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Constrained Experimental Designs
Part II: Analysis of Projection Designs

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Constrained Experimental Designs
Part II: Analysis of Projection Designs

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ABSTRACT

In this report, we discuss the analysis of projection designs proposed in the Center for Quality and Productivity Improvement Report Series #53. We show that analyzing projection designs is essentially the same as analyzing some traditional unconstrained designs such as factorial designs and composite designs.

KEYWORDS: Projection design, constrained design, mixture design, first-order design, second-order design

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Chapter 3

Analyses of the Projection Designs

3.1 Introduction

Let y denote the response and ξ_1, ξ_2, ξ_3 denote the proportions of the three constituents in a mixture. Suppose we want to fit the following planar model:

$$y = \gamma_o + \gamma_1\xi_1 + \gamma_2\xi_2 + \gamma_3\xi_3 + \varepsilon \tag{3.1}$$

Here ε is the error term which is assumed to be i.i.d. and has mean zero and common variance σ^2. Since ξ_1, ξ_2 and ξ_3 are proportions, they are subject to the following constraints:

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

Because of the constraint $\xi_1 + \xi_2 + \xi_3 = 1$, the representation (3.1) is not unique. In other words, different sets of γ's can give the same response surface. In the estimation context, the problem is that the design matrix is singular. To be precise, let D_ξ be the $n \times 4$ design matrix consisting of the column of 1's, ξ_1, ξ_2 and ξ_3. Also let $\mathbf{y}$ be the $n \times 1$ vector of observations at the design points. Then the least-squares estimator $\hat{\gamma} = (\hat{\gamma}_o, \hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3)^t$ is the solution of the following normal equation:

$$D_\xi^t D_\xi \gamma = D_\xi^t \mathbf{y}$$

If D_ξ were nonsingular, then

$$\hat{\gamma} = (D_\xi^t D_\xi)^{-1} D_\xi^t \mathbf{y}$$

When the design variables are subject to some constraints, D_ξ is singular and therefore the inverse of $D_\xi^t D_\xi$ does not exist. There are several standard methods to deal with this problem. The first method is to use the generalized inverse of $D_\xi^t D_\xi$. The second method is to add extra constraints to make D_ξ nonsingular. The last method is to find a parameterization of the model so that the resulting design matrix is nonsingular. The last method is commonly used in the context of mixture designs. See e.g. Cornell (1981). For example, the model (3.1) can be written as:

$$\begin{aligned} E(y) &= \gamma_o + \gamma_1\xi_1 + \gamma_2\xi_2 + \gamma_3\xi_3 \\ &= \gamma_o(\xi_1 + \xi_2 + \xi_3) + \gamma_1\xi_1 + \gamma_2\xi_2 + \gamma_3\xi_3 \\ &= (\gamma_o + \gamma_1)\xi_1 + (\gamma_o + \gamma_2)\xi_2 + (\gamma_o + \gamma_3)\xi_3 \end{aligned}$$

Letting $\gamma_i^* = \gamma_o + \gamma_i$:

$$E(y) = \gamma_1^*\xi_1 + \gamma_2^*\xi_2 + \gamma_3^*\xi_3 \tag{3.2}$$

For the parameterization (3.2), the corresponding design matrix will be nonsingular. For a review of the three methods mentioned above, see Seber (1977) and Cornell (1981).

In the context of constrained designs, the three methods mentioned above have the disadvantages discussed below. The method of generalized inverse involves quite complicated computations. The variance of the estimates has a complex form and therefore is difficult to study. In the second method, the suitable extra constraints are not readily found. For the last method, different parameterizations have to be considered for different forms of constraints. Therefore, the computation and the study of the variance properties are difficult.

In this chapter, we will propose a method of analyzing the projection designs. The idea is to link the design and the response surface in the constrained space with a standard design in the unconstrained space. To illustrate the idea, let us consider a simple example. Suppose we are considering a relationship between an average response $E(y) = \eta$ and the levels of two variables x_1, x_2 in the constrained design space defined by:

$$x_1 + x_2 = 0, \text{ and } -1 \leq x_1, x_2 \leq 1.$$

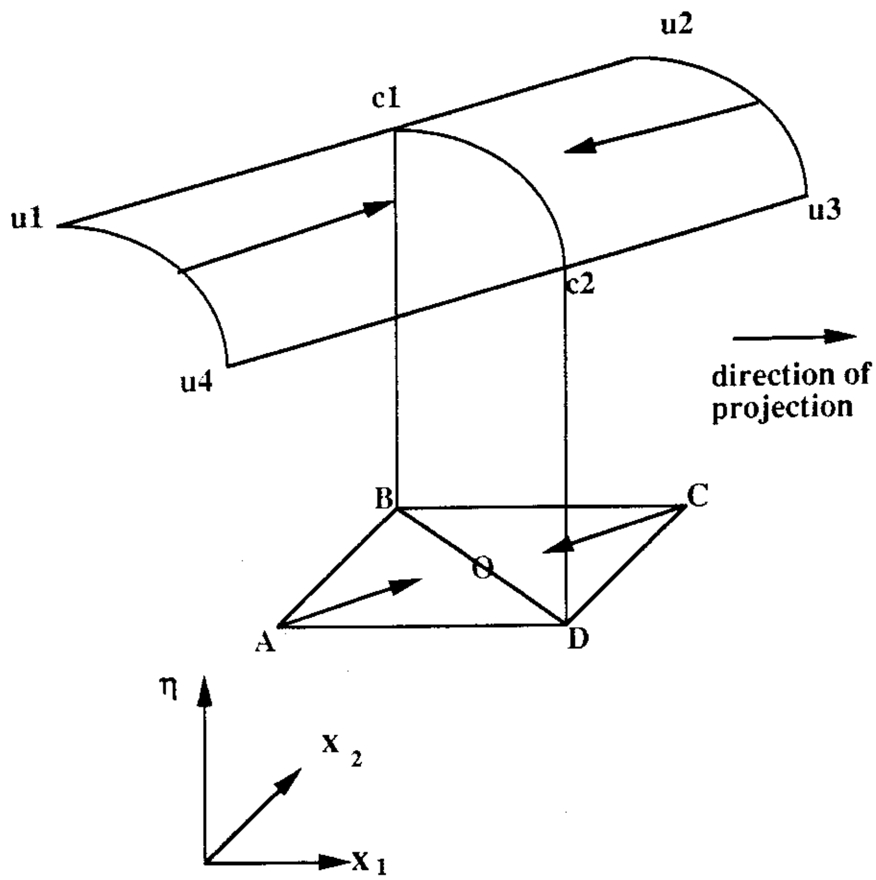

Figure 3.1: Link between a unconstrained design and its projection design

In Figure 3.1, the line segment which passes through B,O and D defines the constrained design space. The 2^2 projected factorial (PF) design consists of one point at B, one point at D and 2 points at O. This design is the projection of the 2^2 design, which consists of four points A,B,C and D. The arrows indicate the direction of the projection. We are now interested in the response surface c_1c_2 over the constrained space BOD. To transform the problem to the unconstrained space, we can imagine that we could run experiments over the unconstrained space but all the information is contained in the constrained space. To do this we can assume that the response surface is a cylinder over the unconstrained region as shown in Figure 3.1. The cylinder $u_1u_2u_3u_4$ has the same values along the direction of projection. Now the two problems are equivalent in the sense that if we know the cylinder then we know c_1c_2, and if we know c_1c_2 then we know the cylinder. Now we can treat the problem as if there were no constraints on the design variables but the response surface were a cylinder.

A cylindrical response surface can be represented by a response surface model in which the coefficients are subject to constraints. To estimate this cylinder over ABCD, the appropriate estimation method is the restricted least-squares (see e.g. Seber (1977)). If we perform ordinary least-squares estimation instead, the corresponding fitted response surface over ABCD would be different from that estimated from the restricted least-squares method. We shall show that this difference is very small and in some cases zero over the constrained space BOD, and that to an adequate approximation, the projection design can be analyzed by ordinary least-squares method as if the data came from the unconstrained design.

3.2 Model and Estimation

We need the following notation to begin with:

$\mathbf{y}$:	$n \times 1$ vector of observations;
D_z :	$n \times k$ full rank design matrix in variables z_i
R :	$r \times k$ full rank matrix of constraints
D_x :	$n \times k$ design matrix in variable x_i

Let $P_z = I - R^t(RR^t)^{-1}R$, $D_x = D_zP_z$. It is easy to verify that $D_xR^t = \mathbf{0}$. Therefore, D_x is of rank k-r.

