

# OPTIMAL RESTRICTIONS ON REGRESSION PARAMETERS FOR LINEAR MIXTURE MODEL<sup>1)</sup>

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## Abstract

A method of finding optimal linear restriction on regression parameters in linear model for mixture experiments in the sense of minimizing integrated mean squared error is studied. We use the formulation of optimal restrictions on regression parameters for estimating responses proposed by Park(1981) by transforming mixture components to mathematically independent variables.

## 1. Introduction

Mixture problem is a special type of experimental design problem in which the response  $Y$ (or responses) depends only on the relative proportions of the design factors(or components) and not on the absolute amounts of these components. If  $x_i$  is the proportion of the  $i$ -th component, then a mixture problem with  $q$  components is characterized by the constraints

$$\begin{aligned}x_1 + x_2 + \cdots + x_q &= 1 \\ x_i &\geq 0\end{aligned}\tag{1}$$

The functional relationship is assumed to be approximated by the linear mixture

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model,

$$y(x) = x' \beta + \varepsilon \quad (2)$$

where  $x$  is a  $q$ -vector of input mixture variables,  $x' = (x_1, x_2, \dots, x_q)$ , and  $\beta = (\beta_1, \beta_2, \dots, \beta_q)$  is a  $q$ -vector of unknown regression parameters. Note that the possible mixtures are restricted to the regular  $(q-1)$  dimensional simplex.

The error,  $\varepsilon$ , is assumed to be identically and independently distributed with mean zero and unknown variance,  $\sigma^2$ . For all observations the model (2) may be conveniently expressed as

$$y = X\beta + \varepsilon \quad (3)$$

where  $y$  is the  $n$ -vector of observed responses,  $X$  is the  $n \times q$  design matrix, and  $\varepsilon$  is the  $n$ -vector of errors. The least squares estimator for  $\beta$  is

$$\hat{\beta} = (X'X)^{-1}X'y.$$

Suppose  $q$  linear restrictions are imposed on the parameter space, such that,

$$C\beta = 0$$

in which  $C$  is an  $r \times q$  matrix of rank  $r (\leq q)$ . Let  $\tilde{\beta}$  be the least squares estimator of  $\beta$  in (3) under the restrictions  $C\beta = 0$ . It is well known (see Searle(1971)) that  $\tilde{\beta}$  has the form of

$$\tilde{\beta} = \hat{\beta} - (X'X)^{-1}C'[C(X'X)^{-1}C']^{-1}C\hat{\beta}.$$

The objective of this paper is to propose the optimal linear restriction on regression parameters in mixture model. Park(1981) proposed how to find the optimal restrictions on regression parameters when the response estimator is the major concern. However, because of the inherent constraints described in (1), the method cannot be applied directly. So we consider a transformation to use his optimal restrictions on mixture experiments.

## 2. Transforming of mixture components

The factor space of the  $q$  mixture component proportions is represented by a  $(q-1)$ -dimensional regular simplex defined according to (1). Instead of working directly with the  $q$  linearly dependent mixture components  $x_1, x_2, \dots, x_q$ , let us redefine the system in terms of  $(q-1)$  mathematically independent variables  $z_1, z_2, \dots, z_{q-1}$ . To do so we suggest the following transformation that was originally due to Claringbold(1955) .

$$V \equiv (qX - J)\Theta$$

where  $J$  is  $n \times q$  matrix that has all elements 1 , and  $\Theta$  is  $q \times q$  matrix defined by

$$\Theta = \begin{bmatrix} q-1 & 0 & 0 & \dots & 0 & s \\ -1 & (q-2)l & 0 & & 0 & s \\ -1 & -l & (q-3)m & & 0 & s \\ -1 & -l & -m & & 0 & s \\ \vdots & \vdots & & \ddots & \vdots & \vdots \\ -1 & -l & -m & & t & s \\ -1 & -l & -m & & -t & s \end{bmatrix}$$

and the elements  $l, m, \dots, t$  and  $s$  in  $\Theta$  are defined in a manner to force the sum of squares of the elements in each column inside the brackets to be  $q(q-1)$ . Then we define  $Z$  as

$$Z = VQ \tag{4}$$

where  $Q$  is  $q \times q$  matrix defined by

$$Q = \text{diag} \left\{ \frac{1}{q(q-1)}, \frac{1}{q(q-2)l}, \frac{1}{q(q-3)m}, \dots, \frac{1}{qt}, 0 \right\}$$

to make the ranges of the transformed variables uniform. This transformation change the design matrix  $X$  into  $Z$  where

$$Z = (z_1, z_2, \dots, z_q)', \quad z_i = (z_{i1}, z_{i2}, \dots, z_{iq})'$$

$$-1 \leq z_{ij} \leq 1, \quad j=1, 2, \dots, q-1, \quad z_{iq} = 0, \quad i=1, 2, \dots, q.$$

