
8.29	$4 \times 3 \times 3 \times 3 \times 3/32$	56.4	90.1	
8.30	$3 \times 3 \times 3 \times 3 \times 3/32$	58.8	90.4	
8.31	$3 \times 3 \times 3 \times 2/18$	26.9	80.1	lin. eff. orth.
8.32	$3 \times 3 \times 2 \times 2/18$	28.1	82.1	lin. eff. orth.
8.33	$3 \times 2 \times 2 \times 2/18$	28.9	76.8	lin. eff. orth.
8.34	$3 \times 3 \times 3 \times 3/27$	55.6*	87.8	lin. + quadr. eff. orth.
8.35	$3 \times 3 \times 3 \times 2/27$	39.2*	84.3	lin. + quadr. eff. orth.
8.36	$3 \times 3 \times 2 \times 2/27$	44.8*	85.8	lin. + quadr. eff. orth.
8.37	$3 \times 3 \times 3/15$ Box Behnken	47.8*	68.1	lin. + interact. terms orth.
8.38	$3 \times 3 \times 3 \times 3/27$ Box Behnken	26.1*	51.6	lin. + interact. terms orth.
8.39	$3 \times 3 \times 3 \times 3/15$ saturated design	39.2	80.2	
8.40	$3 \times 3 \times 3 \times 3 \times 3/21$ saturated design	52.5	88.6	clumpwise orthogonal
8.41	$3 \times 3 \times 3 \times 2/18$ Webb design	39.6	86.0	clumpwise orthogonal
8.42	$3 \times 3 \times 3 \times 3 \times 3/27$ Mitchell and Bayne	65.9	95.2	

Table 7.5. (part 2) *D*- and *G*-efficiencies of 45 designs.

*) Exact value of the *G*-efficiency.

7.4. Judging the designs

7.4.1. Group I. Designs 8.1, 8.2, 8.3 and 8.4 of Table 7.3a

Design 8.1 has, given the limited number of points, excellent qualities. The value of $|\mathbf{r}|$ is rather large, the VIF's are small.

We also refer to Section 4.2, where design 8.1 has been discussed in detail.

The nature of the clumpwise orthogonality can be evaluated with the matrix \mathbf{XTXI} of design 8.1 of the Appendix.

Design 8.2 and 8.3 have both been derived from 8.1 through collapsing.

We see that collapsing produces an increase in $\sigma_{\hat{\beta}}^2$, average $\sigma_{\hat{\beta}}^2$, $\text{trace}(\mathbf{r}^{-1})$, largest VIF and the largest $|\rho|$. See also Table 7.4a. A decrease is found in $|\mathbf{r}|$.

All these characteristics indicate that collapsing reduces the design quality, although designs 8.2 and 8.3 are still acceptable since their characteristics have reasonable values.

Although we used design 8.2 in Section 4.7 we see that design 8.3 has some advantages over design 8.2 because $\text{trace}(\mathbf{r}^{-1})$ and largest $|\rho|$ are smaller, whereas $|\mathbf{r}|$ and the D -efficiency is larger than the same values of design 8.2, although $\max(\sigma_{\hat{\beta}_{pp}}^2/\sigma^2)$ of design 8.3 is the largest.

We tried to find a $3 \times 2 \times 2/8$ design with a higher D -efficiency using the method given in Section 5.7 but we were not successful; we either found smaller D -efficiencies or we had a singular $\mathbf{X}'\mathbf{X}$ matrix. For further details of the designs we refer to the Appendix.

It is again pointed out that \mathbf{r} , \mathbf{r}^{-1} , VIF's and d are independent of the scaling of the X_p .

7.4.2. Group II and group IV. Designs 8.5, 8.6, 8.11 and 8.12

The design characteristics of the designs mentioned above can be found in Tables 7.3b and 7.3c.

We treat these four designs as one group since they are all orthogonal. Details of each design can be found in the Appendix.

We have $\det(\mathbf{X}'\mathbf{X}) = N^P$ because of orthogonality.

All variances of $\hat{\beta}$ are equal to $\sigma^2/N = \sigma^2/16 = 0.063\sigma^2$, if the scaling $\sum_{i=1}^N X_{pi}^2 = N$ is used. Because we choose the collapsing procedure as in Table 5.5, the designs 8.6 and 8.12 are orthogonal. The variances of $\hat{\beta}$ in Tables 7.4b and 7.4d show that collapsing has hardly an effect on these values. For the designs considered we have

$$|\mathbf{r}| = 1, \text{trace}(\mathbf{r}^{-1}) = P - 1, \text{VIF} = 1, \text{largest } |\rho| = 0 .$$

These are the best possible values thanks to the orthogonality of the designs.

The 4 designs considered have reasonable D - and G - efficiencies.

7.4.3. Group III. Designs 8.7, 8.8, 8.9 and 8.10 of Table 7.3b

The four designs have an excellent quality with high D -efficiencies and satisfactory G -efficiencies. The excellent quality is also evident since, $\text{trace}(\mathbf{r}^{-1})$, largest VIF, d and largest $|\rho|$ have small values, whereas $|\mathbf{r}|$ is fairly large. It is also striking that collapsing has a favourable effect since the values mentioned above show an increase in D -efficiency, G -efficiency, $|\mathbf{r}|$ and a decrease in $\text{trace}(\mathbf{r}^{-1})$, largest VIF and d , when comparing design 8.7 with design 8.10.

The explanation is that (8.10) is 'closer' to the D -optimal $3 \times 3 \times 3$ design, since (8.10) has only factors with 3 levels, whereas (8.7), (8.8) and (8.9) have at least one factor with four levels.

It is also interesting to have a look at Table 7.4c. We see that collapsing hardly affects $\sigma_{\hat{\beta}_p}^2$ and $\sigma_{\hat{\beta}_{pq}}^2$ but decreases $\sigma_{\hat{\beta}_0}^2$ and $\sigma_{\hat{\beta}_{pp}}^2$.

The nature of the clumpwise orthogonality is evident from the relevant $(\mathbf{X}'\mathbf{X})^{-1}$ matrices in the Appendix. We see that the linear effects are orthogonal to all others.

7.4.4. Group V. Designs 8.13a, 8.14a, 8.15a, 8.13b, 8.14b, 8.15b of Table 7.3d

This group of designs contains two subgroups. The a -group was obtained using the design generators and collapsing.

The b -group was obtained using properties of the D -optimal $3 \times 3 \times 2 \times 2$ design. See also Section 5.7.

It is hardly possible to establish which group of designs is the best.

Although the b -group has a better D - and G -efficiency than the a -group, we see that the a -group has better values as regards $|\mathbf{r}|$, $\text{trace}(\mathbf{r}^{-1})$, largest VIF, largest $|\rho|$, and $(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$.

Table 7.4e reveals why the latter value is smallest for the a -group. It is because $\sigma_{\hat{\beta}_0}^2$ and $\sigma_{\hat{\beta}_{pp}}^2$ are for the a -group considerably smaller than for the b -group.

The comparison of the *a*-group and *b*-group clearly reveals that it is not sufficient to compare designs using only the *D*- and *G*-efficiency.

Other design characteristics especially those giving measures of non orthogonality such as $|\mathbf{r}|$, $\text{trace}(\mathbf{r}^{-1})$ and the largest VIF must also be taken into account.

Both groups of designs have clumpwise orthogonality. The nature of it can be judged by considering the $(\mathbf{X}'\mathbf{X})^{-1}$ matrices of the relevant designs in the Appendix.

7.4.5. Group VI. Designs 8.16, 8.17, 8.18 and 8.19 of Table 7.3e

Inspection of Table 7.3e shows that this group of designs has acceptable characteristics such as a high *D*-efficiency, small VIF's and small values for the largest $|\rho|$.

Collapsing has in this case a negligible effect on the design quality, although design 8.16 appears to have slightly better characteristics than the three others especially since it has a better *G*-efficiency.

Table 7.4f shows that collapsing decreases $(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$. This decrease is caused by the decrease in $\sigma_{\hat{\beta}_0}^2$ and $\sigma_{\hat{\beta}_{pp}}^2$ through collapsing. The decrease in $\sigma_{\hat{\beta}_{pp}}^2$ is understandable since a parameter β_{pp} is more accurately estimated, if three instead of four levels are used in the range -1 to $+1$.

7.4.6. Group VII. Designs 8.20, ..., 8.24 of Table 7.3f

We again see the same pattern as in group VI, namely a high *D*-efficiency, small VIF's and small values for the largest $|\rho|$.

We also see, as in group VI a decrease in $(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$ through collapsing.

Table 7.4g clearly shows that this decrease is caused by a decrease of $\sigma_{\hat{\beta}_0}^2$ and $\sigma_{\hat{\beta}_{pp}}^2$.

7.4.7. Group VIII. Designs 8.25, ..., 8.30 of Table 7.3g

This group of designs has excellent properties with good values for *D*- and *G*-efficiency, small VIF's and small values for the largest $|\rho|$.

We again see a slight decrease in $(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$, also caused by a decrease in $\sigma_{\hat{\beta}_0}^2$ and $\sigma_{\hat{\beta}_{pp}}^2$ through collapsing, as Table 7.4h clearly shows.

7.4.8. Group IX. Designs 8.31, 8.32 and 8.33 of Table 7.3h

It is striking that the effects of collapsing are negligible. Comparing the three designs we see that 8.32 appears to be better than 8.31 since $(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$ has decreased and so has $\text{trace}(\mathbf{r}^{-1})$ even allowing for the fact that P for 8.32 is one less than for 8.31. The largest $|\rho|$ value has not changed and $|\mathbf{r}|$ of 8.32 is larger than $|\mathbf{r}|$ of 8.31.

Design 8.32 also has the best D -efficiency. The only negative point of design 8.32 is that $\max(\sigma_{\hat{\beta}_{pp}}^2 / \sigma^2)$ has increased.

Comparing 8.31 with 8.33 we see that these designs are of equal quality since most of the characteristics have the same value. Even the $\text{trace}(\mathbf{r}^{-1})$ values are equivalent because their difference equals the difference in P of the designs 8.31 and 8.33.

The fact that collapsing had hardly an effect can be explained. Collapsing was namely carried out on the factors Q and U of design 8.31.

When we examine the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix of design 8.31 in the Appendix, we see that the linear and quadratic effects of Q and U are orthogonally estimated and that the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix contains many zero's.

In Table 6.6 we see that the linear effect of a collapsed two-level factor equals minus the quadratic effect of the original three-level factor.

The linear effect of the collapsed two-level factor will therefore remain orthogonal to all other effects. Only parts of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix corresponding to cross-product terms, especially cross-product terms containing the collapsed factor, will change. Summarizing we may state that the designs 8.31, 8.32 and 8.33 have a good structure since many of their characteristics have acceptable values.

For instance the $\sigma_{\hat{\beta}}^2$ values are small and $|\mathbf{r}|$ is rather large for the three designs, because all linear effects are orthogonally estimated. It is also interesting to have a look at Table 7.4i. It is difficult to find a pattern. Some variances increase, others decrease through collapsing.

7.4.9. Group X. Designs 8.34, 8.35 and 8.36 of Table 7.3i

Again we find that collapsing has a very small effect.

Design 8.35 has slightly less quality than design 8.34. This is obvious when we compare the various characteristic values. Comparing 8.34 with 8.36, we see that they are of the same quality since nearly all their characteristics have the same value. Collapsing has again a small

effect because all the linear and quadratic effects of design 8.34 are orthogonally estimated. This property is not affected by collapsing. See also Section 7.4.8. The designs have an excellent quality since $\sigma_{\hat{\beta}}^2$, VIF's and $|\rho|$ have a small, whereas $|\mathbf{r}|$ has a large value. The D - and G -efficiency have acceptable values. Inspection of Table 7.4j reveals that nearly all $\sigma_{\hat{\beta}_{pq}}$ values decrease when we compare design (8.36) with (8.34).

7.4.10. Group XI. Miscellaneous designs 8.37, . . . , 8.42 of Table 7.3j

Although the orthogonal polynomials were, except for design 8.42, constructed in such a way that $\sum_{i=1}^N Pl_i^2 = \sum_{i=1}^N Pq_i^2 = N$, we do not, for all p , have $\sum_{i=1}^N X_{ip}^2 = N$ for designs 8.37–8.40 since these designs were not derived from orthogonal main-effect designs.

Designs 8.37 and 8.38 have a good quality because their design characteristics have excellent values i.e. a high value of $|\mathbf{r}|$, the $\text{trace}(\mathbf{r}^{-1})$ is very close to its minimum value $P - 1$, small VIF's and small values of $|\rho|$. However the D -efficiency is small since designs 8.37 and 8.38 were designed for spherical experimental regions while the D -efficiency was calculated for a hypercube. The linear and interaction effects are orthogonally estimated.

Design 8.38 contains a fifth factor, namely blocks. It is indicated by the variable x_t ; in design 8.38. This variable has the value 0 for experimental units 1, 2, . . . , 9, a value 1 for units 10, 11, . . . , 18 and a value 2 for units 19, 20, . . . , 27. It is surprising that no orthogonal polynomials were used in *Box and Behnken* (1960). As a result the estimate of $\hat{\beta}_0$ was correlated with the estimates $\hat{\beta}_{pp}$.

We have avoided this correlation since the $\hat{\beta}_{pp}$ are only mutually correlated and not correlated with $\hat{\beta}_0$, $\hat{\beta}_p$ and $\hat{\beta}_{pq}$, as the matrices \mathbf{XTXI} of design 8.37 and 8.38 clearly show.

Designs 8.39 and 8.40 appear to have acceptable properties because their VIF's and largest $|\rho|$ are rather small. The qualities of design 8.39 are less evident when we compare it with design 8.24, a $3 \times 3 \times 3 \times 3/16$ design.

Design 8.40 is of a lesser quality than design 8.30, a $3 \times 3 \times 3 \times 3 \times 3/32$ design, especially since $|\mathbf{r}|$ and $\text{trace}(\mathbf{r}^{-1})$ of 8.30 have much better values. Further discussion of designs 8.39 and 8.40 will be done in the next section.

Design 8.41 has good properties, such as small VIF's, $\text{trace}(\mathbf{r}^{-1})$ and $|\rho|$. The only objection to this design is the fact that a particular $\hat{\beta}$ is correlated with all other $\hat{\beta}$'s with the exception of $\hat{\beta}_0$ and $\hat{\beta}_4$.

Design 8.41 will be compared to design 8.31, also a $3 \times 3 \times 3 \times 2/18$ design, in the next section. Design 8.42, constructed by *Mitchell and Bayne* (1978), has excellent properties. It will be compared with design 8.30 and 8.40 in the next section.

7.5. Comparison between groups of designs

The designs of group I are a class by themselves because they are small designs, since they only consist of 8 experimental units.

Since all other designs considered have at least 15 experimental units, it serves no purpose to compare the designs of group I with the designs of other groups.

The groups II, III, . . . , VII all consist of designs with 16 experimental units.

We shall compare these groups by considering the “leading” design in each group. The word “leading” is used because it refers to the first design in each group, from which all the other designs in a group have been derived through collapsing.

The design characteristics of these leading designs have been given in Tables 7.5a and 7.5b.

All variances in these tables are based on the scale $-1 \leq x_m \leq +1$, for $m = 1, 2, \dots, k$.

When we examine these tables we see that the 6 groups consist of two categories, namely

Category 1 with three factors: Group II, III

and

Category 2 with four factors: Group IV, V, VI, VII.

The first design in each category is orthogonal and the design characteristics therefore have excellent values.

Looking at the designs of Table 7.5 we see that the design quality decreases somewhat when we go from group II to group III, although the D -efficiency design of 8.7 is higher than the D -efficiency of design 8.5.

Design number	8.5	8.7	8.11
Group	II	III	IV
Design	$4 \times 4 \times 2/16$	$4 \times 4 \times 4/16$	$4 \times 2 \times 2 \times 2/16$
<i>D</i> -efficiency	82.0	87.8	90.1
<i>P</i> : number of parameters in model	9	10	12
$\max(\sigma_{\hat{\beta}_p}^2 / \sigma^2)$	0.113	0.084	0.113
$\max(\sigma_{\hat{\beta}_{pq}}^2 / \sigma^2)$	0.203	0.118	0.113
$\max(\sigma_{\hat{\beta}_{pp}}^2 / \sigma^2)$	0.316	0.647	0.316
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.178	0.308	0.108
$ \mathbf{r} $	1.000	0.387	1.000
$\text{trace}(\mathbf{r}^{-1})$	8.00	11.40	11.00
largest VIF	1.00	1.53	1.00
<i>v</i> : degrees of freedom for replication	–	–	–
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	0.902	1.084	0.950
largest $ \rho $	0	0.339	0
<i>N</i> : number of experimental units	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	62.3	57.7	78.9
remarks	orth. design	clumpw. orth.	orth. design

Table 7.5a. Design characteristics of “leading” designs with 16 experimental units.

Design number	8.13a	8.13b	8.16	8.20
Group	V	V	VI	VII
Design	$4 \times 4 \times 2 \times 2/16$	$4 \times 4 \times 2 \times 2/16$	$4 \times 4 \times 4 \times 2/16$	$4 \times 4 \times 4 \times 4/16$
<i>D</i> -efficiency	75.2	84.6	87.5	84.9
<i>P</i> : number of parameters in model	13	13	14	15
$\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$	0.139	0.125	0.110	0.144
$\max(\sigma_{\hat{\beta}_{pq}}^2/\sigma^2)$	0.298	0.141	0.124	0.127
$\max(\sigma_{\hat{\beta}_{pp}}^2/\sigma^2)$	0.316	0.633	0.738	0.836
$(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$	0.176	0.238	0.266	0.355
$ \mathbf{r} $	0.314	0.192	0.301	0.193
$\text{trace}(\mathbf{r}^{-1})$	14.82	15.95	15.77	18.13
largest VIF	1.47	2.00	1.42	1.76
<i>v</i> : degrees of freedom for replication	-	-	-	-
$d = \max(\mathbf{f}'(\mathbf{x}) (\mathbf{X}'\mathbf{X})^{-1} \mathbf{f}(\mathbf{x}))$	2.527	1.411	1.862	2.451
largest $ \rho $	0.436	0.500	0.445	0.385
<i>N</i> : number of experimental units	16	16	16	16
<i>G</i> -efficiency = $100 P/Nd$	32.2	57.6	47.0	38.3
remarks	clumpw. orth.	clumpw. orth.		

Table 7.5b. Design characteristics of "leading" designs with 16 experimental units.

It is striking that in each category we see a more or less stable value of $\max(\sigma_{\hat{\beta}_p}^2/\sigma^2)$, a decrease in $\max(\sigma_{\hat{\beta}_{pq}}^2/\sigma^2)$ and an increase in $\max(\sigma_{\hat{\beta}_{pp}}^2/\sigma^2)$. The value of $(\text{trace}(\mathbf{X}'\mathbf{X})^{-1})/P$ increases within each category.

We see that $|\mathbf{r}|$ decreases within category 1 and fluctuates in category 2.

In each category we find increases of $\text{trace}(\mathbf{r}^{-1})$. If we ignore design 8.13a, we see that the *G*-efficiency decreases within each category. Summarizing we may conclude that the design quality within a category decreases slightly with increasing values of *P*. Nevertheless the designs of Table 7.5 are very useful for practical work because $\sigma_{\hat{\beta}}^2$, $\text{trace}(\mathbf{r}^{-1})$ and VIF's are rather small.

Considering all the designs 8.5–8.24 we have found that their quality varies a great deal.

However, there is one other important aspect as regards designs 8.5–8.24.

We have experienced again and again that experimenters are reluctant to carry out many experiments. These 23 designs are therefore very useful for practical purposes since the number of experimental units is only 16, whereas the experimenter can examine up to 4 factors while each of these has 2, 3 or 4 levels.

Attention is again drawn to the fact the two-level factors may be quantitative or qualitative, the factors with 3 or 4 levels are quantitative.

It is also interesting to compare the designs of group IX, 8.31, 8.32 and 8.33 with designs having 16 experimental units and which have the same number of factors and levels.

We first compare design 8.12 with design 8.33. Although design 8.33 has 18 and design 8.12 has 16 experimental units, we prefer design 8.12 since its design characteristics have more favourable values and because we can use it to calculate an estimate of σ^2 . We now compare design 8.15a and 8.15b with design 8.32. Design 8.32 appears to be slightly better because most design characteristics have better values.

If an experimenter very much wants a design to be as small as possible design 8.15a or 8.15b should be recommended.

When we compare design 8.19 to design 8.31 it is obvious by studying the design characteristics that design 8.19 is to be preferred if only to avoid the fairly large $|\rho|$ of 0.655 for design 8.31.

Design 8.19 also has a better D - and G -efficiency than design 8.31.

We now compare design 8.34 with design 8.38. The latter design has 17 parameters in the model, two more than design 8.34, because the effect of three blocks has been taken into account. Although both designs are of an excellent quality, we prefer design 8.34 because 4 scale independent design characteristics, namely $|\mathbf{r}|$, $\text{trace}(\mathbf{r}^{-1})$, largest VIF and largest $|\rho|$ have better values. Moreover the variances of $\hat{\beta}$ of design 8.34 are much smaller than those of design 8.38.

It was already pointed out in Section 7.4.10 that design 8.38 was constructed for a spherical region. The small D -efficiency of 51.6% indicates that this design performs poorly for a cubical experimental region.

Design 8.34 is also to be preferred from the experimenter's point of view since it contains 5

points in the extreme vertices of the experimental region, namely $(0\ 0\ 0\ 0)$, $(2\ 0\ 0\ 2)$, $(0\ 2\ 0\ 2)$, $(0\ 0\ 2\ 2)$ and $(2\ 2\ 2\ 0)$. These can be very interesting for the subject which is being studied.

The next comparison to be made refers to the designs 8.10, a $3 \times 3 \times 3/16$ design and 8.37, a $3 \times 3 \times 3/15$ Box Behnken design.

It is obvious that design 8.10 is to be preferred to 8.37 since many of its characteristics such as D -efficiency, G -efficiency, $\sigma_{\hat{\beta}_p}$ and $\sigma_{\hat{\beta}_{pq}}$ have better values than those of design 8.37.

The small D -efficiency of design 8.37 shows that this design, constructed for a spherical region, performs poorly, just as design 8.38, for a cubical region.

When we compare design 8.39 with design 8.24, we see that the latter has on the whole the best design characteristics and it is therefore to be preferred.

Although design 8.40 has the advantage that it has a smaller number of experimental units than design 8.30, it is clear that design 8.30 has the best design characteristics. Design 8.42 has on the whole better values for the design characteristics than design 8.30. Design 8.30 however, does have a center point which is an advantage from a practical point of view.

Design 8.41 has on the whole better characteristics than design 8.31.

A disadvantage of design 8.41, as already mentioned in Section 7.4.10, is that nearly all $\hat{\beta}$'s are mutually correlated, whereas the linear effects of 8.31 are orthogonal. However both designs are useful for practical purposes.

It is also interesting to compare design 8.41 with design 8.19. Design 8.41 has slightly better characteristics than design 8.19, but since their D - and G -efficiencies are nearly the same, it is difficult to decide which of them is the best design.

Table 7.6 gives a summary of some recommended designs, if a choice from similar designs has to be made.

Designs compared		Designs recommended
8.10	$3 \times 3 \times 3/16$	8.10
8.37	$3 \times 3 \times 3/15$	
8.12	$3 \times 2 \times 2 \times 2/16$	8.12
8.33	$3 \times 2 \times 2 \times 2/18$	
8.15a	$3 \times 3 \times 2 \times 2/16$	8.32
8.15b	$3 \times 3 \times 2 \times 2/16$	
8.32	$3 \times 3 \times 2 \times 2/18$	
8.19	$3 \times 3 \times 3 \times 2/16$	8.19 or 8.41
8.31	$3 \times 3 \times 3 \times 2/18$	
8.41	$3 \times 3 \times 3 \times 2/18$	
8.24	$3 \times 3 \times 3 \times 3/16$	8.24
8.39	$3 \times 3 \times 3 \times 3/15$	
8.30	$3 \times 3 \times 3 \times 3 \times 3/32$	8.30 or 8.42
8.40	$3 \times 3 \times 3 \times 3 \times 3/21$	
8.42	$3 \times 3 \times 3 \times 3 \times 3/27$	
8.34	$3 \times 3 \times 3 \times 3/27$	8.34
8.38	$3 \times 3 \times 3 \times 3/27$	

Table 7.6. Some recommended designs.

Appendix 7A

The use of eigenvalues and eigenvectors of \mathbf{r} .

The matrix \mathbf{r} is a real symmetric matrix.

A theorem from the matrix algebra states that

$$\mathbf{V}'\mathbf{r}\mathbf{V} = \mathbf{D} , \quad (7.9)$$

where \mathbf{V} is an orthonormal matrix the columns of which are the eigenvectors of \mathbf{r} .

\mathbf{D} is a diagonal matrix with diagonal elements equal to the eigenvalues λ_p of \mathbf{r} .

Because \mathbf{V} is an orthonormal matrix we have $\mathbf{V}'\mathbf{V} = \mathbf{V}\mathbf{V}' = \mathbf{I}$, where \mathbf{I} is the identity matrix.

Multiplying (7.9) on the left by \mathbf{V} and on the right by \mathbf{V}' we obtain

$$\mathbf{r} = \mathbf{V}\mathbf{D}\mathbf{V}' , \text{ or}$$

$$\mathbf{r}^{-1} = \mathbf{V}\mathbf{D}^{-1}\mathbf{V}' ,$$

and it follows that

$$r_{pp}^{-1} = V_{p1}^2 \lambda_1^{-1} + V_{p2}^2 \lambda_2^{-1} + \dots + V_{p,P-1}^2 \lambda_{P-1}^{-1} . \quad (7.10)$$

The V_{pq} are the elements of \mathbf{V} with $p, q = 1, 2, \dots, (P - 1)$.

Expression (7.10) shows that r_{pp}^{-1} , the p^{th} diagonal element of the matrix \mathbf{r}^{-1} and equal to the VIF, can be written as a function of the elements of the eigenvectors and eigenvalues of

\mathbf{r} . We shall now illustrate (7.10) with a numerical example.

