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Constrained Experimental Designs
Part I: Construction of Projection Designs

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Constrained Experimental Designs
Part I: Construction of Projection Designs

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ABSTRACT

Experimental design is a powerful tool for quality improvement. In some situations, however, the design variables are subject to multiple linear constraints. These situations arise quite frequently in the oil industry, the alloy industry, and the food industry. In this paper, we propose a class called *projection designs* which can be used when the design variables are constrained by linear relations. Fundamental issues such as region of interest and scaling of design variables are discussed. Then the construction of projection designs are illustrated.

KEYWORDS: Projection designs, constrained designs, mixture experiments, fractionating, blocking

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Chapter 1

Introduction

1.1 The Problem

A common problem in quality and productivity improvement is to determine what the cause and effect relationship is between some factors such as temperature, pressure and some response such as yield or performance. Such an investigation can be greatly benefited by well-designed experiments, where informative data are generated. When the factors can be varied independently, some well-known designs such as 2^k factorial designs and composite designs are valuable. Their theoretical properties are well understood and they have stood the test of time in the practical world.

However, the situation is further complicated if the factors are constrained by some linear relations and therefore cannot be varied independently. A common example is the blending problem. For example, suppose we are interested in blending three gasoline stocks, and the objective is to find the proportion of each which yield the highest mileage per gallon. If ξ_1, ξ_2 and ξ_3 are the proportions of the three gasoline stocks, they are subject to the constraint:

$$\xi_1 + \xi_2 + \xi_3 = 1, \quad 0 \leq \xi_i \leq 1 \tag{1.1}$$

and in this case the problem is referred to as a mixture experiment.

In some situations, more than one constraint may occur. In the gasoline-blending problem, for example, to allow certain types of engine tests to be performed, the blended gasoline may be required to have an octane number of 90 in each of the runs. Suppose the octane number T can, to a sufficient approximation, be related to the proportions by the linear relationship:

$$T = 50\xi_1 + 120\xi_2 + 40\xi_3$$

Then the design variables must satisfy the following two equality constraints simultaneously:

$$\begin{cases} \xi_1 + \xi_2 + \xi_3 & = & 1 \\ 50\xi_1 + 120\xi_2 + 40\xi_3 & = & 90 \end{cases}$$

In this thesis, we are concerned with design of experiments when the factors are subject to multiple linear constraints. A class of designs called **projection designs** will be introduced and their analyses and properties will be discussed.

The outline of this chapter is as follows. In Section 1.2, we discuss some desirable properties of experimental designs; in 1.3, issues concerning the region of operability and region of interest; in 1.4, the scopes of constrained and unconstrained designs and in 1.5, the problem of scaling (coding) the design variables. These are fundamental issues, however, they seem to have received inadequate attention in the context of mixture experiments. In Section 1.6, we will review some literature on mixture experiments and in Section 1.7 we will discuss the general idea of the projection designs and present an outline of the thesis.

1.2 Desirable Properties of Experimental Designs

Roughly speaking, a good experimental design is one which benefits the underlying investigation the most. Experimental design is a powerful tool in many diverse fields. Since different circumstances produce different objectives, criteria for good designs must be multifaceted. Box and Draper (1975) discussed some desirable properties of good designs, any or all of which might be important, depending on the experimental context.

The designs should

1. Generate a satisfactory distribution of information throughout the region of interest, R.

2. Ensure that the fitted value at $\mathbf{x}$, $\hat{y}(\mathbf{x})$, be as close as possible to the true value at $\mathbf{x}, \eta(\mathbf{x})$.
3. Give good detectability of lack of fit.
4. Allow transformations to be estimated.
5. Allow experiments to be performed in blocks.
6. Allow designs of increasing order to be built up sequentially.
7. Provided an internal estimate of error.
8. Be insensitive to wild observations and to violation of the usual normal theory assumptions.
9. Require a minimum number of experimental runs.
10. Provide simple data patterns that allow ready visual appreciation.
11. Ensure simplicity of calculation.
12. Behave well when errors occur in the settings of the predictor variables, the x's.
13. Not require an impractically large number of levels of the predictor variables.
14. Provide a check on the "constancy of variance" assumption.

Although these properties were discussed in the context of experimental designs without constraints, they apply equally when the experimental space is constrained.

1.3 Region of Operability and Region of Interest

Issues about the *region of operability* and the *region of interest* were discussed by Box (1982) and also by Box and Draper (1987 p.495). The concepts were illustrated with the following example. Suppose it is desired to study some chemical systems, with the objective of obtaining a higher value for a response η such as yield. Initially yield is believed to be some function $\eta = g(\boldsymbol{\chi})$ of k continuous input variables $\boldsymbol{\chi} = (\chi_1, \chi_2, \ldots, \chi_k)$ such as reaction time, temperature or concentration. It is usually known initially that the system can be operated at some point $\boldsymbol{\chi}_o$ in the space of $\boldsymbol{\chi}$ and is expected to be capable of operating over some much more extensive region O called the operability region, which is usually unknown or poorly known. The response function $\eta = g(\boldsymbol{\chi})$ is also unknown or is inaccessible. See Figure 1.1. Suppose then that, over some immediate region of interest R in the neighborhood of $\boldsymbol{\chi}_o$, it is guessed that a graduating function, such as a dth degree polynomial in χ_i,

$$\eta \doteq \mathbf{z}^t \boldsymbol{\beta}$$

might provide a locally adequate approximation to the true function $\eta = g(\boldsymbol{\chi})$, where $\mathbf{z}$ is a p-dimensional vector of input variables:

$$\mathbf{z}^t = (f_1(\boldsymbol{\chi}), f_2(\boldsymbol{\chi}), \ldots, f_p(\boldsymbol{\chi}))$$

and $\boldsymbol{\beta}$ is a vector of coefficients which may be adjusted to approximate the unknown true response function $\eta = g(\boldsymbol{\chi})$. Then progress may be achieved by using a sequence of such approximations. For example, when a first degree polynomial approximation could be employed it might, via the method of steepest ascent, be used to find a new region of interest R_1 where the yield was higher. Also a maximum in many variables is often represented by some rather complicated ridge system and a second degree polynomial approximation, when suitably analyzed, might be used to describe and exploit such a system.

The above discussion by Box applies equally to the constrained experiments. As an example, let us look at the simple situation, a mixture experiment, in which only three ingredients are blended. The constrained region (1.1) can be represented by the triangle shown in Figure 1.2.

In most situations, the operability region O is *not* the whole constrained region. For example, it is obvious that no cake can be made with 100% eggs and a good cook may be fairly sure that amount of baking powder must be between 2% and 10% in order for any cake to turn out at all. Although it is known that the experiment can only be conducted in a subregion of the constrained space, it is usually difficult to describe this operability region