Let  $Z_A$  be the matrix  $Z$  in (4) with the  $q$ th column removed and augmented on the left side with an  $n \times 1$  column of 1's. At the points of the design in the  $\underline{z}_1, \underline{z}_2, \dots, \underline{z}_{q-1}$  system, observed values of the response are collected and are used for the estimation of the parameters in the vector  $\gamma$  in the model

$$y = Z_A \gamma + \varepsilon \quad (5)$$

and observed response,  $y$ , that is determined by

$$y(\underline{z}) = \underline{z}' \gamma + \varepsilon$$

where  $\underline{z}'$  is a row of the matrix  $Z_A$  in (5).

The vector of parameter estimate is

$$\hat{\gamma} = (Z_A' Z_A)^{-1} Z_A' y$$

and the fitted model in  $\underline{z}$  is

$$\hat{y}(\underline{z}) = \underline{z}' \hat{\gamma}.$$

The variance of  $\hat{y}(\underline{z})$  is given by

$$\text{var}[\hat{y}(\underline{z})] = \underline{z}' (Z_A' Z_A)^{-1} \underline{z} \sigma^2.$$

Suppose a set of linear restrictions are imposed on the parameter space, i.e.,

$$L\gamma = 0 \quad (6)$$

in which  $L$  is an  $r \times q$  matrix of rank  $r (\leq q)$ . Let  $\tilde{\gamma}$  be the least squares estimator of  $\gamma$  under the restriction (6). It is well known (see Searle(1971)) that  $\tilde{\gamma}$  has the form of

$$\begin{aligned} \tilde{\gamma} &= \{I - (Z_A' Z_A)^{-1} L' [L (Z_A' Z_A)^{-1} L']^{-1} L\} \hat{\gamma} \\ &= B \tilde{\gamma} \end{aligned} \quad (7)$$

$$\text{where } B = I - (Z_A' Z_A)^{-1} L' [L (Z_A' Z_A)^{-1} L']^{-1} L \quad (8)$$

And the fitted value is

$$\tilde{y}(\underline{z}) = \underline{z}' \tilde{\gamma}. \quad (9)$$

It is easy to show that

$$\begin{aligned} \text{var}(\tilde{\gamma}) &= \sigma^2(Z_A'Z_A)^{-1} \\ &\quad - \sigma^2(Z_A'Z_A)^{-1}L'[L(Z_A'Z_A)^{-1}L']^{-1}L(Z_A'Z_A)^{-1} \end{aligned}$$

and

$$\begin{aligned} \text{MSE}[\tilde{y}(\underline{z})] &= E(\underline{z}'\tilde{\gamma} - \underline{z}'\gamma)^2 \\ &= \sigma^2\underline{z}'B(Z_A'Z_A)^{-1}B'\underline{z} + \underline{z}'GL\gamma\gamma'L'G'\underline{z} \end{aligned}$$

where  $B$  is given in (8) and  $G$  is given by

$$G = (Z_A'Z_A)^{-1}L'[L(Z_A'Z_A)^{-1}L']^{-1}$$

### 3. Formulation of optimal restrictions

To contrast the precision of  $\tilde{y}(\underline{z})$  with that of  $\hat{y}(\underline{z})$ , we examine the difference,

$$\begin{aligned} D(\underline{z}) &= \text{var}[\hat{y}(\underline{z})] - \text{MSE}[\tilde{y}(\underline{z})] \\ &= \{ \text{var}[\hat{y}(\underline{z})] - \text{var}[\tilde{y}(\underline{z})] \} - \{ \text{squared bias of } \tilde{y}(\underline{z}) \} \\ &= \sigma^2\underline{z}'\{ (Z_A'Z_A)^{-1}L'[L(Z_A'Z_A)^{-1}L']^{-1}L(Z_A'Z_A)^{-1} \} \underline{z} - \underline{z}'GL\gamma\gamma'L'G'\underline{z} \end{aligned}$$