DESIGN GENERATORS

$$P1_i := \frac{2 \cdot A_i + B_i}{\sqrt{5}}$$

$$Pq_i := \frac{A_i \cdot B_i}{i_i}$$

$$R1_i := \frac{A_i \cdot B_i \cdot C_i \cdot D_i + A_i \cdot B_i \cdot C_i}{\sqrt{2}}$$

$$S1_i := \frac{B_i \cdot C_i + A_i \cdot B_i \cdot D_i}{\sqrt{2}}$$

$$Q1_i := \frac{C_i + D_i}{\sqrt{2}}$$

$$Qq_i := \frac{C_i \cdot D_i}{i_i}$$

$$Rq_i := \frac{D_i}{i_i}$$

$$Sq_i := \frac{A_i \cdot C_i \cdot D_i}{i_i}$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := x0_i \quad X_{i,2} := Qq_i$$

$$X_{i,3} := Pq_i \quad X_{i,4} := Rq_i$$

$$X_{i,5} := Sq_i \quad X_{i,6} := Q1_i \quad X_{i,7} := R1_i$$

$$X_{i,8} := P1_i \cdot S1_i \quad X_{i,9} := Q1_i \cdot R1_i \quad X_{i,10} := P1_i$$

$$X_{i,11} := S1_i \quad X_{i,12} := P1_i \cdot Q1_i \quad X_{i,13} := P1_i \cdot R1_i$$

$$X_{i,14} := Q1_i \cdot S1_i \quad X_{i,15} := R1_i \cdot S1_i$$

ELEMENTS OF DESIGN MATRIX

$$DM_{i,1} := \frac{3 + P1_i \cdot \sqrt{5}}{2}$$

$$DM_{i,2} := \left[1 + \frac{Q1_i}{\sqrt{2}} \right]$$

$$DM_{i,3} := \left[1 + \frac{R1_i}{\sqrt{2}} \right]$$

$$DM_{i,4} := \left[1 + \frac{S1_i}{\sqrt{2}} \right]$$

DESIGN MATRIX

$$DMT = \begin{bmatrix} 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 2 & 2 & 0 & 2 & 0 & 0 & 2 \\ 1 & 2 & 1 & 0 & 0 & 1 & 2 & 1 & 2 & 1 & 0 & 1 & 1 & 0 & 1 & 2 \end{bmatrix}$$

-1	2.467	-0.025	-1.486	0.05	2.102	-0.163	-0.061	0.49	1.41	-0.346	1.093	-0.16	-0.439	-2.933
	-0.025	3.839	0.026	0.322	-0.037	3.907	0.003	-5.378	0.045	2.388	-0.145	-1.017	-0.301	0.05
	-1.486	0.026	3.715	-0.053	-3.839	-0.065	-0.723	-0.677	-1.469	0.479	-1.403	0.166	0.624	2.972
	0.05	0.322	-0.053	1.357	0.074	0.67	-0.007	-1.244	-0.089	0.68	0.269	-1.128	0.601	-0.101
	2.102	-0.037	-3.839	0.074	5.429	0.092	-1.022	0.957	2.077	-0.677	1.983	-0.235	-0.883	-4.203
	-0.163	3.907	-0.065	0.67	0.092	6.994	-0.724	-8.224	-0.238	3.815	0.181	-2.12	0.409	0.327
	-0.061	0.003	0.723	-0.007	-1.022	-0.724	2.091	-0.592	-0.186	0.418	-0.977	0.021	0.585	0.123
	0.49	-5.378	-0.677	-1.244	0.957	-8.224	-0.592	13.253	0.996	-6.543	0.435	3.935	-2.497	-0.98
	1.41	0.045	-1.469	-0.089	2.077	-0.238	-0.186	0.996	2.504	-0.705	1.011	0.282	-1.086	-2.82
	-0.346	2.388	0.479	0.88	-0.677	3.815	0.418	-6.543	-0.705	4.526	-0.308	-2.782	1.766	0.693
	1.093	-0.145	-1.403	0.289	1.983	0.181	-0.977	0.435	1.011	-0.308	2.517	-0.914	-0.146	-2.187
	-0.16	-1.017	0.166	-1.128	-0.235	-2.12	0.021	3.935	0.282	-2.782	-0.914	3.568	-1.901	0.319
	-0.439	-0.301	0.624	0.601	-0.883	0.409	0.585	-2.497	-1.086	1.766	-0.146	-1.901	3.098	0.879
	-2.933	0.05	2.972	-0.101	-4.203	0.327	0.123	-0.98	-2.82	0.593	-2.187	0.319	0.879	5.867

Table 7.7. $A_4 \times 3 \times 3 \times 3 / 16$ design

For this numerical example we make use of a $4 \times 3 \times 3 \times 3/16$ design in Table 7.7. It was constructed using design generators but later discarded because of its low D -efficiency. To save space we only present the design generators, the column vectors of the \mathbf{X} matrix and the matrix \mathbf{r}^{-1} in Table 7.7. We take this design because it contains a large VIF namely a VIF equal to 13.253, the eighth diagonal element of \mathbf{r}^{-1} . A routine from the software package "Turbo-Pascal" was used to calculate the eigenvectors and eigenvalues of \mathbf{r} . See Table 7.9. The variables of the regression equation of the $4 \times 3 \times 3 \times 3/16$ design and the corresponding VIF's are given in Table 7.8.

Variable	VIF
$X_{i,2} = Qq_i$	2.467
$X_{i,3} = Pq_i$	3.839
$X_{i,4} = Rq_i$	3.715
$X_{i,5} = Sq_i$	1.357
$X_{i,6} = Ql_i$	5.429
$X_{i,7} = Rl_i$	6.994
$X_{i,8} = Pl_iSl_i$	2.091
$X_{i,9} = Ql_iRl_i$	13.253
$X_{i,10} = Pl_i$	2.504
$X_{i,11} = Sl_i$	4.626
$X_{i,12} = Pl_iQl_i$	2.517
$X_{i,13} = Pl_iRl_i$	3.568
$X_{i,14} = Ql_iSl_i$	3.098
$X_{i,15} = Rl_iSl_i$	5.867

Table 7.8. Variables and VIF's of the $4 \times 3 \times 3 \times 3/16$ design of Table 7.7.

Eigenvalues λ_p	$\lambda_1 =$	$\lambda_2 =$	$\lambda_3 =$	$\lambda_4 =$	$\lambda_5 =$	$\lambda_6 =$	$\lambda_7 =$
Variable	1.54211	2.57438	2.01729	1.04954	0.06205	0.29149	1.40980
Qq_i	-0.3498	0.0568	0.2598	-0.2265	-0.2849	0.2767	-0.1953
Pq_i	0.0195	0.2974	-0.2234	-0.2169	-0.0985	0.1269	-0.3757
Rq_i	0.5469	0.0487	0.3184	-0.0328	0.3903	0.2228	-0.1193
Sq_i	0.1559	0.0399	0.0136	0.7147	-0.0347	-0.0769	-0.1228
Ql_i	0.4193	0.1085	0.4580	-0.0023	-0.5178	-0.2233	-0.0691
Rl_i	-0.0722	0.4211	-0.1341	0.2354	-0.1497	-0.2260	0.3535
Pl_iSl_i	-0.1131	0.3268	0.2411	0.1388	0.0923	0.6228	0.5037
Ql_iRl_i	0.0113	0.5253	-0.2363	-0.1211	0.0956	-0.1551	0.0807
Pl_i	-0.3088	0.1092	0.1844	0.2473	-0.2761	0.2553	-0.3868
Sl_i	0.2213	0.2025	-0.0022	-0.4460	-0.0236	0.0612	0.0172
Pl_iQl_i	-0.0161	0.1981	0.2759	-0.1312	-0.2578	-0.2932	0.2221
Pl_iRl_i	0.2674	0.1984	0.0439	0.1120	0.1028	0.1722	-0.1592
Ql_iSl_i	0.0099	0.4112	-0.2184	0.0996	0.0891	-0.0247	-0.3887
Rl_iSl_i	-0.3793	0.1788	0.5287	-0.0224	0.5345	-0.3921	-0.1601

Table 7.9. Eigenvectors and eigenvalues of the r matrix of the $4 \times 3 \times 3 \times 3/16$ design of

Table 7.7.

(Part one)

Eigenvalues λ_p Variable	$\lambda_8 =$ 0.03738	$\lambda_9 =$ 1.02428	$\lambda_{10} =$ 0.93970	$\lambda_{11} =$ 1.72300	$\lambda_{12} =$ 0.18243	$\lambda_{13} =$ 0.72178	$\lambda_{14} =$ 0.42476
Qq_i	0.0550	0.6805	-0.0477	0.0036	0.0619	0.2415	0.1704
Pq_i	-0.2856	0.0073	0.5320	-0.1372	-0.3707	-0.3529	0.0415
Rq_i	-0.0701	0.0124	-0.0711	-0.2990	-0.0131	0.1284	0.5135
Sq_i	-0.0740	0.3904	0.0704	0.2499	0.1906	-0.3998	0.1392
Ql_i	0.0953	0.0004	0.0061	-0.3058	0.0152	-0.0505	-0.4177
Rl_i	-0.4450	0.1085	-0.2866	-0.2013	-0.3513	0.2686	0.1328
Pl_i, Sl_i	-0.0215	-0.0913	0.2141	-0.0512	0.1463	-0.1306	-0.2390
Ql_i, Rl_i	0.6888	0.1227	-0.1578	-0.1485	0.0212	-0.2426	0.1342
Pl_i	0.0815	-0.5180	-0.3899	-0.0123	-0.1046	-0.1368	0.2232
Sl_i	-0.3658	0.0359	-0.4763	0.4096	0.2198	-0.3511	-0.0714
Pl_i, Ql_i	0.0351	-0.2502	0.4049	0.4167	0.1486	0.1169	0.4778
Pl_i, Rl_i	0.2253	0.0300	-0.0134	0.5713	-0.4929	0.3518	-0.2532
Ql_i, Sl_i	-0.1389	-0.1224	0.0936	-0.0500	0.5850	0.4390	-0.1820
Rl_i, Sl_i	-0.1059	0.0331	0.0057	0.0052	-0.1013	-0.1344	-0.1961

Table 7.9. Eigenvectors and eigenvalues of the r matrix of the $4 \times 3 \times 3 \times 3/16$ design of

Table 7.7.

(Part two)

The smallest eigenvalue is $\lambda_8 = 0.03738$. See Table 7.9, part two. The largest three elements in absolute value of the associated eigenvector are: 0.6880, -0.4450, -0.3658 corresponding with Ql_i, Rl_i, Rl_i and Sl_i , which means that the majority of non orthogonality is being produced by these three variables.

It is interesting to calculate the large VIF = 13.253, corresponding to Ql_i, Rl_i , from the eigenvector elements and eigenvalues of the matrix r .

We find, according to expression (7.10),

$$\begin{aligned}
r_{88}^{-1} &= (0.0113)^2 \cdot (1.54211)^{-1} + (0.5253)^2 \cdot (2.57438)^{-1} + \dots + (0.6888)^2 \cdot (0.03738)^{-1} + \\
&+ \dots + (0.1342)^2 \cdot (0.42476)^{-1} \\
&= 13.256 .
\end{aligned}$$

We can see that $r_{88}^{-1} = 13.256$ is built up as a sum of 14 elements. The eighth and largest of these equals $(0.6888)^2 (0.03738)^{-1} = 12.692$, which shows that the eigenvector $\lambda_8 = 0.03738$ has a very large effect on the VIF of $\hat{\beta}_{23}$, the parameter associated with $QI_i RI_i$. The other VIF's can likewise be examined.

In Table 7.10 we present the largest 5 VIF's of the design in Table 7.7 together with the largest element from equation (7.10).

Table 7.10 shows how the largest VIF's are built up. It appears that both λ_8 and λ_5 , the latter being the second smallest eigenvector, have a large effect on the largest 5 VIF's.

Table 7.10 also shows that the variables involved with the largest VIF's are related with factors which were collapsed. These factors therefore contribute most to non orthogonality.

The only non-collapsed factor, namely P , does not occur in Table 7.10.

Variable	VIF	Largest element from equation (5.14)
$X_{i,9} = QI_i RI_i$	13.253	$V_{QIRI,8}^2 \lambda_8^{-1} = (0.6888)^2 (0.03738)^{-1} = 12.692$
$X_{i,7} = RI_i$	6.994	$V_{RI,8}^2 \lambda_8^{-1} = (0.4450)^2 (0.03738)^{-1} = 5.297$
$X_{i,15} = RI_i SI_i$	5.867	$V_{RISI,5}^2 \lambda_5^{-1} = (0.5345)^2 (0.06205)^{-1} = 4.604$
$X_{i,6} = QI_i$	5.429	$V_{QI,5}^2 \lambda_5^{-1} = (0.5178)^2 (0.06205)^{-1} = 4.321$
$X_{i,11} = SI_i$	4.626	$V_{SI,8}^2 \lambda_8^{-1} = (0.3658)^2 (0.03738)^{-1} = 3.580$

Table 7.10. Largest five VIF's with largest elements from (7.10).

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SUMMARY

In this thesis nearly 40 small designs for quantitative factors are developed.

A literature review about fractional replication is presented in Chapter 1 and some arguments are given as to why this research was undertaken, such as

- i) Experimenters want to carry out small experiments.
- ii) Scientists require freedom of choice as regards the number of levels for each factor.
- iii) The existing designs for quantitative factors usually have only 3 or 5 levels for each factor.

General aspects of linear regression theory and experimental design such as the linear regression model, D - and G -efficiency, the techniques of replacement and collapsing are dealt with in Chapter 2.

Chapter 3 presents methods to find D -optimal experimental designs for the incomplete quadratic model in which d variables have linear and quadratic terms, but the other $(k - d)$ variables have only linear terms. All $\binom{k}{2}$ linear \times linear interactions are however included in the model.

These D -optimal designs were constructed to be able to calculate the D -efficiencies of a large number of designs developed in Chapters 4, 5 and 6.

The 2^3 design is used in Chapter 4 to construct a design with one four-level factor and two two-level factors using 8 experimental units. Such a design is indicated as a $4 \times 2 \times 2/8$ design. Moreover, two $3 \times 2 \times 2/8$ designs were constructed in Chapter 4.

A measure of orthogonality, the variance inflation factor, is introduced.

Two applications of the designs developed, are given.

Chapter 5 deals with two methods to construct designs with 16 experimental units.

The first method uses the new concept of 'design generator'. The second method applies properties of D -optimal designs as developed in Chapter 3. The latter method is also used to construct designs with 32 experimental units.

The P.C. package "MATH CAD" is introduced to calculate the various characteristics of the new designs. An application of a $3 \times 3 \times 3 \times 3 \times 3/32$ design is presented.

In Chapter 6 some new designs with two- and three-level factors are developed using orthogonal columns of some main-effect designs. The new 39 and 6 existing designs are discussed and compared in Chapter 7, using various design characteristics such as D - and G -efficiency, variances of parameter estimators, variance inflation factors, trace $(\mathbf{X}'\mathbf{X})^{-1}$, etc. It appears that many new designs have excellent design characteristics.

The details of all the new designs are presented in the appendix. These details facilitate a choice if a design is to be used in a practical application.

SAMENVATTING

In dit proefschrift worden bijna 40 kleine proefschema's voor kwantitatieve factoren ontwikkeld.

Een literatuuroverzicht over gedeeltelijke herhalingen wordt gegeven in Hoofdstuk 1 en enkele redenen worden genoemd waarom dit onderzoek werd opgezet zoals

- i) Onderzoekers wensen kleine proefschema's uit te voeren.
- ii) Personen werkzaam in research en ontwikkeling, wensen keuzevrijheid aangaande het aantal te kiezen niveaus per factor.
- iii) De bestaande proefschema's voor kwantitatieve factoren hebben meestal slechts 3 of 5 niveaus per factor.

Algemene aspecten van lineaire regressie theorie en proefopzetten, zoals het lineaire regressiemodel, D - en G -efficiëncy, de techniek van vervanging en inklappen, komen ter sprake in Hoofdstuk 2.

Hoofdstuk 3 behandelt methoden om D -optimale proefopzetten te vinden voor het onvolledige kwadratische model waarin d variabelen lineaire en kwadratische termen hebben, maar waarbij de andere $(k - d)$ variabelen slechts lineaire termen hebben. Alle $\binom{k}{2}$ lineaire \times lineaire interacties zijn echter in het model opgenomen.

Deze D -optimale schema's werden geconstrueerd om de D -efficiëncies van een groot aantal nieuwe schema's, die in de Hoofdstukken 4, 5 en 6 werden ontwikkeld, te kunnen berekenen. Het 2^3 proefschema wordt in Hoofdstuk 4 gebruikt om een proefschema van 8 experimentele eenheden met één factor op vier niveaus en twee factoren elk op twee niveaus, te construeren. Zo'n schema wordt aangegeven als een $4 \times 2 \times 2/8$ proefopzet.

In Hoofdstuk 4 worden bovendien twee $3 \times 2 \times 2/8$ proefschema's geconstrueerd.

Een orthogonaliteitsmaat, de variantie vergrotende factor, wordt geïntroduceerd. Er worden twee toepassingen van de ontwikkelde schema's gegeven.

Hoofdstuk 5 bevat een tweetal methoden om schema's met 16 experimentele eenheden te construeren.

De eerste methode gebruikt het nieuwe begrip 'design generator'. De tweede past eigenschappen van de D -optimale proefopzetten toe, zoals die werden ontwikkeld in Hoofdstuk 3.

De laatstgenoemde methode wordt ook gebruikt om enkele schema's met 32 experimentele eenheden te maken.

Het P.C. software pakket "MATH CAD" wordt geïntroduceerd om waarden van kenmerken der nieuwe schema's te berekenen.

Er wordt een toepassing van een $3 \times 3 \times 3 \times 3 \times 3/32$ schema gegeven. Enkele nieuwe schema's met factoren op 2 en 3 niveaus worden ontwikkeld in Hoofdstuk 6, waarbij orthogonale kolommen van een aantal hoofd-effect schema's worden gebruikt.

De 39 nieuwe en 6 bestaande schema's worden besproken en vergeleken in Hoofdstuk 7, waarbij men diverse kenmerken van proefschemas gebruikt, zoals *D*- en *G*-efficiëntie, varianties van parameter schatters, variantie vergrotende factoren, het spoor van $(X'X)^{-1}$, enz. Het blijkt dat veel nieuwe schema's uitstekende kenmerken bezitten.

De bijzonderheden van alle nieuwe schema's zijn gegeven in de appendix. Deze details vergemakkelijken een keuze, indien een proefschemas in een praktische toepassing moet worden gebruikt.

CURRICULUM VITAE

Pieter Martinus Upperman was born in Emmen, the Netherlands, on the 9th of June 1929. He obtained his grammar school certificate at the 'Christelijk Lyceum' of Zwolle in 1948 and studied geodesy at the Technical University of Delft, where he obtained his engineering degree in geodesy in 1953.

The author was then for one year employed by the Department of Geodesy of the Technical University of Delft, where he worked on the application of statistical methods to land surveying problems.

Mr. Upperman worked as a surveyor in Nigeria from 1954 to 1961 on triangulation, mining leases and aerial survey.

He worked as a statistician for the 'Nederlandse Philips Bedrijven B.V.' at Eindhoven from 1961 to 1989 and was during the last 10 years of this period in charge of the Statistical Department of the Center for Quantitative Methods.

In 1989 he founded "Upperman Quality Engineering Consultancy" which provides support as regards experimental design, statistical process control and sampling inspection, to industry.

APPENDIX OF THE THESIS

**DESIGNS WITH A SMALL NUMBER OF RUNS
FOR
FACTORIAL EXPERIMENTS**

P.M. UPPERMAN

APPENDIX

Designs for experiments with factors having two, three or four levels

This Appendix contains all the designs which have been mentioned in the previous chapters. All the designs have been discussed in Chapter 7. Some of the designs have been treated in more detail in Chapters 4, 5 and 6. Table I can be used to locate a particular design.

Design number	Design	Page	Design number	Design	Page
8.1	$4 \times 2 \times 2/8$	A1	8.21	$4 \times 4 \times 4 \times 3/16$	A29,30
8.2	$3 \times 2 \times 2/8$	A2	8.22	$4 \times 4 \times 3 \times 3/16$	A31,32
8.3	$3 \times 2 \times 2/8$	A3	8.23	$4 \times 3 \times 3 \times 3/16$	A33,34
8.4	$3 \times 2 \times 2/8$	A4	8.24	$3 \times 3 \times 3 \times 3/16$	A35,36
8.5	$4 \times 4 \times 2/16$	A5	8.25	$4 \times 4 \times 4 \times 4/32$	A37
8.6	$4 \times 3 \times 2/16$	A6	8.26	$4 \times 4 \times 4 \times 4 \times 3/32$	A38
8.7	$4 \times 4 \times 4/16$	A7	8.27	$4 \times 4 \times 4 \times 3 \times 3/32$	A39
8.8	$4 \times 4 \times 3/16$	A8	8.28	$4 \times 4 \times 3 \times 3 \times 3/32$	A40
8.9	$4 \times 3 \times 3/16$	A9	8.29	$4 \times 3 \times 3 \times 3 \times 3/32$	A41
8.10	$3 \times 3 \times 3/16$	A10	8.30	$3 \times 3 \times 3 \times 3 \times 3/32$	A42
8.11	$4 \times 2 \times 2 \times 2/16$	A11	8.31	$3 \times 3 \times 3 \times 2/18$	A43
8.12	$3 \times 2 \times 2 \times 2/16$	A12	8.32	$3 \times 3 \times 2 \times 2/18$	A44
8.13a	$4 \times 4 \times 2 \times 2/16$	A13	8.33	$3 \times 2 \times 2 \times 2/18$	A45
8.13b	$4 \times 4 \times 2 \times 2/16$	A14			
8.14a	$4 \times 3 \times 2 \times 2/16$	A15	8.34	$3 \times 3 \times 3 \times 3/27$	A46
8.14b	$4 \times 3 \times 2 \times 2/16$	A16			
8.15a	$3 \times 3 \times 2 \times 2/16$	A17	8.35	$3 \times 3 \times 3 \times 2/27$	A47
8.15b	$3 \times 3 \times 2 \times 2/16$	A18			
8.16	$4 \times 4 \times 4 \times 2/16$	A19,20	8.36	$3 \times 3 \times 2 \times 2/27$	A48
8.17	$4 \times 4 \times 3 \times 2/16$	A21,22	8.37	$3 \times 3 \times 3/15$ (Box Behnken)	A49
8.18	$4 \times 3 \times 3 \times 2/16$	A23,24	8.38	$3 \times 3 \times 3 \times 3/27$ (Box Behnken)	A50
8.19	$3 \times 3 \times 3 \times 2/16$	A25,26	8.39	$3 \times 3 \times 3 \times 3/15$ (Rechtschaffner)	A51,52
8.20	$4 \times 4 \times 4 \times 4/16$	A27,28	8.40	$3 \times 3 \times 3 \times 3 \times 3/21$ (Rechtschaffner)	A53,54,55
			8.41	$3 \times 3 \times 3 \times 2/18$ (Webb)	A56
			8.42	$3 \times 3 \times 3 \times 3 \times 3/27$ (Mitchell and Bayne)	A57

Table I. Index to the designs.