Suppose we are interested in fitting the observational model:

$$\mathbf{y} = D_x\gamma + \varepsilon \tag{3.3}$$

$$\text{subject to: } D_x R^t = \mathbf{0} \tag{3.4}$$

Here γ is a k $\times$ 1 vector of coefficients and ε is a vector of random errors with $E(\varepsilon) = \mathbf{0}$ and $\mathrm{var}(\varepsilon) = \sigma^2 I$. Since D_x has rank k-r, we run into the problem that the design matrix is less than full rank. To get around this problem, we can express the model in terms of D_z:

$$\begin{aligned} E(\mathbf{y}) &= D_x\gamma \\ &= D_z P_z \gamma \\ &= D_z \gamma^* \end{aligned}$$

Since $\gamma^* = P_z\gamma$, γ^* are subject to the constraints $R\gamma^* = \mathbf{0}$. Strictly speaking, γ^* should be estimated by the restricted least-squares estimators $\hat{\gamma}_R$:

$$\hat{\gamma}_R = \hat{\gamma} - (D_z^t D_z)^{-1} R^t (R(D_z^t D_z)^{-1} R^t)^{-1} R\hat{\gamma}$$

where $\hat{\gamma}$ is the ordinary least-squares estimators:

$$\hat{\gamma} = (D_z^t D_z)^{-1} D_z^t \mathbf{y}$$

However, the difference between $\hat{\gamma}_R$ and $\hat{\gamma}$ is small in the following sense. Let:

$$\begin{aligned} RSS &= (\mathbf{y} - D_z\hat{\gamma})^t(\mathbf{y} - D_z\hat{\gamma}) \\ RSS_R &= (\mathbf{y} - D_z\hat{\gamma}_R)^t(\mathbf{y} - D_z\hat{\gamma}_R) \\ S_R^2 &= (RSS_R - RSS)/r \\ S^2 &= RSS/(n-k) \end{aligned}$$

When $A\gamma^* = \mathbf{0}$ by the standard theory in hypothesis testing for linear models (See e.g. Seber (1977), Chapter 4), we have:

$$\begin{aligned} E(S_R^2) &= \sigma^2 \\ E(S^2) &= \sigma^2 \end{aligned}$$

Define

$$F = \frac{S_R^2}{S^2}$$

then F has F-distribution and:

$$E(F) = 1$$

Therefore when $R\gamma^* = \mathbf{0}$, $\hat{\gamma}_R$ and $\hat{\gamma}$ are close in the sense that the difference of the resulting residual sum of squares $RSS_R - RSS$ is due to the random errors, that is, $S_R^2 \simeq \sigma^2$ or $F \simeq 1$.

In the following sections, we will show the estimations for the first and second order model fit into the above general theory.

3.2.1 Fitting First-Order Model

Recall $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t$ is a coded projection design point that satisfies $A\mathbf{x} = \mathbf{0}$, where A is an m $\times$ q matrix of constraints. This point is obtained by projecting an appropriate unconstrained design point $\mathbf{z} = (z_1, z_2, \ldots, z_q)^t$, i.e., $\mathbf{x} = P\mathbf{z}$ where $P = I - A^t(AA^t)^{-1}A$.

Suppose we are interested in fitting the first order model for the q-factor projection design:

$$\begin{aligned} \eta &= \gamma_o + \gamma_1 x_1 + \gamma_2 x_2 + \ldots + \gamma_q x_q \\ &= (1, \mathbf{x}^t)\gamma \end{aligned}$$

Here $\gamma = (\gamma_o, \gamma_1, \gamma_2, \ldots, \gamma_q)^t$.

Let D_z be the n $\times$ (q+1) matrix of the n unconstrained design points augmented by adding a column of 1's in the first column. The matrix D_x is similarly defined except that the projection design points $\mathbf{x}$ are used. These two matrices are related by a projection:

$$D_x = D_z P_z$$

where

$$P_z = \begin{pmatrix} 1 & \cdot \\ \cdot & P \end{pmatrix}$$

Here the dot . means a block of zeros with appropriate dimensions. Since P is a projection, it is easy to verify that P_z is also a projection. The matrix D_x is subject to the constraints $D_x R^t = \mathbf{0}$, where R is the matrix A augmented by adding a column of 0's in the first column. Then the first-order observational model is:

$$E(\mathbf{y}) = D_x\gamma \tag{3.5}$$

Or writing $\gamma^* = P_z\gamma$, (3.5) can be written as:

$$E(\mathbf{y}) = D_z\gamma^* \tag{3.6}$$

subject to the constraints $R\gamma^* = \mathbf{0}$.

We are going to show that:

If D_z is an orthogonal design, that is, $D_z^tD_z = nI$, then the least-squares estimators in the constrained space of γ are $\hat{\gamma} = (D_z^tD_z)^{-1}D_z\mathbf{y}$.

In fact, the restricted least-squares estimators $\hat{\gamma}_R$ in model (3.6) are (see Seber(1977) p.85):

$$\hat{\gamma}_R = \hat{\gamma} - (D_z^tD_z)^{-1}R^t(R(D_z^tD_z)^{-1}R^t)^{-1}(R\hat{\gamma}) \tag{3.7}$$

But $D_z^tD_z = nI$, therefore:

$$\hat{\gamma}_R = (I - R^t(RR^t)^{-1}R)\hat{\gamma} = P_z\hat{\gamma}$$

Therefore, the fitted model is:

$$\hat{\mathbf{y}} = D_zP_z\hat{\gamma}$$

Recall that $D_zP_z = D_x$, therefore the fitted model is exactly:

$$\hat{\mathbf{y}} = D_x\hat{\gamma}$$

Therefore in the constrained space, the restricted least-squares estimators $\hat{\gamma}_R$ is **exactly** the same as the ordinary least-squares estimators $\hat{\gamma}$ if an orthogonal unconstrained design D_z is projected.

Also under the usual assumptions that the model is an adequate representation, and that the errors of the observations are independent and have constant variance σ^2, the covariance matrix of $\hat{\gamma}$ is:

$$\mathrm{var}(\hat{\gamma}) = \sigma^2(D_z^tD_z)^{-1} = \frac{\sigma^2}{n}I$$

Therefore,

$$\begin{aligned} \text{var}(\hat{\mathbf{y}}) &= \text{var}(D_x\hat{\gamma}\ ) \\ &= \tfrac{\sigma^2}{n} D_x D_x^t \\ &= \tfrac{\sigma^2}{n} D_z P_z D_z^t \end{aligned}$$

Recall that m is the number of constraints, n is the number of observations and $q+1$ is the number of parameters needed to be estimated. The analysis of variance is summarized in Table 3.1:

Source	Sum of Squares	d.f.	Exp. Mean Square
Due to γ_o	ny^2	1	
Linear Effects	$n\hat{\gamma}\ ^tP\hat{\gamma}$	$q-m$	$\sigma^2 + \frac{n}{q-m}\gamma\ ^tP\gamma$
Residual	$\sum_1^n (y-\hat{y})^2$	$n-1-q+m$	σ^2
Total	$\sum_1^n y^2$	n	

Table 3.1: Analysis of Variance for First Order Projection Designs.

An Example

Suppose we want to make a blended gasoline from 5 gasoline stocks A,B,C,D and E. The design variables $\xi_1, \xi_2, \xi_3, \xi_4$ and ξ_5 are the proportions of the different stocks respectively and that the response of interest is miles per gallon (MPG). Suppose further that in order that engine tests can be performed under experimental conditions, all experiments are required to have a certain fixed octane number $T_o = 79$. The octane number T is, to an adequate approximation, a linear function of the proportions of the different stocks:

$$T = 20\xi_1 + 40\xi_2 + 100\xi_3 + 70\xi_4 + 50\xi_5$$

Then the design variables have to satisfy the following two constraints:

$$\begin{cases} \xi_1 + \xi_2 + \xi_3 + \xi_4 + \xi_5 &= 1 \\ 20\xi_1 + 40\xi_2 + 100\xi_3 + 70\xi_4 + 50\xi_5 &= 79 \end{cases} \tag{3.8}$$

Suppose we wish to experiment around a standard mixture of 5% A, 5% B, 50% C, 30% D and 10% E. Thus the center of the design is at $c^t = (c_1, c_2, c_3, c_4, c_5) = (5\%, 5\%, 50\%, 30\%, 10\%)$. Suppose further that the region of interest specified by the experimenter is $c_i \pm r_i$, where:

$$r_1 = 2\%, \quad r_2 = 2\%, \quad r_3 = 10\%, \quad r_4 = 5\%, \quad r_5 = 4\%$$

Then, the scaled variables:

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

must satisfy the constraints:

$$\begin{cases} 0.02x_1 + 0.02x_2 + 0.1x_3 + 0.05x_4 + 0.04x_5 & = 0 \\ (0.02)20x_1 + (0.02)40x_2 + (0.1)100x_3 + (0.05)70x_4 + (0.04)50x_5 & = 0 \end{cases}$$

Recall that α is the size parameter and its value will be computed later. When simplified, the constraints become:

$$\begin{cases} 2x_1 + 2x_2 + 10x_3 + 5x_4 + 4x_5 & = 0 \\ 4x_1 + 8x_2 + 100x_3 + 35x_4 + 20x_5 & = 0 \end{cases} \tag{3.9}$$

Now if there were no constraints, the following 2^{5-1} design might be employed:

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

To obtain the projection design which satisfies the constraints (3.9), we regress each row of Z onto the two constraint vectors and take residuals. Using the notation in Chapter 2, the matrix of constraints is A, where:

$$A = \begin{pmatrix} 2 & 2 & 10 & 5 & 4 \\ 4 & 8 & 100 & 35 & 20 \end{pmatrix}$$

The projection matrix is $P = I - A^t(AA^t)^{-1}A$. Then the projection design X in the scaled variables is:

$$
\begin{aligned}
100X &= 100ZP \\
&= \begin{pmatrix}
-76.68 & -77.65 & -2.76 & -47.75 & 143.74 \\
132.93 & -69.33 & 19.53 & -31.78 & -40.91 \\
-52.57 & 140.77 & 3.93 & -23.05 & -25.12 \\
31.59 & 55.22 & 30.66 & -123.31 & 34.08 \\
10.56 & -21.80 & 5.57 & -25.86 & 24.03 \\
94.71 & -107.35 & 32.30 & -126.12 & 83.23 \\
-90.78 & 102.75 & 16.69 & -117.39 & 99.02 \\
118.82 & 111.06 & 38.99 & -101.42 & -85.63 \\
-56.09 & -64.13 & -41.20 & 159.54 & -36.30 \\
28.06 & -149.68 & -14.48 & 59.28 & 22.90 \\
-157.44 & 60.42 & -30.08 & 68.01 & 38.69 \\
52.17 & 68.74 & -7.79 & 83.98 & -145.96 \\
-94.31 & -102.16 & -28.44 & 65.20 & 87.85 \\
115.29 & -93.84 & -6.15 & 81.17 & -96.81 \\
-70.20 & 116.26 & -21.75 & 89.89 & -81.01 \\
13.95 & 30.71 & 4.98 & -10.37 & -21.81
\end{pmatrix}
\end{aligned}
$$

In the matrix X, the largest number is 1.5954. Thus, in order for the design to lie just inside the region of interest, the size parameter should be $\alpha = 1/1.5954 = 0.63$. The projection design in the original variables $\xi_i = \alpha r_i x_i + c_i$ is shown in Table 3.2.

