A NOTE ON MIXTURE DESIGNS DERIVED FROM FACTORIALS[1]

BY

M.S. RAMACHANDRA MURTHY AND J.S. MURTY

Osmania University, Hyderabad

(Received : February, 1980)

SUMMARY

The present paper provides an expression for the relation between the estimates of parameters of a linear model fitted through factorial design and those of the linear model fitted through the corresponding mixture design.

1. INTRODUCTION

Experiments for the study of response surfaces in which the response depends only on the relative proportions of the predictor variables x_i, in each combination, but not on their amounts, are termed as experiments with mixtures (Scheffe 1958, 1963). If x_i is the proportion of the ith component in an n component mixture, then

$$\sum_{i=1}^{n} x_i=1,\ x_i \geqslant 0,\ i=1, 2, \ldots, n. \qquad \ldots(1.1)$$

x_i's are called mixture variables. Experimental designs for mixture experiments where in proportions for each component vary over the entire range 0 to 1 have been studied by Scheffe (1958, 1963) and Murty and Das (1968). Scheffe suggested the first and second degree polynomial functions for the response surfaces of mixture experiments, as

$$y_1=\sum_{i=1}^{n} \beta_i x_i \qquad \ldots(1.2)$$

[1]This work was first presented at the 33rd Annual Conference of the Indian Society of Agricultural Statistics held at Trichur in Dec., 1979. It was later included in [4].

and

$$M=\frac{1}{n(n-1)}\begin{bmatrix} n-1 & -1 & -1, & \cdots & -1 \\ 0 & (n-2)f & -f, & \cdots & -f \\ 0 & 0 & (n-3)g, & -g, & -g, \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot\cdot & k & -k \\ S & S & \cdots\cdots & S & S \end{bmatrix} \quad ..(2.2)$$

in which the letters f, g, k, ... S are determined such that the sum of squares of each row is 1. Becker (1969) suggested an alternative transformation with

$$M=\begin{bmatrix} \left[1-\frac{1}{n\pm\sqrt{n}}, \frac{-1}{n\pm\sqrt{n}}\right]_{n-1} & \pm\frac{1}{\sqrt{n}}\, J_{n-1} \\ \frac{1}{\sqrt{n}}\, J'_{n-1} & \frac{1}{\sqrt{n}} \end{bmatrix} \quad ...(2.3)$$

where

$[a, b]_r$: is $r\times r$ matrix with a as every diagonal element and every off diagonal element as b, and

J_{n-1} : $(n-1)x1$ vector with every element unity.

Thompson and Myers (1968) suggested a matrix M in which the last row has different elements rather than identical elements as in (2.2) and (2.3).

3. The Linear Model

Let w_{iu} denote the level of the i^{th} factor in the u^{th} combination ($i=1, 2, ..., n-1$; $u=1, 2, .., N$) of W and y_u the corresponding response. Assuming that y_u is linearly related with ($w_{1u}, w_{2u}, ..., w_{(n-1)u}$), the linear model (1.4) in w's will be

$$E(Y)=(J : W)\, B \quad ...(3.1)$$

where

Y' : $(y_1, y_2, \ldots\ y_N)$

W : $Nxn-1$ factorial design matrix

B' : $(b_0. b_1, \ldots, b_{n-1})$.

The least squares estimate of B is

$$\hat{B}\begin{bmatrix} \bar{y} \\ (W'W)^{-1}W'y \end{bmatrix}. \quad ...(3.2)$$

If on the other hand, the response y_u is linearly related to $(x_{1u}, x_{2u}, \ldots, x_{nu})$, the model (1.2) will be

$$E(Y) = X\beta \quad \ldots(3.3)$$

where

X : $N x n$ mixure design matrix, and

β' : $(\beta_1, \beta_2, \ldots, \beta_n)$ is a vector of unknown parameters.

The least squares estimate of β is

$$\hat{\beta} = (X'X)^{-1} X'Y. \quad \ldots(3.4)$$

Since X and W are related by (2.1), we derive below the relation between $\hat{\beta}$ and $\hat{B}$.

From (3.1) and (3.3), using (2.1),

$$(J\ W)\ \hat{B} = [(WO)\ M + J\,x'_0]\ \hat{\beta}. \quad \ldots(3.5)$$

Writing $\quad M = \begin{bmatrix} M_1 \\ M_2 \end{bmatrix} \quad \ldots(3.6)$

we get

$$(JW)\ \hat{B} = (WM_1 + J\,x'_0)\ \hat{\beta} \quad \ldots(3.7)$$

$$= (J : W) \begin{pmatrix} x'_0 \\ M_1 \end{pmatrix} \hat{\beta} \quad \ldots(3.7)$$

Assuming that $(J : W)$ is of rank n

$$\hat{\beta} = \begin{pmatrix} x'_0 \\ M_1 \end{pmatrix}^{-1} \hat{B} \quad \ldots(3.8)$$