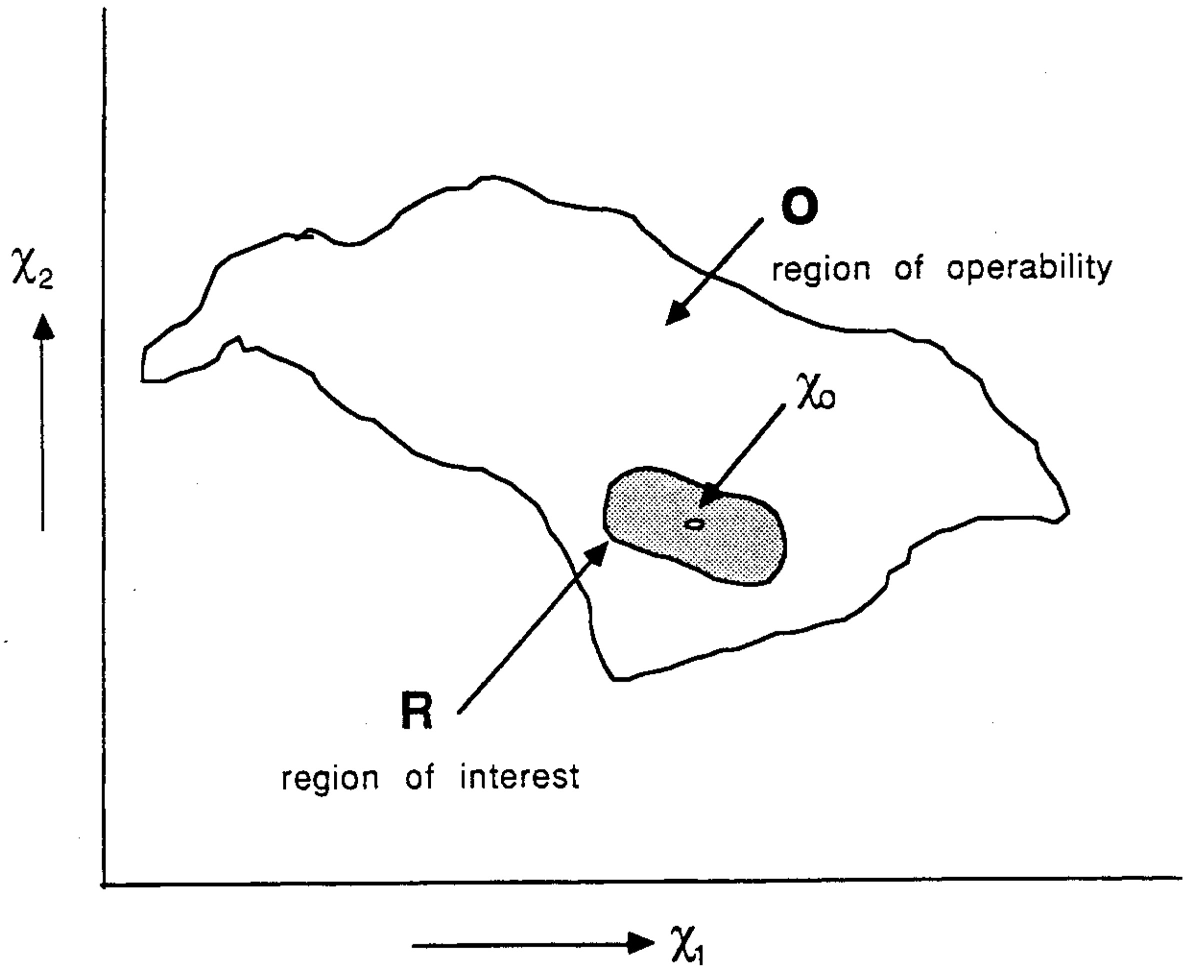

Figure 1.1: Operability Region and Region of Interest

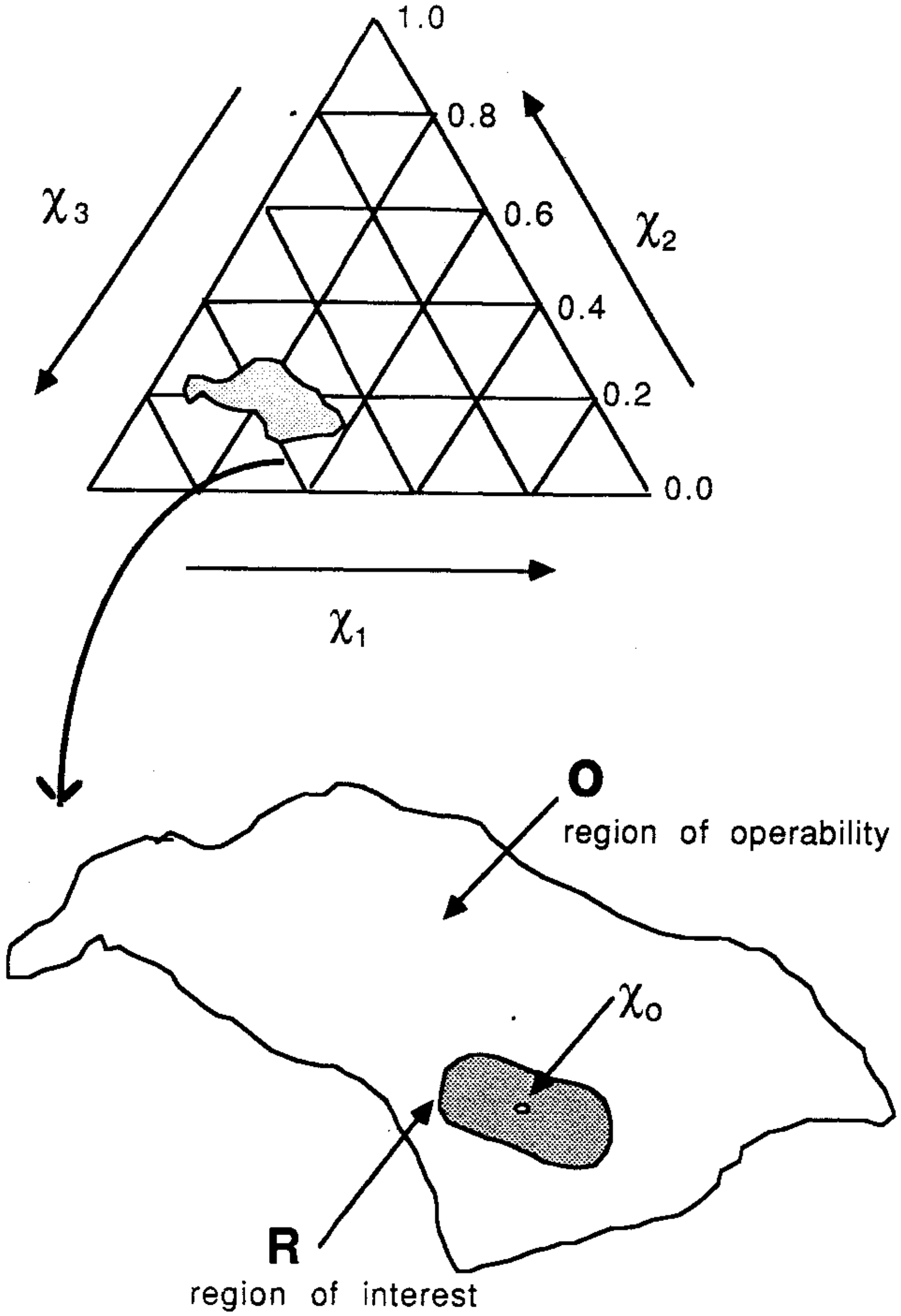

Figure 1.2: Operability Region in the Constrained Space Defined by $\xi_1 + \xi_2 + \xi_3 = 1$

mathematically since it is poorly known. Furthermore, in the whole operability region, a very complex function may be needed to approximate the true surface involving an excessive number of experiments. Therefore, the exploration of the whole operability region is seldom a sensible objective. Instead, we can explore a smaller subregion of interest R, which may change as the investigation progresses. The region of interest is usually the immediate neighborhood of the best condition known at the moment, and the size of the region reflects the prior knowledge of the experimenter.

1.4 Constrained and Unconstrained Designs

Strictly speaking, all designs are subject to constraints. For example, the temperature required to bake a cake must be above the room temperature (we have to turn on the oven!) and below 600°F (the highest temperature possible for my oven). In some chemical experiments, the system may explode if the pressure and temperature are too high. In the context of traditional experimental designs, these inequality constraints are not explicitly dealt with, since the region of interest is usually much smaller than the constrained region. Therefore, unconstrained designs in this thesis refer to the situations where the design variables are tacitly assumed to vary over region not subject to equality constraints, even though inequality constraints may be present in a more extended region. On the other hand, constrained designs refer to designs for which equality constraints must be explicitly taken account of.

1.5 Scaling the Design Variables

So that standard designs can be applied to different experimental situations, they are usually coded. For instances, the levels of design variables in two level factorial designs are usually coded to -1 and 1. More general designs which have q variables and n design points may be written in terms of coded variables $x_{1u}, x_{2u}, \ldots, x_{qu}$ such that:

$$\sum_{u=1}^{n} x_{iu} = 0, \quad \frac{\sum_{u=1}^{n} x_{iu}^2}{n} = 1$$

where $i = 1, 2, \ldots, q$. That is, the variables are coded so that the mean is zero and the "variance" is unity. In this coding we can then arrange, for example, the distribution of information so that it is uniform on a hypersphere about the origin. Without such a standardization of the units, the properties of different designs cannot be directly compared. The coded variables x_1, x_2 etc. may then be related to experimental variables such as Flour Proportion F, Egg Proportion E etc. by the linear relations:

$$x_1 = \frac{F - F_o}{S_F} \quad x_2 = \frac{E - E_o}{S_E}$$

where F_o, E_o, S_F, S_E are suitable chosen constants. Although scaling is discussed mostly in the context of designs without constraints, it should be done in the situation of constrained designs. In a cake mix experiment for example, suppose the region of interest is: baking powder $B = 3\% \pm 2\%$, flour $F = 40\% \pm 10\%$ and so on. Although in this case B and F are in the same units (%), they should be standardized in a manner similar to the last paragraph, since the range of baking powder (4%) and the range of the flour (20%) are very different.

However, there is a complication in specifying the region of interest in the constrained space because the design variables cannot be varied independently and consequently the choice of range for one variable limits the choice of range of the others. When the constraints are complex, the experimenter may not be able to understand the constrained region well enough to specify the ranges for the design variables which are consistent with the constraints. For illustration, suppose the experimental variables ξ_1 and ξ_2 are constrained by:

$$2\xi_1 + \xi_2 = 4 \tag{1.2}$$

Suppose the experimenter thinks that it is appropriate to conduct a design centered at $(\xi_1, \xi_2) = (1, 2)$ and within the region of interest:

$$\xi_1 = 1 \pm 1 \quad \xi_2 = 2 \pm 4$$

The constrained space (1.2) is shown in Figure 1.3. If there were no constraints, the region of interest is represented by the box in Figure 1.3. With the constraint, the region of interest may be taken as the intersection of the line $2\xi_1 + \xi_2 = 4$ and the box:

$$0 \leq \xi_1 \leq 2, \quad -2 \leq \xi_2 \leq 6$$

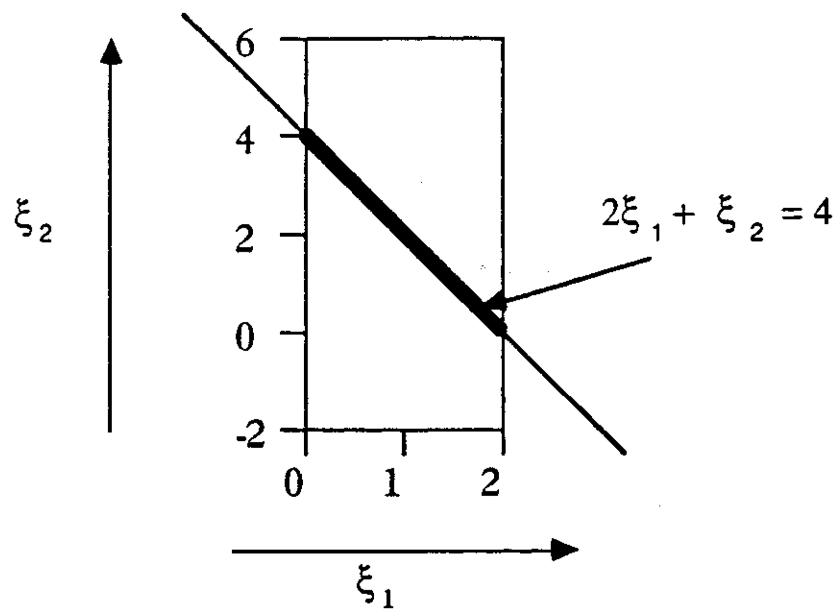

Figure 1.3: The Region of Interest under the Constraint $2\xi_1 + \xi_2 = 4$

This region of interest in the constrained space is the thick line shown in Figure 1.3. In this region, the range of ξ_1 is from 0 to 2 but the range of ξ_2 is from 0 to 4, which is different from what the experimenter initially had specified. Of course, the problem is that the initial ranges of the design variables are not consistent. If we insist the range of ξ_1 be 1 ± 1, then by the constraint $2\xi_1 + \xi_2 = 4$, the range of ξ_2 must be 2 ± 2.