Again, the ranges of the variables in the design are not exactly the same as those given by the experimenter. In particular, for the reasons already discussed in Section 1.5, the range of ξ_3 in the design is quite different from what is given initially. Suppose with better understanding of the constrained space, the experimenter ran the design and and obtained the 16 responses y_i shown in the last column of Table 3.2.

run #	$100\xi_1$	$100\xi_2$	$100\xi_3$	$100\xi_4$	$100\xi_5$	y_i
1	4.04	4.03	49.83	28.50	13.60	50.6
2	6.67	4.13	51.22	29.00	8.97	49.8
3	4.34	6.76	50.25	29.28	9.37	34.8
4	5.40	5.69	51.92	26.14	10.85	44.6
5	5.13	4.73	50.35	29.19	10.60	41.1
6	6.19	3.65	52.02	26.05	12.09	55.5
7	3.86	6.29	51.05	26.32	12.48	40.8
8	6.49	6.39	52.44	26.82	7.85	45.3
9	4.30	4.20	47.42	35.00	9.09	34.7
10	5.35	3.12	49.09	31.86	10.57	45.9
11	3.03	5.76	48.11	32.13	10.97	32.6
12	5.65	5.86	49.51	32.63	6.34	33.5
13	3.82	3.72	48.22	32.04	12.02	41.4
14	6.45	3.82	49.61	32.54	7.57	40.5
15	4.12	6.46	48.64	32.82	7.97	25.3
16	5.17	5.39	50.31	29.68	9.45	40.8

Table 3.2 The Projection Design for the Gasoline Example

To fit the first-order model:

$$\hat{y} = \hat{\gamma}_o + \hat{\gamma}_1 x_1 + \hat{\gamma}_2 x_2 + \hat{\gamma}_3 x_3 + \hat{\gamma}_4 x_4 + \hat{\gamma}_5 x_5$$

we can analyze now the data as if the responses y_i in Table 3.2 came from the original 2^{5-1} design. The estimates $\hat{\gamma}_i$ are thus obtained simply from the sums of products of the response vector with the appropriate columns in the 2^{5-1} design. For example:

$$\begin{aligned} \hat{\gamma}_o &= \bar{y} = 41.08 \\ \hat{\gamma}_2 &= \tfrac{1}{16}(-y_1 - y_2 + y_3 + y_4 - y_5 - y_6 + y_7 + y_8 \\ &\quad -y_9 - y_{10} + y_{11} + y_{12} - y_{13} - y_{14} + y_{15} + y_{16}) \\ &= -3.87 \end{aligned}$$

and the fitted equation in terms of the scaled variables x_i is:

$$\hat{y} = 41.08 + 3.42x_1 - 3.87x_2 + 0.26x_3 - 4.24x_4 + 2.95x_5$$

Using the relationship :

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

we can express the fitted equation in terms of the original variables ξ_i's:

$$\hat{y} = 69.47 + 271.43\xi_1 - 307.14\xi_2 + 4.13\xi_3 - 134.6\xi_4 + 117.06\xi_5$$

subject to the constraints (3.8).

As we have seen in Table 3.2, the levels of the constrained variables ξ_i's are quite "irregular" numbers. Furthermore, the columns of the designs are linearly dependent. If we analyze the design in terms of ξ_i's, the computations would have been difficult. It is very interesting that we can get around these difficulties and estimate the coefficients as if the design were the 2^{5-1} design.

3.2.2 Fitting a Second-Order Model

Recall that $\mathbf{z} = (z_1, z_2, \ldots, z_q)^t$ are the unconstrained design variables, A is an $m \times q$ matrix of constraints, and $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t$ are the scaled constrained design variables obtained by:

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

where $P = I - A^t(AA')^{-1}A$.

Suppose we are interested in fitting the second-order model:

$$\eta = \gamma_o + \sum_{i=1}^{q} \gamma_i x_i + \sum_{i=1}^{q} \gamma_{ii} x_i^2 + \sum_{i<j} \gamma_{ij} x_i x_j \tag{3.10}$$

$$\text{subject to: } A\mathbf{x} = \mathbf{0}$$

Let $\mathbf{y}$ be the vector of responses observed at the design points, D_z and D_x be the design matrix in z's and x's corresponding to the second-order model (3.10). That is, the design matrix D_z is formed by the columns of $1, z_1, \ldots, z_q, z_1^2, \ldots, z_q^2, z_1 z_2, \ldots, z_{q-1} z_q$. Similarly, the design matrix D_x is formed by the columns of $1, x_1, \ldots, x_q, x_1^2, \ldots, x_q^2, x_1 x_2, \ldots, x_{q-1} x_q$. We shall show that there is a projection matrix P_z such that:

$$D_x = D_z P_z \tag{3.11}$$

To see that, we need the properties of derived power and Schläflian matrix. See Aitken (1948), Aitken (1949) and Box and Hunter (1957) for more details. Some review and the proof of (3.11) are included in Appendix 3.A.

Since there is a projection P_z such that $D_x = D_z P_z$, as discussed in Section 3.1,γ can, to an adequate approximation, be estimated by $\hat{\gamma} = (D_z^t D_z)^{-1} D_z^t y$, which are the least-squares estimates as if the data came from the unconstrained design. The analysis of variance can be done by the standard regression technique. In the following example, we demonstrate numerically how close the approximate least-squares estimates and the exact least-squares estimates are.

An Example

Let us look at the cake example discussed in Section 2.3. Recall that the constraints are:

$$\begin{cases} \xi_1 + \xi_2 + \xi_3 + \xi_4 = 100 \\ 2\xi_1 + \xi_2 + \xi_3 = 130 \end{cases}$$

The composite design Z is projected onto the constrained space. The projection design and the responses are shown in Table 3.3.

	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	y
1	−1	−1	−1	−1	0	0	0	0	40	20	30	10	89
2	1	−1	−1	−1	1/2	−1/2	−1/2	1/2	42	18	28	12	74
3	−1	1	−1	−1	−1/2	3/2	−1/2	−1/2	38	26	28	8	28
4	1	1	−1	−1	0	1	−1	0	40	24	26	10	54
5	−1	−1	1	−1	−1/2	−1/2	3/2	−1/2	38	18	36	8	77
6	1	−1	1	−1	0	−1	1	0	40	16	34	10	59
7	−1	1	1	−1	−1	1	1	−1	36	24	34	6	28
8	1	1	1	−1	−1/2	1/2	1/2	−1/2	38	22	32	8	76
9	−1	−1	−1	1	1/2	−1/2	−1/2	1/2	42	18	28	12	75
10	1	−1	−1	1	1	−1	−1	1	44	16	26	14	25
11	−1	1	−1	1	0	1	−1	0	40	24	26	10	53
12	1	1	−1	1	1/2	1/2	−3/2	1/2	42	22	24	12	58
13	−1	−1	1	1	0	−1	1	0	40	16	34	10	63
14	1	−1	1	1	1/2	−3/2	1/2	1/2	42	14	32	12	27
15	−1	1	1	1	−1/2	1/2	1/2	−1/2	38	22	32	8	75
16	1	1	1	1	0	0	0	0	40	20	30	10	90
17	2	0	0	0	1/2	−1/2	−1/2	1/2	42	18	28	12	73
18	−2	0	0	0	−1/2	1/2	1/2	−1/2	38	22	32	8	75
19	0	2	0	0	−1/2	3/2	−1/2	−1/2	38	26	28	8	29
20	0	−2	0	0	1/2	−3/2	1/2	1/2	42	14	32	12	27
21	0	0	2	0	−1/2	−1/2	3/2	−1/2	38	18	36	8	78
22	0	0	−2	0	1/2	1/2	−3/2	1/2	42	22	24	12	57
23	0	0	0	2	1/2	−1/2	−1/2	1/2	42	18	28	12	75
24	0	0	0	−2	−1/2	1/2	1/2	−1/2	38	22	32	8	77
25	0	0	0	0	0	0	0	0	40	20	30	10	88

Table 3.3: The Design and the Responses for the Cake Example

Suppose we are interested in fitting the second-order model:

$$\begin{aligned}\eta \;=\;& \gamma_o + \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 + \gamma_4 x_4 + \gamma_{11} x_1^2 + \gamma_{22} x_2^2 + \\ & \gamma_{33} x_3^2 + \gamma_{44} x_4^2 + \gamma_{12} x_1 x_2 + \gamma_{13} x_1 x_3 + \gamma_{14} x_1 x_4 + \\ & \gamma_{23} x_2 x_3 + \gamma_{24} x_2 x_4 + \gamma_{34} x_3 x_4\end{aligned} \tag{3.12}$$

