Jour. Ind. Soc. Ag. Statistics
Vol. XL, No. 1 (1988), pp. 15-22

MIXTURE *X* PROCESS VARIABLES DESIGN WITH RESTRICTED SIMPLEX

RAKESH KUMARI
D.A.V. College, Dehradun
and
SUKHPAL SINGH
J.V. College, Baraut

(Received : November, 1986)

SUMMARY

Designs and models for mixture *X* process variables experiments have been suggested by Scheffe, Murty and Das, and some others. These designs are suitable when the experimenter is interested in the entire factor space. Sometimes the requirement of the variables may demand a restricted simplex. In this investigation a mixture *X* process variables design with restricted simplex has been constructed from a central composite design given by George and Das, through an empirical transformation. It is illustrated by an example. Estimates of the parameters of a quadratic model together with the variances and covariances of these estimates are also derived.

Keywords : Mixture variables; Process variables; Central composite design; Restricted simplex; Empirical transformation.

Introduction

In mixture experiments the response depends on the proportion of the components (constituents) present but not on the total amount. Suppose we have k components in the mixture and x_i $(i = 1, 2, \ldots, k)$ represents the proportion of the ith components, then

$$x_i \geqslant 0, \qquad i = 1, 2, 3, \ldots, k$$

and

$$\sum_{i=1}^{k} x_i = 1.$$

Scheffe [3], [4] did a pioneering work in the mixture experiments by introducing simplex lattice and simplex centroid designs. He also extended his study to the case where it is desired to subject the mixtures to the experimentation in which p factors (not component of the mixture) are varied in addition to the k proportions of the mixture. These p factors which do not form any component of the mixture are called process variables and the k factors of the mixture as mixture variables. Design for this requirement are termed as process X mixture variables designs. Scheffe defined a complete simplex centroid X factorial design as the one in which at each point of the simplex-centroid design, a complete factorial experiment is conducted. Further Murty and Das [2] evolved symmetric simplex X factorial experiments. The above two designs represent the simplex uniformly and are suitable when the experimenter is interested in the entire factor space. One drawback of these designs is that they require a large number of points.

Sometimes the requirement of the mixture variables may demand a restricted simplex, for example one factor may constitute the major proportion and the others a small proportion of the mixture i.e. the experimental region may be nearer the vertices of the simplex. In other cases it may be nearer the edges or around the centre. These requirements with a smaller number of points can be satisfied by constructing a mixture X process variables design from a response surface design through an emperical transformation i.e. by changing the origin and scale of the variables suitably. If a rotatable design is used as the basic design, the levels of the variables are very often fractional or even irrational and are not equispaced. This creates some inconvenience in the construction of mixture X process (MXP) variables design. We can get rid of this difficulty by adopting the central composite response surface design given by George and Das [1] in which the levels of the different factors are equispaced.

2. Central Composite Design

The experimental points of this design in v factors are divided into three sets (a) set of 2^v or a fraction (for which no four or less factor interaction is in the indentity group) of it having $\pm$ 1 as levels (b) set of

$2v$ star points having ± 2 as levels (c) set of m central points having zero as the level of each factor. Following are the relations satisfied by this design,

$$\sum_{u=1}^{N} x_{iu}^2 = n + 8 = N\omega_2, \qquad i = 1, 2, \ldots, v$$

$$\sum_{u=1}^{N} x_{iu}^4 = n + 32 = cN\omega_4, \qquad i = 1, 2, \ldots, v$$

$$\sum_{u=1}^{N} x_{iu}^2 \; x_{ju}^2 = n = N\omega_4, \qquad \neq i = 1, 2, \ldots, v$$

where n is the number of points in the set under (a) and $N = (n+2v+m)$ is the total number of treatment combinations in this design, sum of squares with at least one 'x' with odd powers is zero.

3. Construction of Mixture X Process Variables Design

If the design is to be constructed in p process variables and k mixture variables, then we start with a central composite design in $v = p + k - 1$ factors. In this design each factor is present at five equispaced levels $-2, -1, 0, 1, 2$ in coded form.

Let Pu $(X_{1u}, X_{2u}, \ldots, X_{pv}, X_{p+1, u}, \ldots, X_{p+k-1, u})$ be the uth ($u = 1, 2, \ldots, N$) point of the design. We use the transformations $X_{iu} = Z_{iu}$, for $i = 1, 2, \ldots, p$

and $\quad X_{iu} + K = X'_{ju} \quad$ for $i = p + 1, p + 2, \ldots, p + k - 1$

$$j = 1, 2, \ldots, k - 1 \; K \geqslant 2.$$

By virtue of the above transformation all X'_{ju} are non-negative. Further let $\sum_{j=1}^{k-1} X'_{ju} = a_u$ and a_m is the greatest among a_u, and p_0 be the lower bound of the components of the factor which constitute the major proportion of the mixture. An integer 'a' is selected such that a $\geqslant a_m/(1-p_0)$. After choosing 'a' add a new factor X'_k to the design such that $X'_{ku} = a - a_u$ and hence $\sum_{j=1}^{k} X'_{ju} = a$. Next by dividing each $X'_{ju} = (j = 1, 2, \ldots, k)$ by the quantity 'a', we get the proportions of the mixture variables. Thus, the uth point of the process X mixture variable design is given by

$$P_u = (Z_{1u}, Z_{2u}, \ldots, Z_{pu}, x_{1u}, x_{2u}, \ldots, x_{ku})$$

where $x_{ju} = (X_{ju}/a)$ $(j = 1, 2, \ldots, k)$. Hence the kth mixture variable which is present in major proportion on the simplex is restricted near the vertices.

