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Report No. 55

Constrained Experimental Designs
Part III: Steepest Ascent and Properties of Projection Designs

Ian Hau and George Box

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C Q P I
UNIVERSITY OF WISCONSIN

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Report Series
in Quality and Productivity

Constrained Experimental Designs
Part III: Steepest Ascent and Properties of Projection Designs

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ABSTRACT

Steepest ascent is an important tool for process improvement. This report discusses how to use the steepest ascent method in the context of constrained designs. The properties of the projection designs proposed in the Center for Quality and Productivity Improvement Report Series #53 are also discussed.

KEYWORDS: Projection designs, mixture design, steepest ascent, rotatability, process improvement

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Table of Contents

Chapter 4

Steepest Ascent under Constraints

4.1 Steepest Ascent

When the design variables are not constrained, designs such as 2^q factorial designs and composite designs are very valuable. These designs have desirable theoretical properties and they have stood the test of time in practice. Since Scheffé (1958) introduced the simplex-lattice designs, mixture experiments have been treated quite differently from the classical unconstrained designs. In the previous chapters, we have discussed how the constrained design problem and the unconstrained design problem should be treated in similar ways: issues about coding and region of interest for constrained design problems should be considered the same way as that for the unconstrained design problems; the constrained (projection) designs are constructed based upon the well-known unconstrained designs; the analyses of the projection designs are the same as that of the unconstrained designs; methods for orthogonal blocking and fractionating available for unconstrained designs can be used in the same way for the constrained designs.

In this chapter we discuss another useful tool, determination of the direction of steepest ascent, used in response surface methodology. It turns out that the steepest ascent procedure used for the unconstrained design problems can be used, after slight modification, for the constrained design problems.

Suppose we want to improve a process by finding a setting of the factors where the response of interest is optimal. At the early stage of the investigation, we are usually far from the optimum. However, it is almost never a feasible solution to approximate the unknown surface over a large region. First, the extent of this region is unknown and second, the number of experiments required to give a reasonable approximation of the surface would be impractically large. What we may do is to fit a simple graduate function such as a planar model over a smaller subregion of interest. From the planar model, we may be able to find a direction pointing to a more profitable region in which we may explore more carefully. When the factors are not constrained, this goal can be achieved by a technique called *steepest ascent* (Box and Wilson (1951)). In this section, we propose a method for finding the steepest ascent direction when the factors $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t$ are subject to the constraints $A\mathbf{x} = \mathbf{0}$.

Suppose we have the following fitted planar model:

$$\hat{y} = \hat{\gamma}_o + \hat{\gamma}_1 x_1 + \ldots + \hat{\gamma}_q x_q \tag{4.1}$$

Let A be the matrix of constraints and $P = I - A^t(AA^t)^{-1}A$ be the projection onto the constrained space $A\mathbf{x} = \mathbf{0}$. Also let $\hat{\boldsymbol{\gamma}}_1 = (\hat{\gamma}_1, \ldots, \hat{\gamma}_q)^t$. Then the steepest ascent direction is proportional to

$$\hat{\boldsymbol{\gamma}}_1^* = P\hat{\boldsymbol{\gamma}}_1 = (\hat{\gamma}_1^*, \hat{\gamma}_2^*, \ldots, \hat{\gamma}_q^*)^t,$$

as a result of the following theorem:

Let $\mathbf{x}_o$ be a $q \times 1$ vector such that $A\mathbf{x}_o = \mathbf{0}$, and for some $k > 0$, let $\triangle\mathbf{x}^t = (k\hat{\gamma}_1^*, k\hat{\gamma}_2^*, \ldots, k\hat{\gamma}_q^*)$. Then $\mathbf{x}^* = \mathbf{x}_o + \triangle\mathbf{x}$ is the solution to the following problem:

$$\max_{\mathbf{x}} \{\hat{y}(\mathbf{x}) - \hat{y}(\mathbf{x}_o)\} \tag{4.2}$$

subject to:

$$(\mathbf{x} - \mathbf{x}_o)^t(\mathbf{x} - \mathbf{x}_o) = r^2 \tag{4.3}$$

$$\textit{and} \qquad A\mathbf{x} = \mathbf{0} \tag{4.4}$$

Here r is some real number.