We have shown that the coefficients in (3.12) can be estimated as if the responses came from the composite design Z. The design matrix D_z is formed by the columns of 1, $z_1, z_2, z_3, z_4, z_1^2, z_2^2, z_3^2, z_4^2, z_1z_2, z_1z_3, z_1z_4, z_2z_3, z_2z_4$ and z_3z_4, where z_1 to z_4 are shown in Table 3.3. Let the estimates of the coefficients be $\hat{\gamma}$, where:

$$\hat{\gamma}^{\,t} = (\hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3, \hat{\gamma}_4, \hat{\gamma}_1^2, \hat{\gamma}_2^2, \hat{\gamma}_3^2, \hat{\gamma}_4^2, \hat{\gamma}_{12}, \hat{\gamma}_{13}, \hat{\gamma}_{14}, \hat{\gamma}_{23}, \hat{\gamma}_{24}, \hat{\gamma}_{34})$$

As discussed before, the approximate least-squares estimates $\hat{\gamma}$ are:

$$\hat{\gamma} = (D_z^tD_z)^{-1}D_z^t\mathbf{y}$$

As a result, the fitted equation is:

$$\begin{aligned} \hat{y} = {} & 88.00 - 1.20x_1 - 0.96x_2 + 3.38x_3 - 0.96x_4 - \\ & 3.82x_1^2 - 15.32x_2^2 - 5.45x_3^2 - 3.32x_4^2 + 13.31x_1x_2 + \\ & 2.69x_1x_3 - 6.69x_1x_4 + 7.06x_2x_3 + 12.44x_2x_4 + 3.06x_3x_4 \end{aligned} \quad (3.13)$$

subject to the constraints:

$$\begin{cases} x_1 + x_2 + x_3 + x_4 = 0 \\ 2x_1 + x_2 + x_3 = 0 \end{cases}$$

The contour of the fitted surface is shown in Figure 3.2.

To compare the approximate least-squares estimates in (3.13) with the exact least-squares estimates, let us express the model (3.12) in terms of design variables which are linearly independent. From the constraints, we have:

$$\begin{aligned} x_3 &= -(2x_1 + x_2) \\ x_4 &= x_1 \end{aligned} \quad (3.14)$$

Substituting (3.14) into (3.12), we obtain a model in terms of the linearly independent variables x_1 and x_2 as follows:

$$\eta = \beta_o + \beta_1x_1 + \beta_2x_2 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{12}x_1x_2 \quad (3.15)$$

where:

$$\begin{aligned} \beta_o &= \gamma_o \\ \beta_1 &= \gamma_1 - 2\gamma_3 + \gamma_4 \\ \beta_2 &= \gamma_2 - \gamma_3 \\ \beta_{11} &= \gamma_{11} + 4\gamma_{33} + \gamma_{44} - 2\gamma_{13} + \gamma_{14} - \gamma_{34} \\ \beta_{22} &= \gamma_{22} + \gamma_{33} - \gamma_{23} \\ \beta_{12} &= 4\gamma_{33} + \gamma_{12} - \gamma_{13} - 2\gamma_{23} + \gamma_{24} - \gamma_{34} \end{aligned}$$

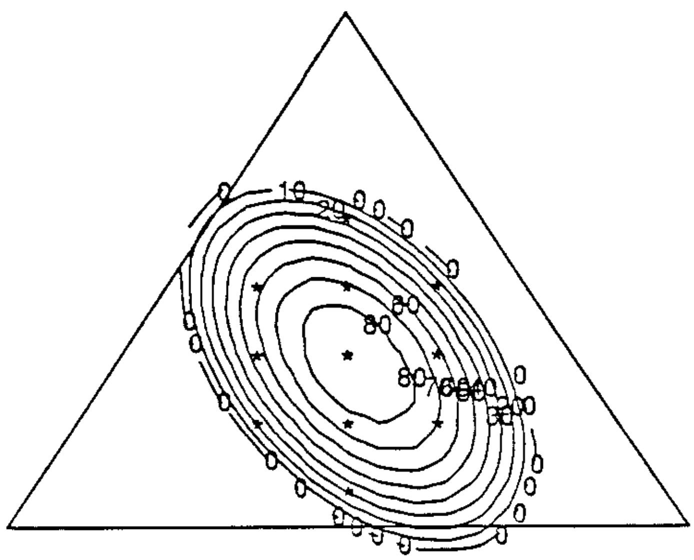

Figure 3.2: Contour of the Fitted Surface in the Cake Example

Substituting the estimates γ in (3.13), we obtain the fitted equation with the approximate least-squares estimates as follows:

$$\hat{y} = 88.0 - 8.92x_1 - 4.34x_2 - 47.13x_1^2 - 27.86x_2^2 - 15.91x_1x_2 \qquad (3.16)$$

The mean residual sum of squares s_1 from the fitted equation (3.16) is

$$s_1 = \sqrt{\frac{\text{RSS}}{df}} = 3.60$$

where RSS is the residual sum of squares and df is the degree of freedom (which is $25 - 6 = 19$ in this example).

If we use the exact least-squares procedure to fit the model (3.15) directly, the fitted equation is:

$$\hat{y} = 88.0 - 8.92x_1 - 4.33x_2 - 48.92x_1^2 - 28.43x_2^2 - 17.11x_1x_2 \qquad (3.17)$$

and the mean residual sum of squares s_2 from (3.17) is:

$$s_1 = \sqrt{\frac{\text{RSS}}{df}} = 3.48$$

As we can see in this example, the approximate least-squares estimates and the the exact least-squares estimates are very close.

3.3 Economical Second-Order Projection Designs

In the previous sections, we have seen that if we need a dth (d=1,2) order constrained design, we can begin with a dth order unconstrained design and project it onto the constrained space. We have shown that certain properties of the unconstrained design are preserved in the constrained design after the projection. For example: analyzing first order constrained designs is exactly the same as analyzing the original unconstrained designs if first order orthogonal designs are projected; analyzing second order projection designs is, to an adequate approximation, the same as analyzing the original second order unconstrained designs; the constrained designs can be fractionated and blocked in the same way as the unconstrained designs.

However, we may not need to project a full second order unconstrained design to get a full second order constrained design. In fact, we can construct more economical constrained designs by projecting resolution V factorial designs onto the constrained space. This is because when the coded design variables $\mathbf{x}$ are constrained by $A\mathbf{x} = \mathbf{0}$, we do not need all the terms in the full second order model (3.12) to describe a full second order surface in the constrained space. For example, suppose there are three variables x_1, x_2 and x_3 and they are constrained by $x_1 + x_2 + x_3 = 0$. The full second order model has the following form:

$$\begin{aligned} \eta &= \gamma_o + \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 + \gamma_{12} x_1 x_2 + \gamma_{13} x_1 x_3 + \gamma_{23} x_2 x_3 \\ &\quad + \gamma_{11} x_1^2 + \gamma_{22} x_2^2 + \gamma_{33} x_3^2 \end{aligned} \tag{3.18}$$

Since $x_1 + x_2 + x_3 = 0$, we have:

$$\begin{aligned} x_1 &= -(x_2 + x_3) \\ x_2 &= -(x_1 + x_3) \\ x_3 &= -(x_1 + x_2) \end{aligned}$$

Therefore,

$$x_1^2 = -x_1(x_2 + x_3) = -x_1 x_2 - x_1 x_3$$

Hence the model (3.18) can be written in the following **canonical** form:

$$\eta = \gamma_o + \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 + \gamma_{12}^* x_1 x_2 + \gamma_{13}^* x_1 x_3 + \gamma_{23}^* x_2 x_3$$

where:

$$\begin{aligned} \gamma_{12}^* &= \gamma_{12} - \gamma_{11} - \gamma_{22} \\ \gamma_{13}^* &= \gamma_{13} - \gamma_{11} - \gamma_{33} \\ \gamma_{23}^* &= \gamma_{23} - \gamma_{22} - \gamma_{33} \end{aligned}$$

In general, we can describe a second order surface in the constrained space by the canonical polynomial which includes only the "main effect" terms and the "two-factor interaction" terms. Since resolution V factorial designs can estimate all "main effects" and "two-factor" interactions, we can construct economical second order constrained designs by projecting resolution V factorial designs onto the constrained space. In this section, we consider the estimations of the second order canonical models when the 2^{q-p} designs are projected.

