OPERABILITY REGION AND OPTIMUM ROTATABLE DESIGNS

By ANIS CH. MUKHOPADHYAY

Indian Statistical Institute

SUMMARY. For exploring the relationship between response and a number of design variables or factors, we are usually interested in a small part of the factor space which may be termed 'operability region'. Assuming the operability region to be spherical and a spherical weight density function with positive weight density over the operability region and zero outside, it is possible to construct optimum designs which minimise weighted mean square bias due to inadequacy of the response function fitted in representing the true response, by using the results of Draper and Lawrence (1967). In particular, optimum second order designs which minimise the weighted mean square bias due to the presence of third order terms in the true response function have been considered in this paper. These designs are nothing but second order rotatable designs defined in the operability region with moments of order 5 all zero and a specific value for λ_4, depending on the particular weight density function assumed. In general situations where design variables are subject to a linear constraint and particularly in mixture experiments, a procedure is given for constructing optimum rotatable designs in a spherical operability region which forms a subspace of the hyperplane defined by the linear constraint. Some optimum properties of the response surface designs so constructed for mixture experiments are studied.

1. Introduction

1.0. Draper and Lawrence (1967) have proved that rotatable designs may be so selected as to minimise the weighted mean square bias, besides ensuring the same variance of estimated response at equidistant points from the origin in the factor space, privided a spherical density is assumed for weight function. The term 'optimum rotatable design' has been used in this paper in precisely the same sense, i.e., in the sense of a rotatable design having minimum weighted mean square bias for a particular spherical weight density function assumed. The results of Draper and Lawrence (1967) may be stated clearly as follows : Suppose as the response function a polynomial of degree d_1 is being fitted, while we want to guard it against a polynomial of degree $d_2 (d_2 > d_1)$. The weighted mean square bias due to the inadequacy of the chosen polynomial of degree d_1 in representing the true response is minimum, provided the moments of the design equal the moments of the weight density function upto and including order d_1+d_2. Moreover, if the weight density is spherical this optimality is achieved if the design is rotatable of order d, where (i) $d_1+d_2 = 2d$ or (ii) $d_1+d_2 = 2d+1$, and in case (ii) moments of order $2d+1$ should be all zero.

1.1. In practice we are never interested in the whole factor space. We want to explore the nature of the response function in a certain region about a fixed point in the factor space, usually chosen to be the origin. Moreover, the concept of weight function brings along with it, as a natural consequence, the idea of a domain in the factor space where the weight density is positive. This domain of the factor space where the weight density is positive has been called 'operability region'. The term 'operability region' has been used in similar sense by previous authors. This is actually the region where the experiment is to be performed. For a spherical weight density defined in a bounded region, the same bounded region which is also the operability region is spherical. For any design to be optimum within this operability region, it is required that (i) the design points all lie within this region and (ii) they give rise to moments equal to the corresponding moments of the weight density function upto a certain order.

2. Some particular spherical weight densities

2.0. Spherical weight function referred to in the previous section may be of various types. In particular, we may consider the following two simple types,[1] viz.,

(A) *Uniform distribution in a finite spherical region :*

$$f(x_1, x_2, \ldots, x_k) = c_1 \quad \text{for} \quad x_1^2+\ldots+x_k^2 \leqslant R^2 \qquad \ldots \quad (2.0.1)$$
$$= 0, \quad \text{otherwise}$$

where c_1 is a constant so adjusted that (2.0.1) is a density function.

(B) *Truncated normal distribution in a finite spherical region :*

$$f(x_1, x_2, \ldots, x_k) = c_2 e^{-\frac{1}{2}(x_1^2+\cdots+x_k^2)} \quad \text{for} \quad x_1^2 + \ldots + x_k^2 \leqslant R^2 \qquad \ldots \quad (2.0.2)$$
$$= 0, \quad \text{otherwise}$$

where c_2 is a constant so adjusted that (2.0.2) is a density function. In (2.0.1) same weight is given to all the points in the region, while in (2.0.2) weight of a point diminishes with increase in distance from the origin.

