A NEW MEASURE OF ROTATABILITY OF RESPONSE SURFACE DESIGNS

ANANT M. KSHIRSAGAR[1] AND JOANNA CHUNG-IN CHENG[1]

University of Michigan

Summary

This paper proposes a new measure of rotatability of a response sur-
face design. It is based on a comparison between the design moments of
a given design and the design moments of a rotatable design closest to the
given design in the least squares sense. This measure is easier to calculate
than Khuri's measure. An alternative easier non-geometrical way of deriving
Khuri's measure is also presented. Both measures are calculated to illustrate
some designs considered by Khuri.

Key words: Rotatability; response surface designs; design moments.

1. Introduction

Rotatability as defined by Box & Hunter (1957) is an important property
of response surface designs. It ensures equal precision of estimated responses at
equal distances from the centroid of the design. Box & Hunter derived certain
conditions on the moments of a design matrix that must be satisfied for rotata-
bility. Khuri (1988) and Draper & Gutterman (1988) have suggested measures of
departure from rotatability. Khuri uses a geometrical approach, projecting a vec-
tor associated with the design matrix on the cone of rotatability, after expressing
the vector in a canonical form.

In this paper we suggest an alternative measure of the rotatability of a de-
sign. This measure is based on the design moments and is easier to calculate. We
given an explicit formula for this measure and compare it with Khuri's measure.
Incidentally, we derive Khuri's measure by an alternative analytical method that
does not require geometrical concepts.

2. Moments of a Design

Consider a response surface model of degree d in the levels $x_1, \ldots, x_k$ of k
factors and N experimental runs. The model for the response variable y is then

$$E(y) = \mathbf{x}^{[d]'}\beta,$$

where $\mathbf{x}^{[d]}$ is the 'derived power vector of degree d' or Schlaffian associated with the vector

$$\mathbf{x}' = [1, x_1, \ldots, x_k]$$

as defined by Box & Hunter (1957) (see also Myers, 1971). It is in fact a vector such that

$$\mathbf{x}^{[d]'}\mathbf{x}^{[d]} = (\mathbf{x}'\mathbf{x})^d.$$

For example, $x^{[2]'} = [1, \sqrt{2}x_1, \ldots, \sqrt{2}x_k, x_1^2, \ldots, \sqrt{2}x_1 x_2, \ldots]$ and is obtained from the terms in the expansion of $(\mathbf{x}'\mathbf{x})^d$. Let x_{iu} be the level of the ith factor in the uth run and let X be a matrix with N rows, the uth row of which equals $\mathbf{x}_u^{[d]'}$. The moment of order $\delta = \delta_1 + \cdots + \delta_k$ of this design is then

$$M(\delta_1, \ldots, \delta_k) = \sum_{u=1}^{N} x_{1u}^{\delta_1} \ldots x_{ku}^{\delta_k}.$$

If δ is even, this is called an even moment. Box & Hunter showed that the design moments of such a design are obtained from the generating function

$$\Phi(\mathbf{t}) = \mathbf{t}^{[d]'} X'X \mathbf{t}^{[d]} = \sum_{u=1}^{N} \left(1 + \sum_{i=1}^{k} t_i x_{ui}\right)^{2d},$$

where $\mathbf{t}' = [1, t_1, \ldots, t_k]$. The coefficient of $t_1^{\delta_1} \ldots t_k^{\delta_k}$ in $\Phi(\mathbf{t})$ is

$$a(\delta_1, \ldots, \delta_k)M(\delta_1, \ldots, \delta_k) \qquad (\delta \le 2d),$$

where

$$a(\delta_1, \ldots, \delta_k) = \frac{(2d)!}{(2d - \delta)! \prod_{i=1}^{k}(\delta_i!)}. \qquad (2.1)$$