Recall that $\mathbf{z}^t = (z_1, z_2, \ldots, z_q)$ are the unconstrained design variables, A is an $m \times q$ matrix of constraints, $P = I - A^t(AA^t)^{-1}A$, $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t = P\mathbf{z}$ are the constrained design variables. Let

$$\begin{aligned} f(\mathbf{z}) &= (z_1 z_2, z_1 z_3, \ldots, z_{q-1} z_q)^t \\ f(\mathbf{x}) &= (x_1 x_2, x_1 x_3, \ldots, x_{q-1} x_q)^t \\ \boldsymbol{\gamma}_1 &= (\gamma_1, \gamma_2, \ldots, \gamma_q)^t \\ \boldsymbol{\gamma}_2 &= (\gamma_{12}, \gamma_{13}, \ldots, \gamma_{q-1.q})^t \end{aligned}$$

For example, when $q = 4$:

$$\begin{aligned} f(\mathbf{x}) &= (x_1 x_2, x_1 x_3, x_1 x_4, x_2 x_3, x_2 x_4, x_3 x_4)^t \\ \boldsymbol{\gamma}_2 &= (\gamma_{12}, \gamma_{13}, \gamma_{14}, \gamma_{23}, \gamma_{24}, \gamma_{34})^t \end{aligned}$$

When $\mathbf{x}$ is subject to one or more equality constraints $A\mathbf{x} = \mathbf{0}$, the following canonical polynomial can describe a full second-order surface in the constrained space:

$$\begin{cases} \eta = \gamma_o + \mathbf{x}^t \boldsymbol{\gamma}_1 + f(\mathbf{x})^t \boldsymbol{\gamma}_2 \\ \qquad \text{subject to: } A\mathbf{x} = \mathbf{0} \end{cases} \tag{3.19}$$

The canonical polynomial (3.19) is used widely in the context of mixture experiments. See e.g. Cornell (1981).

Let Z_1 be the $n \times q$ matrix of unconstrained design points consisting of the columns $z_1, z_2, \ldots, z_q$. Let Z_2 be the matrix consisting of the columns $z_1 z_2, z_1 z_3, \ldots, z_{q-1} z_q$, and $\mathbf{y} = (y_1, y_2, \ldots, y_n)^t$ be the vector of responses. Assume that the unconstrained design has the following properties:

$$\begin{cases} \mathbf{1}^t Z_1 = \mathbf{0} \\ \mathbf{1}^t Z_2 = \mathbf{0} \\ Z_1^t Z_2 = \mathbf{0} \\ Z_1^t Z_1 = nI \\ Z_2^t Z_2 = nI \end{cases} \tag{3.20}$$

For example, the 2^q and the 2^{q-p} designs have the above properties. Let:

$$\begin{cases} \hat{\beta}_o = \bar{y} \\ \hat{\boldsymbol{\beta}}_1 = (Z_1^t Z_1)^{-1} Z_1^t \mathbf{y} = \frac{1}{n} Z_1^t \mathbf{y} \\ \hat{\boldsymbol{\beta}}_2 = (Z_2^t Z_2)^{-1} Z_2^t \mathbf{y} = \frac{1}{n} Z_2^t \mathbf{y} \end{cases} \tag{3.21}$$

We shall show that the least-squares estimates $\hat{\gamma}_o, \hat{\boldsymbol{\gamma}}_1, \hat{\boldsymbol{\gamma}}_2$ of the coefficients in (3.19) are just linear transformations of $\hat{\beta}_o, \hat{\boldsymbol{\beta}}_1, \hat{\boldsymbol{\beta}}_2$ in the following forms:

$$\begin{cases} \hat{\boldsymbol{\gamma}}_1 &= \hat{\boldsymbol{\beta}}_1 \\ \hat{\boldsymbol{\gamma}}_2 &= M\hat{\boldsymbol{\beta}}_2 \\ \hat{\gamma}_o &= \hat{\beta}_o - \mathbf{a}^t\hat{\boldsymbol{\gamma}}_2 \end{cases} \tag{3.22}$$

where the matrix M and the vector $\mathbf{a}$ are to be computed. We will illustrate the estimation procedure for the model (3.19) by an example in next section. Then the method for computing M and $\mathbf{a}$ in general will be given in Section 3.3.2. The analysis of variance will be discussed in Section 3.3.3.

3.3.1 An Example: Second-Order PF Design under Mixture Constraint

Suppose that $q = 3$ and we want to run a second order PF design for a q-component mixture experiment, i.e., we want to run an experiment with q factors $\xi_1, \xi_2, \ldots, \xi_q$, where the factors are subject to the constraints:

$$\begin{cases} \xi_1 + \xi_2 + \ldots + \xi_q = 1 \\ 0 \le \xi_i \le 1 \quad i = 1, 2, \ldots, q. \end{cases}$$

Suppose we want to run the mixture experiment using the 2^3 design given in Section 2.1 and the responses are shown in Table 3.4:

Z_1			X_1			ξ			
z_1	z_2	z_3	x_1	x_2	x_3	ξ_1	ξ_2	ξ_3	y
−1	−1	−1	0	0	0	1/3	1/3	1/3	148
1	−1	−1	4/3	−2/3	−2/3	2/3	1/6	1/6	155
−1	1	−1	−2/3	4/3	−2/3	1/6	2/3	1/6	152
1	1	−1	2/3	2/3	−4/3	1/2	1/2	0	166
−1	−1	1	−2/3	−2/3	4/3	1/6	1/6	2/3	125
1	−1	1	2/3	−4/3	2/3	1/2	0	1/2	112
−1	1	1	−4/3	2/3	2/3	0	1/2	1/2	152
1	1	1	0	0	0	1/3	1/3	1/3	149

Table 3.4: The Mixture Experiment and Responses

The actual experiments are run at $(\xi_1, \xi_2, \xi_3)^t$ and their responses $\mathbf{y}$ are in the last column. Following the notation in the last section, let Z_1 be the matrix consisting of the first three columns in Table 3.4, Z_2 be the matrix consisting of the product terms (z_1z_2, z_1z_3, z_2z_3), which corresponds to the two-factor interaction terms from the 2^3 design. Then:

$$\hat{\beta}_o = \bar{y} = 144.875$$

$$\hat{\boldsymbol{\beta}}_1 = \frac{1}{n} Z_1^t y = (0.625, 9.875, -10.375)^t$$

$$\hat{\boldsymbol{\beta}}_2 = \frac{1}{n} Z_2^t y = (2.125, -4.625, 6.125)^t$$

Here, $n = 2^q = 8$ is the number of design points.

We are interested in fitting the second order canonical polynomial:

$$\begin{aligned} \eta &= \gamma_o + \mathbf{x}^t \boldsymbol{\gamma}_1 + f(\mathbf{x})^t \boldsymbol{\gamma}_2 \\ &= \gamma_o + \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 + \gamma_{12} x_1 x_2 + \gamma_{13} x_1 x_3 + \gamma_{23} x_2 x_3 \end{aligned}$$

We will show later that the least-squares estimates $\hat{\gamma}_i$ of γ_i can be computed through $\hat{\beta}_i$ as follows:

$$\begin{cases} \hat{\boldsymbol{\gamma}}_1 &= \hat{\boldsymbol{\beta}}_1 \\ \hat{\boldsymbol{\gamma}}_2 &= M \hat{\boldsymbol{\beta}}_2 \\ \hat{\gamma}_o &= \hat{\beta}_0 - \mathbf{a}^t \hat{\boldsymbol{\gamma}}_2 \end{cases}$$

where $\mathbf{a} = -(1/3, 1/3, 1/3)$ and M is:

$$M = \begin{pmatrix} 2 & 1/2 & 1/2 \\ 1/2 & 2 & 1/2 \\ 1/2 & 1/2 & 2 \end{pmatrix}$$

Therefore,

$$\hat{\boldsymbol{\gamma}}_1 = \hat{\boldsymbol{\beta}}_1 = (0.625, 9.875, -10.375)^t$$

$$\hat{\boldsymbol{\gamma}}_2 = M \hat{\boldsymbol{\beta}}_2 = (5.0, -5.125, 11.0)^t$$

$$\hat{\gamma}_o = \hat{\beta}_0 - \mathbf{a}^t \hat{\boldsymbol{\gamma}}_2 = 144.875 - (-3.625) = 148.5$$

Hence, the fitted canonical polynomial is:

$$\begin{aligned} \hat{y} = & \; 148.5 + 0.625 x_1 + 9.875 x_2 - 10.375 x_3 \\ & +5.0 x_1 x_2 - 5.125 x_1 x_3 + 11.0 x_2 x_3 \end{aligned}$$

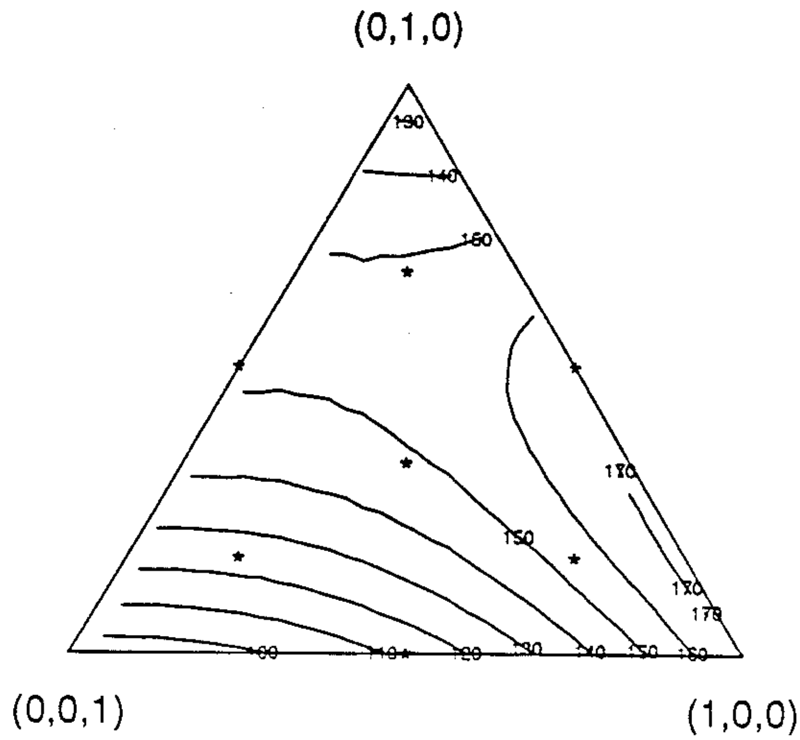

Figure 3.3: The Estimated Response Surface in the Mixture Example

The contour of the fitted response surface is shown in Figure 3.3.