Proof Note that Model (4.1) can be written as:

$$\begin{aligned}\hat{y} &= \hat{\gamma}_o + \mathbf{x}^t \hat{\boldsymbol{\gamma}}_1 \\ &= \hat{\gamma}_o + \mathbf{x}^t P \hat{\boldsymbol{\gamma}}_1\end{aligned}$$

Therefore, we have:

$$\hat{y} = \hat{\gamma}_o + \mathbf{x}^t \hat{\boldsymbol{\gamma}}_1^* \tag{4.5}$$

Note that $\mathbf{x}^*$ is the solution to (4.2), subject to (4.3) alone (Seber (1977) p.235). Therefore, it suffices to prove $A\mathbf{x}^* = \mathbf{0}$. However, $A\triangle\mathbf{x} = kAP\hat{\boldsymbol{\gamma}}_1 = \mathbf{0}$. Therefore, $A\mathbf{x}^* = A(\mathbf{x}_o + \triangle\mathbf{x}) = A\mathbf{x}_o = \mathbf{0}$. □

The theorem applies also for general constraints as follows. Suppose we have the following planar model in ξ_i:

$$\hat{y} = \hat{\gamma}_o + \hat{\gamma}_1\xi_1 + \ldots + \hat{\gamma}_q\xi_q \tag{4.6}$$

and the design variables $\xi = (\xi_1, \xi_2, \ldots, \xi_q)^t$ are subject to general constraints $A\xi = \mathbf{d}$. We can transform ξ to $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t$ by:

$$\mathbf{x} = \xi - \mathbf{c}$$

where $\mathbf{c} = (c_1, c_2, \ldots, c_q)^t$ is a point in the constrained space, i.e., $A\mathbf{c} = \mathbf{d}$. Then $A\mathbf{x} = A(\xi - \mathbf{c}) = \mathbf{0}$ and the model (4.6) becomes:

$$\hat{y} = (\hat{\gamma}_o + \mathbf{c}^t\hat{\boldsymbol{\gamma}}_1) + \hat{\gamma}_1 x_1 + \ldots + \hat{\gamma}_q x_q$$

where $\hat{\boldsymbol{\gamma}}_1 = (\hat{\gamma}_1, \hat{\gamma}_2, \ldots, \hat{\gamma}_q)^t$. By the theorem above, $\hat{\boldsymbol{\gamma}}_1^* = P\hat{\boldsymbol{\gamma}}_1$ is the steepest ascent direction.

4.2 An Example

Let us look at the tensile strength of a mixture which is a composite system of graphite, boron and epoxy. Let η be the tensile strength ($10^3 psi$), ξ_1, ξ_2 and ξ_3 be the proportions of graphite, boron and epoxy respectively. Suppose the experimenter thinks that the region of interest is roughly:

$$c_i \pm r_i \quad i = 1, 2, 3.$$

where $(c_1, c_2, c_3) = (1/6, 1/6, 2/3)$, and $r_i = 2/15$ for $i = 1, 2, 3$. The coded