We wish to find an  $r \times q$  restriction matrix  $L$ , and the corresponding biased estimator in (7) that maximizes the difference between integrated MSE's of  $\hat{y}(\underline{z})$  and  $\tilde{y}(\underline{z})$  over the region  $R$  under a weighting function  $W(\underline{z})$ ,

$$\begin{aligned} J &= \int_R \{ \text{var}[\hat{y}(\underline{z})] - \text{MSE}[\tilde{y}(\underline{z})] \} dW(\underline{z}) \\ &= \int_R D(\underline{z}) dW(\underline{z}) \end{aligned} \tag{10}$$

subject to linear restrictions  $L\gamma = 0$ .

To determine the restriction matrix  $L$ , we first note that the constraint  $L(Z_A'Z_A)^{-1}L = I_r$  may be imposed without loss of generality. Observe that, since  $L(Z_A'Z_A)^{-1}L' = HH'$  for an  $r \times r$  nonsingular matrix  $H$  and

$\tilde{\chi}(L) = \tilde{\chi}(H^{-1}L)$  in (7), it follows that for every  $L$  there exists a corresponding  $L_1$  such that  $\tilde{\chi}(L) = \tilde{\chi}(L_1)$  and  $L_1(Z_A'Z_A)L_1' = I_r$ . If we let

$$M = \int_R \underline{z} \underline{z}' dW(\underline{z}), \text{ then}$$

$$J = IV - IB$$

where

$$\begin{aligned} IV &= \int_R \{ \text{var}[\hat{y}(\underline{z})] - \text{var}[\tilde{y}(\underline{z})] \} dW(\underline{z}) \\ &= \sigma^2 \text{tr}[(Z_A'Z_A)^{-1}L'L(Z_A'Z_A)^{-1}M] \end{aligned}$$

$$\begin{aligned} IB &= \int_R [\text{squared bias of } \tilde{y}(\underline{z})] dW(\underline{z}) \\ &= \gamma'L'L(Z_A'Z_A)^{-1}M(Z_A'Z_A)^{-1}L'L\gamma \end{aligned}$$

Thus,  $J$  is the difference between the integrated difference of  $\text{var}[\hat{y}(\underline{z})] - \text{var}[\tilde{y}(\underline{z})]$  and the integrated squared bias of  $\tilde{y}(\underline{z})$ . Therefore, in essence, we are looking for a restriction matrix  $L$  from which the gain in precision of  $\hat{y}(\underline{z})$  over  $\tilde{y}(\underline{z})$  in terms of variance is not offset by the squared bias over the region  $R$ .

We can now respecify the class of estimators of interest as  $\tilde{\chi} = (I - (Z_A'Z_A)^{-1}L'L)\hat{\chi}$  for all  $L$  such that  $L(Z_A'Z_A)^{-1}L = I_r$  and  $L\gamma = 0$ . A problem is raised in evaluation of  $J$ , for  $J$  is a function of the unknown vector  $\gamma$ . Suppose  $\gamma = \delta \underline{a}$ , where  $\underline{a}$  are the direction conines of  $\gamma$  and  $\delta$  is the length of vector  $\gamma$ ,  $\delta = (\gamma'\gamma)^{\frac{1}{2}}$ . Since  $\underline{a}$  is completely unknown, one might wish to average  $J$  in (10) over an all directions in such a way that the distribution over all directions is uniform. Note that  $IB$  is the only term in  $J$  that involves  $\gamma$ , so consider the average of  $IB$  over all possible directions. Since  $IB$  is a scalar, we can write

$$\begin{aligned}
IB &= \text{tr}[\gamma' L' L (Z_A' Z_A)^{-1} M (Z_A' Z_A)^{-1} L' L \gamma] \\
&= \delta^2 \text{tr}[L' L (Z_A' Z_A)^{-1} M (Z_A' Z_A)^{-1} L' L \alpha \alpha']
\end{aligned}$$