2.1. *First few moments of weight densities* (2.0.1) *and* (2.0.2) :

(i) *Weight density* (2.0.1) :

$$E(x_i^2) = \frac{R^2}{k+2}, \; E(x_i^4) = \frac{3R^4}{(k+4)(k+2)}$$

and
$$\underset{(i\neq j)}{E}(x_i^2 x_j^2) = \frac{R^4}{(k+4)(k+2)}; \quad i, j = 1, 2, \ldots, k \qquad \ldots \quad (2.1.1)$$

all other moments of order $\leqslant 5$ are zero.

(ii) *Weight density* (2.0.2) :

$$E(x_i^2) = \frac{P_{k+2}(R^2)}{P_k(R^2)}$$

$$E(x_i^4) = 3\underset{(i\neq j)}{E}(x_i^2 x_j^2) = \frac{3P_{k+4}(R^2)}{P_k(R^2)}; \quad i, j = 1, 2, \ldots k \qquad \ldots \quad (2.1.2)$$

where $P_n(R^2) = P\{\chi_n^2 \leqslant R^2\}$, χ_n^2 following χ^2 distribution with n d.f. All other moments of order $\leqslant 5$ are zero.

[1] It is to be noted that Draper and Lawrence (1967) too proceeded on similar lines. The designs given by them were all based on a weight density which was multivariate normal and consequently in spite of their stress on a finite region of interest, the operability region spanned the whole factor space. But minimisation of weighted mean square bias over the whole factor space may not give a useful design. Moreover, for all the designs given by them $\lambda_4 = 1$. But λ_4 should be desirably < 1 so that the variance of the estimate of response does not differ markedly in the neighbourhood of the origin.

3. Optimum second order rotatable designs

3.0. Let us consider optimum designs for $d_1 = 2$ and $d_2 = 3$. Optimum design will obviously depend on the weight density function assumed. For any chosen weight density function, optimum second order rotatable design, besides satisfying the general conditions of second order rotatability with moments of order 5 being zero should have λ_4 equal to a specific value $\frac{\underset{i \neq j}{E}(x_i^2 x_j^2)}{[E(x_i^2)]^2}$ given by the weight density assumed (of course this value of λ_4 must satisfy the usual non-singularity condition) and the design points should be all distributed in the operability region ($\sum_{i=1}^{k} x_i^2 \leqslant R^2$) defined by positive weight density. Let us now investigate the optimum designs for the weight densities (2.0.1) and (2.0.2).

(i) *Weight density* (2.0.1) : Moments (2.1.1) yield

$$\lambda_4 = \frac{k+2}{k+4}. \qquad \ldots \quad (3.0.1)$$

This value of λ_4 clearly satisfies non-singularity condition. With weight density (2.0.1), optimum second order rotatable design should be second order rotatable with moments of order 5 equal to zero and $\lambda_4 = \frac{k+2}{k+4}$. In any design so chosen with N points let $\mu_2 = \sum_{s=1}^{N} x_{is}^2/N$ for all i, $i = 1, 2, \ldots, k$ (N being the number of design points) define the second order moment. Equating μ_2 to $E(x_i^2)$ in (2.1.1) we get $R^2 = (k+2)\mu_2$. So, operability region is defined by $\sum_{i=1}^{k} x_i^2 \leqslant (k+2)\mu_2$. Or, for any given operability region $\sum_{i=1}^{k} x_i^2 \leqslant R^2$, the scale factor, i.e., the factor by which the design points in any chosen optimum design with μ_2 as the second moment of the design, are to be multiplied is given by $a = \frac{R}{\sqrt{\mu_2(k+2)}}$. The only other very important condition to be satisfied is that the design points in any optimum design so chosen must all lie in the operability region.

(ii) *Weight density* (2.0.2) : Moments (2.1.2) yield

$$\lambda_4 = \frac{P_{k+4}(R^2)P_k(R^2)}{[P_{k+2}(R^2)]^2}. \qquad \ldots \quad (3.0.2)$$

By Cauchy Schwartz's inequality the value of λ_4 in (3.0.2) is $> \frac{k}{k+2}$. The scale factor for any predetermined operability region is

$$a = \frac{1}{\sqrt{\mu_2}} \cdot \sqrt{\frac{P_{k+2}(R^2)}{P_k(R^2)}}.$$

3.1. *Optimality of central composite designs given by Box and Hunter* (1957). Let us consider a central composite design defined by Box and Hunter (1957) with

n_c = number of points from 2^k factorial design so chosen as to retain all main effects and interactions of order $\leqslant 4$ unconfounded.

n_a = number of star points = $2k$.