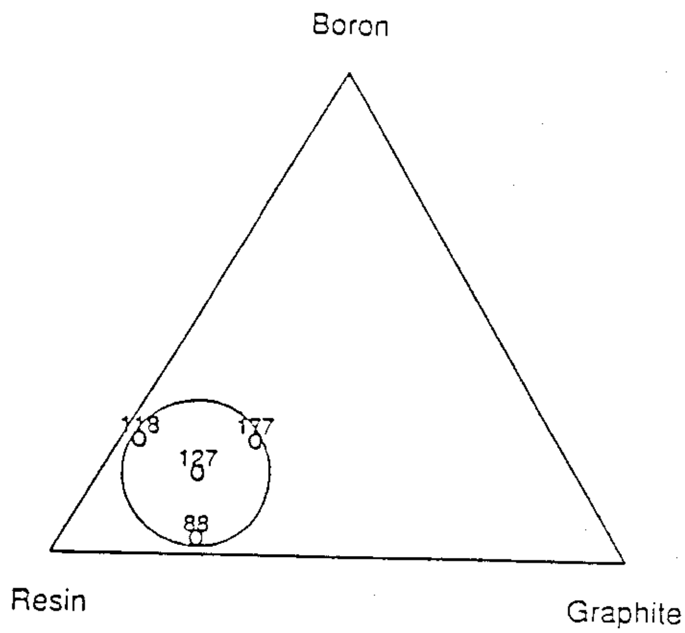

Figure 4.1: Region of interest, 2^{3-1} PF design points and their responses.

variables x_i defined by:

$$x_i = \frac{\xi_i - c_i}{\alpha r_i} \tag{4.7}$$

are constrained by:

$$x_1 + x_2 + x_3 = 0 \tag{4.8}$$

Suppose the experimenter believes that, within the region of interest, a planar model may provide an adequate approximation of the response surface. To obtain a projection design in the coded variables x_i, we may project a 2^{3-1} design onto the constrained space (4.8). The 2^{3-1} design and its projection are shown in columns 2 to 7 of Table 4.1. Now we can transform the design in the coded variables x_i to the original variables ξ_i using the relationship in (4.7). Since the largest absolute value in x_i is $4/3$, the size parameter α should be $3/4$. Now the relationship (4.7) can be simplified to:

$$\xi_i = 0.1x_i + c_i \quad i = 1, 2, 3. \tag{4.9}$$

The projection design in ξ_i is shown in columns 8 to 10 of Table 4.1, and the responses at these design points are given in the last column. The design is shown in Figure 4.1.

run #	z_1	z_2	z_3	x_1	x_2	x_3	ξ_1	ξ_2	ξ_3	y
0	-1	-1	-1	0	0	0	0.167	0.167	0.666	126.9
1	1	1	-1	2/3	2/3	$-4/3$	0.233	0.233	0.534	177.5
2	1	-1	1	2/3	$-4/3$	2/3	0.233	0.033	0.734	88.4
3	-1	1	1	$-4/3$	2/3	2/3	0.033	0.233	0.734	118.1

Table 4.1

The estimation results are summarized in Table 4.2:

Parameter	Computation	Estimates
$\hat{\gamma}_o$	$\bar{y} = (y_1 + y_2 + y_3 + y_4)/4$	127.7
$\hat{\gamma}_1$	$(-y_1 + y_2 + y_3 - y_4)/4$	5.225
$\hat{\gamma}_2$	$(-y_1 + y_2 - y_3 + y_4)/4$	20.075
$\hat{\gamma}_3$	$(-y_1 - y_2 + y_3 + y_4)/4$	-24.475