As a second example, suppose the experimental variables ξ_1, ξ_2 and ξ_3 must satisfy the following constraint:

$$\xi_1 + \xi_2 + \xi_3 = 6$$

This constrained space is shown in Figure 1.4. The experimenter thinks that the region of interest may be:

$$\begin{aligned} 1 \leq & \;\; \xi_1 \;\; \leq 5 \\ 2 \leq & \;\; \xi_2 \;\; \leq 3 \\ 2.5 \leq & \;\; \xi_3 \;\; \leq 3.5 \end{aligned} \tag{1.3}$$

The bounds defined for ξ_i are shown by the thick lines in Figure 1.4. The feasible region of interest defined by these bounds is the shaded area. The ranges of the variables in this region are:

$$\begin{aligned} 1 \leq & \;\; \xi_1 \;\; \leq 1.5 \\ 2 \leq & \;\; \xi_2 \;\; \leq 2.5 \\ 2.5 \leq & \;\; \xi_3 \;\; \leq 3 \end{aligned}$$

Although the ranges of the variables initially given are extensive, the ranges of the variables in the feasible region are quite small. For example, the actual feasible range for ξ_1 is only from 1 to 1.5, which is quite different from the initial range 1 to 5. Thus, it is impossible to obtain a constrained design with the ranges specified in (1.3).

When there are more design variables and several constraints, it may not be easy for the experimenter to come up with a reasonable and consistent region of interest in one attempt. In that case, specifying a region of interest should be an iterative investigation. The experimenter may specify a region of interest and come up with a constrained design in the way to be discussed in Chapter 2. Then the experimenter should see if the ranges of the design variables of the design are reasonable. If not, the region of interest should be modified and a new design should be constructed. The procedure should be continued until a design with satisfactory ranges is found. We shall come back to this point in Chapter 2.

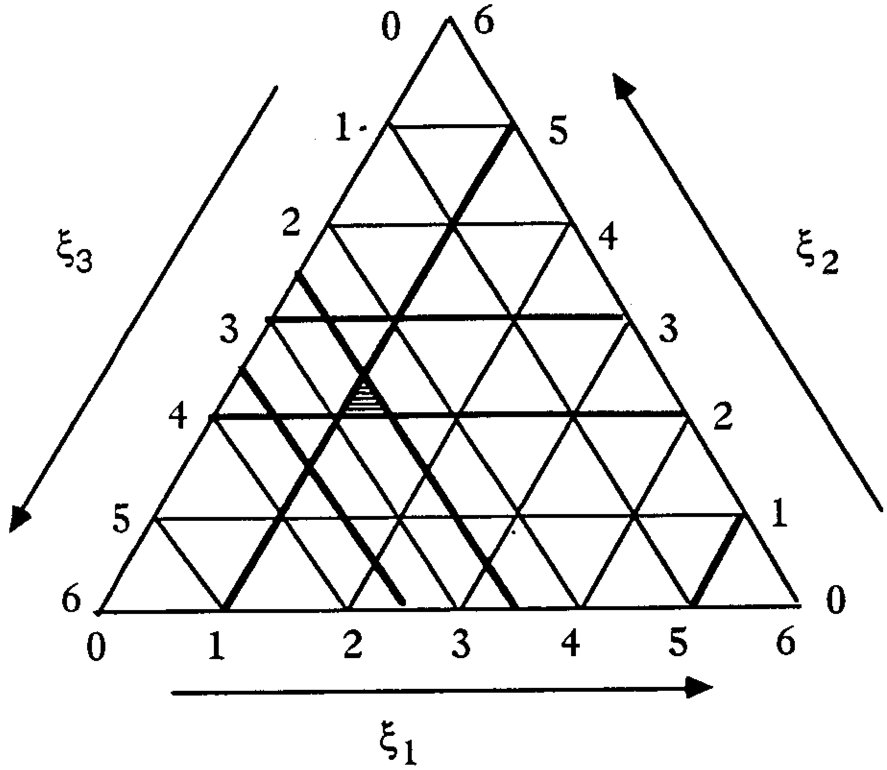

Figure 1.4: The constrained Space Defined by $\xi_1 + \xi_2 + \xi_3 = 6$

1.6 Mixture Experiments

A *Mixture experiment* is one where the factors are subject to the special constraint:

$$\xi_1 + \xi_2 + \ldots + \xi_q = 1 \quad 0 \leq \xi_i \leq 1$$

Cornell (1981) and Khuri and Cornell (1987) have given reviews of the literature in this area. In the following, we will give a brief introduction to some fundamental mixture designs.

1.6.1 Simplex-Lattice Designs

In 1958 Scheffé introduced the simplex-lattice designs which generated a great interest in the area of design and analysis of mixture experiments. The {q,m} simplex-lattice design consists of points that can fit a polynomial of order m in q variables. The coordinates of the points are defined by the following combinations of component proportions; the proportions assumed by each component will take the m+1 equally spaced values from 0 to 1, that is,

$$\xi_i = 0, \frac{1}{m}, \frac{2}{m}, \ldots, 1. \tag{1.4}$$

and the {q,m} simplex-lattice consists of all possible combinations of the components where the proportion (1.4) for each component is used. For example: the {3,2} simplex-lattice designs consists of the six points on the boundary of the triangle:

$$\begin{aligned}(\xi_1, \xi_2, \xi_3) &= (1,0,0), (0,1,0), (0,0,1), \\ &\quad (1/2,1/2,0), (1/2,0,1/2), (0,1/2,1/2)\end{aligned}$$

This design is shown in Figure 1.5.

1.6.2 Simplex-Centroid Designs

In a q-component simplex-centroid design, the points correspond to the q permutations of $(1,0,\ldots,0)$, and C_2^q permutations of $(1/2,1/2,0,\ldots,0),\ldots$ and so on, with finally the overall centroid point $(1/q,1/q,\ldots,1/q)$. For example, the 3-component simplex-centroid design consists of the seven points

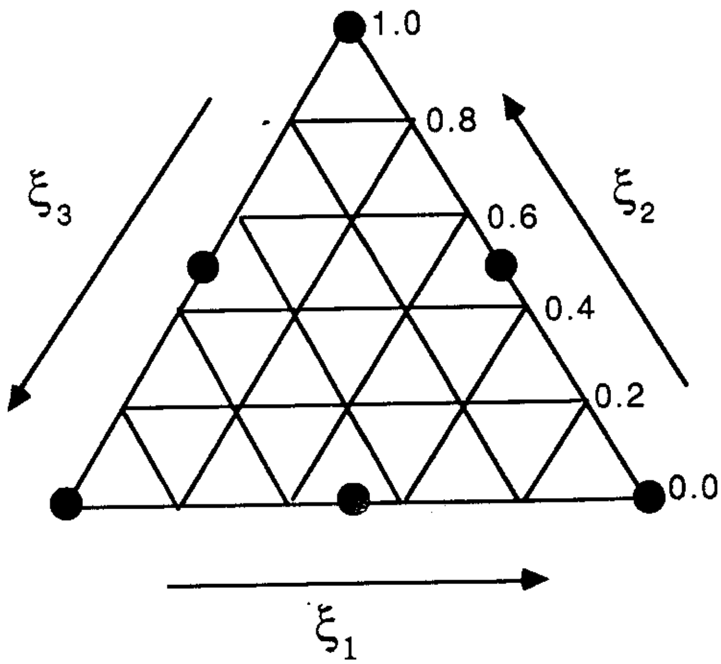

Figure 1.5: The {3,2} Simplex-Lattice Design

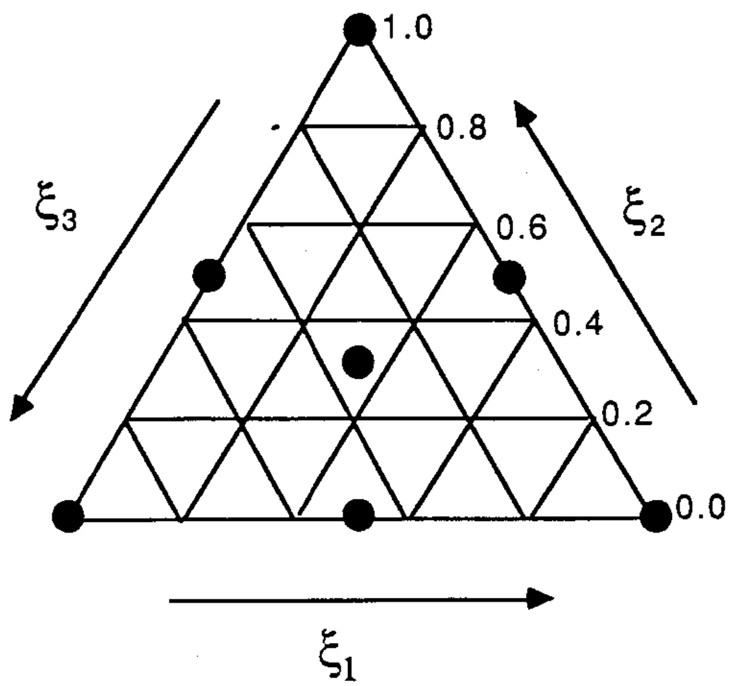

Figure 1.6: The 3-Component Simplex-Centroid Design

as follows:

$$\begin{aligned}(\xi_1, \xi_2, \xi_3) &= (1,0,0),(0,1,0),(0,0,1),\\ &\quad (1/2,1/2,0),(1/2,0,1/2),(0,1/2,1/2),(1/3,1/3,1/3)\end{aligned}$$

The design is shown in Figure 1.6.