For a rotatable design Box & Hunter showed that $\Phi(\mathbf{t})$ is of the form

$$\Phi_R(\mathbf{t}) = \sum_{j=0}^{d} a_{2j}\left(\sum_{i=1}^{k} t_i^2\right)^j$$

for some a_{2j}s . Therefore the moments $M_R(\delta_1, \ldots, \delta_k)$ of a rotatable design are of the form

$$M_R(\delta_1, \ldots, \delta_k) = \theta_\delta C(\delta_1, \ldots, \delta_k) I(\delta_1, \ldots, \delta_k), \qquad (2.2)$$

where

$$\theta_\delta = \frac{a_\delta 2^{\delta/2}(\delta/2)!(2d - \delta)!}{(2d)!},$$

$$C(\delta_1,\ldots,\delta_k) = \frac{\prod_i \delta_i!}{2^{\delta/2}\prod_i(\delta_i/2)!},$$

$$I(\delta_1,\ldots,\delta_k) = \begin{cases} 1 & \text{if every } \delta_i \text{ is even,} \\ 0 & \text{otherwise.} \end{cases}$$

As in Khuri (1988) we assume that $\sum_u x_{iu} = 0$, $\sum x_{iu}^2 = 1$ for all i; otherwise we define

$$x_{iu} = \frac{x_{iu}^* - \bar{x}_i^*}{\left[\sum_{u=1}^{N}(x_{iu}^* - \bar{x}_i^*)^2\right]^{1/2}}$$

for the original levels x_{iu}^* and work with these transformed values. This, as Khuri (1988) explains, is necessary to have our measures of rotatability invariant with respect to origin and scale. As a result, in addition to the obvious property $M(0,\ldots,0) = N$, our design D has

$$M(0,\ldots,0,1,\ldots,0) = 0, \quad M(0,\ldots,0,2,0,\ldots,0) = 1$$

where the 1 and 2 in the last two moments are in the ith places $(i = 1,\ldots,k)$.

3. A New Measure of Rotatability

To define this measure of rotatability for the design D, we consider a rotatable design D_R, for which

$$M_R(0,\ldots,0,1,\ldots,0) = 0, \quad M_R(0,\ldots,0,2,0,\ldots,0) = 1$$

(like those moments of D) and the arbitrary θ_δ (or a_δ) in its other moments are such that the sum of squares of the differences in the coefficients of $t_1^{\delta_1}\ldots t_k^{\delta_k}$ in $\Phi(t)$ and $\Phi_R(t)$ is minimum. The design D_R is then closest to the given design D in a least squares sense. The quantity

$$\Psi = \sum a^2(\delta_1,\ldots,\delta_k)[M(\delta_1,\ldots,\delta_k) - M_R(\delta_1,\ldots,\delta_k)]^2$$

$$= \sum a^2(\delta_1,\ldots,\delta_k)[M(\delta_1,\ldots,\delta_k) - \theta_\delta C(\delta_1,\ldots,\delta_k)I(\delta_1,\ldots,\delta_k)]^2,$$

where the summation extends over all $(\delta_1,\ldots,\delta_k)$ and is thus minimised with respect to θ_δ. Separating the odd and even order moments in Ψ, excluding all $(\delta_1,\ldots,\delta_k)$ such that $\delta = 0$ or 1 (as $M = M_R$ for these values) and observing that $M_R = 0$ if δ is odd, we can easily see that the value of θ_δ that minimises Ψ and gives the rotatable design D_r that is closest to D, is

$$\hat{\theta}_\delta = \frac{\sum'' M(\delta_1,\ldots,\delta_k)C(\delta_1,\ldots,\delta_k)/(\prod \delta_i!)^2}{\sum'' C^2(\delta_1,\ldots,\delta_k)/(\prod \delta_i!)^2},$$

where $\sum''$ denotes summation over all $(\delta_1,\ldots,\delta_k)$ such that each δ_i is even or zero and $\sum \delta_i = \delta$. The minimum value of Ψ, using this optimum $\hat\theta_\delta$ is easily seen to be