Table 4.2

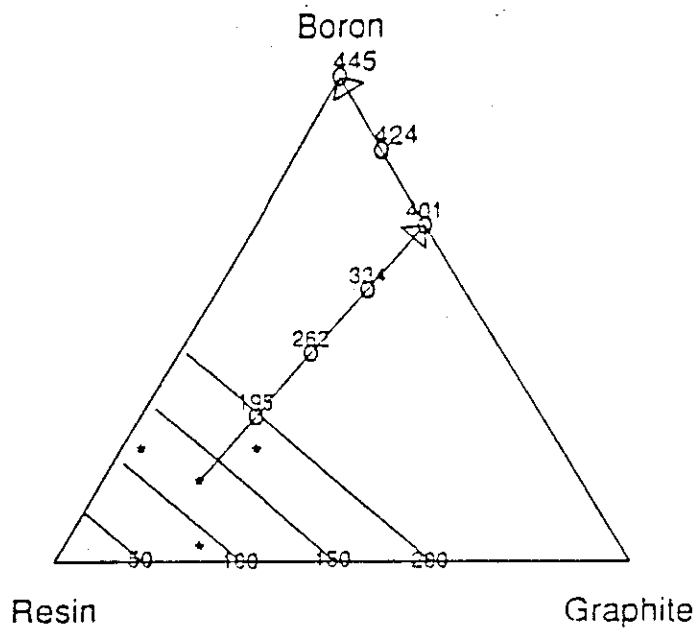

Figure 4.2: Contour of fitted surface and the steepest ascent path

Therefore, the fitted model in the scaled constrained variables is:

$$\begin{aligned} \hat{y} &= \hat{\gamma}_o + \hat{\gamma}_1 x_1 + \hat{\gamma}_2 x_2 + \hat{\gamma}_3 x_3 \\ &= 127.7 + 5.225 x_1 + 20.075 x_2 - 24.475 x_3 \end{aligned} \tag{4.10}$$

Using the relation (4.9), we can express the fitted model (4.10) in the original proportions ξ_i:

$$\begin{aligned} \hat{y} &= (\bar{y} - 10\mathbf{c}^t\hat{\boldsymbol{\gamma}}_1) + 10\hat{\gamma}_1\xi_1 + 10\hat{\gamma}_2\xi_2 + 10\hat{\gamma}_3\xi_3 \\ &= 218.7 + 52.25\xi_1 + 200.75\xi_2 + 244.75\xi_3 \end{aligned} \tag{4.11}$$

The contour of the fitted surface (4.11) is shown in Figure 4.2.

Let $\bar{\gamma} = (\hat{\gamma}_1 + \hat{\gamma}_2 + \hat{\gamma}_3)/3$, then the steepest ascent direction is given by $\hat{\boldsymbol{\gamma}}_1^* = P\hat{\boldsymbol{\gamma}}_1$, i.e.,

$$\begin{aligned} (\hat{\gamma}_1^*, \hat{\gamma}_2^*, \hat{\gamma}_3^*) &= (\hat{\gamma}_1 - \bar{\gamma}, \hat{\gamma}_2 - \bar{\gamma}, \hat{\gamma}_3 - \bar{\gamma}) \\ &= (50, 198, -247) \end{aligned}$$

and the steepest ascent path has the coordinates:

$$(0.167, 0.167, 0.666) + k(50, 198, -247)$$

For example, if the step sizes k are taken to be 0.00067, 2×0.00067, 3×0.00067, 4×0.00067, the exploratory runs and their responses are as shown in Table 4.3.

Exploratory runs no.	ξ_1	ξ_2	ξ_3	y
0 (center)	0.167	0.167	0.666	126.9
1	0.2	0.3	0.5	194.9
2	0.23	0.44	0.33	266.4
3	0.27	0.57	0.16	333.9
4	0.30	0.70	0	401.8
5 (modified	0.15	0.85	0	423.6
6 direction)	0	1	0	444.6

Table 4.3

Since the responses of the four exploratory runs are continuously increasing by significant amounts, we may want to have more runs along the steepest ascent path. However, the 4th exploratory run $(0.3, 0.7, 0)$ hits the boundary of the constrained region, namely, $\xi_3 = 0$. To modify the steepest ascent direction, we adopt the strategy proposed by Box and Draper (1987, Chapter 6). We need to project $(\hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3)$ onto the subspace defined by the constraints:

$$\begin{cases} \xi_1 + \xi_2 + \xi_3 & = & 0 \\ \xi_3 & = & 0 \end{cases} \tag{4.12}$$

The projection of $(\hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3)$ onto the constrained region (4.12) gives the modified steepest ascent path $(-k, k, 0)$. The experimenter decides to make two more runs along the modified direction

$$(0.3, 0.7, 0) + (-k, k, 0)$$

with $k = 0.147$ and $k = 2 \times 0.147$. These are runs 5 and 6 in Table 4.3. As a conclusion, run 6 (100% boron) is the optimal setting.