----- (8.1) A 4x2x2/8 design -----

DESIGN GENERATORS

ELEMENTS OF DESIGN MATRIX

$$P_{i,1} := \frac{2 \cdot A_i + B_i}{\sqrt{5}}$$

$$Q_{i,1} := C_i$$

$$DM_{i,1} := \frac{1 + P_{i,1} \cdot \sqrt{5}}{2}$$

$$DM_{i,3} := \frac{1 + R_i}{2}$$

$$P_{i,2} := \frac{A_i \cdot B_i}{i}$$

$$DM_{i,2} := \frac{1 + Q_{i,1}}{2}$$

$$R_{i,1} := \frac{B_i \cdot C_i}{i}$$

DESIGN MATRIX

$$DM^T = \begin{bmatrix} 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := x_{0,i}$$

$$X_{i,2} := P_{i,1}$$

$$X_{i,3} := Q_{i,1} \cdot R_{i,1}$$

$$X_{i,4} := P_{i,2}$$

$$X_{i,5} := Q_{i,1}$$

$$X_{i,6} := P_{i,1} \cdot R_{i,1}$$

$$X_{i,7} := R_{i,1}$$

$$X_{i,8} := P_{i,1} \cdot Q_{i,1}$$

$$|XTX| = 8.59 \cdot 10^6$$

$$XTX = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 3.578 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3.578 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 3.578 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3.578 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 3.578 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3.578 & 8 \end{bmatrix}$$

$$XTXI = \begin{bmatrix} 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.156 & -0.07 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.07 & 0.156 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.125 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.156 & -0.07 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.07 & 0.156 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.156 & -0.07 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.07 & 0.156 \end{bmatrix}$$

$$\text{tr}(XTXI) = 1.188$$

$$r = \begin{bmatrix} 1 & 0.447 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.447 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0.447 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.447 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0.447 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.447 & 1 & 0 \end{bmatrix}$$

$$|r| = 0.512$$

$$r^{-1} = \begin{bmatrix} 1.25 & -0.559 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.559 & 1.25 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.25 & -0.559 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.559 & 1.25 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.25 & -0.559 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.559 & 1.25 & 0 \end{bmatrix}$$

$$\text{tr}[r^{-1}] = 8.5$$

$$\rho = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -0.447 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.447 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -0.447 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.447 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -0.447 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.447 & 1 \end{bmatrix}$$

----- (8.2) A 3x2x2/8 design -----

DESIGN GENERATORS

$$P1_i := \frac{A_i - A_j B_i}{\sqrt{2}}$$

$$Pq_i := -B_i$$

ELEMENTS OF DESIGN MATRIX

$$DM_{i,1} := 1 + \frac{P1_i}{\sqrt{2}}$$

$$DM_{i,2} := \frac{1 + Q_i}{2}$$

$$Q_i := G_i$$

$$R_i := A_i G_i$$

$$DM_{i,3} := \frac{1 + R_i}{2}$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := \times 0_i$$

$$X_{i,3} := -Q_i \cdot R_i$$

$$X_{i,5} := Q_i$$

$$X_{i,7} := R_i$$

$$X_{i,2} := P1_i$$

$$X_{i,4} := Pq_i$$

$$X_{i,6} := P1_i \cdot R_i$$

$$X_{i,8} := P1_i \cdot Q_i$$

DESIGN MATRIX

$$DM^T = \begin{bmatrix} 0 & 2 & 1 & 1 & 0 & 2 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

$$|XTX| = 2.097 \cdot 10^6$$

$$XTX = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 5.657 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5.657 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 5.657 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.657 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 5.657 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5.657 & 8 \end{bmatrix}$$

$$XTX^{-1} = \begin{bmatrix} 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.25 & -0.177 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.177 & 0.25 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.125 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.25 & -0.177 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.177 & 0.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.25 & -0.177 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.177 & 0.25 \end{bmatrix}$$

$$tr(XTX^{-1}) = 1.75$$

$$r = \begin{bmatrix} 1 & 0.707 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.707 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0.707 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.707 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0.707 \\ 0 & 0 & 0 & 0 & 0 & 0.707 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$|r| = 0.125$$

$$r^{-1} = \begin{bmatrix} 2 & -1.414 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1.414 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1.414 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1.414 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & -1.414 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1.414 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

$$tr[r^{-1}] = 13$$

$$\rho = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -0.707 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.707 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -0.707 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.707 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -0.707 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.707 & 1 \end{bmatrix}$$

----- (B.3) A 3x2x2/8 design -----

DESIGN GENERATORS

$$P1_i := \frac{3 \cdot A_i + B_i - A_i \cdot B_i}{\sqrt{11}} \quad Q_i := C_i$$

$$Pq_i := \left[\begin{array}{c} B_i - A_i \cdot B_i \\ A_i - 3 \cdot \frac{B_i - A_i \cdot B_i}{2} \end{array} \right] \cdot \sqrt{\frac{2}{11}}$$

$$R_i := B_i \cdot C_i$$

ELEMENTS OF DESIGN MATRIX

$$OH_{i,1} := \frac{5 + P1_i \cdot \sqrt{11}}{4} \quad OH_{i,3} := \frac{1 + R_i}{2}$$

$$DH_{i,2} := \frac{1 + Q_i}{2}$$

DESIGN MATRIX

$$OH^T = \begin{bmatrix} 0 & 2 & 1 & 2 & 0 & 2 & 1 & 1 & 2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}$$

$$|XTX| = 4.437 \cdot 10^6$$

$$XTX = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 2.412 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.412 & 8 & -5.117 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -5.117 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 2.412 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.412 & 8 & 0 & -4.364 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 2.412 & 0 \\ 0 & 0 & 0 & 0 & 0 & -4.364 & 2.412 & 8 & 0 \end{bmatrix}$$

$$XTX^{-1} = \begin{bmatrix} 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.148 & -0.075 & -0.048 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.075 & 0.25 & 0.16 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.048 & 0.16 & 0.227 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.145 & -0.065 & 0.012 & -0.039 & 0 \\ 0 & 0 & 0 & 0 & -0.065 & 0.215 & -0.039 & 0.129 & 0 \\ 0 & 0 & 0 & 0 & 0.012 & -0.039 & 0.145 & -0.065 & 0 \\ 0 & 0 & 0 & 0 & -0.039 & 0.129 & -0.065 & 0.215 & 0 \end{bmatrix}$$

$$\text{tr}(XTX^{-1}) = 1.469$$

$$r = \begin{bmatrix} 1 & 0.302 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.302 & 1 & -0.64 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.64 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0.302 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.302 & 1 & 0 & -0.545 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0.302 & 0 \\ 0 & 0 & 0 & 0 & -0.545 & 0.302 & 1 & 0 \end{bmatrix}$$

$$|r| = 0.264$$

$$r^{-1} = \begin{bmatrix} 1.182 & -0.603 & -0.386 & 0 & 0 & 0 & 0 & 0 \\ -0.603 & 2 & 1.279 & 0 & 0 & 0 & 0 & 0 \\ -0.386 & 1.279 & 1.818 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.156 & -0.518 & 0.094 & -0.311 & 1.031 \\ 0 & 0 & 0 & -0.518 & 1.719 & -0.311 & 1.031 & 0 \\ 0 & 0 & 0 & 0.094 & -0.311 & 1.156 & -0.518 & 0 \\ 0 & 0 & 0 & -0.311 & 1.031 & -0.518 & 1.719 & 0 \end{bmatrix}$$

$$\text{tr}[r^{-1}] = 10.75$$

$$\rho = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -0.392 & -0.263 & 0 & 0 & 0 & 0 \\ 0 & -0.392 & 1 & 0.671 & 0 & 0 & 0 & 0 \\ 0 & -0.263 & 0.671 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -0.368 & 0.081 & -0.221 \\ 0 & 0 & 0 & 0 & -0.368 & 1 & -0.221 & 0.6 \\ 0 & 0 & 0 & 0 & 0.081 & -0.221 & 1 & -0.368 \\ 0 & 0 & 0 & 0 & -0.221 & 0.6 & -0.368 & 1 \end{bmatrix}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{array}{ll} X_{i,1} := x0_i & X_{i,2} := P1_i \\ X_{i,3} := Q_i \cdot R_i & X_{i,4} := Pq_i \\ X_{i,5} := Q_i & X_{i,6} := P1_i \cdot R_i \\ X_{i,7} := R_i & X_{i,8} := P1_i \cdot Q_i \end{array}$$

----- (8.4) A 3x2x2/8 design -----

DESIGN GENERATORS

$$P1_i := \frac{A_i + B_i}{\sqrt{2}}$$

$$Pq_i := A_i - B_i$$

$$R_i := B_i - C_i$$

$$Q_i := C_i$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := x0_i$$

$$X_{i,2} := P1_i$$

$$X_{i,3} := Q_i R_i$$

$$X_{i,4} := Pq_i$$

$$X_{i,5} := Q_i$$

$$X_{i,6} := P1_i \cdot R_i$$

$$X_{i,7} := -R_i$$

$$X_{i,8} := P1_i \cdot Q_i$$

ELEMENTS OF DESIGN MATRIX

$$DM_{i,1} := 1 + \frac{P1_i}{\sqrt{2}}$$

$$DM_{i,3} := \frac{1 + R_i}{2}$$

$$DM_{i,2} := \frac{1 + Q_i}{2}$$

DESIGN MATRIX

$$DM^T = \begin{bmatrix} 0 & 1 & 1 & 2 & 0 & 1 & 1 & 2 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

$$|X^T X| = 2.097 \cdot 10^6$$

$$X^T X = \begin{bmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 5.657 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5.657 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 5.657 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.657 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 & 5.657 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5.657 & 8 \end{bmatrix}$$

$$X^T X^{-1} = \begin{bmatrix} 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.25 & -0.177 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.177 & 0.25 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.125 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.25 & -0.177 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.177 & 0.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.25 & -0.177 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.177 & 0.25 \end{bmatrix}$$

$$tr(X^T X^{-1}) = 1.75$$

$$r = \begin{bmatrix} 1 & 0.707 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.707 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0.707 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.707 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0.707 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.707 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$|r| = 0.125$$

$$r^{-1} = \begin{bmatrix} 2 & -1.414 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1.414 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1.414 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1.414 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & -1.414 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1.414 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

$$tr[r^{-1}] = 13$$

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -0.707 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.707 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -0.707 & 0 \\ 0 & 0 & 0 & 0 & -0.707 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -0.707 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.707 & 1 \end{bmatrix}$$

----- (8.6) A 4x3x2/16 design -----

DESIGN GENERATORS

$$P1_i := \frac{2 \cdot A_i + B_i}{\sqrt{5}} \quad Q1_i := \frac{C_i + D_i}{\sqrt{2}}$$

$$Pq_i := A_i - B_i \quad Qq_i := C_i - D_i$$

$$R_i := A_i - B_i - C_i - D_i$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := x0_i \quad X_{i,2} := P1_i$$

$$X_{i,3} := Q1_i \quad X_{i,4} := R_i$$

$$X_{i,5} := Pq_i \quad X_{i,6} := Qq_i$$

$$X_{i,7} := P1_i \cdot Q1_i \quad X_{i,8} := P1_i \cdot R_i$$

$$X_{i,9} := Q1_i \cdot R_i$$

ELEMENTS OF DESIGN MATRIX

$$DM_{i,1} := \frac{3 + P1_i \cdot \sqrt{5}}{2} \quad DM_{i,3} := \frac{1 + R_i}{2}$$

$$DM_{i,2} := 1 + \frac{Q1_i}{\sqrt{2}}$$

DESIGN MATRIX

$$DMT = \begin{bmatrix} 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 & 0 & 2 & 1 & 3 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$|XTX| = 6.872 \cdot 10^{10}$$

$$XTX = \begin{bmatrix} 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 \end{bmatrix}$$

$$NTXI = \begin{bmatrix} 0.063 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.063 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.063 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.063 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.063 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.063 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.063 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.063 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.063 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.063 \end{bmatrix}$$

$$tr(NTXI) = 0.563$$

$$r = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$|r| = 1$$

$$r^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$tr[r^{-1}] = 8$$

$$p = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

------(8.8) A 4x4x3/16 design -----

DESIGN MATRIX

$$\begin{aligned} xp^T &= (0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 1 \ 3 \ 0 \ 2 \ 0 \ 2) & x1_i &= (2xp_i - 3)/3 \\ xq^T &= (0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 1 \ 0 \ 3 \ 2 \ 1 \ 0 \ 3 \ 2) & x2_i &= (2xq_i - 3)/3 \\ xr^T &= (0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2 \ 1 \ 1) & x3_i &= (xr_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} X &= \begin{matrix} 1 & & 2 & & 2 & & 2 \\ 1,1 & & x := x1 & & x := x2 & & x := x3 \\ & & 1,2 & & 1,3 & & 1,4 \end{matrix} \\ X &= \begin{matrix} := x1 \times x2 & X := x1 \times x3 & X := x2 \times x3 \\ 1,5 & 1,6 & 1,7 \end{matrix} \\ X &= \begin{matrix} := x1 & X := x2 & X := x3 \\ 1,8 & 1,9 & 1,10 \end{matrix} \end{aligned}$$

$$XTX = \begin{bmatrix} 16 & 12.444 & 12.444 & 12 & -1.778 & -1.333 & -2.667 & 0 & 0 & 0 \\ 12.444 & 12.049 & 10.469 & 10.222 & -1.383 & -1.926 & -0.889 & 0 & 0 & 0 \\ 12.444 & 10.469 & 12.049 & 10.222 & -2.568 & 0.444 & -2.074 & 0 & 0 & 0 \\ 12 & 10.222 & 10.222 & 12 & 0 & -1.333 & -2.667 & 0 & 0 & 0 \\ -1.778 & -1.383 & -2.568 & 0 & 10.469 & -0.889 & 0.444 & 0 & 0 & 0 \\ -1.333 & -1.926 & 0.444 & -1.333 & -0.889 & 10.222 & 0 & 0 & 0 & 0 \\ -2.667 & -0.889 & -2.074 & -2.667 & 0.444 & 0 & 10.222 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.444 & -1.778 & -1.333 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1.778 & 12.444 & -2.667 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1.333 & -2.667 & 12 \end{bmatrix}$$

$$\left| \frac{XTX}{16} \right| = 1.852 \cdot 10^{-4}$$

$$XTX^{-1} = \begin{bmatrix} 0.3 & -0.225 & -0.225 & -0.106 & 4.796 \cdot 10^{-6} & 0.019 & 0.037 & 0 & 0 & 0 \\ -0.225 & 0.607 & -0.199 & -0.131 & 0.003 & 0.077 & -0.081 & 0 & 0 & 0 \\ -0.225 & -0.199 & 0.678 & -0.194 & 0.092 & -0.114 & 0.007 & 0 & 0 & 0 \\ -0.106 & -0.131 & -0.194 & 0.481 & -0.083 & 0.025 & 0.051 & 0 & 0 & 0 \\ -4.796 \cdot 10^{-6} & 0.003 & 0.092 & -0.083 & 0.116 & -0.004 & -0.008 & 0 & 0 & 0 \\ 0.019 & 0.077 & -0.114 & 0.025 & -0.004 & 0.123 & -0.005 & 0 & 0 & 0 \\ 0.037 & -0.081 & 0.007 & 0.051 & -0.008 & -0.005 & 0.116 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.084 & 0.015 & 0.013 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.015 & 0.087 & 0.021 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.013 & 0.021 & 0.089 \end{bmatrix}$$

$$\text{tr}(XTX^{-1}) = 2.882$$

$$|r| = 0.4$$

$$r^{-1} = \begin{bmatrix} 1.439 & -0.473 & -0.351 & 0.015 & -0.376 & -0.389 & 0 & 0 & 0 \\ -0.473 & 1.607 & -0.516 & 0.453 & -0.557 & 0.024 & 0 & 0 & 0 \\ -0.351 & -0.516 & 1.442 & -0.46 & 0.139 & 0.274 & 0 & 0 & 0 \\ 0.015 & 0.453 & -0.46 & 1.216 & -0.04 & -0.079 & 0 & 0 & 0 \\ 0.376 & -0.557 & 0.139 & -0.04 & 1.24 & -0.047 & 0 & 0 & 0 \\ -0.389 & 0.024 & 0.274 & -0.079 & -0.047 & 1.13 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.043 & 0.183 & 0.154 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.183 & 1.082 & 0.256 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.154 & 0.256 & 1.073 \end{bmatrix}$$

$$\text{tr}[r^{-1}] = 11.27$$

$$\rho = \begin{bmatrix} 1 & -0.408 & -0.386 & -0.217 & 1.971 \cdot 10^{-5} & 0.076 & 0.126 & 0 & 0 & 0 \\ -0.408 & 1 & -0.311 & -0.243 & 0 & 0.11 & 0.281 & -0.305 & 0 & 0 \\ -0.386 & -0.311 & 1 & -0.359 & 0 & 0.124 & -0.394 & 0.025 & 0 & 0 \\ -0.217 & -0.243 & -0.359 & 1 & -0.348 & 0.104 & 0.214 & 0 & 0 & 0 \\ -1.971 \cdot 10^{-5} & 0 & 0 & -0.348 & 1 & -0.033 & -0.067 & 0 & 0 & 0 \\ 0.076 & 0.281 & -0.394 & 0.104 & -0.033 & 1 & -0.04 & 0 & 0 & 0 \\ 0.126 & -0.305 & 0.025 & 0.214 & -0.067 & -0.04 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0.172 & 0.143 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.172 & 1 & 0.238 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.143 & 0.238 & 1 \end{bmatrix}$$

----- (8.9) A 4x3x3/16 design -----

DESIGN MATRIX

$$\begin{aligned} x_p^T &= (0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 1 \ 3 \ 0 \ 2 \ 0 \ 2) & x_{1i} &= (2xp_i - 3)/3 \\ x_q^T &= (0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 1 \ 0 \ 2 \ 1 \ 1 \ 0 \ 2 \ 1) & x_{2i} &= (xq_i - 1) \\ x_r^T &= (0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2 \ 1 \ 1) & x_{3i} &= (xr_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} X_{1.1} & := 1 & X_{1.2} & := x_1 & X_{1.3} & := x_2 & X_{1.4} & := x_3 \\ X_{1.5} & := x_1 \cdot x_2 & X_{1.6} & := x_1 \cdot x_3 & X_{1.7} & := x_2 \cdot x_3 \\ X_{1.8} & := x_1 & X_{1.9} & := x_2 & X_{1.10} & := x_3 \end{aligned}$$

$$\left| \frac{X^T X}{16} \right| = 2.217 \cdot 10^{-4}$$

$$X^T X = \begin{bmatrix} 16 & 12.444 & 12 & 12 & -2.667 & -1.333 & -2 & 0 & 0 & 0 \\ 12.444 & 12.049 & 10.222 & 10.222 & -2.074 & -1.926 & -0.222 & 0 & 0 & 0 \\ 12 & 10.222 & 12 & 10 & -2.667 & 0.667 & -2 & 0 & 0 & 0 \\ -2.667 & -2.074 & -2.667 & -0.667 & 10.222 & -0.222 & 0.667 & 0 & 0 & 0 \\ -1.333 & -1.926 & 0.667 & -1.333 & -0.222 & 10.222 & -0.667 & 0 & 0 & 0 \\ -2 & -0.222 & -2 & -2 & 0.667 & -0.667 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.444 & -2.667 & -1.333 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.667 & 12 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1.333 & -2 & 12 \end{bmatrix}$$

$$X^T X^{-1} = \begin{bmatrix} 0.461 & -0.245 & -0.122 & -0.143 & 0.027 & 0.006 & 0.032 & 0 & 0 & 0 \\ -0.245 & 0.629 & -0.198 & -0.133 & 0.011 & 0.076 & -0.097 & 0 & 0 & 0 \\ -0.122 & -0.198 & 0.511 & -0.138 & 0.048 & -0.101 & 0.036 & 0 & 0 & 0 \\ -0.143 & -0.133 & -0.138 & 0.461 & -0.072 & 0.026 & 0.039 & 0 & 0 & 0 \\ 0.027 & 0.011 & 0.048 & -0.072 & 0.115 & -0.005 & -0.007 & 0 & 0 & 0 \\ 0.006 & 0.076 & -0.101 & 0.026 & -0.005 & 0.123 & -0.004 & 0 & 0 & 0 \\ 0.032 & -0.097 & 0.036 & 0.039 & -0.007 & -0.004 & 0.12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.086 & 0.021 & 0.013 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.021 & 0.091 & 0.018 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.013 & 0.018 & 0.088 \end{bmatrix}$$

$$\text{tr}(X^T X^{-1}) = 2.684$$

$$|r| = 0.413$$

$$r^{-1} = \begin{bmatrix} 1.491 & -0.528 & -0.355 & 0.055 & 0.372 & -0.466 & 0 & 0 & 0 \\ -0.528 & 1.532 & -0.414 & 0.259 & 0.557 & -0.194 & 0 & 0 & 0 \\ -0.355 & -0.414 & 1.382 & -0.392 & 0.145 & 0.213 & 0 & 0 & 0 \\ -0.055 & 0.259 & -0.392 & 1.129 & -0.048 & -0.07 & 0 & 0 & 0 \\ -0.372 & -0.557 & 0.145 & -0.048 & 1.24 & -0.036 & 0 & 0 & 0 \\ -0.466 & 0.194 & 0.213 & -0.07 & -0.036 & 1.144 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.075 & 0.261 & 0.161 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.241 & 1.092 & 0.211 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.161 & 0.211 & 1.053 \end{bmatrix}$$

$$\text{tr}[r^{-1}] = 11.159$$

$$P = \begin{bmatrix} 1 & -0.455 & -0.251 & -0.311 & 0.119 & 0.025 & 0.138 & 0 & 0 & 0 \\ -0.455 & 1 & -0.349 & -0.248 & 0.042 & 0.274 & -0.353 & 0 & 0 & 0 \\ -0.251 & -0.349 & 1 & -0.285 & 0.197 & -0.404 & 0.145 & 0 & 0 & 0 \\ -0.311 & -0.248 & -0.285 & 1 & -0.314 & 0.111 & 0.168 & 0 & 0 & 0 \\ 0.119 & 0.042 & 0.197 & -0.314 & 1 & -0.04 & -0.061 & 0 & 0 & 0 \\ 0.025 & 0.274 & -0.404 & 0.111 & -0.04 & 1 & -0.03 & 0 & 0 & 0 \\ 0.138 & -0.353 & 0.145 & 0.168 & -0.061 & -0.03 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0.241 & 0.151 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.241 & 1 & 0.196 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.151 & 0.196 & 1 \end{bmatrix}$$

----- (8.10) A 3x3x3/16 design -----

DESIGN MATRIX

$$\begin{aligned} \mathbf{x}_p^T &= (0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 1 \ 2 \ 1 \ 2 \ 0 \ 1 \ 0 \ 1) & \mathbf{x}_{1j} &= (\mathbf{x}_{p_j} - 1) \\ \mathbf{x}_q^T &= (0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 1 \ 0 \ 2 \ 1 \ 1 \ 0 \ 2 \ 1) & \mathbf{x}_{2j} &= (\mathbf{x}_{q_j} - 1) \\ \mathbf{x}_r^T &= (0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2 \ 1 \ 1) & \mathbf{x}_{3j} &= (\mathbf{x}_{r_j} - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} \mathbf{x}_{1.1} &= 1 & \mathbf{x}_{1.2} &= \mathbf{x}_1 & \mathbf{x}_{1.3} &= \mathbf{x}_2 & \mathbf{x}_{1.4} &= \mathbf{x}_3 \\ \mathbf{x}_{1.5} &= \mathbf{x}_1 \cdot \mathbf{x}_2 & \mathbf{x}_{1.6} &= \mathbf{x}_1 \cdot \mathbf{x}_3 & \mathbf{x}_{1.7} &= \mathbf{x}_2 \cdot \mathbf{x}_3 \\ \mathbf{x}_{1.8} &= \mathbf{x}_1 & \mathbf{x}_{1.9} &= \mathbf{x}_2 & \mathbf{x}_{1.10} &= \mathbf{x}_3 \end{aligned}$$

$$\mathbf{X} \mathbf{X}^T = \begin{bmatrix} 16 & 12 & 12 & 12 & -2 & -2 & -2 & 0 & 0 & 0 \\ 12 & 12 & 10 & 10 & -2 & -2 & 0 & 0 & 0 & 0 \\ 12 & 10 & 12 & 10 & -2 & 0 & -2 & 0 & 0 & 0 \\ 12 & 10 & 10 & 12 & 0 & -2 & -2 & 0 & 0 & 0 \\ -2 & -2 & -2 & 0 & 10 & 0 & 0 & 0 & 0 & 0 \\ -2 & 0 & -2 & 0 & -2 & 0 & 10 & 0 & 0 & 0 \\ -2 & 0 & -2 & -2 & 0 & 0 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 12 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 12 \end{bmatrix} \quad \left| \frac{\mathbf{X} \mathbf{X}^T}{16} \right| = 2.687 \cdot 10^{-4}$$

$$\mathbf{X} \mathbf{X}^T \mathbf{X}^{-1} = \begin{bmatrix} 0.413 & -0.152 & -0.152 & -0.152 & 0.022 & 0.022 & 0.022 & 0 & 0 & 0 \\ -0.152 & 0.484 & -0.141 & -0.141 & 0.038 & 0.038 & -0.087 & 0 & 0 & 0 \\ -0.152 & -0.141 & 0.484 & -0.141 & 0.038 & -0.087 & 0.038 & 0 & 0 & 0 \\ 0.022 & 0.038 & 0.038 & -0.087 & 0.12 & -0.005 & -0.005 & 0 & 0 & 0 \\ 0.022 & 0.038 & -0.087 & 0.038 & -0.005 & 0.12 & -0.005 & 0 & 0 & 0 \\ 0.022 & -0.087 & 0.038 & 0.038 & -0.005 & -0.005 & 0.12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.089 & 0.018 & 0.018 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.018 & 0.089 & 0.018 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.018 & 0.018 & 0.089 \end{bmatrix}$$

tr($\mathbf{X} \mathbf{X}^T \mathbf{X}^{-1}$) = 2.491

|r| = 0.427

$$\mathbf{r}^{-1} = \begin{bmatrix} 1.451 & -0.424 & -0.424 & 0.206 & 0.206 & -0.47 & 0 & 0 & 0 & 0 \\ -0.424 & 1.451 & -0.424 & 0.206 & -0.47 & 0.206 & 0 & 0 & 0 & 0 \\ -0.424 & -0.424 & 1.451 & -0.47 & 0.206 & 0.206 & 0 & 0 & 0 & 0 \\ 0.206 & 0.206 & -0.47 & 1.166 & -0.053 & -0.053 & 0 & 0 & 0 & 0 \\ 0.206 & -0.47 & 0.206 & -0.053 & 1.166 & -0.053 & 0 & 0 & 0 & 0 \\ -0.47 & 0.206 & 0.206 & -0.053 & -0.053 & 1.166 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.071 & 0.214 & 0.214 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.214 & 1.071 & 0.214 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.214 & 0.214 & 1.071 & 0 \end{bmatrix}$$

tr(\mathbf{r}^{-1}) = 11.065

$$\mathbf{p} = \begin{bmatrix} 1 & -0.34 & -0.34 & -0.34 & 0.098 & 0.098 & 0.098 & 0 & 0 & 0 \\ -0.34 & 1 & -0.292 & -0.292 & 0.158 & 0.158 & -0.362 & 0 & 0 & 0 \\ -0.34 & -0.292 & 1 & -0.292 & 0.158 & -0.362 & 0.158 & 0 & 0 & 0 \\ -0.34 & -0.292 & -0.292 & 1 & -0.362 & 0.158 & 0.158 & 0 & 0 & 0 \\ 0.098 & 0.158 & 0.158 & -0.362 & 1 & -0.045 & -0.045 & 0 & 0 & 0 \\ 0.098 & 0.158 & -0.362 & 0.158 & -0.045 & 1 & -0.045 & 0 & 0 & 0 \\ 0.098 & -0.362 & 0.158 & 0.158 & -0.045 & -0.045 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 1 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 1 \end{bmatrix}$$

------(8.16) A 4x4x4x2/16 design -----

DESIGN MATRIX

$$\begin{aligned} xp^A &= (0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 2\ 2\ 3\ 3\ 3\ 3\ 3) & x1_1 &= (2xp_1-3)/3 \\ xq^A &= (0\ 0\ 1\ 1\ 3\ 3\ 3\ 2\ 3\ 0\ 0\ 0\ 0\ 3\ 3\ 3) & x2_1 &= (2xq_1-3)/3 \\ xr^A &= (0\ 3\ 1\ 3\ 0\ 1\ 3\ 0\ 3\ 0\ 2\ 0\ 3\ 0\ 1\ 3) & x3_1 &= (2xr_1-3)/3 \\ xs^A &= (0\ 1\ 1\ 0\ 1\ 0\ 1\ 0\ 1\ 1\ 0\ 0\ 1\ 0\ 1\ 0) & x4_1 &= (2xs_1-1) \end{aligned}$$