1.6.3 Extreme Vertices Designs

The simplex designs mentioned above are used to explore the whole constrained region but as discussed before, this is often not a feasible or sensible objective. In most mixture experiments, the operability region is not the whole constrained region. In this situation, McLean and Anderson (1966) recommended an algorithm to generate the coordinates of the vertices resulting from placing lower and upper bounds on some or all of the component proportions. These designs are referred to as extreme vertices designs. However, placing simple upper and lower bounds usually can only define a crude area which may be much larger than the actual operability region. Also when this region is extensive, exploration in this whole region via low degree polynomials may be inappropriate for the reasons discussed previously. Further disadvantages of this approach are that the constructions and the analyses of the designs are relatively complicated.

1.7 Projection Designs

Mixture experiments deal with the special constraint (1.1). We have been unable to find any literature that considered the general single constraint:

$$a_1\xi_1 + a_2\xi_2 + \ldots + a_q\xi_q = d$$

where the a_i's and d are arbitrary real numbers. In this thesis, we consider an even more general problem in which the design variables are subject to multiple linear constraints as follows:

$$\sum_{j=1}^{q} b_{ij}\xi_j = d_i, \quad i = 1, 2, \ldots, m. \tag{1.5}$$

Well-known designs such as factorial designs and composite designs cannot be used as they stand because the design variables do not satisfy the constraints. However, these designs have nice properties and we shall show that it is of interest to construct constrained designs based upon them. This may be done by projecting such designs onto the constrained space, an operation which is easily conducted by a simple application of regression analysis. A natural question which arises is: "If a design which possesses a desirable property in the unconstrained space, will this property be preserved in the projected design?" For example:

- If a design can be conveniently blocked in the unconstrained space, will this property be preserved in the constrained space?
- Could the analysis of the projected design be as simple as that for the original unconstrained design?
- Could procedures such as steepest ascent be carried out in a similar way in the constrained space?

- Could a rotatable constrained design be constructed by projecting a rotatable unconstrained design?

These questions are answered in the subsequent chapters. In Chapter 2, we discuss the construction of the projection designs and methods for fractionating and blocking the projection designs. It turns out that fractionating and blocking projection designs can be conveniently done in the same way as for the unconstrained designs. In Chapter 3 we consider the analyses of the projection designs. We will show that the projection designs can be analyzed as if the data came from the unconstrained design. As a result, the calculations are very simple. In Chapter 4 we discuss steepest ascent in the constrained space. It turns out that the method employed in the unconstrained space again can be adopted with little modification. The rotatability of projection designs will be considered in Chapter 5. Concluding remarks and problems for future research are in Chapter 6.

Chapter 2

Construction of Projection Designs

In this chapter, we discuss the construction of experimental designs which may be used when the design variables are subject to linear constraints. A class of designs called **projection designs** is introduced. For illustration, we begin by constructing a projection design for the mixture problem from a 2^3 factorial design. Next the general construction of projection designs and their blocking and fractionating are discussed. In the last section, we discuss the relationship between the projection designs and classical mixture designs such as simplex-lattice designs.

2.1 An Example

Since the classical mixture designs such as simplex-lattice designs usually cover the whole constrained region, for the sake of comparisons, we will construct the largest projection design within the mixture constrained region in this and the following mixture examples. This is done by assuming the region of interest to be the largest sphere inside the mixture constrained region. Although providing useful comparisons, as discussed in Chapter 1, this might not be very realistic since the region of interest we would wish to explore is usually much smaller than the whole constrained region.

Consider a mixture which contains three constituents: graphite, boron and epoxy and suppose the objective is to find the proportions where the tensile strength is maximized. The proportions of the constituents are denoted as ξ_1, ξ_2 and ξ_3. Since they are proportions, they are subject to the constraint:

$$\begin{cases} \xi_1 + \xi_2 + \xi_3 & = & 1 \\ 0 \leq \xi_i \leq 1 & & i = 1, 2, 3. \end{cases}$$

The objective is to find the proportions where the tensile strength is maximized. Suppose the mixture is currently made of 1/3 of each constituent. Let $\mathbf{c}^t = (c_1, c_2, c_3) = (1/3, 1/3, 1/3)$. The region of interest specified by the experimenter is $c_i \pm r_i$ where $r_i = 1/3$ for $i = 1, 2, 3$.

We know little about the response surface of the tensile strength as a function of the proportions and if there were no constraints, we might begin experimentation by using a 2^3 design Z as follows:

$$Z = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

The next step is to project the Z onto the constrained space so that the design points satisfy the constraint:

$$r_1 x_1 + r_2 x_2 + r_3 x_3 = 0.$$

The $\mathbf{x}^t = (x_1, x_2, x_3)$ are the coded variables and are related to the original variables ξ_i by:

$$x_i = \frac{\xi_i - c_i}{\alpha r_i}$$

where α is a real number to be explained later. Since $r_i = 1/3$, the constraint is equivalent to $x_1 + x_2 + x_3 = 0$. The projection onto this constrained space can be done by regressing each row vector of Z on the constraining vector (1,1,1) and then taking the residuals. In other words we want to "regress out the row mean" from each row vector of Z. Take the first row $(-1,-1,-1)$ for example. The row mean is -1. Therefore, when we regress out the row mean it becomes:

$$(-1-(-1),-1-(-1),-1-(-1)) = (0,0,0)$$

All other rows are obtained in the same way and the design X in the coded variables is:

$$X = \begin{pmatrix} 0 & 0 & 0 \\ 4/3 & -2/3 & -2/3 \\ -2/3 & 4/3 & -2/3 \\ 2/3 & 2/3 & -4/3 \\ -2/3 & -2/3 & 4/3 \\ 2/3 & -4/3 & 2/3 \\ -4/3 & 2/3 & 2/3 \\ 0 & 0 & 0 \end{pmatrix}$$

The design points in the coded variables $\mathbf{x}$ are the row vectors in X. The design in the original variables can now be calculated from:

$$\xi_i = \alpha r_i x_i + c_i \quad i = 1,2,3. \tag{2.1}$$

The α is the size parameter chosen so that the constrained design is within the region of interest, i.e.:

$$c_i - r_i \leq \xi_i \leq c_i + r_i \quad i = 1,2,\ldots,q.$$

To do that, the size parameter α should be chosen so that

$$-1 \leq \alpha x_i \leq 1 \quad i = 1,2,\ldots,q.$$

It is obvious that we should take α to be the inverse of the largest absolute value of the entries of X. In this example, the largest absolute value in X is $4/3$, therefore $\alpha = 3/4$ and:

$$\xi_i = \frac{x_i}{4} + \frac{1}{3} \quad i = 1,2,3.$$

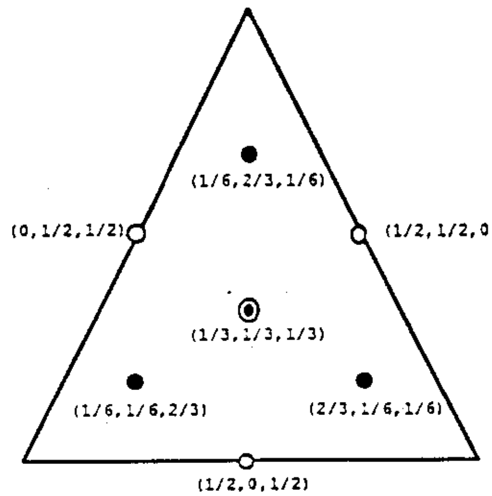

Figure 2.1: The 2^3 Projection Design in the Mixture Case

Take the second row $\mathrm{x}^t = (4/3, -2/3, -2/3)$ of X for example: $\xi_1 = 4/12 + 1/3 = 2/3$, $\xi_2 = -2/12 + 1/3 = 1/6$, and $\xi_3 = \xi_2 = 1/6$. All other rows can be obtained the same way. The design in the original variables is thus:

$$\begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 2/3 & 1/6 & 1/6 \\ 1/6 & 2/3 & 1/6 \\ 1/2 & 1/2 & 0 \\ 1/6 & 1/6 & 2/3 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 1/2 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$$

The design is shown in Figure 2.1.

2.2 Construction of Projection Designs

Suppose we are interested in constructing a design with q factors $\mathbf{x}^t = (x_1, x_2, \ldots, x_q)$ subject to the m constraints:

$$\sum_{j=1}^{q} a_{ij}x_j = 0 \quad i = 1, 2, \ldots, m. \tag{2.2}$$

Or in matrix form:

$$A\mathbf{x} = \mathbf{0} \tag{2.3}$$

where $A = (a_{ij})$ is an m × q matrix of constraints and $\mathbf{0}$ is an m × 1 vector of 0's.

The idea of the construction is to project an appropriate unconstrained design onto the constrained space defined by (2.3). Suppose $\mathbf{z}^t = (z_1, z_2, \ldots, z_q)$ is a design point of the unconstrained design. Let

$$P = I - A^t(AA^t)^{-1}A$$

where I is the q × q identity matrix. Then the constrained design point $\mathbf{x}$ can be obtained by:

$$\mathbf{x} = P\mathbf{z} \tag{2.4}$$

It is easy to check that $\mathbf{x}$ calculated by (2.4) satisfies the constraints (2.3), since:

$$A\mathbf{x} = AP\mathbf{z} = (A - A)\mathbf{z} = \mathbf{0}$$

It may be recognized that $\mathbf{x}$ is the vector of residuals when $\mathbf{z}$ is regressed on the matrix A^t of the constraining vectors.