For the general q-component mixture experiment, the relationships (3.22) still hold for the 2^q PF designs. We only need to determine what $\mathbf{a}$ and M are. It turns out that they can be easily generated. In fact, the vector $\mathbf{a}$ is equal to $-(1/q, 1/q, \ldots, 1/q)^t$. The method for generating M for the q-component mixture case is given in Appendix 3.B. The exact forms of M are also given for $q = 3,4,5$ and 6 as examples.

3.3.2 Estimation of Second Order Canonical Models

Recall that $\mathbf{y}$ is an $n \times 1$ vector of observations, Z_1 is an $n \times q$ matrix of unconstrained design points, Z_2 is an $n \times C_2^q$ matrix of "two-factor interaction" terms obtained from Z_1. Let

$$D_z = (\mathbf{1}, Z_1, Z_2)$$

Assume the design is chosen so that (3.20) are satisfied. The assumptions (3.20) are equivalent to:

$$(D_z^t D_z) = nI$$

Let:

$$D_x = (\mathbf{1}, X_1, Z_2)$$

Note that:

$$\begin{aligned} \mathbf{1}^t X_1 &= \mathbf{1}^t Z_1 P &= \mathbf{0} \\ \mathbf{1}^t Z_2 &= \mathbf{0} & \\ X_1^t Z_2 &= P Z_1^t Z_2 &= \mathbf{0} \end{aligned}$$

Consider the model:

$$\begin{aligned} \eta &= \beta_o + \mathbf{x}^t \boldsymbol{\beta}_1 + f(\mathbf{z})^t \boldsymbol{\beta}_2 \\ &\quad \text{subject to: } A\mathbf{x} = \mathbf{0} \end{aligned} \tag{3.23}$$

We refer to (3.23) as the **ANOVA model** and we will see why in the next section.

The least-squares estimates $\hat{\boldsymbol{\beta}}^t = (\hat{\beta}_0, \hat{\boldsymbol{\beta}}_1^t, \hat{\boldsymbol{\beta}}_2^t)$ of the coefficients in (3.23) are the solutions of the following normal equation:

$$D_x^t D_x \hat{\boldsymbol{\beta}} = D_x^t \mathbf{y} \tag{3.24}$$

We are going to show that $\hat{\boldsymbol{\beta}} = \frac{1}{n}D_z^t\mathbf{y}$ satisfies the normal equation (3.24). In fact:

$$\begin{aligned} D_x^t D_x &= \begin{pmatrix} n & \cdot & \cdot \\ \cdot & X_1^t X_1 & \cdot \\ \cdot & \cdot & Z_2^t Z_2 \end{pmatrix} \\ &= \begin{pmatrix} n & \cdot & \cdot \\ \cdot & nP & \cdot \\ \cdot & \cdot & nI \end{pmatrix} \end{aligned}$$

where the dots in the matrices are blocks of zeros with appropriate dimensions. Therefore:

$$D_x^t D_x D_z^t = n D_x^t$$

As a result:

$$\frac{1}{n} D_x^t D_x D_z^t \mathbf{y} = D_x^t \mathbf{y}$$

That is, the normal equation (3.24) is satisfied and therefore $\hat{\boldsymbol{\beta}}$ are the least-squares estimates of the coefficients in the ANOVA model (3.23).

Now we have the fitted ANOVA model:

$$\begin{aligned} \hat{y} &= \hat{\beta}_o + \mathbf{x}^t \hat{\boldsymbol{\beta}}_1 + f(\mathbf{z})^t \hat{\boldsymbol{\beta}}_2 \\ & \text{subject to: } A\mathbf{x} = \mathbf{0} \end{aligned} \tag{3.25}$$

For prediction purposes, however, it is more convenient to express the fitted surface in terms of the constrained design variables as follows:

$$\begin{aligned} \hat{y} &= \hat{\gamma}_o + \mathbf{x}^t \hat{\boldsymbol{\gamma}}_1 + f(\mathbf{x})^t \hat{\boldsymbol{\gamma}}_2 \\ & \text{subject to: } A\mathbf{x} = \mathbf{0} \end{aligned} \tag{3.26}$$

We will refer to (3.26) as the **prediction model**. Now, we need to find the transformation which relates $f(\mathbf{z})$ to $f(\mathbf{x})$. This is what we are going to do next.

Recall the projection matrix $P = I - A^t(AA^t)^{-1}A$. Denote the ijth element of P as p_{ij}. Let $\otimes$ denote the Kronecker product operator. In Appendix 3.C, a review of the Kronecker product is given. Since $\mathbf{x} = P\mathbf{z}$, we have:

$$\begin{aligned} \mathbf{x} \otimes \mathbf{x} &= P\mathbf{z} \otimes P\mathbf{z} \\ &= (P \otimes P)\mathbf{z} \otimes \mathbf{z} \end{aligned} \tag{3.27}$$

Here:

$$\begin{aligned}
\mathbf{z} \otimes \mathbf{z} &= (z_1\mathbf{z}^t, z_2\mathbf{z}^t, \ldots, z_q\mathbf{z}^t)^t \\
\mathbf{x} \otimes \mathbf{x} &= (x_1\mathbf{x}^t, x_2\mathbf{x}^t, \ldots, x_q\mathbf{x}^t)^t \\
P \otimes P &= \begin{pmatrix} p_{11}P & p_{12}P & \ldots & p_{1q}P \\ p_{21}P & p_{22}P & \ldots & p_{2q}P \\ \vdots & \vdots & \ddots & \vdots \\ p_{q1}P & p_{q2}P & \ldots & p_{qq}P \end{pmatrix}
\end{aligned}$$

From (3.27) we have:

$$x_i x_j = \sum_{k=1}^{q} \sum_{l=1}^{q} p_{ik} p_{jl} z_k z_l$$

By the choice of the design, $z_i^2 = 1$. Thus:

$$x_i x_j = \sum_{k=1}^{q} p_{ik} p_{jk} + \sum_{k<l} (p_{ik} p_{jl} + p_{il} p_{jk}) z_k z_l$$

Since P is a projection matrix, $P^2 = P$. Therefore:

$$\sum_{k=1}^{q} p_{ik} p_{jk} = p_{ij}$$

Hence we have:

$$x_i x_j = p_{ij} + \sum_{k<l} (p_{ik} p_{jl} + p_{il} p_{jk}) z_k z_l \tag{3.28}$$

From (3.28), we can write down the relationship between $f(\mathbf{z})$ and $f(\mathbf{x})$ in matrix form as follows:

$$f(\mathbf{x}) = \mathbf{a} + H f(\mathbf{z}) \tag{3.29}$$

For example, when there are three factors, i.e., $q = 3$:

$$\begin{aligned}
f(\mathbf{x}) &= (x_1x_2, x_1x_3, x_2x_3)^t \\
f(\mathbf{z}) &= (z_1z_2, z_1z_3, z_2z_3)^t \\
\mathbf{a} &= (p_{12}, p_{13}, p_{23})^t
\end{aligned}$$

$$H = \begin{pmatrix} p_{11}p_{22} + p_{12}p_{21} & p_{11}p_{23} + p_{13}p_{21} & p_{12}p_{23} + p_{13}p_{22} \\ p_{11}p_{32} + p_{12}p_{31} & p_{11}p_{33} + p_{13}p_{31} & p_{12}p_{23} + p_{13}p_{32} \\ p_{21}p_{32} + p_{22}p_{31} & p_{21}p_{33} + p_{23}p_{31} & p_{22}p_{23} + p_{23}p_{32} \end{pmatrix}$$

What we want now is to express $f(\mathbf{z})$ in terms of some transformation of $f(\mathbf{x})$. The transformation (3.29) holds for arbitrary multiple linear constraints.

When there is only one constraint, the matrix H is nonsingular. Therefore, if we let $M = H^{-1}$, then:

$$f(\mathbf{z}) = M(f(\mathbf{x}) - \mathbf{a}) \tag{3.30}$$

Since P is symmetric, so is H and hence M is also symmetric. Plugging into the fitted ANOVA model, we have:

$$\begin{aligned}
\hat{\eta} &= \hat{\beta}_o + \mathbf{x}^t\hat{\boldsymbol{\beta}}_1 + f(\mathbf{z})^t\hat{\boldsymbol{\beta}}_2 \\
&= \hat{\beta}_o + \mathbf{x}^t\hat{\boldsymbol{\beta}}_1 + (f(\mathbf{x}) - \mathbf{a})^t M\hat{\boldsymbol{\beta}}_2 \\
&= (\hat{\beta}_o - \mathbf{a}^t M\hat{\boldsymbol{\beta}}_2) + \mathbf{x}^t\hat{\boldsymbol{\beta}}_1 + f(\mathbf{x})^t M\hat{\boldsymbol{\beta}}_2
\end{aligned}$$

Therefore, the least-squares estimates in model (3.26) are:

$$\left\{\begin{aligned}
\hat{\boldsymbol{\gamma}}_1 &= \hat{\boldsymbol{\beta}}_1 \\
\hat{\boldsymbol{\gamma}}_2 &= M\hat{\boldsymbol{\beta}}_2 \\
\hat{\gamma}_o &= \hat{\beta}_o - \mathbf{a}^t\hat{\boldsymbol{\gamma}}_2
\end{aligned}\right.$$

In the q-component mixture case, the matrix $M = H^{-1}$ has a simple form which is given in Appendix 3.B. We can check that by the definition of the inverse of a matrix. When there are multiple constraints, everything is still valid except that H is singular. In that case, the matrix M is not unique. One solution is to use the generalized inverse H^- of H. Algorithms such as singular-value decomposition can be use to compute H^-. Software packages such as S can be used to calculate H^- easily. In the following, we will give two examples.