COLUMN VECTORS OF K-L MATRIX

$$\begin{aligned} X_{i,2} &:= x1_i^2 & X_{i,3} &:= x2_i^2 & X_{i,4} &:= x3_i^2 & X_{i,1} &:= 1 \\ X_{i,5} &:= x1_i \cdot x2_i & X_{i,6} &:= x1_i \cdot x3_i & X_{i,7} &:= x1_i \cdot x4_i & X_{i,8} &:= x2_i \cdot x3_i \\ X_{i,9} &:= x2_i \cdot x4_i & X_{i,10} &:= x3_i \cdot x4_i & & & & \\ X_{i,11} &:= x1_i & X_{i,12} &:= x2_i & X_{i,13} &:= x3_i & X_{i,14} &:= x4_i \end{aligned}$$

$$\left| \frac{KTK}{16} \right| = -7.67 \cdot 10^{-5}$$

$KTK =$

16	12.444	13.333	12.444	-0.444	-0.889	-2	0.445	0.667	3.333	-2	0.667	-0.667	0
12.444	12.049	10.568	9.679	0.543	-0.691	-2	-0.741	-0.074	2.741	-2	1.259	-0.074	0
13.333	10.568	13.037	10.568	-0.938	-0.593	-2.296	0.938	0.963	3.63	0.074	0.963	-0.37	0.889
12.444	9.679	10.568	12.049	-0.444	-1.284	-2.593	1.235	0.074	3.926	-1.407	0.074	-0.074	0
-0.444	0.543	-0.938	-0.444	10.568	-0.741	0.074	-0.593	-2.296	-1.111	1.259	0.074	0.222	-2.222
-0.889	-0.691	-0.593	-1.284	-0.741	9.679	2.741	-0.444	-1.111	-2.593	-0.074	0.222	-1.407	-0.444
-2	-2	-2.296	-2.593	0.074	2.741	12.444	-1.111	-0.444	-0.889	0	-2.222	-0.444	-2
0.445	-0.741	0.938	1.235	-0.593	-0.444	-1.111	10.568	3.63	0.074	0.222	-0.37	0.074	-0.889
0.667	0.074	0.963	0.074	-2.296	-1.111	-0.444	3.63	13.333	0.445	-2.222	0.889	-0.889	0.667
3.333	2.741	3.63	3.926	-1.111	-2.593	-0.889	0.074	0.445	12.444	-0.444	-0.889	0	-0.667
-2	-2	0.074	-1.407	1.259	-0.074	0	0.222	-2.222	-0.444	12.444	-0.444	-0.889	-2
-0.667	1.259	0.963	0.074	0.074	0.222	-2.222	-0.37	0.889	-0.889	-0.444	13.333	0.445	0.667
-0.667	-0.074	-0.37	-0.074	0.222	-1.407	-0.444	0.074	-0.889	0	-0.889	0.445	12.444	3.333
0	0	0.889	0	-2.222	-0.444	-2	-0.889	0.667	-0.667	-2	0.667	3.333	16

tr(KTK) = 3.719

$KTK^{-1} =$

0.986	-0.282	-0.522	-0.356	0.001	0.031	-0.048	0.024	-0.002	0.072	0.086	0.014	0.032	0.032
-0.282	0.493	-0.107	-0.009	-0.046	-0.005	0.016	0.055	-0.003	-0.002	0.038	-0.019	-0.015	0.013
-0.522	-0.107	0.738	-0.012	0.036	-0.04	0.021	-0.039	-0.028	-0.059	-0.127	-0.018	-0.007	-0.052
-0.356	-0.009	-0.012	0.5	0.005	0.007	0.037	-0.048	0.032	-0.051	0.002	0.016	-0.013	0.002
0.001	-0.046	0.036	0.005	0.11	0.012	-3.352 · 10 ⁻⁴	-0.004	0.015	0.01	-0.013	-6.938 · 10 ⁻⁵	-0.003	0.012
0.031	-0.005	-0.04	0.007	0.012	0.124	-0.027	-0.002	0.015	0.027	0.01	-0.004	0.015	0.003
-0.048	0.016	0.021	0.037	-3.352 · 10 ⁻⁴	-0.027	0.097	0.008	-0.002	-0.005	5.026 · 10 ⁻⁵	0.015	-0.005	0.011
0.024	0.055	-0.039	-0.048	-0.004	-0.002	0.008	0.12	-0.033	0.009	0.002	0.004	-0.006	0.012
-0.002	0.003	-0.028	0.032	0.015	0.015	-0.002	-0.033	0.094	-3.789 · 10 ⁻⁴	0.02	-0.006	0.009	-0.001
0.072	-0.002	-0.059	-0.051	0.01	0.027	-0.005	0.009	-3.789 · 10 ⁻⁴	0.103	0.01	0.007	0.002	0.01
0.086	0.038	-0.127	0.002	-0.013	0.01	5.026 · 10 ⁻⁵	0.002	0.02	0.01	0.11	0.003	0.007	0.017
0.014	-0.019	-0.018	0.016	-4.938 · 10 ⁻⁵	-0.004	0.015	0.004	-0.006	0.007	0.003	0.081	-0.003	0.001
0.032	-0.015	-0.007	-0.013	-0.003	0.015	-0.005	-0.006	0.009	0.002	0.007	-0.003	0.009	-0.018
0.032	0.013	-0.052	0.002	0.012	0.003	0.011	0.012	-0.001	0.01	0.017	0.001	-0.016	0.076

------(8,17) A 4x4x3x2/16 design -----

DESIGN MATRIX

$$\begin{aligned} x p^T &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 3 \ 3) & x_{1_i} &= (2xp_i - 3)/3 \\ x q^T &= (0 \ 0 \ 1 \ 1 \ 3 \ 3 \ 3 \ 2 \ 3 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3) & x_{2_i} &= (2xq_i - 3)/3 \\ x r^T &= (0 \ 2 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2) & x_{3_i} &= (xr_i - 1) \\ x s^T &= (0 \ 1 \ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 1 \ 1 \ 0 \ 0 \ 1 \ 0 \ 1 \ 0) & x_{4_i} &= (2xs_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$x_{1,1} := 1$ $x_{1,2} := x_1^2$ $x_{1,3} := x_2^2$ $x_{1,4} := x_3^2$
 $x_{1,5} := x_1 \cdot x_2$ $x_{1,6} := x_1 \cdot x_3$ $x_{1,7} := x_1 \cdot x_4$ $x_{1,8} := x_2 \cdot x_3$
 $x_{1,9} := x_2 \cdot x_4$ $x_{1,10} := x_3 \cdot x_4$ $x_{1,11} := x_1$ $x_{1,12} := x_2$ $x_{1,13} := x_3$ $x_{1,14} := x_4$

X1X :

16	12.444	13.333	12	-0.444	-1.333	-2	1.333	0.667	4	-2	0.667	0	0
12.444	12.049	10.568	9.333	0.543	-1.037	-2	-0.148	0.074	3.111	-2	1.259	0.889	0
13.333	10.568	13.037	10.222	-0.938	-0.741	-2.296	1.926	0.963	4	0.074	0.963	0	0.889
12	0.333	10.222	12	-0.444	-1.333	-2.667	1.333	0	4	-1.333	0	0	0
-0.444	-0.543	-0.938	-0.444	10.568	-0.148	0.074	-0.741	-2.296	-0.444	1.259	0.074	0.444	-2.222
-1.333	-1.037	-0.741	-1.333	-0.148	9.333	3.111	-0.444	-0.444	-2.667	0.889	0.444	-1.333	-1.10
-2	-2.296	-0.074	-2.667	0.074	3.111	12.444	-0.444	-0.444	-1.333	0	-2.222	-1.10	-2
1.333	-0.148	1.926	1.333	-0.741	-0.444	-0.444	10.222	4	0	0.444	0	0	-1.333
0.667	0.074	0.963	0	-2.296	-0.444	-0.444	4	13.333	1.333	-2.222	0.889	-1.333	0.667
4	3.111	4	4	-0.444	-2.667	-1.333	0	1.333	12	-1.10	-1.333	0	0
-2	-2	0.074	-1.333	1.259	0.889	0	0.444	-2.222	-1.10	12.444	-0.444	-1.333	-2
0.667	1.259	0.963	0	0.074	0.444	-2.222	0	0.889	-1.333	-0.444	13.333	1.333	0.667
0	0.889	0	0	0.444	-1.333	-1.10	0	-1.333	0	-1.333	1.333	12	4
0	0	0.889	0	-2.222	-1.10	-2	-1.333	0.667	0	-2	0.667	4	16

$$\left| \frac{X1X}{16} \right| = 4.524 \cdot 10^{-5}$$

$$\text{tr}(X1X) = 3.558$$

X1X1 :

0.881	-0.291	-0.496	-0.241	-0.005	0.041	-0.049	0.005	0.001	0.032	0.077	0.012	0.026	0.024
-0.291	0.514	-0.131	-0.002	-0.044	-0.005	0.017	0.072	-0.006	0.006	0.037	-0.016	-0.04	0.025
-0.496	-0.131	0.746	-0.025	0.043	-0.04	0.021	-0.07	-0.01	-0.047	-0.117	-0.018	0.01	-0.054
-0.241	-0.002	-0.025	0.368	0.006	-0.007	0.037	-0.02	0.025	-0.032	0.007	0.016	-5.546 \cdot 10^{-4}	0.004
-0.005	-0.044	0.043	0.006	0.108	5.994 \cdot 10^{-4}	0.003	-0.004	0.014	-5.85 \cdot 10^{-4}	-0.014	-5.315 \cdot 10^{-4}	-0.004	0.011
0.041	-0.005	-0.04	-0.007	5.994 \cdot 10^{-4}	0.131	-0.035	0.006	0.002	0.027	-0.003	-0.008	0.018	-0.006
-0.049	0.017	0.021	0.037	0.003	-0.035	0.101	0.003	2.734 \cdot 10^{-4}	-0.002	0.003	0.018	-0.012	0.015
0.005	0.072	-0.07	-0.02	-0.004	0.006	0.003	0.132	-0.04	0.016	3.535 \cdot 10^{-4}	0.003	-0.016	0.02
0.001	-0.006	-0.01	0.025	0.014	0.002	2.734 \cdot 10^{-4}	-0.04	0.097	-0.014	0.02	-0.007	0.016	-0.006
0.032	0.006	-0.047	-0.032	-5.85 \cdot 10^{-4}	0.027	-0.002	0.016	-0.014	0.106	-0.001	0.011	-0.002	0.004
0.077	0.037	-0.117	0.007	-0.014	-0.003	0.003	3.535 \cdot 10^{-4}	0.02	-0.001	0.109	0.003	0.006	0.016
0.012	-0.016	-0.018	0.016	-5.315 \cdot 10^{-4}	-0.008	0.018	0.003	-0.007	0.011	0.003	0.083	-0.01	0.003
0.026	-0.04	0.01	-5.546 \cdot 10^{-4}	-0.004	0.018	-0.012	-0.016	0.016	-0.002	0.006	-0.01	0.102	-0.029
0.024	0.025	-0.054	0.004	0.011	-0.006	0.015	0.02	-0.006	0.004	0.016	0.003	-0.029	0.08

DESIGN (8.17) CONTINUED

$$|r| = 0.272$$

$$t_r \begin{bmatrix} \tau \\ r \\ 1 \end{bmatrix} = 16.07$$

A22

$$r^{-1} = \begin{bmatrix} 1.219 & -0.281 & -0.004 & -0.22 & -0.023 & 0.091 & 0.351 & -0.035 & 0.03 & 0.198 & -0.092 & -0.214 & 0.153 \\ -0.281 & 1.437 & -0.059 & 0.196 & -0.169 & 0.103 & -0.309 & -0.053 & -0.215 & -0.568 & -0.092 & 0.046 & -0.302 \\ -0.004 & -0.059 & 1.105 & 0.031 & -0.035 & 0.225 & -0.108 & 0.156 & -0.183 & 0.041 & 0.099 & -0.003 & 0.031 \\ -0.22 & 0.196 & 0.031 & 1.137 & 0.006 & 0.029 & -0.045 & 0.166 & -0.006 & -0.164 & -0.006 & -0.05 & 0.146 \\ -0.023 & -0.169 & -0.035 & 0.006 & 1.212 & -0.372 & 0.056 & 0.019 & 0.275 & -0.036 & -0.087 & 0.186 & -0.075 \\ 0.091 & 0.103 & 0.225 & 0.029 & -0.372 & 1.234 & 0.028 & 0.003 & -0.023 & 0.031 & 0.225 & -0.142 & 0.203 \\ 0.351 & -0.309 & -0.108 & -0.045 & 0.056 & 0.028 & 1.339 & -0.465 & 0.169 & 0.004 & 0.037 & -0.176 & 0.257 \\ -0.035 & -0.053 & 0.156 & 0.166 & 0.019 & 0.003 & -0.465 & 1.295 & -0.172 & 0.25 & -0.098 & 0.202 & -0.089 \\ 0.03 & -0.215 & -0.183 & -0.006 & 0.275 & -0.023 & 0.169 & -0.172 & 1.164 & -0.013 & 0.138 & -0.019 & 0.053 \\ 0.198 & -0.568 & 0.041 & -0.164 & -0.036 & 0.031 & 0.004 & 0.25 & -0.013 & 1.323 & 0.033 & 0.073 & 0.223 \\ -0.092 & -0.092 & 0.099 & -0.006 & -0.087 & 0.225 & 0.037 & -0.098 & 0.138 & 0.033 & 1.105 & -0.132 & 0.047 \\ -0.214 & 0.046 & -0.003 & -0.05 & 0.186 & -0.142 & -0.176 & 0.202 & -0.019 & 0.073 & -0.132 & 1.22 & -0.4 \\ 0.153 & -0.302 & 0.031 & 0.146 & -0.075 & 0.203 & 0.257 & -0.089 & 0.053 & 0.223 & 0.047 & -0.4 & 1.279 \end{bmatrix}$$

$$p = \begin{bmatrix} 1 & -0.432 & -0.612 & -0.424 & -0.015 & 0.121 & -0.165 & 0.013 & 0.004 & 0.106 & 0.247 & 0.043 & 0.086 & 0.09 \\ -0.432 & 1 & -0.212 & -0.004 & -0.187 & -0.019 & 0.074 & 0.275 & -0.027 & 0.025 & 0.156 & -0.079 & -0.175 & 0.123 \\ -0.612 & -0.212 & 1 & -0.047 & 0.153 & -0.128 & 0.078 & -0.223 & -0.039 & -0.166 & -0.412 & -0.073 & 0.035 & -0.223 \\ -0.424 & -0.004 & -0.047 & 1 & 0.028 & -0.03 & 0.193 & -0.089 & 0.13 & -0.161 & 0.034 & 0.089 & -0.003 & 0.026 \\ -0.015 & -0.187 & 0.153 & 0.028 & 1 & 0.005 & 0.025 & -0.037 & 0.137 & -0.005 & -0.134 & -0.006 & -0.042 & 0.121 \\ 0.121 & -0.019 & -0.128 & -0.03 & 0.005 & 1 & -0.304 & 0.044 & 0.015 & 0.232 & -0.028 & -0.075 & 0.153 & -0.06 \\ -0.165 & 0.074 & 0.078 & 0.193 & 0.025 & -0.304 & 1 & 0.022 & 0.003 & -0.02 & 0.025 & 0.193 & -0.116 & 0.162 \\ 0.013 & 0.275 & -0.223 & -0.089 & -0.037 & 0.044 & 0.022 & 1 & -0.353 & 0.135 & 0.003 & 0.03 & -0.138 & 0.197 \\ 0.004 & -0.027 & -0.039 & 0.13 & 0.137 & 0.015 & 0.003 & -0.353 & 1 & -0.14 & 0.191 & -0.082 & 0.161 & -0.069 \\ 0.106 & 0.025 & -0.166 & -0.161 & -0.005 & 0.232 & -0.02 & 0.135 & -0.14 & 1 & -0.01 & 0.122 & -0.016 & 0.043 \\ 0.247 & 0.156 & -0.412 & 0.034 & -0.134 & -0.028 & 0.025 & 0.003 & 0.191 & -0.01 & 1 & 0.027 & 0.058 & 0.172 \\ 0.043 & -0.079 & -0.073 & 0.089 & -0.006 & -0.075 & 0.193 & 0.03 & -0.082 & 0.122 & 0.027 & 1 & -0.114 & 0.039 \\ 0.086 & -0.175 & 0.035 & -0.003 & -0.042 & 0.153 & -0.116 & -0.138 & 0.161 & -0.016 & 0.058 & -0.114 & 1 & -0.32 \\ 0.09 & 0.123 & -0.223 & 0.026 & 0.121 & -0.06 & 0.162 & 0.197 & -0.069 & 0.043 & 0.172 & 0.039 & -0.32 & 1 \end{bmatrix}$$

DESIGN MATRIX

$$\begin{aligned}
 xp^m &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 3) & x1_i &= (2xp_i - 3)/3 \\
 xq^m &= (0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 2 \ 1 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2) & x2_i &= (xq_i - 1) \\
 xr^m &= (0 \ 2 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 2 \ 0 \ 1) & x3_i &= (xr_i - 1) \\
 xs^m &= (0 \ 1 \ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 1 \ 1 \ 0 \ 0 \ 1 \ 0 \ 1) & x4_i &= (2xs_i - 1)
 \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

x	:= 1	x	:= x1	x	:= x2	x	:= x3		
i,1		i,2		i,3		i,4			
x	:= x1 * x2	x	:= x1 * x3	x	:= x1 * x4	x	:= x2 * x3		
i,5		i,6		i,7		i,8			
x	:= x2 * x4	x	:= x3 * x4	x	:= x1	x	:= x2	x	:= x3
i,9		i,10		i,11		i,12		i,13	i,14

XTX =

16	12.444	13	12	-1	-1.333	-2	2	1	4	-2	1	0	0
12.444	12.049	10.333	9.333	-0.111	-1.037	-2	0.222	0.111	3.111	-2	1.889	0.889	0
13	10.333	13	10	-1	-0.667	-2.333	2	1	4	0.333	1	0	1
12	9.333	10	12	-0.667	-1.333	-2.667	2	0	4	-1.333	0	0	0
-1	-0.111	-1	-0.667	10.333	0.222	0.111	-0.667	-2.333	0	1.889	0.333	0	-2.333
-1.333	-1.037	-0.667	-1.333	0.222	9.333	3.111	-0.667	0	-2.667	0.889	0	-1.333	1.10
-2	-2	-2.333	-2.667	0.111	3.111	12.444	0	-1	-1.333	0	-2.333	1.10	-2
2	0.222	2	2	-0.667	-0.667	0	10	4	0	0	0	0	-2
1	0.111	1	0	-2.333	0	-1	4	13	2	-2.333	1	-2	1
4	3.111	4	4	0	-2.667	-1.333	0	2	12	1.10	-2	0	0
-2	-2	0.333	-1.333	1.889	0.889	0	0	-2.333	1.10	12.444	-1	-1.333	-2
1	1.889	1	0	0.333	0	-2.333	0	1	-2	-1	13	2	1
0	0.889	0	0	0	-1.333	1.10	0	-2	0	-1.333	2	12	4
0	0	1	0	-2.333	1.10	-2	-2	1	0	-2	1	4	16

$$|XTX| = 4.292 \cdot 10^{-5}$$

$$tr(XTX) = 3.357$$

XTXi =

0.79	-0.324	-0.356	-0.249	0.01	0.037	-0.048	-0.015	-0.021	0.031	0.056	0.011	0.023	0.018
-0.324	0.523	-0.097	-0.012	-0.03	-0.002	0.011	0.079	-9.376 · 10 ⁻⁴	0.004	0.036	-0.034	-0.039	0.029
-0.356	-0.097	0.554	-0.018	0.022	-0.037	0.022	-0.045	-9.278 · 10 ⁻⁵	-0.042	-0.098	-0.01	0.01	-0.048
-0.249	-0.012	-0.018	0.386	0.003	-0.012	0.043	-0.043	0.045	-0.038	0.011	0.021	0.006	-0.003
0.01	-0.03	0.022	0.003	0.109	-0.005	0.003	-0.004	0.017	-0.008	-0.015	-0.005	-3.873 · 10 ⁻⁴	0.012
0.037	-0.002	-0.037	-0.012	-0.005	0.132	-0.036	0.014	-0.011	0.031	-0.005	-0.003	0.014	-0.004
-0.048	0.011	0.022	0.043	0.003	-0.036	0.102	-0.008	0.01	-0.004	0.004	0.018	-0.01	0.012
-0.015	0.079	-0.045	-0.043	-0.004	0.014	-0.008	0.146	-0.052	0.025	-0.001	7.845 · 10 ⁻⁴	-0.023	0.028
-0.021	-9.376 · 10 ⁻⁴	-9.278 · 10 ⁻⁵	0.045	0.017	-0.011	0.01	-0.052	0.112	-0.029	0.02	-0.011	0.026	-0.013
0.031	0.004	-0.042	-0.038	-0.008	0.031	-0.004	0.025	-0.029	0.114	-0.002	0.02	-0.007	0.006
0.056	0.036	0.098	0.011	-0.015	-0.005	0.004	-0.001	0.02	-0.002	0.109	0.004	0.007	0.015
0.011	-0.034	-0.01	0.021	-0.005	-0.003	0.015	7.845 · 10 ⁻⁴	-0.011	0.02	0.004	0.092	-0.015	0.001
0.023	-0.039	0.01	0.006	-3.873 · 10 ⁻⁴	0.014	-0.01	-0.023	0.026	-0.007	0.007	-0.015	0.106	-0.031
0.018	0.029	-0.048	-0.003	0.012	-0.004	0.012	0.028	-0.013	0.006	0.015	0.001	-0.031	0.083

DESIGN (8,18) CONTINUED

$|r| = 0.23$

$\text{tr} \begin{bmatrix} & -1 \\ r & \end{bmatrix} = 16.564$

A24

$r^{-1} =$

1.239	-0.232	-0.033	-0.147	-0.009	0.058	0.38	-0.005	0.021	0.191	-0.187	-0.21	0.181
-0.232	1.351	-0.048	0.11	-0.176	0.122	-0.217	-5.21 · 10 ⁻⁴	-0.22	-0.533	-0.054	0.053	-0.302
-0.033	-0.048	1.158	0.017	-0.062	0.262	-0.231	0.28	-0.221	0.064	0.129	0.034	-0.018
-0.147	0.11	0.017	1.119	-0.047	0.036	-0.036	0.192	-0.087	-0.168	-0.056	-0.004	0.153
-0.009	-0.176	-0.062	-0.047	1.22	-0.377	0.136	-0.119	0.314	-0.05	-0.029	0.152	-0.053
0.058	0.122	0.262	0.036	-0.377	1.249	-0.082	0.128	-0.043	0.053	0.229	-0.117	0.169
0.38	-0.217	-0.231	-0.036	0.136	-0.082	1.421	-0.582	0.254	-0.011	0.009	-0.244	0.353
-0.005	-5.21 · 10 ⁻⁴	0.28	0.192	-0.119	0.128	-0.582	1.454	-0.352	0.255	-0.148	0.325	-0.188
0.021	-0.22	-0.221	-0.087	0.314	-0.043	0.254	-0.352	1.252	-0.025	0.24	0.085	0.083
0.191	-0.533	0.064	-0.168	-0.05	0.053	-0.011	0.255	-0.025	1.324	0.044	0.082	0.205
-0.187	-0.054	0.129	-0.056	-0.029	0.229	0.009	-0.148	0.24	0.044	1.185	-0.188	0.021
-0.21	0.053	0.034	-0.004	0.152	-0.117	-0.244	0.325	-0.085	0.082	-0.188	1.27	-0.429
0.181	-0.302	-0.018	0.153	-0.053	0.169	0.353	-0.188	0.083	0.205	0.021	-0.429	1.322

$\rho =$

1	-0.504	-0.539	-0.45	0.034	0.116	-0.17	-0.043	-0.072	0.102	0.191	0.039	0.08	0.069
-0.504	1	-0.179	-0.027	-0.125	-0.007	0.046	0.286	-0.004	0.016	0.149	-0.154	-0.167	0.141
-0.539	-0.179	1	-0.038	0.089	-0.137	0.094	-0.157	-3.717 · 10 ⁻⁴	-0.169	-0.398	-0.043	0.041	-0.226
-0.45	-0.027	-0.038	1	0.015	-0.052	0.218	-0.18	0.216	-0.184	0.051	0.11	0.028	-0.014
0.034	-0.125	0.089	0.015	1	-0.04	0.031	-0.029	0.151	-0.073	-0.138	-0.049	-0.004	0.126
0.116	-0.007	-0.137	-0.052	-0.04	1	-0.305	0.103	-0.089	0.254	-0.039	-0.024	0.122	-0.042
-0.17	0.046	0.094	0.218	0.031	-0.305	1	-0.062	0.095	-0.035	0.041	0.189	-0.093	0.132
-0.043	0.286	-0.157	-0.18	-0.029	0.103	-0.062	1	-3.405	0.191	-0.008	0.007	-0.182	0.257
-0.072	-0.004	-3.717 · 10 ⁻⁴	0.216	0.151	-0.089	0.095	-0.405	1	-0.261	0.184	-0.113	0.239	-0.136
0.102	0.016	-0.169	-0.184	-0.073	0.254	-0.035	0.191	-0.261	1	-0.019	0.197	-0.068	0.064
0.191	0.149	-0.398	0.051	-0.138	-0.039	0.041	-0.008	0.184	-0.019	1	0.035	0.064	0.155
0.039	-0.154	-0.043	0.11	-0.049	-0.024	0.189	0.007	-0.113	0.197	0.035	1	-0.153	0.017
0.08	-0.167	0.041	0.028	-0.004	0.122	-0.093	-0.182	0.239	-0.068	0.064	-0.153	1	-0.331
0.069	0.141	-0.226	-0.014	0.126	-0.042	0.132	0.257	-0.136	0.064	0.155	0.017	-0.331	1