In Park(1981), the average of  $\alpha \alpha'$  over all possible directions in such a way that the distribution over all directions is uniform is  $I_q/q$ . Thus, the average of  $IB$  is

$$\frac{\delta^2}{q} \text{tr}[L' L (Z_A' Z_A)^{-1} M (Z_A' Z_A)^{-1} L' L]$$

and the objective function  $J$  for this case may be written as

$$\begin{aligned}
J_a &= \sigma^2 \text{tr}[(Z_A' Z_A)^{-1} L' L (Z_A' Z_A)^{-1} M] \\
&\quad - \frac{\delta}{q} \text{tr}[L' L (Z_A' Z_A)^{-1} M (Z_A' Z_A)^{-1} L' L] \tag{11}
\end{aligned}$$

Now it is of interest to examine the criterion in (11) for some particular moment matrix  $M$ . Define

$$\Lambda^{\frac{1}{2}} = \begin{bmatrix} \Lambda_1^{\frac{1}{2}} & 0 \\ 0 & \Lambda_2^{\frac{1}{2}} \end{bmatrix} \quad \text{and} \quad T = (T_1 : T_2)$$

where  $\Lambda_1^{\frac{1}{2}} = \text{diag}(\lambda_1^{\frac{1}{2}}, \dots, \lambda_{q-r}^{\frac{1}{2}})$ ,  $\Lambda_2^{\frac{1}{2}} = \text{diag}(\lambda_{q-r+1}^{\frac{1}{2}}, \dots, \lambda_q^{\frac{1}{2}})$ ,  $T_1$  is  $q \times (q-r)$ ,  $T_2$  is  $q \times r$  for some  $r \leq q$ ,  $\lambda_i$  are eigen values of  $Z_A' Z_A$ ,  $\lambda_1 \geq \dots \geq \lambda_q > 0$  and  $T$  is the corresponding orthogonal matrix of the eigen vectors.

The rows of  $\Lambda^{\frac{1}{2}} T$  form a basis for  $q$ -Euclidian space and from the condition of  $L(Z_A' Z_A)^{-1} L = I_r$ , we can write

$$L = (DD')^{-1/2} D \Lambda^{1/2} T' \tag{12}$$

where  $D$  is any  $q \times r$  matrix of rank  $r$ .

Suppose now

$$M = \frac{Z_A' Z_A}{n}$$

Then we can show that

$$\begin{aligned} nJ_a &= \sigma^2 \text{tr}[(Z_A' Z_A)^{-1} L' L] - (\delta^2/q) \text{tr}[L' L] \\ &= \sigma^2 r - (\delta^2/q) \text{tr}[\Lambda^{1/2} S_D \Lambda^{1/2}] \\ &= \sigma^2 r - (\delta^2/q) \sum_{i=1}^q s_{ii} \lambda_i \end{aligned}$$

where

$$S_D = D'(DD')^{-1}D = (s_{ij}).$$

Since  $S_D$  is symmetric and idempotent,  $0 \leq s_{ij} \leq 1$  and  $\sum_{i=1}^q s_{ii} = r$ . Therefore, it is easy to see that  $nJ_a$  is maximized by choosing  $s_{ii} = 1$  if  $i = q - r + 1, \dots, q$  and  $s_{ii} = 0$ , otherwise. Consequently,

$$\max [nJ_a] = \sigma^2 r - (\delta^2/q) \sum_{i=q-r+1}^q \lambda_i. \quad (13)$$

Observe that the maximum is attainable if we take

$$D = [0 : I_r] \quad \text{and} \quad S_D = \begin{bmatrix} 0 & 0 \\ 0 & I_r \end{bmatrix}.$$

Substituting this  $D$  into (12), we get the optimal restriction matrix,

$$L^* = \Lambda_2^{\frac{1}{2}} T_2'. \quad (14)$$

Note that the restricted estimator  $\tilde{\gamma}$  with  $L^*$  has the following form,

$$\begin{aligned} \tilde{\gamma}^* &= [I - (Z_A' Z_A)^{-1} L^{*'} L^*] \hat{\gamma} \\ &= [I - T_2 T_2'] \hat{\gamma} \end{aligned}$$

which means that  $\tilde{\gamma}^*$  is nothing but the principal component regression estimator of  $\gamma$ .