In general, we may want to construct a design within the region of interest in the design variables $\xi_1, \xi_2, \ldots, \xi_q$ subject to the constraints:

$$\sum_{j=1}^{q} b_{ij}\xi_j = d_i \quad i = 1, 2, \ldots, m. \tag{2.5}$$

Let $\mathbf{c}^t = (c_1, c_2, \ldots, c_q)$ be a point which satisfies the constraints (2.5). For example, $\mathbf{c}$ may be the current settings of the underlying process. The region of interest is the neighborhood around $\mathbf{c}$ described by:

$$c_j \pm r_j \quad j = 1, 2, \ldots, q.$$

where the r_j's are some positive numbers. As discussed in Chapter 1, we should not study the design in terms of the original variables ξ_i's. Instead, it is more sensible to consider the coded (scaled) variables x_i's:

$$x_i = \frac{\xi_i - c_i}{\alpha r_i} \tag{2.6}$$

where α is a real number explained below. From (2.6),

$$\xi_i = \alpha r_i x_i + c_i \tag{2.7}$$

Substituting (2.7) into the constraints (2.5), we have:

$$\sum_{j=1}^{q} b_{ij}(\alpha r_j x_j + c_j) = d_i$$

Or,

$$\sum_{j=1}^{q} \alpha b_{ij} r_j x_j + \sum_{j=1}^{q} b_{ij} c_j = d_i$$

Since $\mathbf{c}$ satisfies the constraints, $\sum_{j=1}^{q} b_{ij} c_j = d_i$. Letting $a_{ij} = r_j b_{ij}$, the coded variables are subject to the constraints:

$$\sum_{j=1}^{q} a_{ij} x_j = 0$$

which is the same as (2.3). Therefore, we can construct the projection design in the coded variables as in (2.4). Now we need to know α in order to transform the design in the coded variables x_i back to the original design variables ξ_i. Let X be the matrix of all the design points in the coded variables. The α is the largest number such that all the entries of αX are between -1 and 1. Then the design in the original variables, ξ_i's, can be calculated by (2.7).

To see what the size parameter α means, let us study the example in Section 1.5 again. In this example, the design variables ξ_1 and ξ_2 are constrained by:

$$2\xi_1 + \xi_2 = 4$$

The region of interest is:

$$\xi_1 = 1 \pm 1, \quad \xi_2 = 2 \pm 4$$

The coded variables x_1 and x_2 are defined as:

$$x_1 = \frac{\xi_1 - 1}{1\alpha}, \quad x_2 = \frac{\xi_2 - 2}{4\alpha}$$

where α is a suitably chosen size parameter. In terms of the coded variables, the constraint is:

$$x_1 + 2x_2 = 0$$

and the region of interest in this constrained space is:

$$-1 \leq \alpha x_1 \leq 1, \quad -1 \leq \alpha x_2 \leq 1 \quad \text{and} \quad x_1 + 2x_2 = 0$$

This region of interest is shown with a thick line segment in Figure 2.2.

To construct the projection design in the constrained space, we may project the following 2^2 design Z:

$$Z = \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{pmatrix}$$

onto the constrained space. Let $A = (1, 2)$ denote the constraint vector, $P = I - A^t(AA^t)^{-1}A$, then the constrained design $X = ZP$ in the coded variables is:

$$X = \begin{pmatrix} -0.4 & 0.2 \\ 1.2 & -0.6 \\ -1.2 & 0.6 \\ 0.4 & -0.2 \end{pmatrix}$$

The design X is shown in Figure 2.2.

However, not all points in the design lie within the region of interest, which is the thick line segment in the figure. Therefore, we should shrink the design by multiplying the size parameter $\alpha = 5/6$ to the design X:

$$\alpha X = \begin{pmatrix} -1/3 & 1/6 \\ 1 & -1/2 \\ -1 & 1/2 \\ 1/3 & -1/6 \end{pmatrix}$$

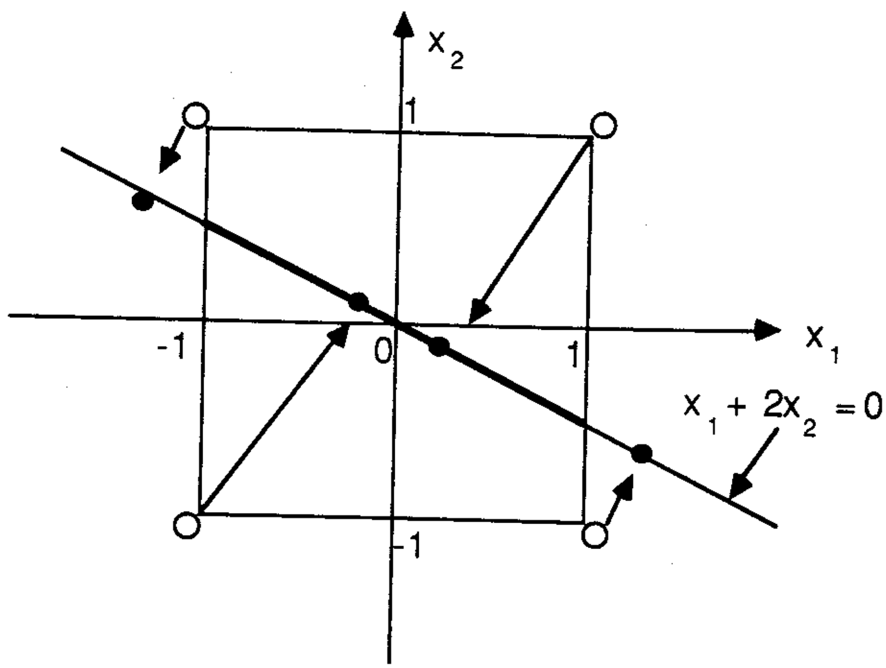

Figure 2.2: The Region of Interest and the Size Parameter

Now all points in αX lie within the region of interest.

As discussed in Section 1.5, the ranges of the design variables in the projection design may be different from what the experimenter initially specified. In the previous example, the range of αx_2 is from -1/2 to 1/2. In terms of the original variable $\xi_2 = 4\alpha x_2 + 2$, the range is 2 ± 2. The reason is that the ranges initially given by the experimenter were not consistent. In practice, it may be difficult for the experimenter to understand the constrained space well enough to specify an adequate region of interest. In those situations, the experimenter should determine the region of interest and then construct the projection design. If the ranges of the resulting design are not satisfactory, the region should be modified and a new projection design should be constructed. By applying this procedure iteratively, we may be able come up with a constrained design which covers an appropriate region.

As a second example, let us consider the 4-component mixture experiment. The factors ξ_1, ξ_2, ξ_3 and ξ_4 are subject to the constraint:

$$\xi_1 + \xi_2 + \xi_3 + \xi_4 = 1$$

Suppose the region of interest is $c_i \pm r_i$ where $c_i = 1/4$ and $r_i = 1/4$ for all $i = 1, 2, 3, 4$. Therefore, the coded variables

$$x_i = \frac{\xi_i - c_i}{\alpha r_i} = \frac{4\xi_i - 1}{\alpha}$$

are subject to the constraint:

$$r_1 x_1 + r_2 x_2 + r_3 x_3 + r_4 x_4 = 0$$

Since $r_i = 1/4$, the constraint in the coded variables is simply:

$$x_1 + x_2 + x_3 + x_4 = 0 \tag{2.8}$$

The constrained design in x_i's can be obtained by projecting the 2^4 factorial design Z onto the constrained space. The 2^4 design Z is shown as follows:

$$
Z = \begin{pmatrix}
-1 & -1 & -1 & -1 \\
1 & -1 & -1 & -1 \\
-1 & 1 & -1 & -1 \\
1 & 1 & -1 & -1 \\
-1 & -1 & 1 & -1 \\
1 & -1 & 1 & -1 \\
-1 & 1 & 1 & -1 \\
1 & 1 & 1 & -1 \\
-1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 \\
-1 & 1 & -1 & 1 \\
1 & 1 & -1 & 1 \\
-1 & -1 & 1 & 1 \\
1 & -1 & 1 & 1 \\
-1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{pmatrix}
$$

Recall that $\mathbf{x}$ is just the vector of residuals when the factorial design point $\mathbf{z}$ is regressed on the constraining vector $A^t = (1, 1, 1, 1)^t$. That means the constrained design X can be obtained by subtracting the row mean from each row of Z. The design X in the coded variables is therefore:

$$X = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 3/2 & -1/2 & -1/2 & -1/2 \\ -1/2 & 3/2 & -1/2 & -1/2 \\ 1 & 1 & -1 & -1 \\ -1/2 & -1/2 & 3/2 & -1/2 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1/2 & 1/2 & 1/2 & -3/2 \\ -1/2 & -1/2 & -1/2 & 3/2 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1/2 & 1/2 & -3/2 & 1/2 \\ -1 & -1 & 1 & 1 \\ 1/2 & -3/2 & 1/2 & 1/2 \\ -3/2 & 1/2 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

In order for all the values in αX to be between -1 and 1, α should be 2/3. Therefore, the design in terms of the original variables can be computed by the formula (2.7) and is shown as follows:

$$\begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 \\ 1/2 & 1/6 & 1/6 & 1/6 \\ 1/6 & 1/2 & 1/6 & 1/6 \\ 5/12 & 5/12 & 1/12 & 1/12 \\ 1/6 & 1/6 & 1/2 & 1/6 \\ 5/12 & 1/12 & 5/12 & 1/12 \\ 1/12 & 5/12 & 5/12 & 1/12 \\ 1/3 & 1/3 & 1/3 & 0 \\ 1/6 & 1/6 & 1/6 & 1/2 \\ 5/12 & 1/12 & 1/12 & 5/12 \\ 1/12 & 5/12 & 1/12 & 5/2 \\ 1/3 & 1/3 & 0 & 1/3 \\ 1/12 & 1/12 & 5/12 & 5/12 \\ 1/3 & 0 & 1/3 & 1/3 \\ 0 & 1/3 & 1/3 & 1/3 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{pmatrix}$$

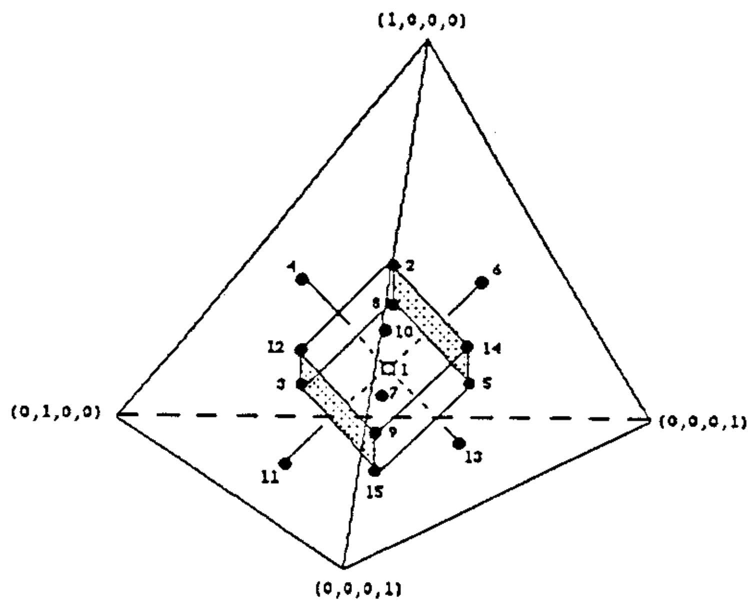

Figure 2.3: The 2^4 Projection Design in the Mixture Case

The arrangement is laid out in Figure 2.3. It is interesting that the resulting design is a central composite design embedded in the constrained region.