DESIGN MATRIX

$$\begin{aligned}
 xp^H &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 1 \ 2 \ 2 \ 2 \ 2) & x1_i &= (xp_i - 1) \\
 xq^H &= (0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 2 \ 1 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2) & x2_i &= (xq_i - 1) \\
 xr^H &= (0 \ 2 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2) & x3_i &= (xr_i - 1) \\
 xs^H &= (0 \ 1 \ 1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 1 \ 1 \ 0 \ 0 \ 1 \ 0 \ 1 \ 0) & x4_i &= (2xs_i - 1)
 \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned}
 x_{i,1} &:= 1 & x_{i,2} &:= x1_i^2 & x_{i,3} &:= x2_i^2 & x_{i,4} &:= x3_i^2 \\
 x_{i,5} &:= x1_i \cdot x2_i & x_{i,6} &:= x1_i \cdot x3_i & x_{i,7} &:= x1_i \cdot x4_i & x_{i,8} &:= x2_i \cdot x3_i \\
 x_{i,9} &:= x2_i \cdot x4_i & x_{i,10} &:= x3_i \cdot x4_i \\
 x_{i,11} &:= x1_i & x_{i,12} &:= x2_i & x_{i,13} &:= x3_i & x_{i,14} &:= x4_i
 \end{aligned}$$

A25

$$XTX = \begin{bmatrix}
 16 & 12 & 13 & 12 & 0 & -1 & -2 & 2 & 1 & 4 & -2 & 1 & 0 & 0 \\
 12 & 12 & 10 & 9 & 0 & -1 & -2 & 0 & 0 & 3 & -2 & 2 & 1 & 0 \\
 13 & 10 & 13 & 10 & 0 & 0 & -2 & 2 & 1 & 4 & 0 & 1 & 0 & 1 \\
 12 & 9 & 10 & 12 & 0 & -1 & -3 & 2 & 0 & 4 & -1 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 10 & 0 & 0 & 0 & -2 & 0 & 2 & 0 & 0 & -2 \\
 -1 & -1 & 0 & -1 & 0 & 9 & 3 & 0 & 0 & -3 & 1 & 0 & -1 & 1 \\
 -2 & -2 & -2 & -3 & 0 & 3 & 12 & 0 & 0 & -1 & 0 & -2 & 1 & -2 \\
 2 & 0 & 2 & 2 & 0 & 0 & 0 & 10 & 4 & 0 & 0 & 0 & 0 & -2 \\
 1 & 0 & 1 & 0 & -2 & 0 & 0 & 4 & 13 & 2 & -2 & 1 & -2 & 1 \\
 4 & 3 & 4 & 4 & 0 & -3 & -1 & 0 & 2 & 12 & 1 & -2 & 0 & 0 \\
 -2 & -2 & 0 & -1 & 2 & 1 & 0 & 0 & -2 & 1 & 12 & 0 & -1 & -2 \\
 1 & 2 & 1 & 0 & 0 & 0 & -2 & 0 & 1 & -2 & 0 & 13 & 2 & 1 \\
 0 & 1 & 0 & 0 & 0 & -1 & 1 & 0 & -2 & 0 & -1 & 2 & 12 & 4 \\
 0 & 0 & 1 & 0 & -2 & 1 & -2 & -2 & 1 & 0 & -2 & 1 & 4 & 16
 \end{bmatrix}$$

$$\left| \frac{XTX}{16} \right| = 4.543 \cdot 10^{-5}$$

$$tr(XTX) = 3.197$$

$$XTX^{-1} = \begin{bmatrix}
 0.724 & -0.235 & -0.354 & -0.266 & -0.013 & 0.048 & -0.054 & -0.01 & -0.02 & 0.031 & 0.056 & 0.001 & 0.025 & 0.011 \\
 -0.235 & 0.41 & -0.081 & -0.01 & 4.444 \cdot 10^{-4} & 0.002 & 0.015 & 0.071 & 0.002 & -4.038 \cdot 10^{-4} & 0.03 & -0.033 & -0.037 & 0.031 \\
 -0.354 & -0.081 & 0.525 & -0.009 & 0.006 & -0.053 & 0.014 & -0.041 & 6.482 \cdot 10^{-4} & -0.04 & -0.073 & -0.003 & 0.01 & -0.044 \\
 -0.266 & -0.01 & -0.009 & 0.397 & 0.009 & -0.02 & 0.058 & -0.039 & 0.038 & -0.04 & -0.003 & 0.023 & -0.004 & 0.002 \\
 -0.013 & 4.444 \cdot 10^{-4} & 0.006 & 0.009 & 0.108 & -0.002 & 0.003 & -0.004 & 0.015 & -0.002 & -0.015 & -0.001 & -0.003 & 0.011 \\
 0.048 & 0.002 & -0.053 & -0.02 & -0.002 & 0.149 & -0.044 & 0.003 & -0.005 & 0.043 & -0.011 & -0.002 & 0.02 & -0.017 \\
 -0.054 & 0.015 & 0.014 & 0.058 & 0.003 & -0.044 & 0.113 & 0.003 & -0.002 & -0.008 & 0.003 & 0.019 & -0.025 & 0.022 \\
 -0.01 & 0.071 & -0.041 & -0.039 & -0.004 & 0.003 & 0.002 & 0.144 & -0.051 & 0.022 & -2.726 \cdot 10^{-4} & 0.002 & -0.024 & 0.029 \\
 -0.02 & 0.002 & 6.482 \cdot 10^{-4} & 0.038 & 0.015 & -0.005 & -0.002 & -0.051 & 0.11 & -0.03 & 0.019 & -0.015 & 0.027 & -0.015 \\
 0.031 & -4.038 \cdot 10^{-4} & -0.04 & -0.04 & -0.002 & 0.043 & -0.068 & 0.022 & -0.03 & 0.12 & -0.017 & 0.021 & -0.006 & 0.001 \\
 0.056 & 0.03 & -0.073 & -0.003 & -0.015 & -0.011 & 0.003 & -2.726 \cdot 10^{-4} & 0.019 & -0.017 & 0.108 & -0.009 & 0.005 & 0.016 \\
 0.001 & -0.033 & -0.003 & 0.023 & -0.001 & -0.002 & 0.019 & 0.002 & -0.015 & 0.021 & -0.009 & 0.092 & -0.018 & 0.001 \\
 0.025 & -0.037 & 0.01 & -0.004 & -0.003 & 0.02 & -0.025 & -0.024 & 0.027 & -0.006 & 0.005 & -0.018 & 0.11 & -0.036 \\
 0.011 & 0.031 & -0.044 & 0.002 & 0.011 & -0.017 & 0.022 & 0.029 & -0.015 & 0.001 & 0.016 & 0.001 & -0.036 & 0.086
 \end{bmatrix}$$

DESIGN (8.19) CONTINUED

$$|r| = 0.219$$

$$tr \begin{bmatrix} & -1 \\ r & \end{bmatrix} = 16.755$$

A26

$$r^{-1} = \begin{bmatrix} 1.229 & -0.218 & -0.003 & 0.002 & 0.011 & 0.091 & 0.382 & 0.012 & -0.002 & 0.18 & -0.207 & -0.223 & 0.213 \\ -0.218 & 1.279 & -0.025 & 0.029 & -0.249 & 0.075 & -0.201 & 0.004 & -0.209 & -0.389 & -0.017 & 0.055 & -0.272 \\ -0.003 & -0.025 & 1.191 & 0.047 & -0.102 & 0.343 & -0.211 & 0.235 & -0.232 & -0.018 & 0.143 & -0.025 & 0.014 \\ 0.002 & 0.029 & 0.047 & 1.083 & -0.021 & 0.036 & -0.042 & 0.175 & -0.025 & -0.161 & -0.012 & -0.03 & 0.14 \\ 0.011 & -0.249 & -0.102 & -0.021 & 1.329 & -0.45 & 0.031 & -0.05 & 0.423 & -0.111 & -0.017 & 0.21 & -0.207 \\ 0.091 & 0.075 & 0.343 & 0.036 & -0.45 & 1.328 & 0.018 & -0.027 & -0.093 & 0.041 & 0.236 & -0.297 & 0.305 \\ 0.382 & -0.201 & -0.211 & -0.042 & 0.031 & 0.018 & 1.406 & -0.569 & 0.232 & -0.003 & 0.025 & -0.263 & 0.364 \\ 0.012 & 0.004 & 0.235 & 0.175 & -0.05 & -0.027 & -0.569 & 1.428 & -0.361 & 0.229 & -0.198 & 0.337 & -0.213 \\ -0.002 & -0.209 & -0.232 & -0.025 & 0.423 & -0.093 & 0.232 & -0.361 & 1.321 & -0.191 & 0.253 & -0.071 & 0.018 \\ 0.18 & -0.389 & -0.018 & -0.161 & -0.111 & 0.041 & -0.003 & 0.229 & -0.191 & 1.272 & -0.108 & 0.056 & 0.213 \\ -0.207 & -0.017 & 0.143 & -0.012 & -0.017 & 0.236 & 0.025 & -0.198 & 0.253 & -0.108 & 1.193 & -0.225 & 0.021 \\ -0.223 & 0.055 & -0.025 & -0.03 & 0.21 & -0.297 & -0.263 & 0.337 & -0.071 & 0.056 & -0.225 & 1.321 & -0.497 \\ 0.213 & -0.272 & 0.014 & 0.14 & -0.207 & 0.305 & 0.364 & -0.213 & 0.018 & 0.213 & 0.021 & -0.497 & 1.374 \end{bmatrix}$$

$$p = \begin{bmatrix} 1 & -0.432 & -0.575 & -0.496 & -0.046 & 0.147 & -0.187 & -0.032 & -0.072 & 0.104 & 0.198 & 0.004 & 0.09 & 0.045 \\ -0.432 & 1 & -0.174 & -0.025 & 0.002 & 0.009 & 0.071 & 0.29 & 0.009 & -0.002 & 0.144 & -0.171 & -0.175 & 0.164 \\ -0.575 & -0.174 & 1 & -0.02 & 0.025 & -0.191 & 0.058 & -0.15 & 0.003 & -0.161 & -0.305 & -0.014 & 0.042 & -0.205 \\ -0.496 & -0.025 & -0.02 & 1 & 0.041 & -0.081 & 0.273 & -0.163 & 0.18 & -0.185 & -0.015 & 0.12 & -0.02 & 0.011 \\ -0.046 & 0.002 & 0.025 & 0.041 & 1 & -0.018 & 0.03 & -0.034 & 0.141 & -0.021 & -0.137 & -0.01 & -0.025 & 0.115 \\ 0.147 & 0.009 & -0.191 & -0.081 & -0.018 & 1 & -0.338 & 0.023 & -0.036 & 0.319 & -0.085 & -0.013 & 0.158 & -0.153 \\ -0.187 & 0.071 & 0.058 & 0.273 & 0.03 & -0.338 & 1 & 0.013 & -0.02 & -0.07 & 0.031 & 0.187 & -0.224 & 0.226 \\ -0.032 & 0.29 & -0.15 & -0.163 & -0.034 & 0.023 & 0.013 & 1 & -0.402 & 0.17 & -0.002 & 0.019 & -0.193 & 0.262 \\ -0.072 & 0.009 & 0.003 & 0.18 & 0.141 & -0.036 & -0.02 & -0.402 & 1 & -0.263 & 0.17 & -0.151 & 0.246 & -0.152 \\ 0.104 & -0.002 & -0.161 & -0.185 & -0.021 & 0.319 & -0.07 & 0.17 & -0.263 & 1 & -0.148 & 0.201 & -0.053 & 0.013 \\ 0.198 & 0.144 & -0.305 & -0.015 & -0.137 & -0.085 & 0.031 & -0.002 & 0.17 & -0.148 & 1 & -0.087 & 0.043 & 0.161 \\ 0.004 & -0.171 & -0.014 & 0.12 & -0.01 & -0.013 & 0.187 & 0.019 & -0.151 & 0.201 & -0.087 & 1 & -0.179 & 0.016 \\ 0.09 & -0.175 & 0.042 & -0.02 & -0.025 & 0.158 & -0.224 & -0.193 & 0.246 & -0.053 & 0.043 & -0.179 & 1 & -0.369 \\ 0.045 & 0.164 & -0.205 & 0.011 & 0.115 & -0.153 & 0.226 & 0.262 & -0.152 & 0.013 & 0.161 & 0.016 & -0.369 & 1 \end{bmatrix}$$

DESIGN MATRIX

$$\begin{aligned} xp^i &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 3 \ 3) & x1_i &= (2xp_i - 3)/3 \\ xq^i &= (0 \ 0 \ 1 \ 1 \ 3 \ 3 \ 3 \ 2 \ 3 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3) & x2_i &= (2xq_i - 3)/3 \\ xr^i &= (0 \ 3 \ 1 \ 3 \ 0 \ 1 \ 3 \ 0 \ 3 \ 0 \ 2 \ 0 \ 3 \ 0 \ 1 \ 3) & x3_i &= (2xr_i - 3)/3 \\ xs^i &= (0 \ 1 \ 3 \ 0 \ 3 \ 0 \ 1 \ 1 \ 3 \ 3 \ 0 \ 0 \ 3 \ 0 \ 3 \ 0) & x4_i &= (2xs_i - 3)/3 \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$x_{i,1} := 1$ $x_{i,2} := x1$ $x_{i,3} := x2$ $x_{i,4} := x3$ $x_{i,5} := x4$
 $x_{i,6} := x1 \cdot x2$ $x_{i,7} := x1 \cdot x3$ $x_{i,8} := x1 \cdot x4$ $x_{i,9} := x2 \cdot x3$
 $x_{i,10} := x2 \cdot x4$ $x_{i,11} := x3 \cdot x4$
 $x_{i,12} := x1^2$ $x_{i,13} := x2^2$ $x_{i,14} := x3^2$ $x_{i,15} := x4^2$

	16	12.444	13.333	12.444	13.333	-0.444	-0.889	0.444	0.445	0.889	1.10	-2	0.667	-0.667	-2
XTX	12.444	12.049	10.568	9.679	10.568	0.543	-0.691	0.642	-0.741	0.099	1.10	-2	1.259	-0.074	-2.593
	13.333	10.568	13.037	10.568	11.457	-0.938	-0.593	0.346	0.938	0.988	0.889	0.074	0.963	-0.37	-1.704
	12.444	9.679	10.568	12.049	9.778	-0.444	-1.284	-0.148	1.235	0.296	0.593	-1.407	0.074	-0.074	-2
	13.333	10.568	11.457	9.778	13.037	-0.346	0.593	-0.247	0.741	0.988	0.296	0.074	0.37	-1.556	-1.111
	-0.444	0.543	-0.938	-0.444	-0.346	10.568	-0.741	0.099	-0.593	0.346	-1.037	1.259	0.074	0.222	-2.296
	-0.889	-0.691	-0.593	-1.284	0.593	-0.741	9.679	1.10	-0.444	-1.037	-0.148	-0.074	0.222	-1.407	2.445
	0.444	0.642	0.346	-0.148	-0.247	0.099	1.10	10.568	-1.037	-0.346	0.593	-2.593	-2.296	2.445	0.074
	0.445	-0.741	0.938	1.235	0.741	-0.593	-0.444	-1.037	10.568	0.889	0.296	0.222	-0.37	0.074	-1.111
	0.889	0.099	0.988	0.296	0.988	0.346	-1.037	-0.346	0.889	11.457	0.741	-2.296	-1.704	-1.111	0.37
	1.10	1.10	0.889	0.593	0.296	-1.037	-0.148	0.593	0.296	0.741	9.778	2.445	-1.111	-2	-1.556
	-2	-2	0.074	-1.407	0.074	1.259	-0.074	-2.593	0.222	-2.296	2.445	12.444	-0.444	-0.889	0.444
	0.667	1.259	0.963	0.074	0.37	0.074	0.222	-2.296	-0.37	-1.704	-1.111	-0.444	13.333	0.445	0.889
	-0.667	-0.074	-0.37	-0.074	-1.556	0.222	-1.407	2.445	0.074	-1.111	-2	-0.889	0.445	12.444	1.10
	-2	-2.593	-1.704	-2	-1.111	-2.296	2.445	0.074	-1.111	0.37	-1.556	0.444	0.889	1.10	13.333

$$\left| \frac{XTX}{16} \right| = 1.855 \cdot 10^{-6}$$

$$\text{tr}(XTXI) = 5.325$$

XTXI	1.586	-0.153	-0.451	-0.502	-0.737	-0.018	0.095	-0.022	0.066	0.03	0.049	0.174	9.694	-10	0.014	-0.002	
	-0.153	0.545	-0.11	-0.046	-0.161	-0.047	0.013	-0.004	0.068	0.036	-0.008	0.067	-0.026	-0.018	0.041	0.008	
	-0.451	-0.11	0.708	-0.058	-0.019	0.06	-0.021	-0.038	-0.037	-0.055	-0.023	-0.123	-0.038	-0.018	0.008	0.008	
	-0.502	-0.046	-0.058	0.526	0.206	-0.003	0.003	0.044	-0.049	0.023	-0.034	-0.004	0.032	-0.013	-0.007	-0.007	
	-0.737	-0.161	-0.019	0.206	0.836	0.012	-0.1	0.023	-0.059	-0.039	0.005	-0.126	0.024	0.037	-0.024	-0.024	
	-0.018	-0.047	0.06	-0.003	0.012	0.113	-2.994	10	-0.01	4.553	-10	-0.017	0.019	-0.032	-0.005	0.001	0.02
	0.095	0.013	-0.021	0.003	-0.1	-2.994	-10	0.127	0.001	0.007	0.02	-0.002	0.024	2.64	-10	0.01	-0.018
	-0.022	-0.004	-0.038	0.044	0.023	-0.01	-0.001	0.12	0.007	0.015	-0.021	0.033	0.027	-0.023	-0.008	-0.008	
	0.066	0.068	-0.037	-0.049	-0.059	4.553	10	0.007	0.007	0.112	-0.002	0.002	0.014	-0.001	-0.005	0.014	0.01
	0.03	0.036	-0.055	0.023	-0.039	-0.017	0.02	0.015	-0.002	0.108	-0.015	0.043	0.017	0.005	-0.01	-0.01	
	0.049	-0.008	-0.023	-0.034	0.005	0.019	-0.002	-0.021	0.002	-0.015	0.126	-0.03	0.002	0.023	0.018	0.018	
	0.174	0.067	-0.123	-0.008	-0.126	-0.032	0.024	0.033	0.014	0.043	-0.03	0.144	0.012	-0.004	-0.004	-0.004	
	9.694	-10	-0.026	-0.038	0.032	0.024	-0.005	2.64	-10	0.027	-0.001	0.017	0.002	0.012	0.087	-0.004	-0.01
	0.014	-0.018	-0.018	-0.013	0.037	0.001	0.01	-0.023	-0.005	0.005	0.023	-0.004	-0.004	-0.004	0.095	-0.002	
	-0.002	0.041	0.008	-0.007	-0.024	0.02	-0.018	-0.008	0.014	-0.01	0.018	-0.008	-0.01	-0.002	0.092	0.092	

DESIGN (8.20) CONTINUED

$|r| = 0.193$

$t_r [r^{-1}] = 18.134$

r^{-1}

1.291	-0.236	-0.108	-0.343	-0.235	0.063	-0.02	0.34	0.187	-0.041	0.359	-0.146	-0.1	0.23
-0.236	1.364	-0.124	-0.036	0.27	-0.088	-0.17	-0.168	-0.256	-0.099	-0.595	-0.191	-0.089	0.039
-0.108	-0.124	1.248	0.441	-0.014	0.014	0.22	-0.245	0.119	-0.165	-0.041	0.179	-0.071	-0.041
-0.343	-0.036	0.441	1.611	0.052	-0.432	0.102	-0.265	-0.182	0.021	-0.609	0.124	0.179	-0.12
-0.235	0.27	-0.014	0.052	1.189	-0.003	-0.107	0.005	-0.187	0.195	-0.367	-0.056	0.016	0.236
0.063	-0.088	0.014	-0.432	-0.003	1.222	-0.011	0.066	0.214	-0.019	0.264	0.003	0.107	-0.203
-0.02	-0.17	0.22	0.102	-0.107	-0.011	1.268	0.077	0.167	-0.213	0.377	0.319	-0.268	-0.092
0.34	-0.168	-0.245	-0.265	0.005	0.066	0.077	1.183	-0.027	0.022	0.162	-0.015	-0.057	0.167
0.187	-0.256	0.119	-0.182	-0.187	0.214	0.167	-0.027	1.232	-0.16	0.507	0.206	0.057	-0.117
-0.041	-0.099	-0.165	0.021	0.195	-0.019	-0.213	0.022	-0.16	1.231	-0.328	0.023	0.248	0.204
0.359	-0.595	-0.041	-0.609	-0.367	0.264	0.377	0.162	0.507	-0.328	1.756	0.149	-0.05	-0.095
-0.146	-0.191	0.179	0.124	-0.056	0.003	0.319	-0.015	0.206	0.023	0.149	1.163	-0.046	-0.138
-0.1	-0.089	-0.071	0.179	0.016	0.107	-0.268	-0.057	0.057	0.248	-0.05	-0.046	1.174	-0.022
0.23	0.039	-0.041	-0.12	0.236	-0.203	-0.092	0.167	-0.117	0.204	-0.095	-0.138	-0.022	1.203

ρ

1	-0.165	-0.426	-0.549	-0.64	-0.042	0.212	-0.051	0.156	0.073	0.111	0.364	0.003	0.035	-0.005
-0.165	1	-0.178	-0.085	-0.238	-0.19	0.05	-0.016	0.275	0.148	-0.032	0.238	-0.119	-0.081	0.185
-0.426	-0.178	1	-0.095	-0.025	0.212	-0.068	-0.129	-0.132	-0.197	-0.076	-0.385	-0.151	-0.07	0.03
-0.549	-0.085	-0.095	1	0.311	-0.011	0.011	0.175	-0.201	0.096	-0.133	-0.028	0.149	-0.059	-0.033
-0.64	-0.238	-0.025	0.311	1	0.038	-0.308	0.071	-0.192	-0.13	0.015	-0.362	0.091	0.13	-0.087
-0.042	-0.19	0.212	-0.011	0.038	1	-0.003	-0.088	0.004	-0.154	0.162	-0.254	-0.047	0.013	0.197
0.212	0.05	-0.068	0.011	-0.308	-0.003	1	-0.009	0.055	0.174	-0.016	0.18	0.003	0.09	-0.168
-0.051	-0.016	-0.129	0.175	0.071	-0.088	-0.009	1	0.063	0.133	-0.171	0.253	0.263	-0.22	-0.074
0.156	0.275	-0.132	-0.201	-0.192	0.004	0.055	0.063	1	-0.022	0.018	0.112	-0.013	-0.049	0.14
0.073	0.148	-0.197	0.096	-0.13	-0.154	0.174	-0.133	-0.022	1	-0.13	0.345	0.172	0.048	-0.096
0.111	-0.032	-0.076	-0.133	0.015	0.162	-0.016	-0.171	0.018	-0.13	1	-0.223	0.019	0.206	0.168
0.364	0.238	-0.385	-0.028	-0.362	-0.254	0.18	0.253	0.112	0.345	-0.223	1	0.104	-0.035	-0.065
0.003	-0.119	-0.151	0.149	0.091	-0.047	0.003	0.263	-0.013	0.172	0.019	0.104	1	-0.04	-0.117
0.035	-0.081	-0.07	-0.059	0.13	0.013	0.09	-0.22	-0.049	0.048	0.206	-0.035	-0.04	1	-0.019
-0.005	0.185	0.03	-0.033	-0.087	0.197	-0.168	-0.074	0.14	-0.096	0.168	-0.065	-0.117	-0.019	1

DESIGN MATRIX

$$\begin{aligned} x p^m &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 3) & x 1_i &= (2x p_i - 3)/3 \\ x q^m &= (0 \ 0 \ 1 \ 1 \ 3 \ 3 \ 3 \ 2 \ 3 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3) & x 2_i &= (2x q_i - 3)/3 \\ x r^m &= (0 \ 3 \ 1 \ 3 \ 0 \ 1 \ 3 \ 0 \ 3 \ 0 \ 2 \ 0 \ 3 \ 0 \ 1 \ 3) & x 3_i &= (2x r_i - 3)/3 \\ x s^m &= (0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 1 \ 2 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 0) & x 4_i &= (x s_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} x_{i,1} &:= x_1 & x_{i,2} &:= x_1^2 & x_{i,3} &:= x_2 & x_{i,4} &:= x_3 & x_{i,5} &:= x_4^2 \\ x_{i,6} &:= x_1 \cdot x_2 & x_{i,7} &:= x_1 \cdot x_3 & x_{i,8} &:= x_1 \cdot x_4 & x_{i,9} &:= x_2 \cdot x_3 \\ x_{i,10} &:= x_2 \cdot x_4 & x_{i,11} &:= x_3 \cdot x_4 \\ x_{i,12} &:= x_1 & x_{i,13} &:= x_2 & x_{i,14} &:= x_3 & x_{i,15} &:= x_4 \end{aligned}$$