$$\Psi_{\min} = \sum a^2(\delta_1,\ldots,\delta_k)M^2(\delta_1,\ldots,\delta_k) - \sum_{\delta=4}^{2d}\sum{}'' \hat\theta_\delta^2(\delta_1,\ldots,\delta_k)C^2(\delta_1,\ldots,\delta_k),$$

where the first summation $\sum$ is over all $(\delta_1,\ldots,\delta_k)$ except when $\delta = 0$ and $\delta = 1$. A measure of rotatability then should compare this $\Psi_{\min}$ with the sum of squares of the coefficients of $t_1^{\delta_1}\ldots t_k^{\delta_k}$ in $\Phi(t)$ of the given design. We therefore propose

$$R = \frac{\sum_{\delta=4}^{2d}\sum{}'' \hat\theta_\delta^2 a^2(\delta_1,\ldots,\delta_k)C^2(\delta_1,\ldots,\delta_k)}{\sum{}' a^2(\delta_1,\ldots,\delta_k)M^2(\delta_1,\ldots,\delta_k)} \times 100\%. \qquad (3.1)$$

The summation in the denominator is over all $(\delta_1,\ldots,\delta_k)$ except when $\delta = 0$, $\delta = 1$ or when only one $\delta_i = 2$, the rest being all equal to 0.

4. Khuri's Measure of Rotatability

The matrix X we defined in Section 1 has $x_u^{[d]'}$ as its uth row. Khuri defines his matrix X in a slightly different way. It has, in the uth row, the elements $1, x_{1u}, x_{2u}, \ldots, x_{ku}, x_{1u}^2, x_{2u}^2, \ldots, x_{1u}x_{2u}, \ldots$ etc. Each element is a product of powers of x_{iu} $(i = 1,\ldots,k)$ such that the degree is d or less. The entries in our matrix X are algebraically very like those of Khuri, apart from the numerical coefficients, which in our case are not all unity. For Khuri's matrix, $X'X$ has the elements $M(\delta_1,\ldots,\delta_k)$ and they occur different numbers of times in $X'X$. Let $f(\delta_1,\ldots,\delta_k)$ be the number of times $M(\delta_1,\ldots,\delta_k)$ occurs on the diagonal of $X'X$ or above it. Khuri then considers the sum of squares Ψ_k of differences of the elements of his $X'X$ (on the diagonal and above it) with the corresponding elements of the $X'X$ matrix of the closest rotatable design D_R, excluding the moments $M(0,\ldots,0)$, $M(0,\ldots,1,0\ldots,0)$ (1 in the ith place; $i = 1,\ldots,k$), $M(0,\ldots,0,2,0,\ldots,0)$, (2 in the ith place; $i = 1,\ldots,k$). He uses a vec notation. But all this amounts to minimising (with respect to θ_δ)

$$\Psi_k = \sum f(\delta_1,\ldots,\delta_k)[M(\delta_1,\ldots,\delta_k) - C(\delta_1,\ldots,\delta_k)\theta_\delta I(\delta_1,\ldots,\delta_k)]^2 \qquad (4.1)$$

where the summation is over all $(\delta_1,\ldots,\delta_k)$ except those corresponding to moments of order 0,1 and pure moments of order 2. This gives the closest rotatable design D_R. Khuri's measure K has an expression very similar to our R, except that $a(\delta_1,\ldots,\delta_k)$ in (3.4) is replaced by $f(\delta_1,\ldots,\delta_k)$. Both these measures R and K are, in a sense, weighted averages of squared differences of the moments of D and those of the closest D_R. Only the weights are different. The measure R has the advantage that $a(\delta_1,\ldots,\delta_k)$ has an explicit formula but for Khuri's K, $f(\delta_1,\ldots,\delta_k)$ must be counted by actually writing down $X'X$.