Example. To illustrate the above procedure we construct a process X mixture variables design in one process and three mixture variables in which the proportion of the major factor is greater than or equal to .70. For this purpose we start with a central composite design in three factors as the basic design.

Basic Design			*Intermediate Design*				*Mixture x Process Variables Design*			
X_1	X_2	X_3	Z_1	X_1'	X_2'	X_3'	Z_1	x_1	x_2	x_3
−1	−1	−1	−1	1	1	18	−1	.05	.05	.90
−1	−1	1	−1	1	3	16	−1	.05	.15	.80
−1	1	−1	−1	3	1	16	−1	.15	.05	.80
−1	1	1	−1	3	3	14	−1	.15	.15	.70
1	−1	−1	1	1	1	18	1	.05	.05	.90
1	−1	1	1	1	3	16	1	.05	.15	.80
1	1	−1	1	3	1	16	1	.15	.05	.80
1	1	1	1	3	3	14	1	.15	.15	.70
2	0	0	2	2	2	16	2	.10	.10	.80
−2	0	0	−2	2	2	16	−2	.10	.10	.80
0	2	0	0	4	2	14	0	.20	.10	.70
0	−2	0	0	0	2	18	0	.00	.10	.90
0	0	2	0	2	4	14	0	.10	.20	.70
0	0	−2	0	2	0	18	0	.10	.00	.90
0	0	0	0	2	2	16	0	.10	.10	.80

In the intermediate design X_1 is replaced by Z_1 and

$$X_1' = X_2 + 2$$

$$X_2' = X_3 + 2.$$

As the maximum of $(X_1' + X_2') = 6$,

$$a \geqslant \frac{6}{1 - .70} = 20.$$

We take $a = 20$ and put $X_3' = 20 - (X_1' + X_2')$. Finally on dividing X_1', X_2' and X_3' by 20, the desired process X mixture variables design is obtained.

For restricting the simplex in other regions, we choose 'a' and K as below :

(1) On choosing $K = 2$ and $a \geqslant 6(k - 1)$, the region will be restricted near the vertices.
(2) On choosing $K = 2$ and $a = a_m$ (or near to the right) the region will be restricted near the vertices and edges both.
(3) On choosing K large and $a = a_m$ (or near to the right) the region will be restricted near the edges.
(4) On choosing K large and $a = k \cdot K$ the region will be restricted around the centre.

4. Analysis

As the mixture x process variables design has been obtained from the central composite design by making a change in the origin and scale in some of the independent variables, the response surface in mixture and process variables can also be obtained from the surface in $(p + k - 1)$ variables by introducing the same transformation.

Supposing that a quadratic model in the (p) process and k mixture variables represents the response surface i.e.

$$y_u = \Sigma \gamma_{ii} Z_{iu}^2 + \Sigma \gamma_{ii'} Z_{iu} Z_{i'u} + \Sigma \beta_{j'} x_{i'u}$$
$$+ \Sigma \beta_{jj'} x_{ju} x_{j'u} + \Sigma \partial_{ij} Z_{iu} x_{ju} + e_u \quad (1)$$

where $i = 1, 2, \ldots, p$ and $j = 1, 2, \ldots, k$

model (1) can be obtained from the following quadratic model in $(p + k - 1)$ independent variables $X_1, X_2, \ldots, X_{p+k-1}$

$$y = B_0 + \Sigma B_n X_{hu} + \Sigma B_{hh} X_{hu}^2 + \Sigma B_{hh'} X_{hu} X_{hu} X_{h'u} + e_u \quad (2)$$

$h, h' = 1, 2, \ldots, p + k - 1.$

The estimates of the parameters in model (2) are given below :

$$\hat{i}_0 = \frac{1}{N}\sum_u y_u - \frac{\omega_2}{N}\left[\frac{\sum_h (\sum_u X_{hu}^2\, y_u) - v\omega_2 \sum_u y_u}{\omega_4\,(c + v - 1) - v\,\omega_2^2}\right]$$

where (i) $v = p + k - 1$

and (ii) c, ω_2 and ω_4 are defined in section (2)

$$\hat{B}_h = \frac{1}{N\omega_2}\sum_u X_{hu}\, y_u,\quad B_{hh'} = \frac{\sum_u X_{hu}\, X_{h'u}\, y_u}{N\omega_4}$$

$$\hat{B}_{hh} = \frac{1}{N\omega_4\,(c-1)}\left[\sum_u X_{hu}\, y_u - \omega_2 \sum_u y_u\right.$$

$$\left. + (\omega_2^2 - \omega_4)\, \frac{\sum_h (\sum_u X_{hu}^2\, y_u) - v\omega_2 \sum_u y_u}{\omega_4\,(c + v - 1) - v\omega_2^2}\right].$$