$n_0 = N - n_c - n_a$ = number of centre points.

For this central composite design

$$\lambda_4 = \frac{N}{n_c + 4(1+\sqrt{n_c})}. \qquad \dots \quad (3.1.1)$$

From (3.1.1) it is obvious that λ_4 for central composite designs may attain any prefixed value (in particular the values given by (3.0.1) and (3.0.2)) at least approximately, by selecting N and consequently n_0 suitably. The relation may be approximately satisfied, because N or n_0 has to be an integer always.

For the optimum central composite design with weight density (2.0.1) we have square of the radius of the operability region, $R^2 = \frac{\sqrt{n_c}}{\sqrt{n_c}+2}(k+4)$. In order that all design points lie within the operability region we must have $R^2 > k$, which reduces to the condition

$$n_c > \frac{k^2}{4}. \qquad \dots \quad (3.1.2)$$

The inequality (3.1.2) is usually trivial. Similarly, for optimum central composite design with weight density (2.0.2) the condition is

$$n_c > 4\left[\frac{P_{k+2}(k)}{P_{k+4}(k)} - 1\right]^2. \qquad \dots \quad (3.1.3)$$

[Since $\frac{P_{k+4}(R^2)}{P_{k+2}(R^2)} \leqslant 1$ always and is an increasing function in R].

3.2. *A class of optimum second order rotatable designs.* With central composite designs of Box and Hunter, any pre-assigned value of λ_4 determined by the weight density chosen can be attained only approximately in most of the cases. Moreover, the number of design points and consequently the number of centre points to be included for such a design becomes fixed. This is a too rigid condition, particularly when the experiment is performed sequentially. But by slightly modifying the central composite design, i.e., by including two sets of star points, it is possible to choose N arbitrarily and the design may be made to satisfy any predetermined value of λ_4 exactly. This modified design is given by

(i) $n_c = 2^{k-p}$ points of a 2^k factorial design with no main effects or interactions of order $\leqslant 4$ confounded;

(ii) $(b, 0, \dots 0) \times 2$ giving $2k$ points;

(iii) $(c, 0, \dots 0) \times 2$ giving $2k$ points;

(iv) $n_0 = N - n_c - 4k$ centre points.

Rotatability condition can be written as

$$b^4 + c^4 = n_c. \qquad \dots \quad (3.2.1)$$

For the design to be optimum, λ_4 should equal some pre-assigned value λ determined by the weight density assumed i.e.

$$\frac{n_c/N}{\dfrac{\{n_c+2(b^2+c^2)\}^2}{N^2}} = \lambda$$

or,

$$\frac{n_c+2(b^2+c^2)}{\sqrt{Nn_c}} = \frac{1}{\sqrt{\lambda}}$$

or,

$$b^2+c^2 = \frac{\sqrt{Nn_c}-n_c\sqrt{\lambda}}{2\sqrt{\lambda}}. \qquad \dots \quad (3.2.2)$$

From (3.2.1) and (3.2.2)

$$b^2-c^2 = \left[\frac{(8\lambda-N)n_c+2\sqrt{\lambda N}n_c^{3/2}-\lambda n_c^2}{4\lambda}\right]^{1/2}. \qquad \dots \quad (3.2.3)$$

Solving (3.2.2) and (3.2.3), b^2 and c^2 are obtained. For this design

$$\mu_2 = \frac{n_c+2(b^2+c^2)}{N} = \sqrt{\frac{n_c}{\lambda N}}. \qquad \dots \quad (3.2.4)$$

For any chosen $N > n_c+4k$ we get the value of μ_2 from (3.2.4) and scale factor $a = \sqrt[4]{\dfrac{\lambda N}{n_c}}\sqrt{f(R^2)}$ where $f(R^2) = E(x_i^2)$ for the spherical weight density assumed.