The constrained designs we have seen are the projections of 2^q factorial designs. This class of projection designs is called 2^q **Projected Factorial (PF)** designs. We will see in the following chapters that PF designs are of particular interest since many nice properties of factorial designs are preserved after projection.

In the following section, we will look at an example with multiple constraints where a composite design is projected.

2.3 Design under Multiple Constraints - A Cake Example

Suppose we want to make a cake with 4 ingredients: sugar, flour, eggs and baking powder. Our objective is to make a cake of certain texture that tastes the best. Let ξ_1, ξ_2, ξ_3 and ξ_4 be the percentages of the ingredients. Suppose it is required that the texture $T = 130$ in some appropriate unit, and that the relation between the percentage of ingredients and the texture T is known to be:

$$T = 2\xi_1 + \xi_2 + \xi_3$$

Therefore, we are interested in designing an experiment to optimize the taste function subject to the known percentage and texture constraints:

$$\left\{ \begin{array}{rcccccccl} \xi_1 & + & \xi_2 & + & \xi_3 & + & \xi_4 & = & 100 \\ 2\xi_1 & + & \xi_2 & + & \xi_3 & & & = & 130 \\ & & 0 & \leq & \xi_i & \leq & 100 & & \end{array} \right. \tag{2.9}$$

Since there are four factors with two constraints, the constrained space is 2-dimensional. The percentage constraint defines a pyramid which is 3-dimensional, shown at the top of Figure 2.4. The texture constraint defines a plane and its intersection with the pyramid is shown by the shaded area. With suitable rotation, the constrained region can be represented by a 2-dimensional plane with the coordinate system shown at the bottom of Figure 2.4.

Suppose the current recipe is $\mathbf{c}^t = (c_1, c_2, c_3, c_4) = (40, 20, 30, 10)$, and the region of interest is $c_i \pm 6$, $i = 1, 2, 3, 4$. Thus the coded variables defined as in (2.6) are constrained by:

$$\left\{ \begin{array}{rcccccccl} x_1 & + & x_2 & + & x_3 & + & x_4 & = & 0 \\ 2x_1 & + & x_2 & + & x_3 & & & = & 0 \end{array} \right. \tag{2.10}$$

Suppose we intend to fit a second order surface over the region of interest. To construct the constrained design, we can project the composite design Z in Table 2.1 onto the constrained space (2.10). Let $\mathbf{z}$ be a design point in

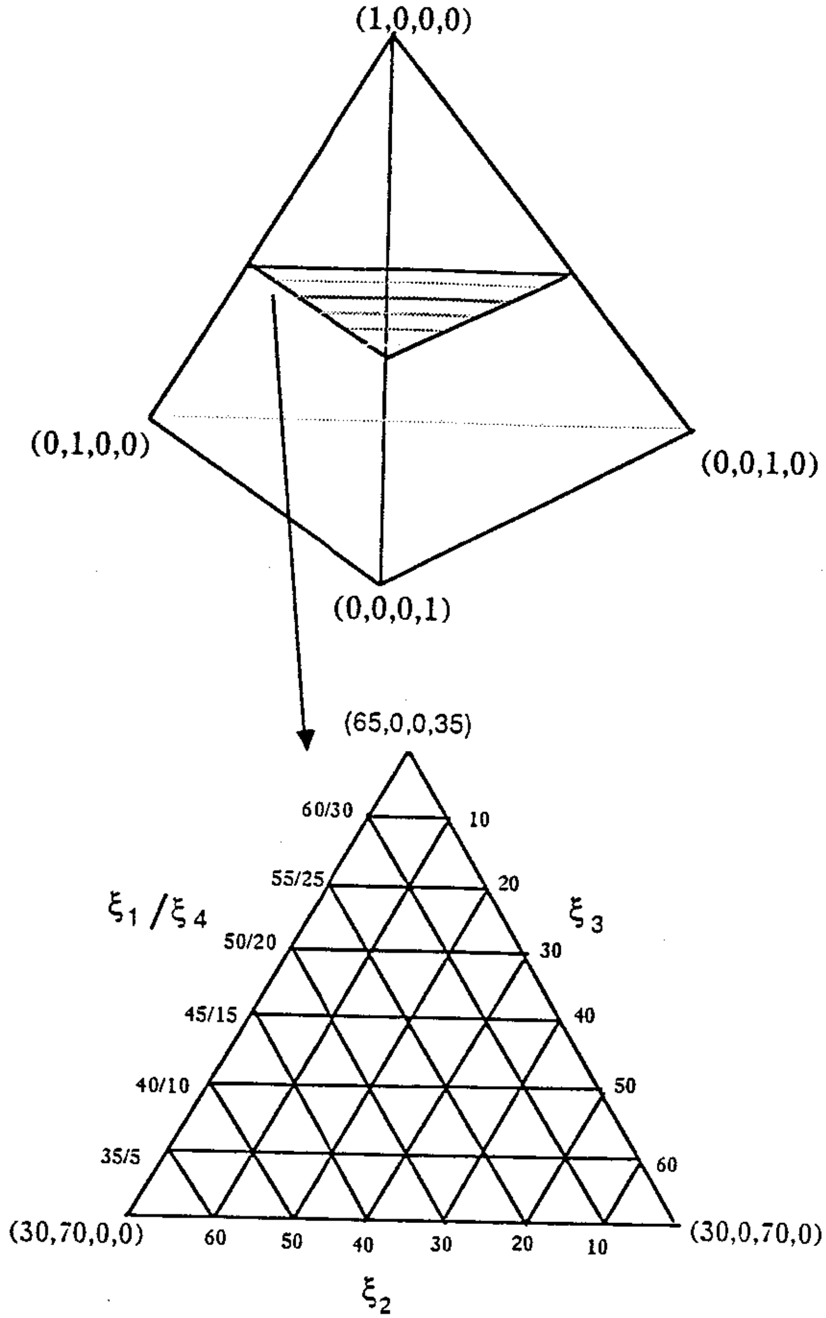

Figure 2.4: The Constrained Region in the Cake Example

the composite design. Then using the previous notation,

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix} \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$\begin{aligned} P &= I - A^T(AA^T)^{-1}A \\ &= \begin{pmatrix} 0.25 & -0.25 & -0.25 & 0.25 \\ -0.25 & 0.75 & -0.25 & -0.25 \\ -0.25 & -0.25 & 0.75 & -0.25 \\ 0.25 & -0.25 & -0.25 & 0.25 \end{pmatrix} \end{aligned}$$

Then a point in the projection design in the coded variables is calculated by:

$$\mathbf{x} = P\mathbf{z}$$

	Z				X				ξ			
run #	z_1	z_2	z_3	z_4	x_1	x_2	x_3	x_4	ξ_1	ξ_2	ξ_3	ξ_4
1	−1	−1	−1	−1	0	0	0	0	40	20	30	10
2	1	−1	−1	−1	1/2	−1/2	−1/2	1/2	42	18	28	12
3	−1	1	−1	−1	−1/2	3/2	−1/2	−1/2	38	26	28	8
4	1	1	−1	−1	0	1	−1	0	40	24	26	10
5	−1	−1	1	−1	−1/2	−1/2	3/2	−1/2	38	18	36	8
6	1	−1	1	−1	0	−1	1	0	40	16	34	10
7	−1	1	1	−1	−1	1	1	−1	36	24	34	6
8	1	1	1	−1	−1/2	1/2	1/2	−1/2	38	22	32	8
9	−1	−1	−1	1	1/2	−1/2	−1/2	1/2	42	18	28	12
10	1	−1	−1	1	1	−1	−1	1	44	16	26	14
11	−1	1	−1	1	0	1	−1	0	40	24	26	10
12	1	1	−1	1	1/2	1/2	−3/2	1/2	42	22	24	12
13	−1	−1	1	1	0	−1	1	0	40	16	34	10
14	1	−1	1	1	1/2	−3/2	1/2	1/2	42	14	32	12
15	−1	1	1	1	−1/2	1/2	1/2	−1/2	38	22	32	8
16	1	1	1	1	0	0	0	0	40	20	30	10
17	2	0	0	0	1/2	−1/2	−1/2	1/2	42	18	28	12
18	−2	0	0	0	−1/2	1/2	1/2	−1/2	38	22	32	8
19	0	2	0	0	−1/2	3/2	−1/2	−1/2	38	26	28	8
20	0	−2	0	0	1/2	−3/2	1/2	1/2	42	14	32	12
21	0	0	2	0	−1/2	−1/2	3/2	−1/2	38	18	36	8
22	0	0	−2	0	1/2	1/2	−3/2	1/2	42	22	24	12
23	0	0	0	2	1/2	−1/2	−1/2	1/2	42	18	28	12
24	0	0	0	−2	−1/2	1/2	1/2	−1/2	38	22	32	8
25	0	0	0	0	0	0	0	0	40	20	30	10

