

A MEASURE OF ROTATABILITY FOR SECOND ORDER RESPONSE SURFACE DESIGNS

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Abstract. The concept of rotatability introduced by Box and Hunter (1957, *Ann. Math. Statist.*, **28**, 195-241) is an important design criterion for response surface design. Recently, a few measures of rotatability that enable us to assess the degree of rotatability for a given response surface design have been introduced. In this paper, a new measure of rotatability for second order response surface designs is suggested, and illustrated for 3^k factorial design and central composite design. Also a short comparison is made between the proposed measure with the previously suggested measures.

Key words and phrases: Rotatability, measure, response surface design, factorial design, central composite design.

1. Introduction

Suppose that an experimenter is concerned with a system involving some response η which depends on several independent variables ξ_1, \dots, ξ_k . In general, the functional relationship between the independent variables and the mean response can be written as $\eta = f(\xi_1, \dots, \xi_k)$, where the explicit form of f is unknown or extremely complicated. Response Surface Methodology (RSM) often involves the approximation of f by a low order polynomial in some region of the independent variables. Usually, the original variables (ξ 's) are coded to the design variables (x 's) in order to locate the origin to the center of region, the latter normally being simple linear functions of the former.

In this paper, we will concentrate on the second order model

$$\eta(\mathbf{x}) = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i < j}^k \beta_{ij} x_i x_j$$

which may be written in matrix notation as

$$(1.1) \quad \eta(\mathbf{x}) = \mathbf{x}'_s \boldsymbol{\beta},$$

in which

$$\begin{aligned}\mathbf{x}' &= (x_1, x_2, \dots, x_k), \\ \mathbf{x}'_s &= (1, x_1, x_2, \dots, x_k, x_1^2, x_2^2, \dots, x_k^2, x_1x_2, \dots, x_{k-1}x_k),\end{aligned}$$

and β is the $m \times 1$ column vector corresponding to the coefficients, where $m = (k+1)(k+2)/2$.

The coefficients in the polynomial are to be estimated, by the method of least squares, from N observations on the response variable,

$$y_u = \eta(\mathbf{x}_u) + \epsilon_u, \quad u = 1, 2, \dots, N$$

where ϵ_u 's are assumed to be uncorrelated and have zero means and constant variance, σ^2 . The β is then estimated by the method of least squares as follows

$$(1.2) \quad \mathbf{b} = (X'X)^{-1}X'\mathbf{y}$$

in which X is the $N \times m$ matrix of values of the m elements of \mathbf{x}_s 's taken at the design points and \mathbf{y} is the $N \times 1$ matrix of observations.

The predicted response value at a particular point $\mathbf{x}' = (x_1, x_2, \dots, x_k)$ in the region of interest R will be denoted by $\hat{y}(\mathbf{x})$. This value is obtained by substituting the elements of β in the model (1.1) by the corresponding elements of \mathbf{b} in (1.2), i.e., $\hat{y}(\mathbf{x}) = \mathbf{x}'_s\mathbf{b}$. The variance function of the predicted value \hat{y} at any point $\mathbf{x}' = (x_1, x_2, \dots, x_k)$ is well known as

$$(1.3) \quad \text{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}'_s(X'X)^{-1}\mathbf{x}_s\sigma^2.$$

$\text{Var}(\hat{y}(\mathbf{x}))$ thus depends on the particular values of the independent variables through the vector \mathbf{x}'_s , and also depends on the design through the matrix $(X'X)^{-1}$.

A design D is said to be rotatable if the variance function (1.3) is a function of only $r^2 = x_1^2 + x_2^2 + \dots + x_k^2$, i.e., the variance of \hat{y} is a function of only distance of \mathbf{x} from the origin, not of direction. Thus, when a design is rotatable, the prediction variance is the same at all points \mathbf{x} that are equidistant from the design center. Consequently, in the space of the input variables, surfaces of constant prediction variance from concentric hyperspheres.

A work which has generated initial interest in the use of RSM is a paper by Box and Wilson (1951). In recent years, interests in RSM have been increased and books on this subject have been written by some authors such as Myers (1976), Box and Draper (1987) and Khuri and Cornell (1987).

The concepts of rotatability was first introduced by Box and Hunter (1957). Since it was first introduced, it has become an important design criterion. If the circumstances are such that exact rotatability is unattainable, it is still a good idea to make the design *nearly rotatable*. Thus it is important to know if a particular design is rotatable or, if it is not, to know *how rotatable it is*. Analogous to rotatability, the concept of slope-rotatability has been advanced by Hader and Park

(1978) and Park (1987). In this concept, the variance of $\partial\hat{y}(\mathbf{x})/\partial x_i$ ($i = 1, \dots, k$) are equal for all \mathbf{x} equidistant from the design origin.