4. Optimum designs when design variables are subject to a linear constraint

4.0. In all the designs in previous sections, design variables have been assumed to vary unconditionally. But it may be that the design variables can assume values only under certain restriction imposed by practical considerations. If this restriction can be expressed mathematically in the form of a linear equation, the part of the factor space admissible for the purpose of experimentation is the hyperplane defined by the same linear equation. An operability region, if any, in this case must lie wholly in the hyperplane which is admissible. So, for these designs under a linear constraint, it is not possible to obtain an optimum rotatable design in all the k variables over an operability region defined in the k dimensional space. But the existence of an optimum rotatable design in $(k-1)$ dimensions for an operability region which forms a part of the admissible hyperplane is proved in the following subsections.

4.1. *Mixture design*. This is a particular type of design described in the above paragraph, where design variables refer to relative proportions of quantities applied with regard to different factors acting as inputs and response is a function of these relative proportions and not of absolute magnitudes of the different factors. For a mixture experiment with k factors, the admissible hyperplane is defined by

$$x_1+x_2 \dots +x_k = 1, \quad x_i \geqslant 0, \quad i = 1, 2, \dots, k. \qquad (4.1.1)$$

The mixture designs known so far are simplex lattice designs and simplex centroid designs (Scheffe, 1958; 1963), extreme vertices designs (Mclean and Anderson, 1966) and optimum designs for $k = 3$ and 4 with uniform weight density defined over the whole admissible simplex (Draper and Lawrence, 1965a; 1965b). These designs are all constructed on the assumption that the whole admissible simplex defined by (4.1.1) is of interest to us and is practically feasible for the purpose of experimentation. Moreover, most of these designs suffer from an arbitrary and uneven distribution of points. But, usually the purpose of experimentation is to obtain an optimum response if one such exists and whether such a unique optimum exists or not to explore the nature of response function in the near optimum region. So, in practice we are not interested in the whole admissible region. Either from practical considerations or guess work, we know tentatively that the optimum response occurs near about the point $P' = (p_1, p_2, ..., p_k)$, with $\sum_{i=1}^{k} p_i = 1$ and $p_i \geqslant 0$, $i = 1, 2, ..., k$ and we are interested in exploring the response function in a well-defined operability region round about the point P'. Within this operability region, assumed to be circular or spherical (of course the region becomes just the segment of a straight line when $k = 2$) which lies completely within the admissible simplex, an optimum rotatable design for a particular choice of a weight density function in $(k-1)$ dimensions can be constructed. To satisfy the essential condition that operability region forms a part of the admissible simplex, the operability region should be defined as

$$\left.\begin{aligned} & \sum_{i=1}^{k} (x_i - p_i)^2 \leqslant r^2 \\ \text{with} \quad & \sum_{i=1}^{k} x_i = 1, \quad x_i \geqslant 0 \quad \text{for } i = 1, 2, ..., k \\ \text{where} \quad & r \leqslant \sqrt{\frac{k}{k-1}} \min(p_1, ..., p_k). \end{aligned}\right\} \quad \ldots \quad (4.1.2)$$

The region (4.1.2) can be written in terms of transformed variables $y_1, ..., y_k$ where $y_i = x_i - p_i$, $i = 1, 2, ..., k$ as

$$\sum_{i=1}^{k} y_i^2 \leqslant r^2 \quad \text{with} \quad y_i \geqslant -p_i \quad \text{for} \quad i = 1, 2, ..., k,$$

$$\sum_{i=1}^{k} y_i = 0$$

and

$$r \leqslant \sqrt{\frac{k}{k-1}} \min(p_1, p_2, ..., p_k).$$

Let us introduce an orthogonal transformation $\xi = Cy$ where $\xi' = (\xi_1, ..., \xi_k)$, $y' = (y_1 ... y_k)$ and C is an orthogonal matrix with first row as $\left(\frac{1}{\sqrt{k}}, \frac{1}{\sqrt{k}}, ..., \frac{1}{\sqrt{k}}\right)$. Then ξ_1 is identically zero and admissible simplex (4.1.1) is a $(k-1)$ dimensional hyperplane defined effectively by the variables $\xi_2, \xi_3, \ldots, \xi_k$. Moreover, $\sum_{i=2}^{k} \xi_i^2 = \sum_{i=1}^{k} y_i^2$. So, the operability region is now a hypersphere in $(k-1)$ dimensions defined by

$$\sum_{i=2}^{k} \xi_i^2 < r^2 \text{ where } r < \sqrt{\frac{k}{k-1}} \min (p_1, \ldots, p_k). \qquad \ldots \quad (4.1.3)$$