Suppose now that

$$M = w \int_R \underline{z} \underline{z}' d\underline{z} ,$$

where  $1/w = \int_R d\underline{z}$  and  $R$  is  $R = \{z: -1 \leq z_i \leq 1 \text{ for all } i\}$ . Then,  $M = cI_q$

where  $c$  is a constant, and

$$\begin{aligned} J_a/c &= \sigma^2 \text{tr}[(Z_A' Z_A)^{-1} L' L (Z_A' Z_A)^{-1}] \\ &\quad - (\delta^2/q) \text{tr}[L' L (Z_A' Z_A)^{-2} L' L]. \end{aligned} \quad (15)$$

Substituting  $L = (DD')^{1/2} D\Lambda^{1/2} T'$  into (15),

$$\begin{aligned} J_a/c &= \sigma^2 \text{tr}[\Lambda^{-1/2} S_D \Lambda^{-1/2}] - (\delta^2/q) \text{tr}[\Lambda^{1/2} S_D \Lambda^{-1} S_D \Lambda^{1/2}] \\ &= \sigma^2 \sum_{i=1}^q s_{ii} \lambda_i^{-1} - (\delta^2/q) \left[ \sum_{i=1}^q s_{ii}^2 + \sum_{i \neq j} s_{ij}^2 (\lambda_i \lambda_j^{-1}) \right]. \end{aligned}$$

Since, in the event of severe collinearity, the values of  $\lambda_q, \lambda_{q-1}, \lambda_{q-2}, \dots$ , etc. are close to zero, it can be seen that  $s_{ii} = 0$  for  $i = 1, 2, \dots, q-r$ ,  $s_{ii} = 1$  for  $i = q-r+1, \dots, q$ , and  $s_{ij} = 0$  for  $i \neq j$  in order to maximize  $J_a$ . This leads to the same optimal matrix  $L^*$  in (14), and

$$\max [J_a/c] = \sigma^2 \sum_{i=q-r+1}^q \lambda_i^{-1} - r\delta^2/q. \quad (16)$$

Note that the criteria (13) and (16) lead to the same optimal number of  $r$ . For (13), we should drop the  $i$ th principal component if and only if

$$\sigma^2 - \frac{\delta^2}{q} \lambda_i > 0 \quad (17)$$

For (16), we should drop the  $i$ th principal component if and only if

$$\frac{\sigma^2}{\lambda_i} - \frac{\delta^2}{q} > 0 \quad (18)$$

which is the same inequality as (17).

We may use the followings as the estimates of  $\sigma^2$  and  $\delta^2$  practically.

$$\hat{\sigma}^2 = \underline{y}'(I - Z_A(Z_A' Z_A)^{-1} Z_A') \underline{y} / (n - q) \quad (19)$$

$$\widehat{\delta}^2 = \widehat{\gamma}' \widehat{\gamma} - \widehat{\sigma}^2 \frac{q}{\lambda_M} \quad (20)$$

where  $\lambda_M$  is the median of  $\lambda_1, \lambda_2, \dots, \lambda_q$ . Note that (19) is equal to  $\mathbf{y}'(I - X(X'X)^{-1}X')\mathbf{y}/(n - q)$  and that the usual unbiased estimator of  $\delta$  is

$$\widehat{\delta}_{UE} = \widehat{\gamma}' \widehat{\gamma} - \widehat{\sigma}^2 \sum_{i=1}^m \lambda_i^{-1} . \quad (21)$$

But the values of  $\lambda_q, \lambda_{q-1}, \lambda_{q-2}, \dots$ , etc. are close to zero, (21) varies extremely and even have a negative value. So we recommend (20) which is robust to the values of  $\lambda_i, i = 1, 2, \dots, q$  as the estimator of  $\delta$ .

We have to transform this optimal restriction,  $L^* \boldsymbol{\gamma} = 0$ , properly, to use for  $\boldsymbol{\beta}$ , the regression parameter in the mixture model (3). The optimal restriction would be

$$C^* \boldsymbol{\beta} = 0, \quad (22)$$

where  $C^* = L^* P^{-1}$ .

$$\text{and } P = \begin{bmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 1 & -(q-1)^{-1} & 1 & 0 & & 0 \\ 1 & -(q-1)^{-1} & -(q-2)^{-1} & 1 & & 0 \\ 1 & -(q-1)^{-1} & -(q-2)^{-1} & -(q-3)^{-1} & & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & -(q-1)^{-1} & -(q-2)^{-1} & -(q-3)^{-1} & \dots & 1 \\ 1 & -(q-1)^{-1} & -(q-2)^{-1} & -(q-3)^{-1} & \dots & -1 \end{bmatrix}$$

#### 4. An example

We can evaluate the optimal restriction (22) by an example. The data for this example are the octane-blending data which appeared in Cornell(1990).