A29

$X T X =$

16	12.444	13.333	12.444	13	-0.444	-0.889	-0.333	0.445	1	0.333	-2	0.667	-0.667	-1
12.444	12.049	10.568	9.679	10.333	0.543	-0.691	-0.037	-0.741	0.111	0.63	-2	1.259	-0.074	-1.889
13.333	10.568	13.037	10.568	11.222	-0.938	-0.593	-0.333	0.938	1	1.519	0.074	0.963	-0.37	-1
12.444	9.679	10.568	12.049	9.444	-0.444	-1.284	-0.926	1.235	0.407	0.926	-1.407	0.074	-0.074	-1
13	10.333	11.222	9.444	13	-0.333	0.778	-0.333	0.778	1	0.333	0.333	0.333	-1.667	-1
-0.444	0.543	-0.938	-0.444	-0.333	10.568	-0.741	0.111	-0.593	-0.333	-1	1.259	0.074	0.222	-2.333
-0.889	-0.691	-0.593	-1.284	0.778	-0.741	9.679	0.63	-0.444	-1	-0.926	-0.074	0.222	-1.407	1.889
-0.333	-0.037	-0.333	-0.926	-0.333	0.111	0.63	10.333	-1	-0.333	0.778	-1.889	-2.333	1.889	0.333
0.445	-0.741	0.938	1.235	0.778	-0.593	-0.444	-1	10.568	1.519	0.407	0.222	-0.37	0.074	-1.222
1	0.111	1	0.407	-1	-0.333	-1	-0.333	1.519	11.222	0.778	-2.333	-1	-1.222	0.333
0.333	0.63	1.519	0.926	0.333	-1	-0.926	0.778	0.407	0.778	9.444	1.889	-1.222	-1	-1.667
-2	-2	0.074	-1.407	0.333	1.259	-0.074	-1.889	0.222	-2.333	1.889	12.444	-0.444	-0.889	-0.333
0.667	1.259	0.963	0.074	0.333	0.074	0.222	-2.333	-0.37	-1	-1.222	-0.444	13.333	0.445	1
-0.667	-0.074	-0.37	-0.074	-1.667	0.222	-1.407	1.889	0.074	-1.222	-1	-0.889	0.445	12.444	0.333
-1	-1.889	-1	-1	-1	-1	-2.333	1.889	0.333	-1.222	0.333	-1.667	-0.333	1	0.333

$|X T X| = 2.315 \cdot 10^{-6}$

$tr(X T X) = 5.008$

$X T X I =$

1.465	-0.204	-0.478	-0.478	-0.56	-0.018	0.092	-0.005	0.054	0.013	0.075	0.158	0.011	0.016	-0.033
-0.204	0.548	-0.095	-0.04	-0.128	0.047	0.01	0.002	0.066	0.035	-0.028	0.068	-0.029	-0.021	0.04
-0.478	-0.095	0.714	-0.045	-0.022	0.05	-0.021	-0.02	-0.034	-0.037	-0.062	-0.109	-0.034	-0.023	0.002
-0.478	-0.04	-0.045	0.522	0.171	5.295 · 10 ⁻⁴	-4.494 · 10 ⁻⁴	0.039	-0.05	0.022	-0.029	-0.013	0.028	-0.009	0.005
-0.56	-0.128	-0.022	0.171	0.652	0.016	-0.091	-0.01	-0.047	-0.033	0.022	-0.117	0.016	0.037	0.01
-0.018	-0.047	0.05	5.295 · 10 ⁻⁴	0.016	0.11	0.003	-0.007	5.345 · 10 ⁻⁴	-0.008	0.017	-0.027	-0.002	1.164 · 10 ⁻⁴	0.018
0.092	0.01	-0.021	-4.494 · 10 ⁻⁴	-0.091	0.003	0.127	-0.004	0.005	0.018	0.008	0.021	-0.001	0.012	-0.017
-0.005	0.002	-0.02	0.039	-0.01	-0.007	-0.006	0.116	0.008	0.01	-0.018	0.026	0.023	-0.019	-0.005
0.054	0.066	-0.034	-0.05	-0.047	5.345 · 10 ⁻⁴	0.005	0.008	-0.113	-0.01	7.93 · 10 ⁻⁴	0.012	-0.002	-0.006	0.014
0.013	0.035	-0.037	0.022	-0.033	-0.008	0.018	0.01	-0.01	0.106	-0.013	0.036	0.009	0.008	-0.007
0.075	-0.028	-0.062	-0.029	0.022	0.017	0.008	-0.018	7.93 · 10 ⁻⁴	-0.013	0.132	-0.021	0.009	0.015	0.014
0.158	0.068	-0.109	-0.013	-0.117	-0.027	0.021	0.026	0.012	0.036	-0.021	0.136	0.007	9.269 · 10 ⁻⁵	-0.004
0.011	-0.029	-0.034	0.028	0.016	-0.002	-0.001	0.023	-0.002	0.009	0.009	0.007	0.085	-0.003	-0.009
0.016	-0.021	-0.023	-0.009	0.037	1.164 · 10 ⁻⁴	0.012	-0.019	-0.006	0.008	0.015	9.269 · 10 ⁻⁵	-0.003	0.092	-0.004
-0.033	0.04	0.002	-0.005	0.01	0.018	-0.017	-0.005	0.014	-0.007	0.014	-0.004	-0.009	-0.004	0.091

DESIGN (8.21) CONTINUED

$|r| = 0.208$

$r_r \begin{bmatrix} -1 \\ r \end{bmatrix} = 17.81$

$r =$

1.299	-0.203	+0.096	-0.308	-0.234	0.048	0.012	0.33	0.179	-0.132	0.366	-0.162	-0.112	0.221
-0.203	1.376	-0.096	-0.047	0.223	-0.091	-0.088	-0.153	-0.171	-0.264	-0.527	-0.171	-0.114	0.01
-0.096	-0.096	1.238	0.411	0.003	-0.002	0.194	-0.249	0.112	-0.136	-0.071	0.16	-0.048	-0.027
-0.308	-0.047	0.411	1.588	0.083	-0.441	-0.049	-0.24	-0.174	0.104	-0.64	0.093	0.205	0.058
-0.234	0.223	0.003	0.083	1.162	0.028	-0.077	0.006	-0.088	0.167	-0.305	-0.024	0.001	0.215
0.048	-0.091	-0.002	-0.441	0.028	1.223	-0.061	0.051	0.183	0.08	0.225	-0.013	0.128	-0.184
0.012	-0.088	0.194	-0.049	-0.077	-0.061	1.195	0.079	0.109	-0.174	0.296	0.271	-0.219	-0.059
0.33	-0.153	-0.249	-0.24	0.006	0.051	0.079	1.193	-0.106	0.008	0.139	-0.021	-0.068	0.169
0.179	-0.171	0.112	-0.174	-0.088	0.183	0.109	-0.106	1.187	-0.13	0.425	0.11	0.094	-0.087
-0.132	-0.264	-0.136	0.104	0.167	0.08	-0.174	0.008	-0.13	1.241	-0.223	0.095	0.165	0.158
-0.366	-0.527	-0.071	-0.64	-0.305	0.225	0.296	0.139	0.425	-0.223	1.656	0.088	0.001	-0.055
-0.162	-0.171	0.16	0.093	-0.024	-0.013	0.271	-0.021	0.11	0.095	0.088	1.138	-0.033	-0.117
-0.112	-0.114	-0.048	0.205	0.001	0.128	-0.219	-0.068	0.094	0.165	0.001	-0.033	1.14	-0.045
0.221	0.01	-0.027	0.058	0.215	-0.184	-0.059	0.169	-0.087	0.158	-0.055	-0.117	-0.045	1.173

A30

$p =$

1	-0.228	-0.467	-0.547	-0.573	-0.044	0.213	-0.013	0.134	0.033	0.171	0.355	0.032	0.042	-0.09
-0.228	1	-0.152	-0.076	-0.215	-0.19	0.038	0.01	0.265	0.144	-0.104	0.249	-0.133	-0.092	0.179
-0.467	-0.152	1	-0.074	-0.032	0.177	-0.07	-0.069	-0.119	-0.134	-0.202	-0.349	-0.136	-0.091	0.008
-0.547	-0.076	-0.074	1	0.293	0.002	-0.002	0.159	-0.205	0.092	-0.11	-0.049	0.135	-0.041	-0.022
-0.573	-0.215	-0.032	0.293	1	0.061	-0.317	-0.035	-0.175	-0.127	0.074	-0.395	0.069	0.152	0.042
-0.044	-0.19	0.177	0.002	0.061	1	0.024	-0.065	0.005	-0.075	0.139	-0.22	-0.02	0.001	0.184
0.213	0.038	-0.07	-0.002	-0.317	0.024	1	-0.05	0.042	0.152	0.065	0.158	-0.011	0.109	-0.154
-0.013	0.01	-0.069	0.159	-0.035	-0.065	-0.05	1	0.066	0.091	-0.143	0.21	0.233	-0.188	-0.05
0.134	0.265	-0.119	-0.205	-0.175	0.005	0.042	0.066	1	-0.089	0.007	0.099	-0.018	0.058	0.143
0.033	0.144	-0.134	0.092	-0.127	-0.075	0.152	0.091	-0.089	1	-0.107	0.303	0.094	0.081	-0.073
0.171	-0.104	-0.202	-0.11	0.074	0.139	0.065	-0.143	0.007	-0.107	1	-0.155	0.08	0.139	0.131
											-4			
0.355	0.249	-0.349	-0.049	-0.395	-0.22	0.158	0.21	0.099	0.303	-0.155	1	0.064	8.301-10	-0.039
0.032	-0.133	-0.136	0.135	0.069	-0.02	-0.011	0.233	-0.018	0.094	0.08	0.064	1	-0.029	-0.101
												-4		
0.042	-0.092	-0.091	-0.041	0.152	0.001	0.109	-0.188	-0.050	0.081	0.139	8.301-10	-0.029	1	-0.039
-0.09	0.179	0.008	-0.022	0.042	0.184	-0.154	-0.05	0.143	-0.073	0.131	-0.039	-0.101	-0.039	1

DESIGN MATRIX

$$\begin{aligned} x p^q &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 3 \ 3) & x1_i &= (2xp_i - 3)/3 \\ x q^q &= (0 \ 0 \ 1 \ 1 \ 3 \ 3 \ 2 \ 3 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3) & x2_i &= (2xq_i - 3)/3 \\ x r^q &= (0 \ 2 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2) & x3_i &= (xr_i - 1) \\ x s^q &= (0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 1 \ 2 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 0) & x4_i &= (xs_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} x_{i,1} &:= x_1 & x_{i,2} &:= x_2 & x_{i,3} &:= x_3 & x_{i,4} &:= x_4 \\ x_{i,6} &:= x_1 \cdot x_2 & x_{i,7} &:= x_1 \cdot x_3 & x_{i,8} &:= x_1 \cdot x_4 & x_{i,9} &:= x_2 \cdot x_3 \\ x_{i,10} &:= x_2 \cdot x_4 & x_{i,11} &:= x_3 \cdot x_4 \\ x_{i,12} &:= x_1 & x_{i,13} &:= x_2 & x_{i,14} &:= x_3 & x_{i,15} &:= x_4 \end{aligned}$$

$\left| \frac{XTX}{16} \right| = 2.264 \cdot 10^{-6}$

	16	12.444	13.333		12	13	-0.444	-1.333	-0.333	1.333	1	1	-2	0.667	0	-1
	12.444	12.049	10.568	9.333	10.333	0.543	-1.037	-0.037	-0.148	0.111	1	-2	1.259	0.889	-1.889	-1
	13.333	10.568	13.037	10.222	11.222	-0.938	-0.741	-0.333	1.926	1	1.889	0.074	0.963	0	0	-1
	12	9.333	10.222	12	9	-0.444	-1.333	-1	1.333	0.333	1	-1.333	0	0	0	-1
	13	10.333	11.222	9	13	-0.333	0.333	-0.333	1.667	1	1	0.333	0.333	-1	-1	-1
	-0.444	0.543	-0.938	-0.444	-0.333	10.568	-0.148	0.111	-0.741	-0.333	-0.333	1.259	0.074	0.444	-2.333	-1
	-1.333	-1.037	-0.741	-1.333	0.333	-0.148	9.333	1	-0.444	-0.333	-1	0.889	0.444	-1.333	2.333	1
	-0.333	-0.037	-0.333	-1	-0.333	0.111	1	10.333	-0.333	0.333	0.333	-1.889	-2.333	2.333	0.333	1
	1.333	-0.148	1.926	1.333	1.667	-0.741	-0.444	-0.333	10.222	1.889	0.333	0.444	0	0	-1.667	1
	1	0.111	1	0.333	1	-0.333	-0.333	-0.333	1.889	11.222	1.667	-2.333	-1	-1.667	0.333	1
	1	1	1.889	1	1	-0.333	-1	0.333	0.333	1.667	9	2.333	-1.667	-1	-1	-1
	-2	-2	0.074	-1.333	0.333	1.259	0.889	-1.889	-0.444	-2.333	2.333	12.444	-0.444	-1.333	-0.333	1
	0.667	1.259	0.963	0	0.333	0.074	0.444	-2.333	0	-1	-1.667	-0.444	13.333	1.333	1	1
	0	0.889	0	0	-1	0.444	-1.333	2.333	0	-1.667	-1	-1.333	1.333	12	1	1
	-1	-1.889	-1	-1	-1	-2.333	2.333	0.333	-1.667	0.333	-1	-0.333	1	1	13	1

tr(XTX) = 4.805

	1.338	-0.215	-0.463	-0.357	-0.538	-0.029	0.103	-0.006	0.029	0.008	0.039	0.147	0.009	0.008	-0.047
	-0.215	0.575	-0.111	-0.033	-0.135	-0.043	6.834 · 10 ⁻⁴	0.003	0.082	0.029	-0.03	0.067	-0.03	-0.045	0.053
	-0.463	-0.111	0.714	-0.055	-0.01	0.055	-0.026	0.021	-0.053	-0.028	-0.051	-0.105	-0.032	-0.01	0.004
	-0.357	-0.033	-0.055	0.395	0.141	0.003	-0.012	-0.034	-0.023	0.014	-0.002	-0.013	-0.027	0.005	0.002
	-0.538	-0.135	-0.01	0.161	0.634	0.018	-0.028	-0.001	-0.047	-0.023	0.023	-0.104	0.02	0.038	0.006
	-0.029	-0.043	0.055	0.003	0.018	0.109	-0.005	-0.005	0.003	-0.009	0.008	-0.027	-0.002	-0.004	0.019
	0.103	6.834 · 10 ⁻⁴	-0.026	-0.012	-0.08	-0.005	0.133	-0.018	0.005	0.004	0.015	0.005	-0.006	0.017	-0.024
	-0.006	0.003	-0.021	0.034	-0.001	-0.005	-0.018	0.118	7.584 · 10 ⁻⁴	0.01	-0.012	0.025	0.025	-0.025	-2.735 · 10 ⁻⁴
	0.029	0.082	-0.053	-0.023	-0.047	0.003	0.005	7.584 · 10 ⁻⁴	0.122	-0.016	0.004	0.007	-0.005	-0.012	0.022
	0.008	0.029	-0.028	0.016	-0.023	-0.009	0.004	-0.01	-0.016	0.109	-0.025	0.038	0.007	0.012	-0.008
	0.039	-0.03	-0.051	-0.002	0.023	0.008	0.015	-0.012	0.004	-0.025	0.138	-0.032	0.014	0.01	0.004
	0.147	0.047	-0.105	-0.013	-0.106	-0.027	0.005	0.025	0.007	0.038	-0.032	0.136	0.004	1.412 · 10 ⁻⁴	-0.002
	0.009	-0.03	-0.032	0.027	0.02	-0.002	-0.006	0.025	-0.005	0.007	0.014	0.004	0.008	-0.008	-0.008
	0.008	-0.045	-0.01	0.005	0.038	0.004	0.017	-0.025	-0.012	0.012	0.01	1.412 · 10 ⁻⁴	-0.008	0.101	-0.015
	-0.047	0.053	0.004	0.002	0.006	0.019	-0.024	-2.735 · 10 ⁻⁴	0.022	-0.008	0.004	-0.002	-0.008	-0.015	0.095

A31

DESIGN (8,22) CONTINUED

$$|r| = 0.191$$

$$\text{tr} \begin{bmatrix} & -1 \\ r & \end{bmatrix} = 18.014$$

1	1.363	-0.236	-0.089	-0.325	-0.213	0.003	0.013	0.401	0.148	-0.139	0.359	-0.17	-0.239	0.291
	-0.236	1.376	-0.131	-0.023	0.246	-0.109	-0.095	-0.233	-0.131	-0.213	-0.508	-0.163	-0.048	0.019
	-0.089	-0.131	1.185	0.435	0.019	-0.065	0.187	-0.124	0.095	-0.013	-0.078	0.171	0.032	0.012
	-0.325	-0.023	0.435	1.545	0.091	-0.377	-0.006	-0.234	-0.121	0.106	-0.579	0.115	0.204	0.034
	-0.213	0.246	0.019	0.091	1.148	-0.045	-0.048	0.028	-0.098	0.074	-0.301	-0.021	-0.044	0.219
	0.003	-0.109	-0.065	-0.377	-0.045	1.228	-0.175	0.053	0.043	0.138	0.048	-0.071	0.178	-0.264
	0.013	-0.095	0.187	-0.006	-0.048	-0.175	1.213	0.008	0.105	-0.113	0.282	0.297	-0.274	-0.003
	0.401	-0.233	-0.124	-0.234	0.028	0.053	0.008	1.237	-0.171	0.036	0.083	-0.06	-0.132	0.253
	0.148	-0.131	0.095	-0.121	-0.098	0.043	0.105	-0.171	1.219	-0.253	0.44	0.083	0.139	-0.094
	-0.139	-0.213	-0.013	0.106	0.074	0.138	-0.113	0.036	-0.253	1.234	-0.332	0.157	0.107	0.045
	0.359	-0.508	-0.078	-0.579	-0.301	0.048	0.282	0.083	0.44	-0.332	1.657	0.057	0.002	-0.022
	-0.17	-0.163	0.171	0.115	-0.021	-0.071	0.297	-0.06	0.083	0.157	0.057	1.168	-0.102	-0.106
	-0.239	-0.048	0.032	0.204	-0.044	0.178	-0.274	-0.132	0.139	0.107	0.002	-0.102	1.215	-0.182
	0.291	0.019	0.012	0.034	0.219	-0.264	-0.003	0.253	-0.094	0.045	-0.022	-0.106	-0.182	1.224

1	1	-0.245	-0.474	-0.491	-0.584	-0.076	0.245	-0.014	0.072	0.021	0.091	0.345	0.027	0.023	-0.133
	-0.245	1	-0.173	-0.07	-0.224	-0.171	0.002	0.01	0.309	0.115	-0.107	0.239	-0.135	-0.186	0.226
	-0.474	-0.173	1	-0.103	-0.015	0.196	-0.084	-0.073	-0.178	-0.101	-0.163	-0.337	-0.129	-0.037	0.015
	-0.491	-0.07	-0.103	1	0.321	0.016	-0.054	0.156	-0.103	0.079	-0.01	-0.056	0.145	0.027	0.01
	-0.584	-0.224	-0.015	0.321	1	0.068	-0.274	-0.004	-0.17	-0.088	0.077	-0.362	0.086	0.149	0.024
	-0.076	-0.171	0.196	0.016	0.068	1	-0.038	-0.041	0.023	-0.082	0.062	-0.218	-0.018	-0.037	0.185
	0.245	0.002	-0.084	-0.054	-0.274	-0.038	1	-0.143	0.043	0.035	0.112	0.034	-0.059	0.145	-0.216
	-0.014	0.01	-0.073	0.156	-0.004	-0.041	-0.143	1	0.006	0.086	-0.092	0.199	0.25	-0.226	-0.003
	0.072	0.309	-0.178	-0.103	-0.17	0.023	0.043	0.006	1	-0.139	0.029	0.058	-0.05	-0.108	0.206
	0.021	0.115	-0.101	0.079	-0.088	-0.082	0.035	0.086	-0.139	1	-0.206	0.309	0.069	0.114	-0.077
	0.091	-0.107	-0.163	-0.01	0.077	0.062	0.112	-0.092	0.029	-0.206	1	-0.232	0.131	0.087	0.037
	0.345	0.239	-0.337	-0.056	-0.362	-0.218	0.034	0.199	0.058	0.309	-0.232	1	0.041	0.001	-0.015
	0.027	-0.135	-0.129	0.145	0.086	-0.018	-0.059	0.25	-0.05	0.069	0.131	0.041	1	-0.086	-0.089
	0.023	-0.186	-0.037	0.027	0.149	-0.037	0.145	-0.226	-0.108	0.114	0.087	0.001	-0.086	1	-0.15
	-0.133	0.226	0.015	0.01	0.024	0.185	-0.216	-0.003	0.206	-0.077	0.037	-0.015	-0.089	-0.15	1

------(8.23) A 4x3x3x3/16 design -----

DESIGN MATRIX

$$\begin{aligned} x p_i^1 &= (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 3 \ 3) & x 1_i &= (2x p_i - 3) / 3 \\ x q_i^1 &= (0 \ 0 \ 1 \ 1 \ 2 \ 2 \ 2 \ 1 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2) & x 2_i &= (x q_i - 1) \\ x r_i^1 &= (0 \ 2 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2) & x 3_i &= (x r_i - 1) \\ x s_i^1 &= (0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 1 \ 2 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 0) & x 4_i &= (x s_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$x_{i,1} := 1$ $x_{i,2} := x_1^2$ $x_{i,3} := x_2^2$ $x_{i,4} := x_3^2$ $x_{i,5} := x_4^2$
 $x_{i,6} := x_1 \cdot x_2$ $x_{i,7} := x_1 \cdot x_3$ $x_{i,8} := x_1 \cdot x_4$ $x_{i,9} := x_2 \cdot x_3$
 $x_{i,10} := x_2 \cdot x_4$ $x_{i,11} := x_3 \cdot x_4$
 $x_{i,12} := x_1$ $x_{i,13} := x_2$ $x_{i,14} := x_3$ $x_{i,15} := x_4$

A33

XTX =

16	12.444	13	12	13	13	-1	-1.333	-0.333	2	1	1	-2	1	0	-1
12.444	12.049	10.333	9.333	10.333	10.333	-0.111	-1.037	-0.037	0.222	0.111	1	-2	1.889	0.889	-1.889
13	10.333	13	10	11	-1	-0.667	-0.333	-0.333	2	1	2	0.333	1	0	-1
12	9.333	10	12	9	-0.667	-1.333	-1	2	0	1	-1.333	0	0	0	-1
13	10.333	11	9	13	-1	0.333	-0.333	2	1	1	0.333	1	-1	-1	-1
-1	-0.111	-1	-0.667	-1	10.333	0.222	0.111	-0.667	-0.333	0	1.889	0.333	0	-2.333	0
-1.333	-1.037	-0.667	-1.333	0.333	0.222	9.333	1	-0.667	0	-1	0.889	0	-1.333	2.333	0.333
-0.333	-0.037	-0.333	-1	-0.333	0.111	1	10.333	0	-1	0.333	-1.889	-2.333	2.333	0.333	0.333
2	0.222	2	2	2	-0.667	-0.667	0	10	2	0	0	0	0	0	-2
1	0.111	1	0	1	-0.333	0	-1	2	11	2	-2.333	-1	-2	1	1
1	1	2	1	1	0	-1	0.333	0	2	9	2.333	-2	-1	-1	-1
-2	-2	0.333	-1.333	0.333	1.889	0.889	-1.889	0	-2.333	2.333	12.444	-1	-1.333	-0.333	0.333
1	1.889	1	0	1	0.333	0	-2.333	0	-1	-2	-1	13	2	1	1
0	0.889	0	0	-1	0	-1.333	2.333	0	-2	-1	-1.333	2	12	1	1
-1	-1.889	-1	-1	-1	-2.333	2.333	0.333	-2	1	-1	-0.333	1	1	13	1

$\frac{|XTX|}{16} = 2.162 \cdot 10^{-6}$

$tr(XTX) = 4.625$

XTX1 =

1.249	-0.263	-0.329	-0.352	-0.534	-0.029	0.101	-0.002	-0.007	-0.003	0.04	0.134	0.029	0.004	-0.056
-0.263	0.588	-0.068	-0.046	-0.127	-0.029	-0.001	-0.006	0.095	0.017	-0.029	0.058	-0.047	-0.043	0.061
-0.329	-0.068	0.532	-0.057	-0.012	0.032	-0.024	-0.019	-0.017	-0.03	-0.044	-0.09	-0.024	-0.01	0.007
-0.352	-0.046	-0.057	0.413	0.154	-0.003	-0.012	0.043	-0.041	0.042	-0.01	-0.001	0.033	0.007	-0.008
-0.534	-0.127	-0.012	0.154	0.634	-0.039	-0.08	-0.009	-0.062	-0.02	0.018	-0.111	-0.006	0.041	0.013
-0.029	-0.029	0.032	-0.003	0.039	0.112	-0.01	-0.009	0.007	-0.013	0.007	-0.033	-0.008	1.895 · 10 ⁻⁴	0.023
0.101	-0.001	-0.024	-0.012	-0.08	-0.01	0.133	-0.016	0.006	4.639 · 10 ⁻⁴	0.017	0.005	3.582 · 10 ⁻⁴	0.016	-0.025
-0.002	-0.006	-0.019	0.043	-0.009	-0.009	-0.016	0.123	-0.01	0.024	-0.015	0.033	0.032	-0.024	-0.006
-0.007	0.095	-0.017	-0.041	-0.042	0.007	0.006	-0.01	0.132	-0.028	0.01	-2.94 · 10 ⁻⁴	-0.012	-0.012	0.031
-0.003	0.017	-0.03	0.042	-0.02	-0.013	4.639 · 10 ⁻⁴	0.024	-0.032	0.124	-0.035	0.046	0.013	0.015	-0.019
0.04	-0.029	-0.044	-0.01	0.018	0.007	0.017	-0.015	0.01	-0.035	0.143	-0.034	0.015	0.008	0.007
0.134	0.058	-0.09	-0.001	-0.111	-0.033	0.005	0.033	-2.94 · 10 ⁻⁴	0.046	-0.034	0.142	0.013	-3.035 · 10 ⁻⁴	-0.008
0.029	-0.047	-0.024	0.035	-0.006	-0.008	3.582 · 10 ⁻⁴	0.032	-0.012	0.013	0.015	0.013	0.097	-0.013	-0.014
0.004	-0.043	-0.01	0.007	0.041	1.895 · 10 ⁻⁴	0.016	-0.024	-0.012	0.015	0.008	-3.035 · 10 ⁻⁴	-0.013	0.103	-0.015
-0.056	0.061	0.007	-0.008	0.013	0.023	-0.025	-0.006	0.031	-0.019	0.007	-0.008	-0.014	-0.015	0.1