<div align="center">

TABLE 1

Moments of D and D_R; frequencies of f and coefficients a

</div>

Moment	$f(\delta_1,\delta_2)$	δ	$a(\delta_1,\delta_2)$	$M_R(\delta_1,\delta_2) = \theta_\delta C(\delta_1,\delta_2)I$
$M(0,0) = n$	1	0	1	$M_R(0,0) = n$
$M(1,0) = M(0,1) = 0$	1	1	4	$M_R(1,0) = M_R(0,1) = 0$
$M(1,1)$	2	2	12	$M_R(1,1) = 0$
$M(2,0) = M(0,2) = 1$	2	2	6	$M_R(2,0) = M_R(0,2) = 1$
$M(2,1), M(1,2)$	2	3	12	$M(2,1) = M(1,2) = 0$
$M(2,2)$	2	4	6	θ_4
$M(3,0), M(0,3)$	1	3	4	$M_R(3,0) = M_R(0,3) = 0$
$M(3,1), M(1,3)$	1	4	4	$M_R(3,1) = M_R(1,3) = 0$
$M(4,0), M(0,4)$	1	4	1	$M_R(4,0) = M_R(0,4) = 3\theta_4$

5. Rotatability of a Second Order Design, with Two Factors

For $d = 2$ and $k = 2$, Khuri's $X'X$ matrix (when $\sum x_i = 0$, $\sum x_i^2 = 1$) is

$$
\begin{bmatrix}
n & 0 & 0 & 1 & 1 & M(1,1) \\
 & 1 & M(1,1) & M(2,0) & M(1,2) & M(2,1) \\
 & & 1 & M(2,1) & M(0,3) & M(1,2) \\
 & & & M(4,0) & M(2,2) & M(3,1) \\
 & & & & M(0,4) & M(1,3) \\
 & & & & & M(2,2)
\end{bmatrix}
$$

Table 1 shows the frequencies $f(\delta_1,\delta_2)$ of $M(\delta_1,\delta_2)$ in the above matrix and the coefficients $a(\delta_1,\delta_2)$ as defined in (2.1), and the corresponding values $M_R(\delta_1,\delta_2)$ of a rotatable design, as given by (2.2).

Khuri's Ψ_k then becomes

$$
\begin{aligned}
\Psi_k &= \sum f(\delta_1,\delta_2)[M(\delta_1,\delta_2) - M_R(\delta_1,\delta_2)]^2 \\
&= 2M^2(1,1) + 2M^2(2,1) + 2M^2(1,2) + M^2(3,0) + M^2(0,3) \\
&\quad + M^2(3,1) + M^2(1,3) + 2[M(2,2) - \theta_4]^2 \\
&\quad + [M(4,0) - 3\theta_4]^2 + [M(0,4) - 3\theta_4]^2.
\end{aligned}
$$

Minimising Ψ_k with respect to θ_4, we find that the closest D_R has

$$
\hat{\theta}_4 = \frac{1}{20}[2M(2,2) + 3M(4,0) + 3M(0,4)].
$$

Hence,

$$
K = \frac{100\% \times 20 \times \hat{\theta}_4^2}{\sum_{\delta=2}^{4}{}' f(\delta_1,\delta_2)M^2(\delta_1,\delta_2)},
$$

TABLE 2

Roquemore designs

Design	310	311A	311B
K	94.89%	99.40%	98.99%
R	97.16%	99.82%	98.46%

where the summation $\sum'$ excludes $M(0,2)$ and $M(2,0)$. Therefore,

$$K = \frac{100\% \times [2M(2,2) + 3M(4,0) + 3M(0,4)]^2}{20[2M^2(1,1) + 2M^2(1,2) + 2M^2(2,1) + 2M^2(2,2) + M^2(3,0) \atop + M^2(0,3) + M^2(3,1) + M^2(1,3) + M^2(4,0) + M^2(0,4)]}. \quad (5.1)$$