From the above results the following construction procedure[2] for mixture designs can be given :

We can construct an optimum design in $\xi_2, \ldots, \xi_k$ in the above operability region, for a suitable choice of the weight density function. To any design point obtained for the factors $\xi_2, \xi_3, \ldots, \xi_k$ we can add $\xi_1 = 0$ and the corresponding design point in variables $y_1, y_2, \ldots, y_k$ can be written with the help of the transformation

$$y = C'\xi$$

and the corresponding design point in the original design variables $x_1, x_2, \ldots, x_k$ is given by $x' = (x_1, x_2, \ldots, x_k)$ where

$$x' = y+P = C'\xi+P. \qquad \ldots \quad (4.1.4)$$

When nothing is known about the nature of response in a mixture experiment so that each design variable has to be given the same weight initially we can choose P' as the centroid $\left(\frac{1}{\sqrt{k}}, \ldots, \frac{1}{\sqrt{k}}\right)$ of the admissible simplex (4.1.1) i.e. where each design variable is given the same value. In this case, operability region may have the maximum area or content and r can be any quantity $\leqslant \frac{1}{\sqrt{k(k-1)}}$. Depending on the results of this experimentation, we can revise P' and explore a smaller operability region with this point in the central position and in this way we can proceed. In all these cases, however small the chosen operability region may be, it can be magnified for the purpose of constructing a design and exploring the nature of response.

The non-uniqueness in the representation of the response function as pointed out by Scheffe (1958, 1963) can be overcome by considering the response as a polynomial in $\xi_2, \ldots, \xi_k$ and fitting it by method of least square. The apparent arbitrariness in the form of the transformation matrix C is not a problem. The expectation and variance of an estimated response does not depend on the form of C.[3] Some further properties of the design so constructed which are considered important are enumerated here with proof.

(I) The spherical weight distribution in $y_1, y_2, \ldots, y_k$ defined over the hyperplane $\sum_{i=1}^{k} y_i = 0$ remains unaltered by any choice of an orthogonal matrix C with first row $\left(\frac{1}{\sqrt{k}}, \ldots, \frac{1}{\sqrt{k}}\right)$.

[2]The construction procedure described here has appeared in a recently published paper by William O. Thompson and Raymond H. Mayers (1968) without the corresponding inequality restrictions on the operability region given by (4.1.2) or (4.1.3), which are deemed very important in so far as the construction of an optimum design in a well-defined spherical operability region is the objective of the present paper.

[3]This result has been proved by Thompson and Mayers (1968) and so is not included here.

Proof : Writing $\xi = Cy$, $\xi_1 = 0$, a spherical weight density is considered in $\xi_2, \xi_3, \ldots, \xi_k$, so that the required probability, say, T of

$$\left\{\sum_{i=1}^{k} y_i^2 < l^2, \sum_{i=1}^{k} y_i = 0\right\}$$

is the same as

$$P\left\{\sum_{i=2}^{k} \xi_i^2 < l^2, \quad \xi_1 = 0\right\} \qquad \ldots \quad (4.1.5)$$

where l is a constant.