DESIGN (8.23) CONTINUED

$|r| = 0.161$

$\tau r \begin{bmatrix} -1 \\ r \end{bmatrix} = 18.566$

$r =$

1.393	-0.164	-0.123	-0.305	-0.145	-0.005	-0.032	0.455	0.085	-0.133	0.31	-0.262	-0.231	0.339
-0.164	1.296	-0.154	-0.029	0.158	-0.112	-0.095	-0.083	-0.156	-0.204	-0.491	-0.134	-0.055	0.041
-0.123	-0.154	1.238	0.416	-0.015	-0.061	0.241	-0.223	0.239	-0.052	-0.009	0.219	0.044	-0.048
-0.305	-0.029	0.416	1.545	0.194	-0.378	-0.045	-0.204	-0.102	0.083	-0.603	-0.031	0.221	0.071
-0.145	0.158	-0.015	0.194	1.152	-0.097	-0.097	0.07	-0.141	0.068	-0.371	-0.089	0.002	0.268
-0.005	-0.112	-0.061	-0.378	-0.097	1.229	-0.158	0.056	0.005	0.157	0.052	0.004	0.163	-0.278
-0.032	-0.095	0.241	-0.045	-0.097	-0.158	1.274	-0.104	0.258	-0.146	0.366	0.368	-0.272	-0.072
0.455	-0.083	-0.223	-0.204	0.07	0.056	-0.104	1.286	-0.286	0.093	-0.003	-0.133	-0.132	0.349
0.085	-0.156	0.239	-0.102	-0.141	0.005	0.258	-0.286	1.356	-0.348	0.528	0.156	0.168	-0.225
-0.133	-0.204	-0.052	0.083	0.068	0.157	-0.146	0.093	-0.348	1.278	-0.359	0.163	0.079	0.078
0.31	-0.491	-0.009	-0.603	-0.371	0.052	0.366	-0.003	0.528	-0.359	1.73	0.166	-0.004	-0.102
-0.262	-0.134	0.219	-0.031	-0.089	0.004	0.368	-0.133	0.156	0.163	0.166	1.258	-0.165	-0.185
-0.231	-0.055	0.044	0.221	0.002	0.163	-0.272	-0.132	0.168	0.079	-0.004	-0.165	1.235	-0.181
0.339	0.041	-0.048	0.071	0.268	-0.278	-0.072	0.349	-0.225	0.078	-0.102	-0.185	-0.181	1.296

$p =$

1	-0.307	-0.404	-0.491	-0.6	-0.077	0.247	-0.004	-0.017	-0.007	0.094	0.319	0.083	0.012	-0.158
-0.307	1	-0.122	-0.093	-0.208	-0.115	-0.004	-0.024	0.34	0.062	-0.099	0.2	-0.198	-0.176	0.252
-0.404	-0.122	1	-0.122	-0.021	0.129	-0.089	-0.074	-0.065	-0.117	-0.159	-0.328	-0.105	-0.044	0.032
-0.491	-0.093	-0.122	1	0.301	-0.013	-0.049	0.192	-0.177	0.185	-0.041	-0.006	0.176	0.035	-0.038
-0.6	-0.208	-0.021	0.301	1	0.146	-0.274	-0.032	-0.145	-0.07	0.059	-0.369	-0.022	0.16	0.05
-0.077	-0.115	0.129	-0.013	0.146	1	-0.081	-0.08	0.058	-0.113	0.056	-0.262	-0.074	0.002	0.219
0.247	-0.004	-0.089	-0.049	-0.274	-0.081	1	-0.126	0.044	0.004	0.126	0.036	0.003	0.133	-0.22
-0.004	-0.024	-0.074	0.192	-0.032	-0.08	-0.126	1	-0.081	0.196	-0.115	0.246	0.291	-0.217	-0.056
-0.017	0.34	-0.065	-0.177	-0.145	0.058	0.044	-0.081	1	-0.217	0.073	-0.002	-0.105	-0.105	0.27
-0.007	0.062	-0.117	0.185	-0.07	-0.113	0.004	0.196	-0.217	1	-0.264	0.345	0.12	0.13	-0.17
0.094	-0.099	-0.159	-0.041	0.059	0.056	0.126	-0.115	0.073	-0.264	1	-0.242	0.128	0.063	0.061
0.319	0.2	-0.328	-0.006	-0.369	-0.262	0.036	0.246	-0.002	0.345	-0.242	1	0.113	-0.003	-0.068
0.083	-0.198	-0.105	0.176	-0.022	-0.074	0.003	0.291	-0.105	0.12	0.128	0.113	1	-0.132	-0.145
0.012	-0.176	-0.044	0.035	0.16	0.002	0.133	-0.217	-0.105	0.13	0.063	-0.003	-0.132	1	-0.143
-0.158	0.252	0.032	-0.038	0.05	0.219	-0.22	-0.056	0.27	-0.17	0.061	-0.068	-0.145	-0.143	1

------(5.24) A 3x3x3x3/16 design -----

DESIGN MATRIX

$$\begin{aligned} xp^i &= (0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 2\ 2\ 2\ 2\ 2) & x1_i &= (xp_i - 1) \\ xq^i &= (0\ 0\ 1\ 1\ 2\ 2\ 2\ 1\ 2\ 0\ 0\ 0\ 0\ 2\ 2\ 2) & x2_i &= (xq_i - 1) \\ xr^i &= (0\ 2\ 1\ 2\ 0\ 1\ 2\ 0\ 2\ 0\ 1\ 0\ 2\ 0\ 1\ 2) & x3_i &= (xr_i - 1) \\ xs^i &= (0\ 1\ 2\ 0\ 2\ 0\ 1\ 1\ 2\ 2\ 0\ 0\ 2\ 0\ 2\ 0) & x4_i &= (xs_i - 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} x_{1,1} & := 1 \\ x_{1,2} & := x_1^2 & x_{1,3} & := x_2^2 & x_{1,4} & := x_3^2 & x_{1,5} & := x_4^2 \\ x_{1,6} & := x_1 x_2 & x_{1,7} & := x_1 x_3 & x_{1,8} & := x_1 x_4 & x_{1,9} & := x_2 x_3 \\ x_{1,10} & := x_2 x_4 & x_{1,11} & := x_3 x_4 \\ x_{1,12} & := x_1^3 & x_{1,13} & := x_2^3 & x_{1,14} & := x_3^3 & x_{1,15} & := x_4^3 \end{aligned}$$

XTX =

16	12	13	12	13	0	-1	0	2	1	1	-2	1	0	-1
12	12	10	9	10	0	-1	0	0	0	1	-2	2	1	-2
13	10	13	10	11	0	0	0	2	1	2	0	1	0	-1
12	9	10	12	9	0	-1	-1	2	0	1	-1	0	0	-1
13	10	11	9	13	0	1	0	2	1	1	0	1	-1	-1
0	0	0	0	0	10	0	0	0	0	0	2	0	0	-2
-1	-1	0	-1	1	0	9	1	0	0	-1	1	0	-1	3
0	0	0	-1	0	0	1	10	0	0	1	-2	-2	3	0
2	0	2	2	2	0	0	0	10	2	0	0	0	0	-2
1	0	1	0	1	0	0	0	2	11	2	-2	-1	-2	1
-1	1	2	1	1	0	-1	-1	0	2	9	3	-2	-1	-1
-2	-2	0	-1	0	2	-1	-2	0	-2	3	12	0	-1	0
1	2	1	0	1	0	0	-2	0	-1	-2	0	13	2	1
0	1	0	0	-1	0	-1	3	0	-2	-1	-1	2	12	1
-1	-2	-1	-1	-1	-2	3	0	-2	1	-1	0	1	1	13

$$\left| \frac{XTX}{16} \right| = 2.163 \cdot 10^{-6}$$

$$\text{tr}(XTX) = 4.565$$

X1X1 =

1.257	-0.181	-0.328	-0.397	-0.584	-0.039	0.16	-0.035	-0.002	-0.007	0.039	0.123	0.006	0.006	-0.073
-0.181	0.461	-0.049	-0.042	-0.111	0.001	0.004	0.014	0.085	0.014	-0.033	0.052	-0.044	-0.044	0.057
-0.328	-0.049	0.507	-0.043	-0.02	0.014	-0.048	-0.006	-0.017	-0.017	-0.048	-0.058	-0.013	-0.01	0.031
-0.397	-0.042	-0.043	0.422	0.177	0.004	-0.026	0.048	-0.038	0.032	-0.009	-0.021	0.035	0.001	6.103 · 10 ⁻⁴
-0.584	-0.111	-0.02	0.177	0.661	0.025	-0.121	-0.004	-0.039	-0.014	0.021	-0.1	0.006	0.043	0.026
-0.039	0.001	0.014	0.004	0.025	0.11	-0.009	-0.005	0.006	-0.011	0.012	-0.029	-0.001	-0.002	-0.023
0.16	0.004	-0.048	-0.026	-0.121	-0.009	0.16	-0.024	-0.002	-0.004	0.024	0.005	0.001	0.015	-0.04
-0.035	-0.014	-0.006	0.048	-0.004	-0.005	-0.024	-0.153	-0.002	0.01	-0.03	0.031	0.024	-0.039	0.005
-0.002	0.085	-0.017	-0.038	-0.039	0.006	-0.002	-0.002	0.131	-0.026	0.008	0.002	0.01	-0.015	0.032
-0.007	-0.014	-0.017	0.032	-0.014	-0.011	0.004	0.01	-0.026	0.118	-0.037	0.037	0.005	0.016	-0.019
0.039	-0.033	-0.048	-0.009	0.021	0.012	0.024	-0.03	0.008	-0.037	0.158	-0.053	0.019	0.013	0.005
0.123	0.052	-0.058	-0.021	-0.1	-0.029	0.005	0.031	0.002	0.037	-0.053	0.14	-0.004	-0.005	-0.008
0.006	-0.044	-0.013	0.035	0.006	-0.001	0.001	0.024	-0.01	0.005	0.019	-0.004	0.094	-0.014	-0.011
0.006	-0.044	-0.01	0.001	0.043	-0.002	0.015	-0.039	-0.015	0.016	0.013	-0.005	-0.014	0.109	-0.017
-0.073	0.057	0.011	6.103 · 10 ⁻⁴	0.026	0.023	-0.04	0.005	0.032	-0.019	0.005	-0.008	-0.011	-0.017	0.105

DESIGN (8.24) CONTINUED

$$|r| = 0.145$$

$$tr \begin{bmatrix} & -1 \\ r & \end{bmatrix} = 18.851$$

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$$r^{-1} = \begin{bmatrix} 1.384 & -0.133 & -0.125 & -0.3 & 0.006 & 0.02 & 0.074 & 0.461 & 0.078 & -0.171 & 0.308 & -0.276 & -0.266 & 0.356 \\ -0.133 & 1.236 & -0.117 & -0.049 & 0.068 & -0.223 & -0.029 & -0.085 & -0.088 & -0.225 & -0.308 & -0.076 & -0.056 & 0.063 \\ -0.125 & -0.117 & 1.267 & 0.478 & 0.024 & -0.132 & 0.264 & -0.206 & 0.183 & -0.044 & -0.124 & 0.218 & 0.006 & 0.004 \\ -0.3 & -0.049 & 0.478 & 1.611 & 0.124 & -0.564 & -0.021 & -0.189 & -0.072 & 0.098 & -0.535 & 0.031 & 0.234 & 0.144 \\ 0.006 & 0.068 & 0.024 & 0.124 & 1.104 & -0.087 & -0.053 & 0.059 & -0.117 & 0.111 & -0.32 & -0.016 & -0.027 & 0.256 \\ 0.02 & -0.223 & -0.132 & -0.564 & -0.087 & 1.428 & -0.229 & -0.019 & 0.043 & 0.213 & 0.055 & 0.012 & 0.159 & -0.435 \\ 0.074 & -0.029 & 0.264 & -0.021 & -0.053 & -0.229 & 1.33 & -0.015 & 0.106 & -0.282 & 0.339 & 0.27 & -0.431 & 0.056 \\ 0.461 & -0.085 & -0.206 & -0.189 & 0.059 & -0.019 & -0.015 & 1.276 & -0.268 & 0.074 & 0.022 & -0.11 & -0.158 & 0.356 \\ 0.078 & -0.088 & 0.183 & -0.072 & -0.117 & 0.043 & 0.106 & -0.268 & 1.287 & -0.369 & 0.422 & 0.056 & 0.182 & -0.222 \\ -0.171 & -0.225 & -0.044 & 0.098 & 0.111 & 0.213 & -0.282 & 0.074 & -0.369 & 1.412 & -0.546 & 0.201 & 0.134 & 0.057 \\ 0.308 & -0.308 & -0.124 & -0.535 & -0.32 & 0.055 & 0.339 & 0.022 & 0.422 & -0.546 & 1.639 & -0.055 & -0.062 & -0.098 \\ -0.276 & -0.076 & 0.218 & 0.031 & -0.016 & 0.012 & 0.27 & -0.11 & 0.056 & 0.201 & -0.055 & 1.214 & -0.18 & -0.146 \\ -0.266 & -0.056 & 0.006 & 0.234 & -0.027 & 0.159 & -0.431 & -0.158 & 0.182 & 0.134 & -0.062 & -0.18 & 1.307 & -0.217 \\ 0.356 & 0.063 & 0.004 & 0.144 & 0.256 & -0.435 & 0.056 & 0.356 & -0.222 & 0.057 & -0.098 & -0.146 & -0.217 & 1.355 \end{bmatrix}$$

$$P = \begin{bmatrix} 1 & -0.238 & -0.411 & -0.545 & -0.641 & -0.105 & 0.357 & -0.087 & -0.006 & -0.019 & 0.087 & 0.294 & 0.018 & 0.016 & -0.2 \\ -0.238 & 1 & -0.102 & -0.095 & -0.201 & 0.005 & 0.014 & 0.055 & 0.347 & 0.059 & -0.122 & 0.204 & -0.213 & -0.198 & 0.26 \\ -0.411 & -0.102 & 1 & -0.094 & -0.035 & 0.058 & -0.168 & -0.022 & -0.067 & -0.07 & -0.17 & -0.216 & -0.062 & -0.044 & 0.048 \\ -0.545 & -0.095 & -0.094 & 1 & 0.335 & 0.02 & -0.098 & 0.203 & -0.162 & 0.143 & -0.033 & -0.086 & 0.176 & 0.005 & 0.003 \\ -0.641 & -0.201 & -0.035 & 0.335 & 1 & 0.093 & -0.372 & -0.014 & -0.132 & -0.05 & 0.065 & -0.329 & 0.022 & 0.161 & 0.097 \\ -0.105 & 0.005 & 0.058 & 0.02 & 0.093 & 1 & -0.069 & -0.043 & 0.049 & -0.098 & 0.089 & -0.238 & -0.013 & -0.022 & 0.21 \\ 0.357 & 0.014 & -0.168 & -0.098 & -0.372 & -0.069 & 1 & -0.166 & -0.014 & 0.032 & 0.15 & 0.036 & 0.009 & 0.116 & -0.312 \\ -0.087 & 0.055 & -0.022 & 0.203 & -0.014 & -0.043 & -0.166 & 1 & -0.012 & 0.081 & -0.206 & 0.23 & 0.212 & -0.327 & 0.042 \\ -0.006 & 0.347 & -0.067 & -0.162 & -0.132 & 0.049 & -0.014 & -0.012 & 1 & -0.209 & 0.055 & 0.015 & -0.089 & -0.122 & 0.271 \\ -0.019 & 0.059 & -0.07 & 0.143 & -0.05 & -0.098 & 0.032 & 0.081 & -0.209 & 1 & -0.274 & 0.29 & 0.045 & 0.141 & -0.168 \\ 0.087 & -0.122 & -0.17 & -0.033 & 0.065 & 0.089 & 0.15 & -0.206 & 0.055 & -0.274 & 1 & -0.359 & 0.153 & 0.098 & 0.041 \\ 0.294 & 0.204 & -0.216 & -0.086 & -0.329 & -0.238 & 0.036 & 0.23 & 0.015 & 0.29 & -0.359 & 1 & -0.039 & -0.043 & 0.066 \\ 0.018 & -0.213 & -0.062 & 0.176 & 0.022 & -0.013 & 0.009 & 0.212 & -0.089 & 0.045 & 0.153 & -0.039 & 1 & -0.143 & -0.114 \\ 0.016 & -0.198 & -0.044 & 0.005 & 0.161 & -0.022 & 0.116 & -0.327 & -0.122 & 0.141 & 0.098 & -0.043 & -0.143 & 1 & -0.163 \\ -0.2 & 0.26 & 0.048 & 0.003 & 0.097 & 0.21 & -0.312 & 0.042 & 0.271 & -0.168 & 0.041 & -0.066 & -0.114 & -0.163 & 1 \end{bmatrix}$$

----- (8.25) A 4x4x4x4x4/32 design -----

DESIGN MATRIX

$$xp^T = (0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 1 \ 2 \ 0 \ 2 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 0 \ 2)$$

$$xq^T = (0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 1 \ 3 \ 2 \ 1 \ 1 \ 3 \ 3 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 3 \ 3)$$

$$xr^T = (0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3 \ 3 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3 \ 3 \ 1 \ 0 \ 0 \ 0 \ 3 \ 2 \ 3 \ 2 \ 0 \ 1 \ 0 \ 1 \ 3 \ 2 \ 3 \ 3)$$

$$xs^T = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3 \ 3 \ 3 \ 3 \ 3 \ 3 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 1 \ 0 \ 2 \ 3 \ 2 \ 3 \ 3 \ 2 \ 3 \ 3)$$

$$xt^T = (0 \ 3 \ 3 \ 0 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 0 \ 3 \ 3 \ 0 \ 2 \ 1 \ 0 \ 3 \ 0 \ 2 \ 3 \ 0 \ 1 \ 3 \ 3 \ 0 \ 3 \ 0 \ 1 \ 2)$$

$$x1_i = (2xp_i - 3)/3$$

$$x2_i = (2xq_i - 3)/3$$

$$x3_i = (2xr_i - 3)/3$$

$$x4_i = (2xs_i - 3)/3$$

$$x5_i = (2xt_i - 3)/3$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1_i \quad X_{i,3} := x2_i \quad X_{i,4} := x3_i \quad X_{i,5} := x4_i \quad X_{i,6} := x5_i$$

$$X_{i,7} := x1_i \cdot x2_i \quad X_{i,8} := x1_i \cdot x3_i \quad X_{i,9} := x1_i \cdot x4_i \quad X_{i,10} := x1_i \cdot x5_i$$

$$X_{i,11} := x2_i \cdot x3_i \quad X_{i,12} := x2_i \cdot x4_i \quad X_{i,13} := x2_i \cdot x5_i$$

$$X_{i,14} := x3_i \cdot x4_i \quad X_{i,15} := x3_i \cdot x5_i \quad X_{i,16} := x4_i \cdot x5_i$$

$$X_{i,17} := x1_i \quad X_{i,18} := x2_i \quad X_{i,19} := x3_i \quad X_{i,20} := x4_i \quad X_{i,21} := x5_i$$

----- (8.26) A 4x4x4x4x3/32 design -----

DESIGN MATRIX

$$xp^T = (0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 1 \ 2 \ 0 \ 2 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 0 \ 2)$$

$$xq^T = (0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 0 \ 3 \ 3 \ 0 \ 1 \ 3 \ 2 \ 1 \ 1 \ 3 \ 3 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 3 \ 3)$$

$$xr^T = (0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3 \ 3 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3 \ 3 \ 1 \ 0 \ 0 \ 0 \ 3 \ 2 \ 3 \ 2 \ 0 \ 1 \ 0 \ 1 \ 3 \ 2 \ 3 \ 3)$$

$$xs^T = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 3 \ 3 \ 3 \ 3 \ 3 \ 3 \ 3 \ 3 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 1 \ 0 \ 2 \ 3 \ 2 \ 3 \ 3 \ 2 \ 3 \ 3)$$

$$xt^T = (0 \ 2 \ 2 \ 0 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 2 \ 0 \ 1 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 2 \ 0 \ 2 \ 0 \ 1 \ 1)$$

$$x1_i = (2xp_i - 3)/3$$

$$x2_i = (2xq_i - 3)/3$$

$$x3_i = (2xr_i - 3)/3$$

$$x4_i = (2xs_i - 3)/3$$

$$x5_i = (xt_i - 1)$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1^2 \quad X_{i,3} := x2^2 \quad X_{i,4} := x3^2 \quad X_{i,5} := x4^2 \quad X_{i,6} := x5^2$$

$$X_{i,7} := x1 \cdot x2 \quad X_{i,8} := x1 \cdot x3 \quad X_{i,9} := x1 \cdot x4 \quad X_{i,10} := x1 \cdot x5$$

$$X_{i,11} := x2 \cdot x3 \quad X_{i,12} := x2 \cdot x4 \quad X_{i,13} := x2 \cdot x5$$

$$X_{i,14} := x3 \cdot x4 \quad X_{i,15} := x3 \cdot x5 \quad X_{i,16} := x4 \cdot x5$$

$$X_{i,17} := x1 \quad X_{i,18} := x2 \quad X_{i,19} := x3 \quad X_{i,20} := x4 \quad X_{i,21} := x5$$

----- (8.27) A 4x4x4x3x3/32 design -----

DESIGN MATRIX

$$xp^T = (0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 1\ 3\ 1\ 2\ 0\ 2\ 0\ 3\ 0\ 3\ 1\ 3\ 0\ 2)$$

$$xq^T = (0\ 0\ 3\ 3\ 0\ 0\ 3\ 3\ 0\ 0\ 3\ 3\ 0\ 0\ 3\ 3\ 0\ 1\ 3\ 2\ 1\ 1\ 3\ 3\ 0\ 0\ 2\ 2\ 0\ 0\ 3\ 3)$$

$$xr^T = (0\ 0\ 0\ 0\ 3\ 3\ 3\ 3\ 0\ 0\ 0\ 0\ 3\ 3\ 3\ 3\ 1\ 0\ 0\ 0\ 3\ 2\ 3\ 2\ 0\ 1\ 0\ 1\ 3\ 2\ 3\ 3)$$

$$xs^T = (0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 2\ 2\ 2\ 2\ 2\ 2\ 2\ 2\ 0\ 0\ 1\ 0\ 0\ 1\ 1\ 0\ 1\ 2\ 1\ 2\ 2\ 1\ 2\ 2)$$

$$xt^T = (0\ 2\ 2\ 0\ 2\ 0\ 0\ 2\ 2\ 0\ 0\ 2\ 0\ 2\ 2\ 0\ 1\ 1\ 0\ 2\ 0\ 1\ 2\ 0\ 1\ 2\ 2\ 0\ 2\ 0\ 1\ 1)$$

$$x1_i = (2xp_i - 3)/3$$

$$x2_i = (2xq_i - 3)/3$$

$$x3_i = (2xr_i - 3)/3$$

$$x4_i = (xs_i - 1)$$

$$x5_i = (xt_i - 1)$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1_i \quad X_{i,3} := x2_i \quad X_{i,4} := x3_i \quad X_{i,5} := x4_i \quad X_{i,6} := x5_i$$

$$X_{i,7} := x1_i \cdot x2_i \quad X_{i,8} := x1_i \cdot x3_i \quad X_{i,9} := x1_i \cdot x4_i \quad X_{i,10} := x1_i \cdot x5_i$$

$$X_{i,11} := x2_i \cdot x3_i \quad X_{i,12} := x2_i \cdot x4_i \quad X_{i,13} := x2_i \cdot x5_i$$

$$X_{i,14} := x3_i \cdot x4_i \quad X_{i,15} := x3_i \cdot x5_i \quad X_{i,16} := x4_i \cdot x5_i$$

$$X_{i,17} := x1_i \quad X_{i,18} := x2_i \quad X_{i,19} := x3_i \quad X_{i,20} := x4_i \quad X_{i,21} := x5_i$$

----- (8.28) A 4x4x3x3x3/32 design -----

DESIGN MATRIX

$$xp^T = (0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 0\ 3\ 1\ 3\ 1\ 2\ 0\ 2\ 0\ 3\ 0\ 3\ 1\ 3\ 0\ 2)$$

$$xq^T = (0\ 0\ 3\ 3\ 0\ 0\ 3\ 3\ 0\ 0\ 3\ 3\ 0\ 0\ 3\ 3\ 0\ 1\ 3\ 2\ 1\ 1\ 3\ 3\ 0\ 0\ 2\ 2\ 0\ 0\ 3\ 3)$$

$$xr^T = (0\ 0\ 0\ 0\ 2\ 2\ 2\ 2\ 0\ 0\ 0\ 0\ 2\ 2\ 2\ 2\ 1\ 0\ 0\ 0\ 2\ 1\ 2\ 1\ 0\ 1\ 0\ 1\ 2\ 1\ 2\ 2)$$

$$xs^T = (0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 2\ 2\ 2\ 2\ 2\ 2\ 2\ 2\ 0\ 0\ 1\ 0\ 0\ 1\ 1\ 0\ 1\ 2\ 1\ 2\ 2\ 1\ 2\ 2)$$

$$xt^T = (0\ 2\ 2\ 0\ 2\ 0\ 0\ 2\ 2\ 0\ 0\ 2\ 0\ 2\ 2\ 0\ 1\ 1\ 0\ 2\ 0\ 1\ 2\ 0\ 1\ 2\ 2\ 0\ 2\ 0\ 1\ 1)$$

$$x1_i = (2xp_i - 3) / 3$$

$$x2_i = (2xq_i - 3) / 3$$

$$x3_i = (xr_i - 1)$$

$$x4_i = (xs_i - 1)$$

$$x5_i = (xt_i - 1)$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1^2 \quad X_{i,3} := x2^2 \quad X_{i,4} := x3^2 \quad X_{i,5} := x4^2 \quad X_{i,6} := x5^2$$

$$X_{i,7} := x1 \cdot x2 \quad X_{i,8} := x1 \cdot x3 \quad X_{i,9} := x1 \cdot x4 \quad X_{i,10} := x1 \cdot x5$$

$$X_{i,11} := x2 \cdot x3 \quad X_{i,12} := x2 \cdot x4 \quad X_{i,13} := x2 \cdot x5$$

$$X_{i,14} := x3 \cdot x4 \quad X_{i,15} := x3 \cdot x5 \quad X_{i,16} := x4 \cdot x5$$

$$X_{i,17} := x1 \quad X_{i,18} := x2 \quad X_{i,19} := x3 \quad X_{i,20} := x4 \quad X_{i,21} := x5$$