In practice, it is unlikely that a planar response surface would provide an adequate approximation over the whole constrained region. The purpose of this example is simply to illustrate the steepest ascent method when there are constraints.

Chapter 5

Rotatability of Projection Designs

5.1 Introduction

In the previous chapters, we have seen that constrained design problems can be treated in the manner similar to classical unconstrained design problems. For example, using the principle of projection:

- Constrained designs can be constructed based upon well-known unconstrained designs;
- Constrained designs can be blocked and fractionated by the known methods for unconstrained designs;
- Analyzing constrained designs is as simple as analyzing the original unconstrained designs;
- The steepest ascent method for unconstrained design problems can be adopted with little modification for constrained design problem.

In this chapter, we will show further that rotatability of the original unconstrained designs is preserved in their projection designs.

5.2 Rotatability of Unconstrained Designs

Orthogonality has been widely recognized as an important design principle for first order designs. For design of higher order, Box and Hunter (1957) pointed out that the logical extension of orthogonality is *rotatability* which has since become an important design criterion. The concept of rotatability is as follows. Let $\hat{y}_{\mathbf{x}}$ be the predicted value at the design point $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t$. The variance of $\hat{y}_{\mathbf{x}}$, which is a function of $\mathbf{x}$, is denoted as $\text{var}(\hat{y}_{\mathbf{x}})$. When the design points are arranged in such a way that $\text{var}(\hat{y}_{\mathbf{x}})$ is constant at all points $\mathbf{x}$ that are equidistant from the design center, the design is called a **rotatable design**. Suppose there are n design points $(x_{1u}, x_{2u}, \ldots, x_{qu})$ in q design factors, $u = 1, 2, \ldots, n$, and x_{iu} are scaled so that:

$$\sum_{u=1}^{n} x_{iu} = 0, \quad \sum_{u=1}^{n} x_{iu}^2 = n, \quad i = 1, 2, \ldots, q.$$

The quantity:

$$n^{-1} \sum x_{1u}^p x_{2u}^r \cdots x_{qu}^s,$$

where this and subsequent summations are over $u = 1, 2, \ldots, n$, is called a design moment of order $p + r + \cdots + s$. If multiplied by n, it is called a "sum of powers" (if only one of $p, r, \ldots, s$ is non-zero) or a "sum of products" (if two or more of $p, r, \ldots, s$ are non-zero) of the same order.

For a design to be rotatable, its design moments of different orders must satisfies certain conditions. For example, a third order rotatable design must be such that

$$\sum_{u=1}^{n} x_{iu}^2 = n\lambda_2, \quad i = 1, 2, \ldots, q \tag{5.1}$$

$$\sum_{u=1}^{n} x_{iu}^4 = 3 \sum_{u=1}^{n} x_{iu}^2 x_{ju}^2 = 3n\lambda_4, \quad i \neq j \tag{5.2}$$

$$\sum_{u=1}^{n} x_{iu}^6 = 5 \sum_{u=1}^{n} x_{iu}^2 x_{ju}^4 = 15 \sum_{u=1}^{n} x_{iu}^2 x_{ju}^2 x_{lu}^2 = 15n\lambda_6, \quad i \neq j \neq l \tag{5.3}$$

where $0 \leq i, j, l \leq q$. and all other sums of powers and products up to and including order 2k (where k=3) must be zero. The parameters $\lambda_2, \lambda_4, \lambda_6$ are some adjustable constants. (See Box and Hunter (1957), p.209). For the second order rotatability, $2k = 4$ and we need only (5.1) and (5.2). For the first order rotatability, we need (5.1) only and $2k = 2$.