The variances and covariances of the estimates are shown below

$$V(\hat{B}_0) = \omega_4\,(c + v - 1)\, D\, \sigma^2$$

where

$$D = [N\,\omega_4\,(c + v - 1) - v\,\omega_2^2]^{-1}$$

$$\text{Cov}\,(\hat{B}_0, \hat{B}_{hh}) = -\,\omega_2\, D\, \sigma^2$$

$$V(\hat{B}_h) = \frac{1}{N\omega_2}\,\sigma^2$$

$$V(\hat{B}_{hh}) = \frac{D}{\omega_4\,(c-1)}\,[\omega_4\,(c + v - 2) - (v - 1)\,\omega_2^2]\,\sigma^2$$

$$V(\hat{B}_{hh'}) = \frac{1}{B\omega_4}\,\sigma^2$$

$$\text{Cov}\,(\hat{B}_{hh}, \hat{B}_{h'h'}) = \frac{D}{\omega_4\,(c-1)}\,[\omega_2^2 - \omega_4]\,\sigma_2.$$

The covariances between any other pair of B's are zero.

The variance of a response y_0 estimated through the surface (2) at the point $(X_{10}, X_{20}, \ldots, X_{p+k-10})$ comes out as

$$V(\hat{y}_0) = V(\hat{B}_0) + d^2\left[\frac{1}{N\omega_4} - 2\omega_2 D\right]\sigma^2 + d^4 V(\hat{B}_{hh})$$

$$+ \frac{(c-3)}{N\omega_4 (c-1)} \sigma^2 \Sigma X^2_{h0} \cdot X^2_{h'0} \qquad (3)$$

where

$$d^2 = \sum_h X^2_{h0} .$$

The estimates of the parameters in model (1) can be obtained from those of B's in model (2) by the following relations

$$\hat{\beta}_\omega = \hat{B}_0 + a\,\hat{B}_{p+\omega} - K \sum_{p+k}^{p+k-1} \hat{B}_h + (a^2 - 2aK)\,\hat{B}_{p+\omega,\,p+\omega}$$

$$- aK \sum_{h' \neq p+\omega} \hat{B}_{p+\omega h'} + K^2 \sum_{k<h'=p+1}^{p+k-1} \hat{B}_{hh'}$$

$$\hat{\beta}_k = \hat{B}_0 - K \sum_{h=p+1}^{p+k-1} \hat{B}_h + K^2 \sum_{p+1}^{p+k-1} \hat{B}_{hh} + K^2 \Sigma \hat{B}_{hh'}$$

$$\hat{\beta}_{\omega\omega'} = a^2 (\hat{B}_{p+\omega,\,p+\omega'} - \hat{B}_{p+\omega,\,p+\omega} - \hat{B}_{p+\omega',\,p+\omega})$$

$$\hat{\beta}_{\omega k} = - a^2\, \hat{B}^2_{p+\omega',\,p+\omega}$$

$$\hat{\gamma}_{\mu\mu} = \hat{B}_{\mu\mu}$$

$$\hat{\gamma}_{\mu\mu'} = \hat{B}_{\mu\mu'}$$

$$\hat{\partial}_{\omega\mu} = a\,\hat{B}_{p+\omega\mu} + \hat{B}_\mu - K \sum_{p+k}^{p+k-1} \hat{B}_{h\mu}$$

$$\hat{\partial}_{k\mu} = \hat{B}_\mu - K \sum_{p+1}^{p+k-1} \hat{B}_{\omega\mu}$$

where $\omega = 1, 2, \ldots, (k-1)$.

$\omega' = 1, 2, \ldots, (k-1)$, with $\omega < \omega'$

$\mu = 1, 2, \ldots, p = \mu'$ (but $\mu < \mu'$).

Here it is worth to note that the same estimate will be obtained from model (1) at a specified point and from model (2) at the corresponding point. Thus through central composite design, first a general quadratic model (2) in ($v = p + k - 1$) independent variables can be fitted and then it can be transformed into model (1) having p process and k mixture variables.

5. Variance of the Estimated Response

The variance of the estimated response from model (2) at a specified point is the same as the variance of the estimated response estimated by model (1) at the corresponding point. This follows from the fact that so long as the point at which the response is estimated remains the same, the variance of the estimated response at that point remains unchanged, though the variables might have changed.

ACKNOWLEDGEMENT

The authors wish to express their gratitude to the referee for his valuable comments.

REFERENCES

[1] George, K. C. and Das, M. N. (1968) : A type of central composite response surface design, *J. Ind. Soc. Agri. Stat.*, **20** : 21-29.

[2] Murty, J. S. and Das, M. N. (1968) : Design and analysis of experiments with mixtures, *A.M.S.*, **39** : 1517-1539.

[3] Scheffe, H. (1958) : Experiments with mixtures, *J. Roy. Stat. Soc.*, **B 20**: 344-360.

[4] Scheffe, H. (1963) : Simplex centroid designs for experiments with mixtures, *J. Roy. Stat. Soc.*, **B25** : 235-263.