The optimum value of θ_4 in the measure R we propose is obtained by minimising

$$\Psi = 144[M^2(1,1) + M^2(2,1) + M^2(1,2)] + 36[M(2,2) - \theta_4]^2$$
$$+ 16[M^2(3,0) + M^2(0,3)] + 16[M^2(3,1) + M^2(1,3)]$$
$$+ [M(4,0) - 3\theta_4]^2 + [M(0,4) - 3\theta_4]^2$$

with respect to θ_4, yielding

$$\tilde{\theta}_4 = \frac{1}{18}[M(4,0) + M(0,4) + 12M(2,2)].$$

Substituting this in R we find,

$$R = \frac{100\% \times \frac{1}{6}[M(4,0) + M(0,4) + 12M(2,2)]^2}{(144[M^2(1,1) + M^2(2,1) + M^2(1,2)) + 36[M^2(2,2) + 16[M^2(3,0) \atop + 16M^2(0,3) + 16M^2(3,1) + 16M^2(1,3) + M^2(0,4) + M^2(4,0)]}. \quad (5.2)$$

We use these expressions to find the measure of rotatability of the 3^2 factorial design considered by Khuri that has $n = 9$, $M(1,1) = M(1,2) = M(2,1) = M(3,0) = M(0,3) = M(1,3) = M(3,1) = 0$, $M(2,2) = 1/9$ and $M(4,0) = M(0,4) = 1/6$. From (5.1) and (5.2), for this design, the rotatability index is

$$K = 93.08\%, \quad R = 92.60\%.$$

Khuri has calculated K for Roquemore (1976) designs with $k = 3$ and $d = 2$. We give K and R for these three designs in Table 2.

Finally we consider Scheffé's (1958) mixture design with $k = 3$ factors and the model

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3.$$

For the design, the vertex point, i.e. a point of the type

$$x_i = 1, \quad x_j = 0 \qquad (i \neq j, \; i,j = 1,2,3),$$

is repeated r_a times; the mid-point, i.e. a point of the type

$$x_i = x_j = \tfrac{1}{2}, \quad x_k = 0 \qquad (i \neq j \neq k),$$

is repeated r_b times. Cheng (1991) showed that for this design,

$$R = \frac{3b^2}{b^2 + 68a^2 + 1}, \qquad \text{while} \qquad K = \frac{4b^2}{4b^2 + 24a^2 + 1},$$

where

$$a = \frac{1}{9c^{3/2}}\left(-r_a + \tfrac{1}{8}r_b \right), \quad b = \frac{1}{9c^2}\left(r_a + \tfrac{1}{16}r_b \right), \quad c = \tfrac{2}{3}r_a + \tfrac{1}{6}r_b.$$

6. Conclusions

Note that both the measures of K and R are weighted averages of the squared differences between moments of a given design and those of the closest rotatable design, but the advantage of R is that the weights have an explicit formula, while for k one needs to write the whole $X'X$ matrix and count the frequencies $f(\delta_1, \ldots, \delta_k)$ of the different moments. Our measure R should prove useful in algorithms for the automatic construction of near-optimal designs where approximate rotatability is a desirable additional property.

References

BOX, G.E.P. & HUNTER, J.S. (1957). Multifactor experimental designs for exploring response surfaces. *Ann. Math. Statist.* **28**, 195–241.

CHENG, JOANNA CHUNG-IN. (1991). Some Aspects of Mixture and Response Surface Designs. PhD dissertation, Dept of Biostatistics, University of Michigan, Ann Arbor.

DRAPER, N.R. & GUTTERMAN, I. (1988). An index of rotatability. *Technometrics* **30**, 105–111.

KHURI, A.I. (1988). A measure of rotatability for response-surface designs. *Technometrics* **30**, 95–104.

MYERS, R.H. (1971). *Response Surface Methodology.* Boston: Allyn and Bacon.

ROQUEMORE, K.G. (1976). Hybrid designs for quadratic response surfaces. *Technometrics* **18**, 419–423.

SCHEFFÉ, H. (1958). Experiments with mixtures. *J. Roy. Statist. Soc. Ser. B* **20**, 344–360.