One convenient class of rotatable designs (available for all values of q) is that of the suitably dimensioned central composite designs. These designs in q factors consist of the cube points,

$$(\pm 1, \pm 1, \cdots, \pm 1),$$

the axial points,

$$(\pm\alpha, 0, 0, \ldots, 0), (0, \pm\alpha, 0, \ldots, 0), \ldots, (0, 0, \ldots, 0, \pm\alpha)$$

and the center points $(0, 0, \ldots, 0)$. Suppose the cube is replicated r_c times and the axial points are replicated r_s times. To attain rotatability, the axial points must be located at:

$$\alpha = \left(\frac{2^q r_c}{r_s}\right)^{1/4} \tag{5.4}$$

For example, consider the central composite design in $q = 3$ factors which consist of eight cube points $(\pm 1, \pm 1, \pm 1)$, six axial points $(\pm\alpha, 0, 0)$, $(0, \pm\alpha, 0)$, $(0, 0, \pm\alpha)$ and two center points $(0, 0, 0)$. To attain rotatability, the appropriate choice of α is:

$$\alpha = \left(\frac{2^3 r_c}{r_s}\right)^{1/4} = \left(\frac{2^3 1}{1}\right)^{1/4} = 8^{1/4}$$

5.3 Rotatability of Projection Designs

In this section, we will show that if a k-th order rotatable design is projected onto the constrained space, the resulting projection design is also k-th order rotatable, where k=1,2,3.

Suppose there are q design variables and m constraints. If the original design is rotatable in the q space, then we can rotate the design so that m of its coordinates define the constrained space. Thus the problem is equivalent to dropping m variables from a q variable rotatable design and showing that it is still rotatable in the $q - m$ remaining variables. The proof is shown in the following. Suppose there are n unconstrained design points:

$$\mathbf{z}_u^* = (z_{1u}^*, z_{2u}^*, \ldots, z_{qu}^*)^t \quad u = 1, 2, \ldots, n.$$

Let $\Lambda = \text{diag}(1, 1, \ldots, 1, 0, \ldots, 0)$ be a $q \times q$ diagonal matrix with the first $q - m$ diagonal elements equal to 1, and the remaining m diagonal elements equal to 0. Let the projection of $\mathbf{z}_u^*$ on $z_{ju}^* = 0$, $j = q - m, q - m + 1, \ldots, q$, be $\mathbf{x}_u^*$, i.e., $\mathbf{x}_u^* = \Lambda \mathbf{z}_u^*$. In other words:

$$\mathbf{x}_u^* = (z_{1u}^*, z_{2u}^*, \ldots, z_{q-m.u}^*, 0, 0, \ldots, 0)^t$$

We claim that if $\mathbf{z}_u^*$ is a k-th order rotatable design, then $\mathbf{x}_u^*$ is also a k-th order rotatable design, where k=1,2 and 3.

Assume k=3, i.e., the design $\mathbf{z}_u^*$ is third order rotatable, then the following conditions must be satisfied:

$$\sum_{u=1}^{n} {z_{iu}^*}^2 = n\lambda_2, \quad i = 1, 2, \ldots, q \tag{5.5}$$

$$\sum_{u=1}^{n} {z_{iu}^*}^4 = 3 \sum_{u=1}^{n} {z_{iu}^*}^2 {z_{ju}^*}^2 = 3n\lambda_4, \quad i \neq j \tag{5.6}$$

$$\sum_{u=1}^{n} {z_{iu}^*}^6 = 5 \sum_{u=1}^{n} {z_{iu}^*}^2 {z_{ju}^*}^4 = 15 \sum_{u=1}^{n} {z_{iu}^*}^2 {z_{ju}^*}^2 {z_{lu}^*}^2 = 15n\lambda_6, \quad i \neq j \neq l \tag{5.7}$$

where $0 \leq i, j, l \leq q$, and all other sums of powers and products up to and including order 2k (where k=3) must be zero.