Table 2.1 The Projection Design for the Cake Example

The projection design X in the coded variables is given in Table 2.1. In order for all values in αX to be between −1 and 1, $\alpha = 2/3$ should be chosen. The design in the original variables ξ_i is therefore:

$$\begin{aligned}\xi_i &= \alpha r_i x_i + c_i \\ &= 4x_i + c_i\end{aligned}$$

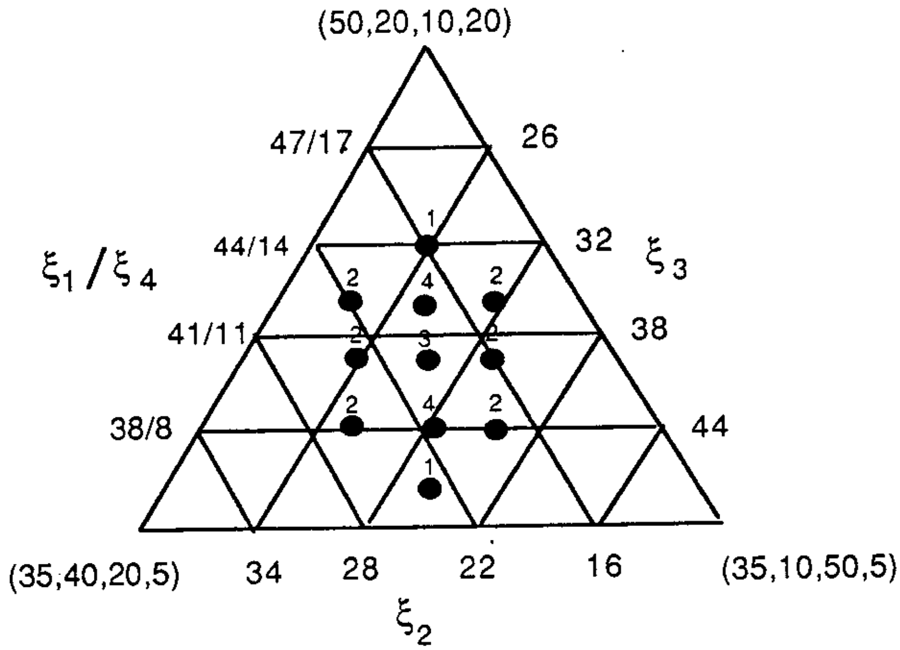

Figure 2.5: The Projection Design in the Cake Example

The design in ξ_i's is shown in the last four columns of Table 2.1. The design points are laid out in Figure 2.5.

Note that the ranges of the design variables are not exactly $c_i \pm 6\%$. For the reasons already explained in Section 1.5, it is impossible to construct a design with exactly these ranges due to the constraints. We suppose, however, the experimenter has modified the region of interest iteratively.

2.4 Fractionating and Blocking the Projection Designs

Consider again the projection of the 2^q factorial designs. These designs were referred to as 2^q Projected Factorial (PF) designs. As discussed in Section 1.2, it is often desirable to allow experiments to be performed in blocks and allow sequential building of designs. One incidental advantage of the factorial designs is that they can be readily fractionated and blocked in convenient ways. It turns out that the *projected* factorial designs can be usefully blocked and fractionated in the same way. For example, let us consider the projected 2^3 factorial design of Section 2.1. Suppose we want to run this design in two fractions. With three factors A, B and C, if there were no constraints, we may want to begin with a half fraction of a 2^3 design. This would be a "first order" design (Box and Wilson (1951)) which allows fitting a planar model which at this stage we might hope to provide a pretty good approximation of the response surface. If, after we have analyzed the results, we found out that the planar model was not really adequate, we might then add the other fraction in order to find out something about the second order terms. To do that, we might first run the fraction using the defining relation $C = AB$ (see Box, Hunter and Hunter (1978)) as follows:

A	B	$C = AB$
-1	-1	1
1	-1	-1
-1	1	-1
1	1	1

The remaining fraction is obtained using the defining relation $C = -AB$. Now we can project these two fractions onto the mixture constrained space. These two fractions in the mixture space are referred to as the 2^{3-1} **Fractional Projected Factorial** designs and are shown in Figure 2.6.

In general, we propose the following way to run the 2^q PF design in p fractions. First generate the 2^{q-p} fractional factorial design. Then project the design onto the constrained space. The resulting design will be called the 2^{q-p} **Fractional Projected Factorial (FPF) Design**. To run the PF designs in blocks, the same idea can be applied. We begin with the factorial designs in the desired number of blocks, then project the different blocks onto the constrained space.

One advantage of the fractional factorial designs is that they are orthogonal and hence their analyses are simple. It turns out that this simplicity can be preserved after projection. In fact, we will show in Chapter 3 that the 2^{q-p} FPF constrained designs can be analyzed as if they were the 2^{q-p}

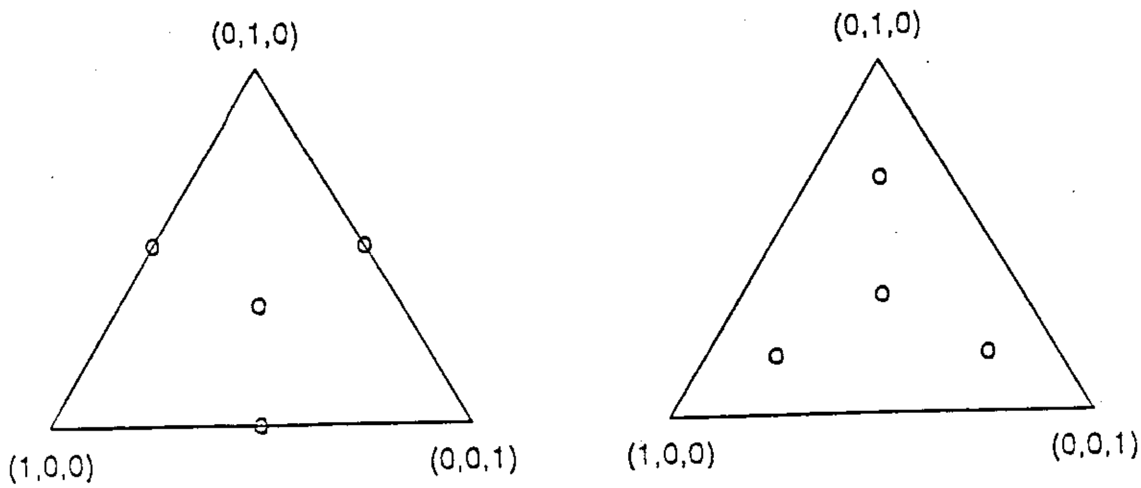

Figure 2.6: The Two Fractions of the 2^3 PF Mixture Design

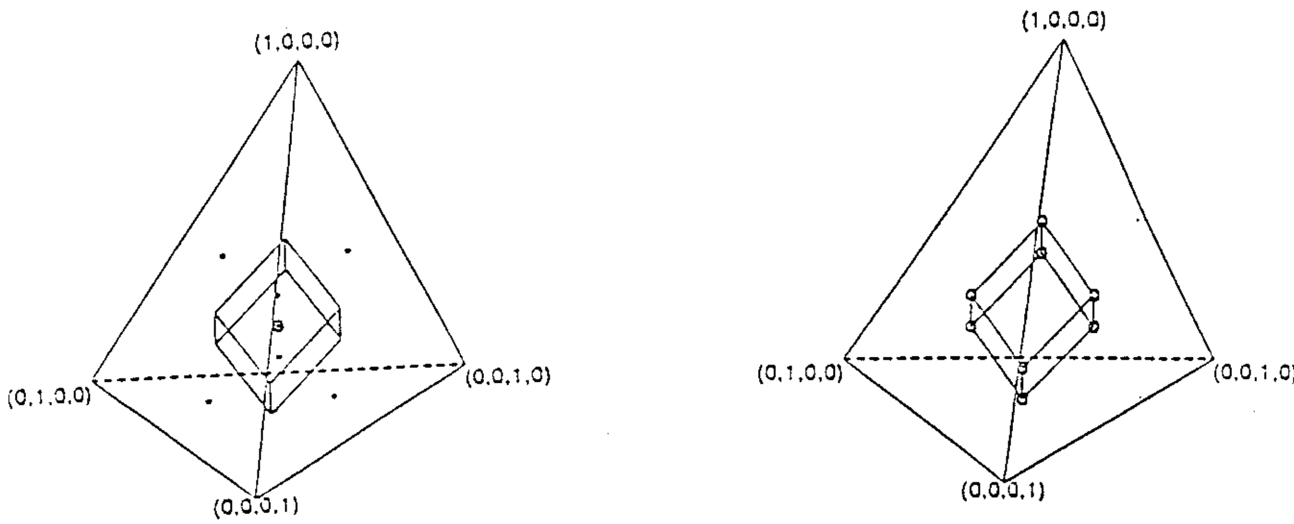

Figure 2.7: The 2^{4-1} FPF Designs in the Mixture Case

unconstrained designs. Similarly, the advantage of orthogonal blocking of factorial designs is also preserved in the projected factorial designs.

As another example, let us see what the 2^{4-1} FPF design in the mixture case looks like. Recall the 2^4 PF mixture design in Section 2.2. If we denote the factors as A,B,C and D and let D=ABC, we get the fraction consisting of the points (rows) 2, 3, 5, 8, 9, 12, 14 and 15. The rest of the points belong to another fraction which can be obtained by letting D=−ABC. Both fractions are laid out in Figure 2.7. It is interesting to note that one fraction corresponds to the "cube points" and the other fraction corresponds to the "star points" and "center points".