<Table 1> Gasoline motor octane ratings

Gasoline Components							Motor Octane at 1.5ml Pb/gal
$x_1$	$x_2$	$x_3$	$x_4$	$x_5$	$x_6$	$x_7$	$y$
0	0.23	0	0	0	0.74	0.03	98.7
0	0.10	0	0	0.12	0.74	0.04	97.8
0	0	0	0.10	0.12	0.74	0.04	96.6
0	0.49	0	0	0.12	0.37	0.02	92.0
0	0	0	0.62	0.12	0.18	0.08	86.6
0	0.62	0	0	0	0.37	0.01	91.2
0.17	0.27	0.10	0.38	0	0	0.08	81.9
0.17	0.19	0.10	0.38	0.02	0.06	0.08	83.1
0.17	0.21	0.10	0.38	0	0.06	0.08	82.4
0.17	0.15	0.10	0.38	0.02	0.10	0.08	83.2
0.21	0.36	0.12	0.25	0	0	0.06	81.4
0	0	0	0.55	0	0.37	0.08	88.1

The original model is

$$y = X\beta + \varepsilon$$

$$\begin{bmatrix} 98.7 \\ 97.8 \\ \vdots \\ 88.1 \end{bmatrix} = \begin{bmatrix} 0 & 0.23 & 0 & 0 & 0 & 0.74 & 0.03 \\ 0 & 0.1 & 0 & 0 & 0.12 & 0.74 & 0.04 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0.55 & 0 & 0.37 & 0.08 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_7 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_{12} \end{bmatrix}$$

To transform  $X$  into  $Z_A$ , we should evaluate  $\Theta$  and  $Q$ ,

$$\Theta = \begin{bmatrix} 6 & 0 & 0 & 0 & 0 & 0 & 2.45 \\ -1 & 5.92 & 0 & 0 & 0 & 0 & 2.45 \\ -1 & -1.18 & 5.80 & 0 & 0 & 0 & 2.45 \\ -1 & -1.18 & -1.45 & 5.61 & 0 & 0 & 2.45 \\ -1 & -1.18 & -1.45 & -1.87 & 5.29 & 0 & 2.45 \\ -1 & -1.18 & -1.45 & -1.87 & -2.65 & 4.58 & 2.45 \\ -1 & -1.18 & -1.45 & -1.87 & -2.65 & -4.58 & 2.45 \end{bmatrix}$$

$$Q = \begin{bmatrix} 0.024 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.024 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.025 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.025 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.027 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.031 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

## 5. Conclusion

This paper discussed the problem of finding optimal restriction on regression parameters for mixture model where the collinearity exists in components. We can apply the optimal restriction proposed by Park(1981) in general regression model after we transform  $q$ -component in  $(q-1)$ -dimensional simplex to  $(q-1)$  mathematically independent variables. The method of transformation may have many choices besides the method we used in this paper. The properties of this optimal restriction can be evaluated by some criteria such as screening strategy in Park(1978).

### References

1. Claringbold, P. J., "Use of the Simplex Design in the Study of the Joint Action of Related Hormones," *Biometrics*, vol. 11, 174-185, 1955.
2. Cornell, J. A., *Experiments with Mixtures: Designs, Models, and the Analysis of Mixture Data*, 2nd ed. John Wiley & Sons, New York, 1990.
3. Park, S. H., "Selecting Contrasts Among Parameters in Scheffe's Mixture Model: Screening Components and Model Reduction," *Technometrics*, vol.20, 273-279, 1978.
4. Park, S. H., "Collinearity and Optimal Restrictions on Regression Parameters for Estimating Responses," *Technometrics*, vol. 23, 289-295, 1981.
5. Searle, S. R., *Linear Models*, New York: Wiley, Inc.,1971.