----- (8.29) A $4 \times 3 \times 3 \times 3 \times 3 / 32$ design -----

DESIGN MATRIX

$$xp^T = (0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 1 \ 2 \ 0 \ 2 \ 0 \ 3 \ 0 \ 3 \ 1 \ 3 \ 0 \ 2)$$

$$xq^T = (0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 1 \ 2 \ 1 \ 1 \ 1 \ 2 \ 2 \ 0 \ 0 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2)$$

$$xr^T = (0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 1 \ 0 \ 0 \ 0 \ 2 \ 1 \ 2 \ 1 \ 0 \ 1 \ 0 \ 1 \ 2 \ 1 \ 2 \ 2)$$

$$xs^T = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 1 \ 0 \ 1 \ 2 \ 1 \ 2 \ 2 \ 1 \ 2 \ 2)$$

$$xt^T = (0 \ 2 \ 2 \ 0 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 2 \ 0 \ 1 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 2 \ 0 \ 2 \ 0 \ 1 \ 1)$$

$$x1_i = (2xp_i - 3) / 3$$

$$x2_i = (xq_i - 1)$$

$$x3_i = (xr_i - 1)$$

$$x4_i = (xs_i - 1)$$

$$x5_i = (xt_i - 1)$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1_i^2 \quad X_{i,3} := x2_i^2 \quad X_{i,4} := x3_i^2 \quad X_{i,5} := x4_i^2 \quad X_{i,6} := x5_i^2$$

$$X_{i,7} := x1_i \cdot x2_i \quad X_{i,8} := x1_i \cdot x3_i \quad X_{i,9} := x1_i \cdot x4_i \quad X_{i,10} := x1_i \cdot x5_i$$

$$X_{i,11} := x2_i \cdot x3_i \quad X_{i,12} := x2_i \cdot x4_i \quad X_{i,13} := x2_i \cdot x5_i$$

$$X_{i,14} := x3_i \cdot x4_i \quad X_{i,15} := x3_i \cdot x5_i \quad X_{i,16} := x4_i \cdot x5_i$$

$$X_{i,17} := x1_i \quad X_{i,18} := x2_i \quad X_{i,19} := x3_i \quad X_{i,20} := x4_i \quad X_{i,21} := x5_i$$

----- (8.30) A $3 \times 3 \times 3 \times 3 \times 3 / 32$ design -----

DESIGN MATRIX

$$xp^T = (0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 1 \ 2 \ 1 \ 1 \ 0 \ 1 \ 0 \ 2 \ 0 \ 2 \ 1 \ 2 \ 0 \ 1)$$

$$xq^T = (0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 1 \ 2 \ 1 \ 1 \ 1 \ 2 \ 2 \ 0 \ 0 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2)$$

$$xr^T = (0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 1 \ 0 \ 0 \ 0 \ 2 \ 1 \ 2 \ 1 \ 0 \ 1 \ 0 \ 1 \ 2 \ 1 \ 2 \ 2)$$

$$xs^T = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 1 \ 0 \ 1 \ 2 \ 1 \ 2 \ 2 \ 1 \ 2 \ 2)$$

$$xt^T = (0 \ 2 \ 2 \ 0 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 2 \ 0 \ 1 \ 1 \ 0 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 2 \ 0 \ 2 \ 0 \ 1 \ 1)$$

$$x1_i = (xp_i - 1)$$

$$x2_i = (xq_i - 1)$$

$$x3_i = (xr_i - 1)$$

$$x4_i = (xs_i - 1)$$

$$x5_i = (xt_i - 1)$$

COLUMN VECTORS OF X-MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1_i^2 \quad X_{i,3} := x2_i^2 \quad X_{i,4} := x3_i^2 \quad X_{i,5} := x4_i^2 \quad X_{i,6} := x5_i^2$$

$$X_{i,7} := x1_i \cdot x2_i \quad X_{i,8} := x1_i \cdot x3_i \quad X_{i,9} := x1_i \cdot x4_i \quad X_{i,10} := x1_i \cdot x5_i$$

$$X_{i,11} := x2_i \cdot x3_i \quad X_{i,12} := x2_i \cdot x4_i \quad X_{i,13} := x2_i \cdot x5_i$$

$$X_{i,14} := x3_i \cdot x4_i \quad X_{i,15} := x3_i \cdot x5_i \quad X_{i,16} := x4_i \cdot x5_i$$

$$X_{i,17} := x1_i \cdot x3_i \cdot x5_i \quad X_{i,18} := x2_i \cdot x3_i \cdot x5_i \quad X_{i,19} := x3_i \cdot x4_i \cdot x5_i \quad X_{i,20} := x4_i \cdot x5_i \quad X_{i,21} := x5_i$$

COLUMN VECTORS OF X-MATRIX

DESIGN MATRIX

$xw^T = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1)$
 $xp^T = (0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 2 \ 2 \ 2 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 2 \ 2 \ 2)$
 $xq^T = (0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 1 \ 2)$
 $xu^T = (0 \ 1 \ 2 \ 2 \ 0 \ 1 \ 1 \ 2 \ 0 \ 1 \ 2 \ 0 \ 2 \ 0 \ 1 \ 0 \ 1 \ 2)$

$X_{1,1} := 1$
 $X_{1,2} := 2 \cdot xw - 1$

$X_{1,3} := \frac{[xp_i - 1] \cdot \sqrt{6}}{2}$
 $X_{1,4} := \left[\begin{matrix} 2 \\ X_{1,3} - 1 \end{matrix} \right] \cdot \sqrt{2}$

$X_{1,5} := \frac{[xq_i - 1] \cdot \sqrt{6}}{2}$
 $X_{1,6} := \left[\begin{matrix} 2 \\ X_{1,5} - 1 \end{matrix} \right] \cdot \sqrt{2}$

$XTX =$
 $|XTX| = 6.149 \cdot 10^{16}$

18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	18	0	0	0	0	0	0	0	0	0	0	0	0	6.364	0
0	0	0	0	18	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	18	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	18	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	18	0	0	0	0	0	0	0	0	11.023	0
0	0	0	0	0	0	0	0	18	0	0	0	0	0	0	0	11.023	0
0	0	0	0	0	0	0	0	0	18	11.023	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	18	4.5	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	18	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	18	0	0	0
0	0	0	6.364	0	0	0	0	11.023	0	0	0	0	0	0	0	18	0

$X_{1,7} := \frac{[xu_i - 1] \cdot \sqrt{6}}{2}$
 $X_{1,8} := \left[\begin{matrix} 2 \\ X_{1,7} - 1 \end{matrix} \right] \cdot \sqrt{2}$

$X_{1,9} := X_{1,2} - X_{1,3}$
 $X_{1,10} := X_{1,2} - X_{1,5}$

$X_{1,11} := X_{1,2} - X_{1,7}$
 $X_{1,12} := X_{1,2} - X_{1,5}$

$X_{1,13} := X_{1,3} - X_{1,7}$
 $X_{1,14} := X_{1,3} - X_{1,7}$

XTX⁻¹

0.056	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0.056	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0.056	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0.069	0	0	0	0	0	0	0.024	0	0	0	0	0	0	-0.039
0	0	0	0	0.056	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.056	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0.056	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0.056	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0.056	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0.056	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0.097	0	0	0	0	0	0	-0.068
0	0	0	0	0.024	0	0	0	0	0	0	0.097	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0.095	-0.016	0.026	-0.065	0	0
0	0	0	0	0	0	0	0	0	0	0	0	-0.016	0.095	-0.065	0.026	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0.026	-0.065	0.106	-0.042	0	0
0	0	0	0	0	0	0	0	0	0	0	0	-0.065	0.026	-0.042	0.106	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.111	0

tr(XTX⁻¹) = 1.069

r

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0.612	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0.612	1	0.25	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0.25	1	0	0	0	0	0
0	0	0.354	0	0	0	0	0	0.612	0	0	0	0	0	0	0	0	1

|r| = 0.164

r⁻¹

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1.25	0	0	0	0	0.433	0	0	0	0	0	0	0	0	0	-0.707
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0.433	0	0	0	0	1.75	0	0	0	0	0	0	0	0	0	-1.225
0	0	0	0	0	0	0	0	1.714	-0.286	0.467	-1.166	0	0	0	0	0	0
0	0	0	0	0	0	0	0	-0.286	1.714	-1.166	0.467	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0.467	-1.166	1.905	-0.762	0	0	0	0	0	0
0	0	0	0	0	0	0	0	-1.166	0.467	-0.762	1.905	0	0	0	0	0	0
0	0	-0.707	0	0	0	0	-1.225	0	0	0	0	0	0	0	0	0	2

tr[r⁻¹] = 18.238

P

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0.293	0	0	0	0	0	0	0	0	0	-0.447
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	-0.167	0.258	-0.645	0	0	0	0	0	-0.655
0	0	0	0	0	0	0	0	-0.167	1	-0.645	0.258	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0.258	-0.645	1	-0.4	0	0	0	0	0	0
0	0	0	0	0	0	0	0	-0.645	0.258	-0.4	1	0	0	0	0	0	0
0	0	0	-0.447	0	0	0	0	-0.655	0	0	0	0	0	0	0	0	1

----- (8.37) A 3x3x3/15 Box Behnken design -----

DESIGN MATRIX

$$\begin{aligned} xp^T &= (0 \ 0 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1) \\ xq^T &= (0 \ 2 \ 0 \ 2 \ 1 \ 1 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2 \ 1 \ 1 \ 1) \\ xr^T &= (1 \ 1 \ 1 \ 1 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 1 \ 1 \ 1) \end{aligned}$$

COLUMN VECTORS OF X-MATRIX

$$\begin{aligned} X_{i,1} &:= 1 \\ X_{i,2} &:= 0.5 \cdot [xp_i - 1] \cdot \sqrt{7.5} \\ X_{i,3} &:= \frac{7 - 30 \cdot xp_i + 15 \cdot xp_i^2}{\sqrt{56}} \\ X_{i,4} &:= 0.5 \cdot [xq_i - 1] \cdot \sqrt{7.5} \\ X_{i,5} &:= \frac{7 - 30 \cdot xq_i + 15 \cdot xq_i^2}{\sqrt{56}} \\ X_{i,6} &:= 0.5 \cdot [xr_i - 1] \cdot \sqrt{7.5} \\ X_{i,7} &:= \frac{7 - 30 \cdot xr_i + 15 \cdot xr_i^2}{\sqrt{56}} \\ X_{i,8} &:= X_{i,2} \cdot X_{i,4} \quad X_{i,9} := X_{i,2} \cdot X_{i,6} \quad X_{i,10} := X_{i,4} \cdot X_{i,6} \end{aligned}$$

$$XTX = \begin{bmatrix} 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 15 & 0 & -1.071 & 0 & -1.071 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1.071 & 0 & 15 & 0 & -1.071 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 15 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1.071 & 0 & -1.071 & 0 & 15 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 14.063 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 14.063 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 14.063 & 0 \end{bmatrix}$$

$|XTX| = 4.675 \cdot 10^{11}$

$$XTXI = \begin{bmatrix} 0.067 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.067 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.067 & 0 & 0.005 & 0 & 0.005 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.067 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.005 & 0 & 0.067 & 0 & 0.005 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.067 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.005 & 0 & 0.005 & 0 & 0.067 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.071 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.071 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.071 & 0 \end{bmatrix}$$

$tr(XTXI) = 0.682$

$$r = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -0.071 & 0 & -0.071 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.071 & 0 & 1 & 0 & -0.071 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -0.071 & 0 & -0.071 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$|r| = 0.984$

$$r^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.011 & 0 & 0.078 & 0 & 0.078 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.078 & 0 & 1.011 & 0 & 0.078 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0.078 & 0 & 0.078 & 0 & 1.011 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$tr[r^{-1}] = 9.033$

$$p = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0.077 & 0 & 0.077 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.077 & 0 & 1 & 0 & 0.077 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0.077 & 0 & 0.077 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

----- (8.39) A 3x3x3x3/15 Saturated design -----

DESIGN MATRIX

$$\begin{aligned} x_p^T &= (0 \ 0 \ 2 \ 2 \ 2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 0 \ 2 \ 1 \ 1 \ 1) \\ x_q^T &= (0 \ 2 \ 0 \ 2 \ 2 \ 2 \ 0 \ 0 \ 2 \ 2 \ 0 \ 1 \ 2 \ 1 \ 1) \\ x_r^T &= (0 \ 2 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 0 \ 2 \ 1 \ 1 \ 2 \ 1) \\ x_s^T &= (0 \ 2 \ 2 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 0 \ 2 \ 2 \ 1 \ 1 \ 1 \ 2) \end{aligned}$$

$$X_{i,1} := -1$$

COLUMN VECTORS OF X-MATRIX.

$$X_{i,2} := \frac{-17 + 15 \cdot x_p}{\sqrt{176}} \quad X_{i,3} := \frac{-17 + 15 \cdot x_q}{\sqrt{176}} \quad X_{i,4} := \frac{-17 + 15 \cdot x_r}{\sqrt{176}}$$

$$X_{i,5} := \frac{-17 + 15 \cdot x_s}{\sqrt{176}} \quad X_{i,6} := \frac{21 - 179 \cdot x_p + 88 \cdot x_p^2}{\sqrt{1232}}$$

$$X_{i,7} := \frac{21 - 179 \cdot x_q + 88 \cdot x_q^2}{\sqrt{1232}} \quad X_{i,8} := \frac{21 - 179 \cdot x_r + 88 \cdot x_r^2}{\sqrt{1232}}$$

$$X_{i,9} := \frac{21 - 179 \cdot x_s + 88 \cdot x_s^2}{\sqrt{1232}} \quad X_{i,10} := X_{i,2} \cdot X_{i,3}$$

$$X_{i,11} := X_{i,2} \cdot X_{i,4} \quad X_{i,12} := X_{i,2} \cdot X_{i,5} \quad X_{i,13} := X_{i,3} \cdot X_{i,4}$$

$$X_{i,14} := X_{i,3} \cdot X_{i,5} \quad X_{i,15} := X_{i,4} \cdot X_{i,5}$$

$$|XTX| = 2.764 \cdot 10^{16}$$

XTX =

15	0	0	0	0	0	0	0	0	0	0	-1.619	-1.619	-1.619	-1.619	-1.619	-1.619
0	15	-1.619	-1.619	-1.619	0	-1.578	-1.578	-1.578	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379
0	-1.619	15	-1.619	-1.619	-1.578	0	-1.578	-1.578	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379
0	-1.619	-1.619	15	-1.619	-1.578	-1.578	0	-1.578	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379
0	-1.619	-1.619	-1.619	15	-1.578	-1.578	-1.578	0	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379	-0.379
0	0	-1.578	-1.578	-1.578	15	9.048	9.048	9.048	9.048	-0.527	-0.527	-0.527	-0.527	-0.527	-0.527	-0.527
0	-1.578	0	-1.578	-1.578	9.048	15	9.048	9.048	9.048	-0.527	0.148	0.148	0.148	-0.527	-0.527	-0.527
0	-1.578	-1.578	0	-1.578	9.048	9.048	15	9.048	9.048	-0.527	0.148	-0.527	0.148	-0.527	-0.527	-0.527
0	-1.578	-1.578	-1.578	0	9.048	9.048	9.048	15	9.048	-0.527	0.148	-0.527	0.148	-0.527	-0.527	-0.527
-1.619	-0.379	-0.379	-0.379	-0.379	-0.527	-0.527	-0.527	-0.527	0.148	17.664	-0.583	-0.583	-0.583	-0.583	-0.583	7.32
-1.619	-0.379	-0.379	-0.379	-0.379	-0.527	0.148	-0.527	0.148	-0.583	17.664	-0.583	-0.583	-0.583	-0.583	-0.583	7.32
-1.619	-0.379	-0.379	-0.379	-0.379	-0.527	0.148	-0.527	-0.583	-0.583	17.664	7.32	-0.583	-0.583	-0.583	-0.583	7.32
-1.619	-0.379	-0.379	-0.379	-0.379	-0.527	0.148	-0.527	-0.583	-0.583	7.32	17.664	-0.583	-0.583	-0.583	-0.583	7.32
-1.619	-0.379	-0.379	-0.379	-0.379	0.148	-0.527	-0.583	-0.583	-0.583	7.32	-0.583	17.664	-0.583	-0.583	-0.583	7.32
-1.619	-0.379	-0.379	-0.379	-0.379	0.148	0.148	-0.527	-0.527	-0.527	7.32	-0.583	-0.583	17.664	-0.583	-0.583	7.32

XTX1 =

$$cr(XTX1) = 1.563$$

0.073	0.012	0.012	0.012	0.012	0.002	0.002	0.002	0.002	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
0.012	0.104	0.032	0.032	0.032	-0.012	0.012	0.012	0.012	0.007	0.007	0.007	0.031	0.031	0.031	0.031	0.031
0.012	0.032	0.104	0.032	0.032	0.012	-0.012	0.012	0.012	0.007	0.007	0.007	0.031	0.031	0.031	0.031	0.031
0.012	0.032	0.032	0.104	0.032	0.012	0.012	-0.012	0.012	0.007	0.007	0.007	0.031	0.031	0.031	0.031	0.031
0.002	-0.012	0.012	0.012	0.012	0.012	0.141	-0.038	-0.038	-0.038	0.012	0.012	-0.007	-0.007	-0.007	-0.007	-0.007
0.002	0.012	-0.012	0.012	0.012	-0.038	0.141	-0.038	-0.038	-0.038	0.012	-0.007	-0.007	-0.007	-0.007	-0.007	-0.007
0.002	0.012	0.012	-0.012	0.012	-0.038	-0.038	0.141	-0.038	-0.007	0.012	-0.007	-0.007	-0.007	-0.007	-0.007	-0.007
0.002	0.012	0.012	0.012	-0.012	-0.038	-0.038	-0.038	0.141	-0.007	-0.007	-0.007	-0.007	-0.007	-0.007	-0.007	-0.007
0.01	0.007	0.007	0.031	0.031	0.031	0.012	0.012	-0.007	0.085	0.008	0.008	0.008	0.008	0.008	0.008	-0.03
0.01	0.007	0.031	0.007	0.031	0.031	0.012	-0.007	0.012	-0.007	0.008	0.085	0.008	0.008	0.008	0.008	-0.03
0.01	0.007	0.031	0.031	0.007	0.031	-0.007	-0.007	-0.007	0.012	0.008	0.008	0.085	-0.03	0.008	0.008	0.008
0.01	0.031	0.007	0.007	0.031	-0.007	0.012	0.012	-0.007	0.008	0.008	-0.03	0.085	0.008	0.008	0.008	0.008
0.01	0.031	0.007	0.031	0.007	-0.007	0.012	-0.007	0.012	0.008	-0.03	0.008	0.008	0.085	0.008	0.008	0.008
0.01	0.031	0.031	0.031	0.007	-0.007	-0.007	-0.007	0.012	-0.03	0.008	0.008	0.008	0.008	0.085	0.008	0.085

DESIGN MATRIX

$$xp^T = (2 \ 0 \ 1 \ 0 \ 0 \ 2 \ 0 \ 1 \ 0 \ 1 \ 2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 0 \ 2 \ 2 \ 2 \ 1 \ 0 \ 2 \ 2 \ 0 \ 0 \ 0)$$

$$xq^T = (2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 2 \ 0 \ 2 \ 1 \ 1 \ 0 \ 0 \ 1 \ 0 \ 1 \ 0 \ 0 \ 2 \ 0 \ 2 \ 2 \ 2 \ 0 \ 2 \ 2 \ 1)$$

$$xr^T = (2 \ 0 \ 2 \ 1 \ 0 \ 2 \ 1 \ 0 \ 0 \ 1 \ 0 \ 2 \ 0 \ 2 \ 2 \ 0 \ 2 \ 2 \ 0 \ 1 \ 0 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2)$$

$$xs^T = (2 \ 0 \ 2 \ 1 \ 2 \ 0 \ 0 \ 0 \ 0 \ 2 \ 0 \ 0 \ 2 \ 1 \ 2 \ 2 \ 0 \ 2 \ 0 \ 0 \ 1 \ 2 \ 2 \ 1 \ 0 \ 2 \ 1)$$

$$xt^T = (2 \ 2 \ 2 \ 2 \ 0 \ 0 \ 1 \ 1 \ 0 \ 0 \ 0 \ 2 \ 2 \ 1 \ 1 \ 2 \ 0 \ 0 \ 2 \ 0 \ 2 \ 0 \ 0 \ 0 \ 2 \ 2 \ 0)$$

$$x1_i := \begin{bmatrix} xp_i - 1 \\ i \end{bmatrix} \quad x2_i := \begin{bmatrix} xq_i - 1 \\ i \end{bmatrix} \quad x3_i := \begin{bmatrix} xr_i - 1 \\ i \end{bmatrix}$$

$$x4_i := \begin{bmatrix} xs_i - 1 \\ i \end{bmatrix} \quad x5_i := \begin{bmatrix} xt_i - 1 \\ i \end{bmatrix}$$

COLUMN VECTORS OF X MATRIX

$$X_{i,1} := 1$$

$$X_{i,2} := x1_i^2 \quad X_{i,3} := x2_i^2 \quad X_{i,4} := x3_i^2 \quad X_{i,5} := x4_i^2 \quad X_{i,6} := x5_i^2$$

$$X_{i,7} := x1_i \cdot x2_i \quad X_{i,8} := x1_i \cdot x3_i \quad X_{i,9} := x1_i \cdot x4_i \quad X_{i,10} := x1_i \cdot x5_i$$

$$X_{i,11} := x2_i \cdot x3_i \quad X_{i,12} := x2_i \cdot x4_i \quad X_{i,13} := x2_i \cdot x5_i$$

$$X_{i,14} := x3_i \cdot x4_i \quad X_{i,15} := x3_i \cdot x5_i \quad X_{i,16} := x4_i \cdot x5_i$$

$$X_{i,17} := x1_i \quad X_{i,18} := x2_i \quad X_{i,19} := x3_i \quad X_{i,20} := x4_i \quad X_{i,21} := x5_i$$

Stellingen

bij het proefschrift

**DESIGNS WITH A SMALL NUMBER OF RUNS
FOR
FACTORIAL EXPERIMENTS**

van

P.M. Upperman

1. Orthogonale "*N*-designs" kunnen met behulp van half-normaal waarschijnlijkheidspapier worden geanalyseerd.

Hoofdstuk 7 van dit proefschrift.

Daniel, C. (1959), The use of Half-Normal Plots in Interpreting Factorial Two-Level Experiments, *Technometrics* 1, 311-341.

Zahn, D.A. (1975), Modifications of and Revised Critical Values for the Half-Normal Plot, *Technometrics* 17, 189-200.

2. Het gebruik van blokindeling bij proefopzetten is niet alleen geschikt om het effect van de experimentele fout te verkleinen, maar kan ook dienen om een onbekende factor, die ongewenste kwaliteitsfluctuaties veroorzaakt, op te sporen.

Upperman, P.M. en Dévény, A.M. (1974), De oplossing van een kwaliteitsprobleem door het gebruik van proefschemas, *Statistica Neerlandica* 28, 153-171.

Upperman, P.M. (1991), Aspecten, principes en toepassingen van proefopzetten, *SIGMA*, No. 3, 8-12.

3. De kwaliteit van een proefopzet wordt niet alleen door statistische kenmerken bepaald, maar ook door de mate waarin ze bruikbaar is voor de onderzoeker.

Boz, G.E.P., Hunter, W.G. and Hunter, J.S. (1978), *Statistics for Experimenters*, John Wiley & Sons, New York.

4. Het construeren van proefschemas, waarbij men sommige eerste orde interacties wel en andere niet kan schatten, is meer een intellectuele dan een praktische bezigheid, omdat men doorgaans of alleen hoofdeffecten, of hoofdeffecten en *alle* eerste orde interacties met een proefopzet wil schatten.

5. Het is aannemelijk dat de receptuur en kwaliteit van bakkerijproducten sterk verbeterd zal worden, indien men op grote schaal de in de laatste decennia ontwikkelde proefopzetten voor mengsels gaat toepassen.

Cornell, J.A. (1990), *Experiments with Mixtures*, John Wiley & Sons, New York.

6. Het rendement van de Nederlandse industrie kan aanmerkelijk worden verhoogd, indien de vakken proefopzetten en variantie-analyse voor studenten in de chemie, electrotechniek, natuurkunde en werktuigbouw tot de verplichte leerstof gaan behoren.

Upperman, P.M. (1985), *Industrial Statistics*, *Statistica Neerlandica*, Vol. 39, No. 2, 203-217.

7. Bij de uitoefening van de geodesie doen zich, met name bij de triangulatie van grote netten, interessante statistische problemen voor inzake verwerking en analyse van waarnemingen.
8. Uitdrukkingen als "De temperatuur was 2 graden lager dan normaal" zoals die wel eens in de maandelijkse weeroverzichten van het NOS-journaal worden gebezigd, zijn voor een leek nauwelijks en voor een statisticus helemaal niet te begrijpen.
9. Om in een ontwikkelingsland te kunnen werken zijn verschillende vaardigheden vereist, die tijdens een schoolopleiding niet aan de orde komen.
10. Het feit dat men van huisartsen en diëtisten soms tegenstrijdige adviezen krijgt inzake aard en samenstelling van het te gebruiken voedsel, doet het vermoeden ontstaan dat de kennis inzake de biochemische mechanismen van het menselijk lichaam, nog in de kinderschoenen staat.