Example 1: Suppose we are running an experiment with 4 factors subject to a single equality constraint as follows:

$$x_1 - x_2 + 2x_3 - x_4 = 0$$

That is, $A = (1, -1, 2, -1)$. Then the projection matrix P:

$$\begin{aligned}
P &= I - A^t(AA^t)^{-1}A \\
&= \begin{pmatrix}
0.857 & 0.143 & -0.286 & 0.143 \\
0.143 & 0.875 & 0.286 & -0.143 \\
-0.286 & 0.286 & 0.429 & 0.286 \\
0.143 & -0.143 & 0.286 & 0.857
\end{pmatrix}
\end{aligned}$$

The H matrix is:

$$H = \begin{pmatrix} 0.755 & 0.204 & -0.102 & -0.204 & 0.102 & 0.082 \\ 0.204 & 0.449 & 0.204 & -0.020 & 0.082 & -0.020 \\ -0.102 & 0.204 & 0.755 & 0.082 & 0.102 & -0.204 \\ -0.204 & -0.020 & 0.082 & 0.449 & 0.204 & 0.020 \\ 0.102 & 0.082 & 0.102 & 0.204 & 0.755 & 0.204 \\ 0.082 & -0.020 & -0.204 & 0.020 & 0.204 & 0.449 \end{pmatrix}$$

Therefore,

$$\begin{aligned} \mathbf{a}^t &= (p_{12}, p_{13}, p_{14}, p_{23}, p_{24}, p_{34}) \\ &= (0.143, -0.286, 0.143, 0.286, -0.143, 0.286) \end{aligned}$$

And the matrix $M = H^{-1}$ is:

$$M = \begin{pmatrix} 2.0 & -1.0 & 0.5 & 1.0 & -0.5 & 0.0 \\ -1.0 & 3.125 & -1.0 & -0.125 & 0.0 & -0.125 \\ 0.5 & -1.0 & 2.0 & 0.0 & -0.5 & 1.0 \\ 1.0 & -0.125 & 0.0 & 3.125 & -1.0 & 0.125 \\ -0.5 & 0.0 & -0.5 & -1.0 & 2.0 & -1.0 \\ 0.0 & -0.125 & 1.0 & 0.125 & -1.0 & 3.125 \end{pmatrix}$$

Example 2: Let us visit the cake example again. Recall that the coded design variables in this example are constrained by:

$$\begin{aligned} x_1 + x_2 + x_3 + x_4 &= 0 \\ 2x_1 + x_2 + x_3 \quad &= 0 \end{aligned}$$

The projection matrix $P = I - A^t(AA^t)^{-1}A$ is shown in Section 2.3. Here A is the matrix of constraints. From P we can calculate H which is as follows:

$$H = \begin{pmatrix} 0.25 & 0.0 & -0.125 & -0.125 & 0.25 & 0.0 \\ 0.0 & 0.25 & -0.125 & -0.125 & 0.0 & 0.25 \\ -0.125 & -0.125 & 0.125 & 0.125 & -0.125 & -0.125 \\ -0.125 & -0.125 & 0.125 & 0.625 & -0.125 & -0.125 \\ 0.25 & 0.0 & -0.125 & -0.125 & 0.25 & 0.0 \\ 0.0 & 0.25 & -0.125 & -0.125 & 0.0 & 0.25 \end{pmatrix}$$

Therefore we have:

$$\begin{aligned}\mathbf{a}^t &= (p_{12}, p_{13}, p_{14}, p_{23}, p_{24}, p_{34}) \\ &= (-0.25, -0.25, 0.25, -0.25, -0.25, -0.25)\end{aligned}$$

and $M = H^-$ is:

$$M = \begin{pmatrix} 0.9 & -0.1 & -0.4 & 0.4 & 0.9 & -0.1 \\ -0.1 & 0.9 & -0.4 & 0.4 & -0.1 & 0.9 \\ -0.4 & -0.4 & 0.4 & -0.4 & -0.4 & -0.4 \\ 0.4 & 0.4 & -0.4 & 2.0 & 0.4 & 0.4 \\ 0.9 & -0.1 & -0.4 & 0.4 & 0.9 & -0.1 \\ -0.1 & 0.9 & -0.4 & 0.4 & -0.1 & 0.9 \end{pmatrix}$$

With $\mathbf{a}$ and M, we can compute the least-squares estimates $\hat{\gamma}$ in the prediction model:

$$\begin{cases} \hat{\boldsymbol{\gamma}}_1 &= \hat{\boldsymbol{\beta}}_1 = (-1.56, -1.69, 2.44, -1.19)^t \\ \hat{\boldsymbol{\gamma}}_2 &= M\hat{\boldsymbol{\beta}}_2 = (28.1, 8.1, -18.1, 29.4, 28.1, 8.1)^t \\ \hat{\gamma}_o &= \hat{\beta}_o - \mathbf{a}^t\hat{\boldsymbol{\gamma}}_2 = 59.43 - (-29.99) = 89.42 \end{cases}$$

Therefore the fitted canonical polynomial for the cake example is:

$$\begin{aligned}\hat{\eta} &= 89.42 - 1.56x_1 - 1.69x_2 + 2.44x_3 - 1.19x_4 + 28.1x_1x_2 + \\ &\quad 8.1x_1x_3 - 18.1x_1x_4 + 29.4x_2x_3 + 28.1x_2x_4 + 8.1x_3x_4\end{aligned} \tag{3.31}$$

3.4 Analysis of Variance for Second-Order PF Designs

When we are concerned with the predictions of the response surface, the prediction model (3.26) is more convenient than the ANOVA model (3.23) since it is tedious to compute $f(\mathbf{z})$ every time. However, if we are interested in the computations at the design points, such as the analysis of variance, the ANOVA model is easier to use because $f(\mathbf{z})$ is readily found. Recall that $D_z = (\mathbf{1}, Z_1, Z_2)$, $D_x = (\mathbf{1}, X_1, Z_2)$ and $\mathbf{y}$ is the $n \times 1$ vector of observations. The fitted ANOVA model (3.25) can be written in the following observational form:

$$\hat{\mathbf{y}} = D_x\hat{\boldsymbol{\beta}} \tag{3.32}$$

where

$$\hat{\boldsymbol{\beta}} = (\hat{\beta}_o, \hat{\boldsymbol{\beta}}_1^t, \hat{\boldsymbol{\beta}}_2^t)^t = \frac{1}{n} D_z^t \mathbf{y}.$$

Under the usual assumptions that the model is an adequate representation and that the errors of the observations are independent and have constant variance σ^2, the variance of $\hat{\boldsymbol{\beta}}$ is simply:

$$\mathrm{var}(\hat{\boldsymbol{\beta}}) = \frac{\sigma^2}{n} I$$

Since there are many choices for the coefficients that can give the same surface, the variance of $\hat{\boldsymbol{\beta}}$ may not be very interesting. We may be more interested in the variance of the fitted values. Since:

$$\hat{\mathbf{y}} = \frac{1}{n} D_x D_z^t \mathbf{y}$$

Therefore:

$$\mathrm{var}(\hat{\mathbf{y}}) = \tfrac{\sigma^2}{n} D_x D_z^t$$

Recall that n is the number of design points, q is the number of factors, m is the number of constraints. The analysis of variance is shown Table 3.5:

Source	Sum of Squares	d.f.	Exp. Mean Square
Due to β_o	$n\bar{y}$	1	
Linear Effects	$n\hat{\boldsymbol{\beta}}_1^t P \hat{\boldsymbol{\beta}}_1$	$q-m$	$\sigma^2 + \frac{n}{q-m}\boldsymbol{\beta}_1^t P \boldsymbol{\beta}_1$
Quadratic Effects	$n\hat{\boldsymbol{\beta}}_2^t \hat{\boldsymbol{\beta}}_2$	C_2^q	$\sigma^2 + \frac{n}{C_2^q}\boldsymbol{\beta}_2^t \boldsymbol{\beta}_2$
Residual	$\sum_1^n (y-\hat{y})^2$	$n-1-q+m-C_2^q$	σ^2
Total	$\sum_1^n y^2$	n	

Table 3.5 ANOVA for the 2nd-Order PF Designs

When σ^2 is unknown, it is estimated by s^2 which is the mean residual sum of squares, i.e.:

$$s^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-1-q+m-C_2^q}$$

Example 1: The ANOVA for a Second Order PF Mixture Design

Let us look at the mixture example given in Section 3.3.1. In this example, $n = 8$, $q = 3$, $m = 1$. Also:

$$
\begin{aligned}
\hat{\beta}_o &= 144.875 \\
\hat{\boldsymbol{\beta}}_1 &= (0.625, 9.875, -10.375)^t \\
\hat{\boldsymbol{\beta}}_2 &= (2.125, -4.625, 6.125)^t \\
P &= \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ -1/3 & 2/3 & -1/3 \\ -1/3 & -1/3 & 2/3 \end{pmatrix}
\end{aligned}
$$