In order for the projection design $\mathbf{x}_u^*$ to be third order rotatable in the $q - m$ space, the equations (5.5), (5.6) and (5.7) must be satisfied and all other sums of powers and products up to 2k = 6 must be zero for $i \neq j \neq l, 0 \leq i, j, l \leq q - m$. This is true given that $\mathbf{z}_u^*$ is third order rotatable, i.e., all these conditions are satisfied for $0 \leq i, j, k \leq q$. Therefore $\mathbf{x}^*$ is third order rotatable.

In general, suppose the constrained design points $\mathbf{x}_u$ must satisfy the m general constraint

$$\sum_{j=1}^{q} a_{ij} x_{ju} = 0, \quad i = 1, 2, \ldots, m$$

or in matrix form:

$$A\mathbf{x}_u = \mathbf{0}$$

where $A = (a_{ij})$ is a $m \times q$ matrix of constraints. Let $P = I - A^t(AA^t)^{-1}A$ be the projection onto the constrained space. Since P is symmetric and idempotent, its q eigenvalues are either one or zero. Furthermore, since P has rank $q-m$, there are $q-m$ eigenvalues equal to one and the others equal to zero. Therefore, there is an orthonormal matrix Q, i.e. $Q^tQ = I$, and a diagonal matrix Λ with $q-m$ diagonal elements equal to 1 and m diagonal elements equal to 0 such that:

$$P = Q^t \Lambda Q \tag{5.8}$$

Or,

$$QP = \Lambda Q \tag{5.9}$$

Without loss of generality, let the first $q-m$ diagonal elements of Λ be 1 and the others be 0, i.e., $\Lambda = \text{diag}(1,1,\ldots,1,0,0,\ldots,0)$. Since $Q^tQ = I$, Q is a rotation. Let

$$\mathbf{x}^* = Q\mathbf{x} \quad \text{and} \quad \mathbf{z}^* = Q\mathbf{z}$$

By (5.9):

$$\Lambda\mathbf{z}^* = \Lambda Q\mathbf{z} = QP\mathbf{z} = Q\mathbf{x} = \mathbf{x}^*$$

Therefore, $\mathbf{x}^*$ is a projection of $\mathbf{z}^*$ onto $z_{ju}^* = 0$, $j = q-m, q-m+1, \ldots, q$. Since $\mathbf{z}$ forms a third order rotatable design and Q is a rotation, $\mathbf{z}^*$ also forms a rotatable design. As a result, the projection $\mathbf{x}^* = \Lambda\mathbf{z}^*$ of $\mathbf{z}^*$ onto the $z_{qu}^* = 0$ is also third order rotatable. Finally, since $\mathbf{x} = Q^t\mathbf{x}^*$ is a rotation of $\mathbf{x}^*$, the projection design $\mathbf{x}$ is third order rotatable. The proofs for the second order and first order rotatability are exactly the same.

As a simple illustration of the result, consider a composite design in three factors which consists of eight cube points with coordinates $(\pm 1, \pm 1, \pm 1)$, six axial points $(\pm\alpha, 0, 0)$, $(0, \pm\alpha, 0)$, $(0, 0, \pm\alpha)$ and two center points $(0,0,0)$. The design is shown on the left hand side of Figure 5.1. As already shown in last section, in order for this design to be second order rotatable, α must equal $8^{1/4} = 1.682$. Suppose this rotatable design is projected onto one axis, say, $z_3 = 0$. Then the projection design consists of two sets of cube points $(\pm 1, \pm 1)$, one set of axial points $(\pm\alpha, 0)$, $(0, \pm\alpha)$ and four center points $(0,0)$. This projection design is shown on the right hand side of Figure 5.1. We see that for the projection design, $\alpha = 8^{1/4}$ is the right distance for rotatability since

$$\alpha = \left(\frac{2^2 r_c}{r_s}\right)^{1/4} = \left(\frac{2^2 2}{1}\right)^{1/4} = 8^{1/4}$$

where r_c and r_s are the number of times the cube and the star points are replicated.