The inverse in (3.8) can be evaluated using a result in Westlake (1968). Suppose the matrix $P = (P_{ij})n, n$ differs from the matrix $Q = (q_{ij})\ n, n$ in the kth column. Then writing $P^{-1} = (p^{ij})$,

$$q^{-1} = (q^{ij}) \text{ and } Z_1 = \sum_{r=1}^{n} P^{ir}\, q_{rk}\ , \text{ we have}$$

$$q^{ij} = P^{ij} - Z_i q^{kj} \text{ for } i \neq k,$$

$$q^{kj} = \frac{P^{kj}}{Z_k} \text{ for } i = k.$$

Now writing $P' = (M'_1\ \ M'_2),\ Q = (M'_1\ \ X_0)$,

and $\quad Z' = (Z_1, Z_2, \ldots, Z_n) = (Mx'_0)$

we get

$$\begin{pmatrix} x_0' \\ M_1 \end{pmatrix}^{-1} = \begin{bmatrix} \frac{m_{n1}}{Z_n}, & m_{11}-\frac{Z_1 m_{n1}}{Z_n}, & m_{21}-\frac{Z_2 m_{n1}}{Z_n}, & \ldots, & m_{n-1,1}-\frac{Z_{n-1} m_{n1}}{Z_n} \\ \frac{m_{n2}}{Z_n}, & m_{12}-\frac{Z_1 m_{n2}}{Z_n}, & m_{22}-\frac{Z_2 m_{n2}}{Z_n} & \ldots, & m_{n-1,2}-\frac{Z_{n-1} m_{n2}}{Z_n} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{m_{nn}}{Z_n}, & m_{1n}-\frac{Z_1 m_{nn}}{Z_n}, & m_{2n}-\frac{Z_2 m_{nn}}{Z_n} & \ldots, & m_{n-1,n}-\frac{Z_{n-1} m_{nn}}{Z_n} \end{bmatrix}$$

$$[M_2'(M_2x_0)^{-1} : M_1' - M_2'(M_2x_0)^{-1} x_0' M_1'] \qquad \ldots(3.9)$$

If we assume $M_2 = \frac{1}{\sqrt{n}} J_{1,n}$ as as in (2.2) and (2.3), then

$M_2x_0 = \frac{1}{\sqrt{n}}$ and

$$\begin{bmatrix} x_0' \\ M_1 \end{bmatrix}^{-1} = [J_{n,1} : (I_n - J_{n1} x_0') M_1'] \qquad \ldots(3.10)$$

Therefore, from (3.9)

$$\hat{\beta} = J_{n,1} : (I_n - J_{n,1} x_0') M_1'] \hat{B} \qquad \ldots(3.11)$$

In particular, if

$$x_0' = \left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right) \text{ i.e.,}$$

if the origin is shifted to the centroid of the simplex and M has the form given in (2.3) then

$$\hat{\beta} = (J : M_1') \hat{B}. \qquad \ldots(3.12)$$

From (3.1) the dispersion matrix of $\hat{B}$ is given by

$$D(\hat{B}) = \begin{bmatrix} J'J & J'W \\ W'J & W'W \end{bmatrix}^{-1} \sigma^2 \qquad \ldots(3.13)$$

When W represents a s^{n-1} factorial design with levels

$$0, \pm k_1, \pm K_2, \ldots \pm \frac{k_{s-1}}{2}$$

it can be easily verified that

$$\left.\begin{aligned} &W'J=0 \text{ and} \\ &W'W=\frac{2NK}{s} I_{n-1,\,n-1} \\ &\text{where} \\ &K=\sum_{i=1}^{\frac{S-1}{2}} k_1^2,\ N=s^{n-1} \end{aligned}\right\} \quad \ldots(3.14)$$

$$\therefore,\quad D(\hat{B})=\begin{bmatrix} \frac{1}{N} & 0 \\ 0 & \frac{s}{2NK} I_{n-1,\,n-1} \end{bmatrix}\sigma^2 \quad \ldots(3.15)$$

From (3.11)

$$D(\hat{B})=[J_{n,\,1} : (I_n-J_{n,\,1}\,x_0')\ M_1']\begin{bmatrix} \frac{1}{N} & 0 \\ 0 & \frac{s}{2NK} I_{n-1,\,n-1} \end{bmatrix}$$

$$\begin{bmatrix} J_{1,\,n}' \\ (I_n-Jx_0')'' \\ M_1 \end{bmatrix}\sigma^2=\frac{JJ'}{N}+\frac{s}{2NK}(I_n-Jx_0')(I_n'-Jx_0')'\,\sigma^2.$$

$$\ldots(3.16)$$

ACKNOWLEDGEMENTS

The authors are thankful to the referee for the suggestions in improving the paper.

REFERENCES

[1] Becker, N.G (1969) : Regression problems when the predictor variables are proportions. *Jour. Roy. Stat. Soc.* B, **31**, 107-12.

[2] Murty, J.S. (1966) : Problems of construction and Analysis of designs of experiments. Ph.D., thesis. Delhi University (unpublished).

[3] Murty, J.S., and Das, M.N. (1968) : Design and Analysis of experiments with mixtures. *Ann. Math. Stat.* **39**, 1517-39.

[4] Ramchandra Murthy, M.S. (1980) : Some studies on the design and analysis of experiments with mixtures. Ph.D., thesis, Osmania University, Hyderabad, (unpublished).

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

[6] Scheffe, H. (1963) : The simplex-centroid designs for experiments with mixtures. *Jour. Roy. Stat. Soc.* **B-25**

[7] Thompson, W.O and Myers, R.H. (1968) : Response surface designs for experiments with mixtures. *Technometrics*, **10**, 739-56.

[8] Westlake, J.R. (1968) : *A hand book of Numerical matrix inversions and solution of linear equation* John Wiley and Sons, Inc. New York.