Therefore, the ANOVA table is shown as follows:

Source	Sum of Squares	d.f.	Mean Squares	F-Value
β_o	167910.1	1		
Linear Effects	1644.3	2	822.2	1370
Quadratic Effects	507.4	3	169.1	282
Residual	1.2	2	0.6	
Total	170063	8		

Table 3.6: ANOVA for the Mixture Experiment in 3.3.1

Example 2: The ANOVA for a Second Order Design under Multiple constraints

In the cake example in Section 3.3.2, the constrained design was the 2^4 PF design. In this example, $n = 16$, $q = 4$, $m = 2$. We have seen that:

$$
\begin{aligned}
\hat{\beta}_o &= 59.44 \\
\hat{\boldsymbol{\beta}}_1 &= (-1.56, -1.69, 2.44, -1.19)^t \\
\hat{\boldsymbol{\beta}}_2 &= (13.31, 2.69, -6.69, 7.06, 12.44, 3.06)^t \\
P &= \begin{pmatrix} 1/4 & -1/4 & -1/4 & 1/4 \\ -1/4 & 3/4 & -1/4 & -1/4 \\ -1/4 & -1/4 & 3/4 & -1/4 \\ 1/4 & -1/4 & -1/4 & 1/4 \end{pmatrix}
\end{aligned}
$$

Plugging these values into Table 3.5, we have the ANOVA as follows:

Source	Sum of Squares	d.f.	Mean Squares	F-Value
Due to β_o	56525	1		
Linear Effects	185	2	92.5	5.7
Quadratic Effects	7090	6	1181.7	73.4
Residual	113	7	16.1	
Total	63913	16		

Table 3.7 ANOVA for the Cake Example

Appendix

3.A Derived Power and Schläflian Matrices

If $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t$, then its derived power of degree 2 is defined to be $\mathbf{x}^{[2]}$, where:

$$\mathbf{x}^{[2]} = (x_1^2, x_2^2, \ldots, x_q^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{q-1}x_q)^t$$

For example, when $q = 3$:

$$\begin{aligned} \mathbf{x} &= (x_1, x_2, x_3)^t \\ \mathbf{x}^{[2]} &= (x_1^2, x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3)^t \end{aligned}$$

Let $\mathbf{x} = (x_1, x_2, \ldots, x_q)^t, \mathbf{z} = (z_1, z_2, \ldots, z_q)^t$ and:

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

where P is an $q \times q$ matrix. Then the Schläflian matrix $P^{[2]}$ is defined such that:

$$\mathbf{x}^{[2]} = P^{[2]}\mathbf{z}^{[2]}$$

It is easily confirmed that:

$$(PK)^{[2]} = P^{[2]}K^{[2]}$$

where K is an another $q \times q$ matrix.

We claim the following result about Schläflian matrices:

If P is a projection, i.e. $P^t = P$ and $P^2 = P$, then so is $P^{[2]}$.

Proof: By the construction of the Schläflian matrix, it is easy to see that $P^{[2]}$ is symmetric. To see $P^{[2]}P^{[2]} = P^{[2]}$, note that $P\mathbf{x} = PP\mathbf{z} = \mathbf{x}$. Therefore:

$$\mathbf{x}^{[2]} = (Px)^{[2]} = P^{[2]}\mathbf{x}^{[2]}$$

Hence:

$$P^{[2]}\mathbf{x}^{[2]} = P^{[2]}P^{[2]}\mathbf{x}^{[2]}$$

Since $\mathbf{x}^{[2]}$ is arbitrary,

$$P^{[2]} = P^{[2]}P^{[2]}$$

Therefore $P^{[2]}$ is also a projection.

The projection P_z in (3.11) can be chosen as follows:

$$P_z = \begin{pmatrix} 1 & . & . \\ . & P & . \\ . & . & P^{[2]} \end{pmatrix}$$

It is straightforward to prove that P_z above is a projection.

3.B Generation of the matrix M in Mixture Cases

The method for generating the matrix M which transforms the factorial contrasts to the least-squares estimates $\hat{\gamma}_2$ in the constrained model is as follows. There are only three different numbers in M: 2, 1/2 and 0. To decide which entry should have which number, first we write down the arrangement of the indices of all two-factor interaction terms as the row headers and column headers. For example, when there are 4 factors, there will be six two-factor interaction terms. Therefore, the row and column headers are 12, 13, 14, 23, 24 and 34 as in Table 3.B.1. To fill up the row corresponding to the index ij in the column header, we look at the indices in the row header. If both i and j appear in the column header, the number "2" should be filled in. If only one (either i or j, regardless of the position) is present, the number "1/2" should be filled in. If neither i nor j is present, the number "0" is filled in. In Table 3.B.1, for example, the row corresponding to the index 14 is 1/2, 1/2, 2, 0, 1/2, and 1/2. This completes the third row. The other rows of M can be completed the same way. In other words, all the diagonal entries of M are equal to 2. When the indices in the column header and the row header have no common index, the corresponding entry is 0. All other entries are 1/2.

	12	13	14	23	24	34
12						
13						
14	1/2	1/2	2	0	1/2	1/2
23						
24						
34						

Table 3.B.1: Example for generating M

In Table 3.B.2 to Table 3.B.5, we give the matrix M for the 2^q mixture PF designs when q =3,4,5 and 6.

	12	13	23
12	2	1/2	1/2
13	1/2	2	1/2
23	1/2	1/2	2

Table 3.B.2: M when $q = 3$

	12	13	14	23	24	34
12	2	1/2	1/2	1/2	1/2	0
13	1/2	2	1/2	1/2	0	1/2
14	1/2	1/2	2	0	1/2	1/2
23	1/2	1/2	0	2	1/2	1/2
24	1/2	0	1/2	1/2	2	1/2
34	0	1/2	1/2	1/2	1/2	2

Table 3.B.3: M when $q = 4$

	12	13	14	15	23	24	25	34	35	45
12	2	1/2	1/2	1/2	1/2	1/2	1/2	0	0	0
13	1/2	2	1/2	1/2	1/2	0	0	1/2	1/2	0
14	1/2	1/2	2	1/2	0	1/2	0	1/2	0	1/2
15	1/2	1/2	1/2	2	0	0	1/2	0	1/2	1/2
23	1/2	1/2	0	0	2	1/2	1/2	1/2	1/2	0
24	1/2	0	1/2	0	1/2	2	1/2	1/2	0	1/2
25	1/2	0	0	1/2	1/2	1/2	2	0	1/2	1/2
34	0	1/2	1/2	0	1/2	1/2	0	2	1/2	1/2
35	0	1/2	0	1/2	1/2	0	1/2	1/2	2	1/2
45	0	0	1/2	1/2	0	1/2	1/2	1/2	1/2	2

Table 3.B.4: M when $q = 5$

	12	13	14	15	16	23	24	25	26	34	35	36	45	46	56
12	2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	0	0	0	0	0	0
13	1/2	2	1/2	1/2	1/2	1/2	0	0	0	1/2	1/2	1/2	0	0	0
14	1/2	1/2	2	1/2	1/2	0	1/2	0	0	1/2	0	0	1/2	1/2	0
15	1/2	1/2	1/2	2	1/2	0	0	1/2	0	0	1/2	0	1/2	0	1/2
16	1/2	1/2	1/2	1/2	2	0	0	0	1/2	0	0	1/2	0	1/2	1/2
23	1/2	1/2	0	0	0	2	1/2	1/2	1/2	1/2	1/2	1/2	0	0	0
24	1/2	0	1/2	0	0	1/2	2	1/2	1/2	1/2	0	0	1/2	1/2	0
25	1/2	0	0	1/2	0	1/2	1/2	2	1/2	0	1/2	0	1/2	0	1/2
26	1/2	0	0	0	1/2	1/2	1/2	1/2	2	0	0	1/2	0	1/2	1/2
34	0	1/2	1/2	0	0	1/2	1/2	0	0	2	1/2	1/2	1/2	1/2	0
35	0	1/2	0	1/2	0	1/2	0	1/2	0	1/2	2	1/2	1/2	0	1/2
36	0	1/2	0	0	1/2	1/2	0	0	1/2	1/2	1/2	2	0	1/2	1/2
45	0	0	1/2	1/2	0	0	1/2	1/2	0	1/2	1/2	0	2	1/2	1/2
46	0	0	1/2	0	1/2	0	1/2	0	1/2	1/2	0	1/2	1/2	2	1/2
56	0	0	0	1/2	1/2	0	0	1/2	1/2	0	1/2	1/2	1/2	1/2	2

Table 3.B.5: M when $q = 6$

3.C Kronecker Product

Let

$$\begin{aligned} A &= (a_{ij}) \quad \text{be a m} \times \text{n matrix} \\ B &= (b_{ij}) \quad \text{be a k} \times \text{l matrix} \end{aligned}$$

Then the Kronecker product $A \otimes B$ is a mk $\times$ nl matrix defined by:

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & \dots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mn}B \end{pmatrix}$$

Let C be a n$\times$u matrix and D be a l$\times$v matrix. The following result is useful:

$$AC \otimes BD = (A \otimes B)(C \otimes D)$$

The proof is straightforward.

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