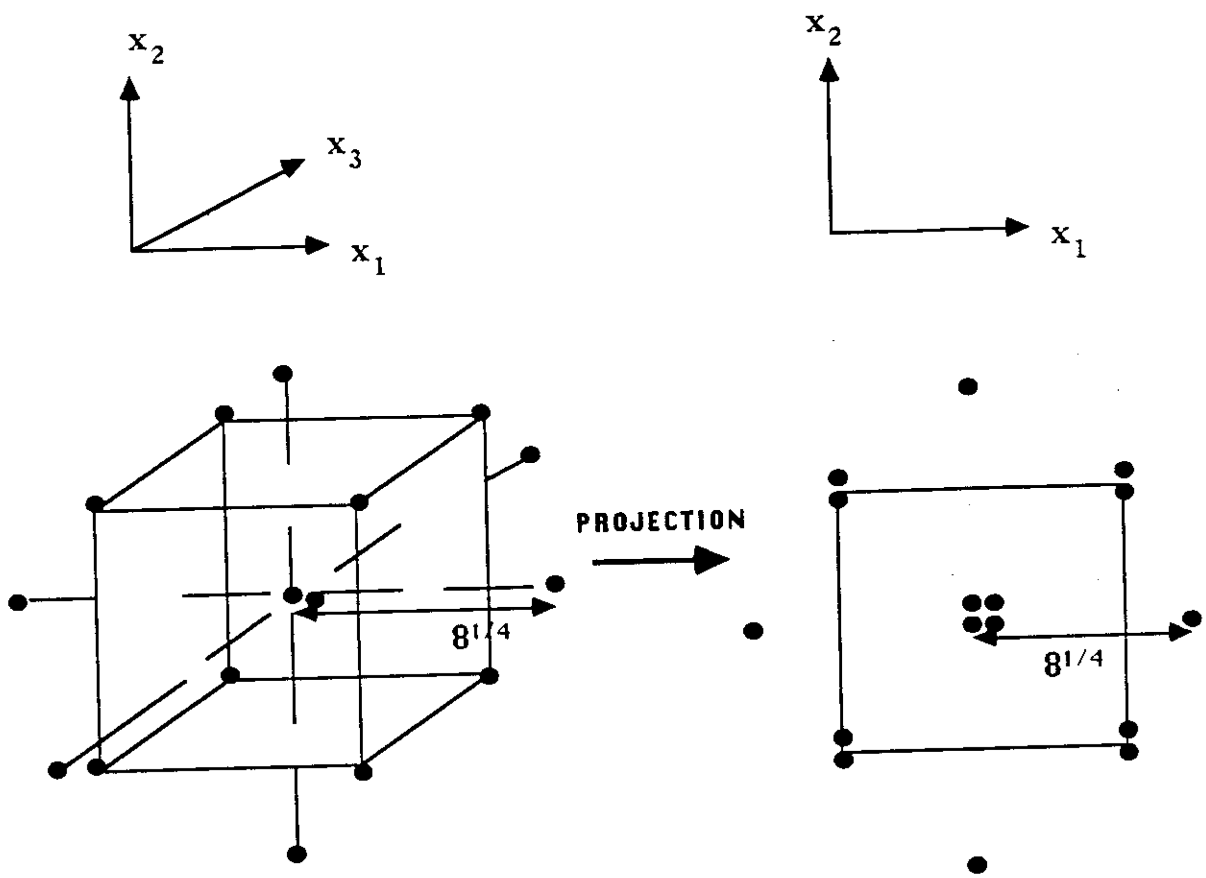

Figure 5.1: The Three-Factor Composite Design and its Projection

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