If we consider another orthogonal transformation

$$\xi^{(1)} = C_1 y, \quad \text{with } \xi^{(1)'} = (\xi_1' = 0, \; \xi_2' \ldots \xi_k')$$

and the same spherical weight density as earlier for $\xi_2' \ldots \xi_k'$ then,

$$T = P\left\{\sum_{i=2}^{k} \xi_i'^2 < l^2, \quad \xi_1' = 0\right\}. \qquad \ldots \quad (4.1.6)$$

Relation between $\xi^{(1)}$ and ξ is

$$\xi^{(1)} = C_1 C' \xi = \begin{pmatrix} 1 & 0 \\ 0 & P \end{pmatrix} \xi$$

where P is a $(k-1)\times(k-1)$ orthogonal matrix

$$\begin{bmatrix} \xi_2' \\ \xi_3' \\ \vdots \\ \xi_k' \end{bmatrix} = P \begin{bmatrix} \xi_2 \\ \xi_3 \\ \vdots \\ \xi_k \end{bmatrix}$$

The weight density for $(\xi_2', \ldots, \xi_k')$ being same as that for $(\xi_2, \ldots, \xi_k)$, the expressions (4.1.5) and (4.1.6) are identical. This proves the statement (I).

(II) For any choice of the orthogonal matrix C with first row $\left(\frac{1}{\sqrt{k}}, \frac{1}{\sqrt{k}}, \ldots, \frac{1}{\sqrt{k}}\right)$ the same minimum weighted mean square bias is obtained.

Proof : As the weight distribution and also the expectation of estimated response remain unaltered for any such choice of C, weighted mean square bias defined as $\int_{0} W(x)\{E\hat{\eta}(x) - \eta(x)\}^2 dx$ will obviously remain the same, where $W(x)$ is the weight density defined in the operability region 0 within the $(k-1)$ dimensional admissible simplex (4.1.1), $\hat{\eta}(x)$ is the estimated response and $\eta(x)$ the true response, x denoting the vector $(x_1, x_2, \ldots, x_k)$.

4.2. *Generalised mixture experiments.* The linear constraint in mixture experiments may be generalised as follows :

$$a_1x_1+a_2x_2 \dots +a_kx_k = c \quad \dots \quad (4.2.1)$$

where a_i's and c are constant with

$$a_i > 0, c > 0, \ x_i \geqslant 0, \ i = 1, 2, \dots, k.$$

The point $P' = (p_1, p_2, \dots, p_k)$ should satisfy the relation

$$a_1p_1+a_2p_2 \dots +a_kp_k = c.$$

With each $p_i \geqslant 0$ we can construct an optimum rotatable design with P' as the central point in a spherical operability region of radius r in $(k-1)$ dimensions defined by (4.2.1). The procedure is exactly same as in ordinary mixture experiments described in Section 4.1 and

$$r \leqslant \sqrt{L}. \min_{1\leqslant i\leqslant k}\left\{\frac{p_i}{\sqrt{L-a_i^2}}\right\} \quad \dots \quad (4.2.2)$$

where

$$L = \sum_{j=1}^{k} a_j^2.$$

Of course, the orthogonal matrix C, transforming y's to ξ's has the first row as

$$\left(\frac{a_1}{\sqrt{L}}, \frac{a_2}{\sqrt{L}} \dots \frac{a_k}{\sqrt{L}}\right).$$

4.3. *Experiments where the linear constraint does not involve all the design variables.* The linear constraint is written as

$$a_1x_1+a_2x_2 \dots +a_kx_k = c \quad \dots \quad (4.3.1)$$

with each $\quad a_i > 0, c > 0 \ x_i \geqslant 0, \ i = 1, 2, \dots, k.$

We have $p(\geqslant 1)$ more design variables, viz., $x_{k+1}, x_{k+2} \dots x_{k+p}$, with no restriction imposed on them.

By choosing suitable scales and origins for the variables $x_{k+1}, x_{k+2} \dots x_{k+p}$, the central point P' is taken to be $(p_1, p_2, \dots, p_k, 0, \dots, 0)$ where $a_1p_1+a_2p_2 \dots +a_kp_k = c$, $p_i \geqslant 0$ for $i = 1, 2, \dots, k$. Here too, an optimum rotatable design can be constructed in the same manner as described in Sections 4.1 and 4.2. r = radius of the spherical operability region should be

$$\leqslant \sqrt{L}. \min_{1\leqslant i\leqslant k}\left\{\frac{p_i}{\sqrt{L-a_i^2}}\right\} \quad \dots \quad (4.3.2)$$

and the transformation matrix C will have the first row as

$$\left(\frac{a_1}{\sqrt{L}}, \frac{a_2}{\sqrt{L}}, \dots, \frac{a_k}{\sqrt{L}}, 0, \dots, 0\right).$$

A proof of the inequalities in r given in (4.1.2), (4.2.2) and (4.3.2) is provided in the appendix.