2.5 Other Projection Designs

We have illustrated our discussion using two types of projection designs so far: the **Projected Factorial** design and the **Projected Composite** design. In the following, we will look at another class called **Projected Koshal** designs.

An interesting question: "what kind of 'de-projected' designs do classical mixture designs such as the simplex-lattice correspond to?" It turns out that if we project the Koshal designs onto the mixture constrained space, we get the simplex-lattice designs. In Section 1.6, we reviewed the simplex-lattices designs and the simplex-centroid designs. See Cornell (1981) for more details for simplex designs. In the following sections, we review the Koshal designs and show their relation with simplex designs.

2.5.1 Simplex Designs and Koshal Designs

Koshal designs were first proposed by Koshal (1933) to determine the maximum of a likelihood function numerically. The designs were modified by Fung (1986) in the response surface context. The m-th order Koshal design with q factors consists of the following points (vectors of length q) and all their permutations.

$$
\begin{array}{llllllll}
(& m, & 0, & 0, & 0, & \ldots, & 0 &) \\
(& m-1, & 1, & 0, & 0, & \ldots, & 0 &) \\
(& m-2, & 2, & 0, & 0, & \ldots, & 0 &) \\
(& m-2, & 1, & 1, & 0, & \ldots, & 0 &) \\
 & & & \vdots & & & & \\
(& 1, & 0, & 0, & 0, & \ldots, & 0 &) \\
(& 0, & 0, & 0, & 0, & \ldots, & 0 &)
\end{array}
$$

In other words, the design consists of all possible vectors of q positive integers, which have sums equal to $0, 1, 2, \ldots$ or m. This design is a saturated design which can estimate all the coefficients of an m-th degree polynomial in q variables. The designs are very useful in pure numerical applications such as that employed by Koshal. However, for the situation when the effect of experimental errors must be considered, the distribution of information of this class of designs are less satisfactory than that obtained from standard response surface designs. See Fung (1986).

2.5.2 Projected Koshal Designs

If we project a Koshal design onto the constrained space, the resulting projection design is called the **Projected Koshal (PK)** design. Let us look at an example with 3 factors ξ_1, ξ_2, ξ_3 in the mixture case. That is:

$$\begin{cases} \xi_1 + \xi_2 + \xi_3 = 1 \\ 0 \leq \xi_i \leq 1, \quad i = 1, 2, 3 \end{cases} \tag{2.11}$$

The second order projected Koshal design is obtained by projecting the following 3-factor 2nd-order Koshal design:

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

The above design is projected onto the mixture constrained space. In order to compare this design with the simplex designs, let us consider the largest possible spherical region of interest centered at (1/3,1/3,1/3). Following the same calculation as in Section 2.1, we obtain the following PK design:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 1/2 \\ 2/3 & 1/6 & 1/6 \\ 1/6 & 2/3 & 1/6 \\ 1/6 & 1/6 & 2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$$

The design is shown in Figure 2.8. If we take the fraction consisting of only the first six points, we get the {3,2} simplex-lattice design. If we add the center point (1/3,1/3,1/3), we obtain the simplex-centroid design. Finally, the full PK design is the 10-point design proposed by Cornell (1986).

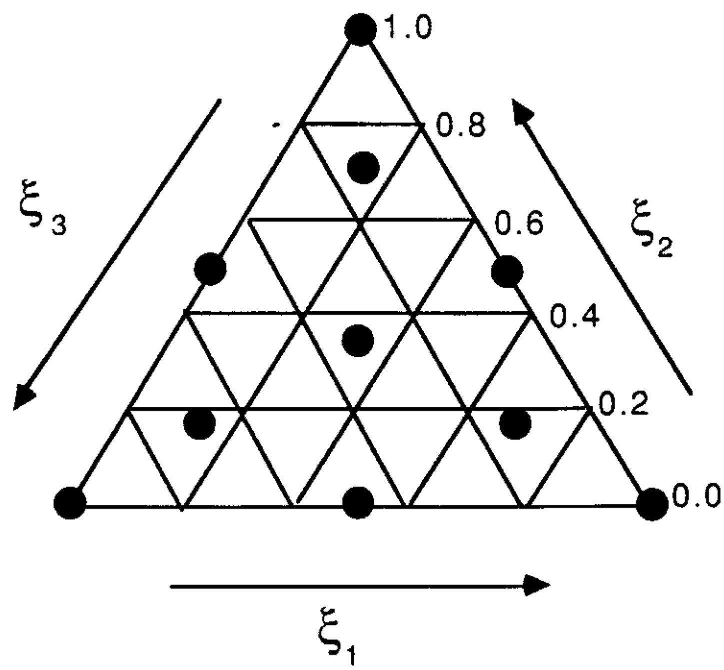

Figure 2.8: The 2nd-order Projected Koshal Design in the Mixture Case

In general, the {q,m} simplex-lattice design is a fraction of the q-factor Projected Koshal design of order m. In fact, the fraction only consists of the points whose coordinates add up to m, i.e., the points in Koshal designs used to estimated the mth-order terms. The points (vectors of length q) which correspond to the m-th order terms are the following points and all their permutations:

$$
\begin{array}{ccccccccc}
(& m, & 0, & 0, & 0, & \ldots, & 0 &) \\
(& m-1, & 1, & 0, & 0, & \ldots, & 0 &) \\
(& m-2, & 2, & 0, & 0, & \ldots, & 0 &) \\
(& m-2, & 1, & 1, & 0, & \ldots, & 0 &) \\
 & & & \vdots & & & &
\end{array}
$$

Note that all the row means are m/q. The projections of these points onto the simplex with center at $(1/q, \ldots, 1/q)$ are:

$$
\begin{array}{rcl}
\frac{1}{m}\left(m - \frac{m}{q}, -\frac{m}{q}, -\frac{m}{q}, -\frac{m}{q}, \cdots, -\frac{m}{q}\right) & + & \left(\frac{1}{q}, \cdots, \frac{1}{q}\right) \\
\frac{1}{m}\left(m - 1 - \frac{m}{q}, 1 - \frac{m}{q}, -\frac{m}{q}, -\frac{m}{q}, \cdots, -\frac{m}{q}\right) & + & \left(\frac{1}{q}, \cdots, \frac{1}{q}\right) \\
\frac{1}{m}\left(m - 2 - \frac{m}{q}, 1 - \frac{m}{q}, 1 - \frac{m}{q}, -\frac{m}{q}, \cdots, -\frac{m}{q}\right) & + & \left(\frac{1}{q}, \cdots, \frac{1}{q}\right) \\
 & \vdots &
\end{array}
$$

When simplified, the points are:

$$
\begin{array}{cccccccc}
(& 1 & 0 & 0 & \cdots & 0 &) \\
(& 1-\frac{1}{m} & \frac{1}{m} & 0 & \cdots & 0 &) \\
(& 1-\frac{2}{m} & \frac{2}{m} & 0 & \cdots & 0 &) \\
(& 1-\frac{2}{m} & \frac{1}{m} & \frac{1}{m} & \cdots & 0 &) \\
 & & & \vdots & & &
\end{array}
$$

and all their permutations. These are the points in $\{q, m\}$ simplex-lattice designs.

Bibliography

[1] Aitken,A.C.(1948), *Determinants and Matrices,* Oliver & Boyd, London.

[2] Aitken,A.C.(1949), *On the Wishart Distribution in Statistics,* Biometrika, **36**, 56-62.

[3] Box,G.E.P.(1982), *Choice of Response Surface Design and Alphabetic Optimality,* Utilitas Mathematica, **21B**, 791-799.

[4] Box,G.E.P. and Draper,N.R.(1959), *"A Basis for the Selection of a Response Surface Design"*, J. Am. Statist. Assoc., **54**, 622-654.

[5] Box,G.E.P. and Draper,N.R.(1975), *"Robust Designs"*, Biometrika, **62**, 347-352.

[6] Box,G.E.P and Draper,N.R.(1982), *"Measures of Lack of Fit for Response Surface Designs and Predictor Variable Transformations"*, Technometrics, **24**, 1-8.

[7] Box,G.E.P and Draper,N.R.(1987), *"Empirical Model-Building and Response Surfaces"*, New York: John Wiley.

[8] Box,G.E.P. and Hunter,J.S.(1957), *Multifactor Experimental Designs for Exploring Response Surfaces,* Ann. Math. Statist., **28**, 195-241.

[9] Box,G.E.P., Hunter,W.G. and Hunter,J.S.(1978), *"Statistics for Experimenters"*, New York: John Wiley.

[10] Box,G.E.P. and Wilson,K.B.(1951), *"On the Experimental Attainment of Optimum Conditions"*, J. Roy. Statist. Soc, **B13**, 1-38, discussion 38-45.

[11] Cornell,J.A.(1981), *"Experiments with Mixtures"*, New York: John Wiley.

[12] Cornell,J.A.(1986), *"A Comparison Between Two Ten-Point Designs for Studying Three Component Mixture System"*, J. Quality Tech., **18**, 1-15.

[13] Cornell,J.A. and Khuri,A.I.,(1987), *"Response Surfaces: Designs and Analyses"*, ASQC Press.

[14] Fung, C. (1986), *"Statistical Topics on Off-Line Quality Control"*, Ph.D. Thesis, University of Wisconsin - Madison.

[15] Koshal, R.S.,(1933), *Application of the Method of Maximum Likelihood to the Improvement of Curves Fitted by the Method of Moments*, J. Roy. Statist. Soc., **B46**, 558-563.

[16] McLean, R.A. and Anderson, V.L. (1966), *"Extreme Vertices Design of Mixture Experiments*, Technometics, **8**, 447-454.

[17] Scheffé,H.(1959) *"Experiments with Mixtures"*, J. Roy. Statist. Soc., **B20**, 344-360.

[18] Scheffé,H.(1963) *"Simplex-Centroid design for Experiments with Mixtures"*, J. Roy. Statist. Soc., **B25**, 235-263.

[19] Seber,G.A.F(1977), *"Linear Regression Analysis"*, New York: John Wiley.