Appendix

Let us define an admissible region by

$$a_1x_1+a_2x_2+\ldots+a_kx_k = c \qquad \ldots \text{(i)}$$

with $c > 0$, $a_i > 0$ and $x_i \geqslant 0$ for all i, $i = 1, 2, \ldots, k$. Then the admissible region is a $(k-1)$ dimensional hyperplane defined only for non-negative value of the variables, with corner points given by

$$\left(\frac{c}{a_1}, 0 \ldots 0\right), \left(0, \frac{c}{a_2}, 0, \ldots 0,\right) \ldots \left(0, \ldots 0, \frac{c}{}\right).$$

An edge of the admissible region is again a $(k-2)$ dimensional hyperplane passing through $(k-1)$ of the k corner points, defined only for non-negative values of the variables. So, the equation of the edge passing through all but i-th corner point is

$$\left.\begin{array}{l} a_1x_1 \ldots +a_{i-1}x_{i-1}+a_{i+1}x_{i+1} \ldots +a_kx_k = c \\ x_i = 0, \quad x_j \geqslant 0, \quad j \neq i, \quad j = 1, 2, \ldots, k. \end{array}\right\} \qquad \ldots \text{(ii)}$$

Now, $P' = (p_1, \ldots, p_k)$ is a point in the admissible region. So, $ap_1 \ldots + ap_k = c$, and $p_i \geqslant 0$, for $i = 1, 2, \ldots, k$. The length of the perpendicular from P' on the edge defined by (ii) is easily found to be

$$\left\{p_i^2+\frac{(a_1p_1+\ldots+a_{i-1}p_{i-1}+a_{i+1}p_{i+1} \ldots +a_kp_k-c)^2}{L-a_i^2}\right\}^{\frac{1}{2}}, \quad \text{where} \quad L = \sum_{j=1}^{k} a_j^2$$

$$= \sqrt{\frac{p_i^2.L}{L-a_i^2}} = \sqrt{L}.p_i \sqrt{\frac{1}{L-a_i}} \qquad \ldots \text{(iii)}$$

writing $a_1 = a_2 \ldots = a_k = c = 1$, this length of the perpendicular is $\sqrt{\frac{k}{k-1}}\, p_i$.

Operability region is just a hypersphere with P' as the centre and lying wholly within the admissible region. For this reason, the radius of the hypersphere must be less than or equal to the minimum of the perpendicular lengths obtained in (iii).

If besides the k variables which must satisfy the relation (i), $p(\geqslant 1)$ new variables are introduced with no restriction imposed on them, the situation remains unchanged excepting that the dimension of the admissible region is increased by p. The equations of the edges given by (ii) will still hold good and the length of the perpendicular from $P' = (p_1, \ldots, p_k, 0, \ldots, 0)$ on the edge (ii) is given by the same expression (iii).

References

Box, G. E. P. and Hunter, J. S. (1957): Multifactor experimental designs for exploring response surfaces. *AMS*, **28**, 195-241.

Draper, N. R. and Lawrence, W. E. (1967): Sequential designs for spherical weight functions. *Technometrics*, **9**, 517-530.

——— (1965a): I. Mixture designs for three factors. *JRSS* B, **27**, 450-465. II. Mixture designs for four factors. *JRSS* B, **27**, 473-478.

——— (1965b): Designs which minimise model inadequacies in cuboidal regions of interest. *Biometrika*, **52**, 111-118.

McLean, R. A. and Anderson, V. L. (1966): Extreme vertices designs for mixture experiments. *Technometrics*, **8**, 447-454.

Scheffe, H. (1958): Experiments with mixture. *JRSS* B, **20**, 344-366.

——— (1963): The simplex centroid design for experiment with mixtures. *JRSS* B, **25**, 235-251.

Thompson, William O. and Myers, Raymond H. (1968): Response surface designs for experiments with mixtures. *Technometrics*, **10**.

Paper received : December, 1968.