Recently, Khuri (1988), Draper and Guttman (1988), and Draper and Pukelsheim (1990) suggest the measures of rotatability that enable us to assess the degree of rotatability for a given design. In this paper, another measure of rotatability, $R_k(D)$, is introduced and illustrated.

2. Proposed measure of rotatability

In this chapter, a general measure of rotatability is proposed. This measure will enable us to appreciate the degree of rotatability for a given response surface design. Let

$$(2.1) \quad V(\mathbf{x}) = \frac{N}{\sigma^2} \text{Var}(\hat{y}(\mathbf{x}))$$

where $\text{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}'_s (X'X)^{-1} \mathbf{x}_s \sigma^2$.

In the k -dimensional space ($k \geq 2$), $V(\mathbf{x})$ can be expressed in terms of spherical coordinates of $(\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta)$ where

$$(2.2) \quad \begin{aligned} x_1 &= \rho \cos \phi_1, \\ x_2 &= \rho \sin \phi_1 \cos \phi_2, \\ &\vdots \\ x_{k-1} &= \rho \sin \phi_1 \sin \phi_2 \cdots \sin \phi_{k-2} \cos \theta, \\ x_k &= \rho \sin \phi_1 \sin \phi_2 \cdots \sin \phi_{k-2} \sin \theta \end{aligned}$$

and $\rho \geq 0$, $0 \leq \phi_1, \phi_2, \dots, \phi_{k-2} \leq \pi$, $0 \leq \theta < 2\pi$. (See Fleming (1977), p. 218.) The absolute value of the Jacobian of this transformation is

$$|J| = \rho^{k-1} \sin^{k-2} \phi_1 \sin^{k-3} \phi_2 \cdots \sin^2 \phi_{k-3} \sin \phi_{k-2}.$$

If we substitute (2.2) into (2.1), then (2.1) will be expressed as a function of $\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta$, i.e., $V(\mathbf{x}) = w(\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta)$. Let

$$(2.3) \quad \bar{w}(\rho) = \frac{1}{I_k} \int_0^{2\pi} \int_0^\pi \cdots \int_0^\pi w(\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta) d\Omega$$

where $d\Omega = \sin^{k-2} \phi_1 \cdots \sin \phi_{k-2} d\phi_1 d\phi_2 \cdots d\phi_{k-2} d\theta$, and

$$I_k = \int_0^{2\pi} \int_0^\pi \cdots \int_0^\pi d\Omega = \frac{2\pi^{k/2}}{\Gamma(k/2)}.$$

$\bar{w}(\rho)$ means the averaged value of $V(\mathbf{x})$ over all the points on the hypersphere of radius ρ centered at the origin. To be rotatable,

$$w(\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta) = \bar{w}(\rho) \quad \text{for all } \rho, \phi_i, \theta.$$

For a given design, the discrepancy from rotatability at ρ can be expressed as

$$(2.4) \quad h(\rho) = \int_0^{2\pi} \int_0^\pi \cdots \int_0^\pi [w(\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta) - \bar{w}(\rho)]^2 d\Omega.$$

If the region of interest is $0 \leq \rho \leq 1$, the proposed measure will be

$$(2.5) \quad P_k(D) = \frac{1}{1 + R_k(D)}$$

where

$$(2.6) \quad R_k(D) = \frac{1}{E_k} \int_0^1 \rho^{k-1} h(\rho) d\rho,$$

and E_k is a positive constant depending only on k . Let us take E_k to be

$$E_k = \int_0^1 \rho^{k-1} I_k d\rho = \frac{1}{k} I_k$$

for convenience. By this way, $R_k(D)$ represents the average of $(w - \bar{w})^2$ over the region of integration. $P_k(D)$ is 1 if and only if a design is rotatable, and it is smaller than one for a nonrotatable design. Note that $P_k(D)$ is invariant with respect to the rotation of the coordinate axes, since $\bar{w}(\rho)$, $h(\rho)$ and $R_k(D)$ are invariant with respect to the rotation of the coordinate axes.

Now, we introduce the following fact which is useful for evaluating our measure.

- (1) $\int d\Omega = 2\pi^{k/2}/\Gamma(k/2)$,
- (2) $\int x_i^2 d\Omega = \rho^2 I_k/k$,
- (3) $\int x_i^2 x_j^2 d\Omega = (1/3) \int x_i^4 d\Omega = \rho^4 I_k/k(k+2)$ ($i \neq j$),
- (4) $\int x_i^2 x_j^2 x_l^2 d\Omega = (1/3) \int x_i^4 x_j^2 d\Omega = (1/15) \int x_i^6 d\Omega = \rho^6 I_k/k(k+2)(k+4)$ ($i \neq j \neq l$),
- (5) $\int x_i^2 x_j^2 x_l^2 x_m^2 d\Omega = (1/3) \int x_i^4 x_j^2 x_l^2 d\Omega = (1/9) \int x_i^4 x_j^4 d\Omega = (1/15) \int x_i^6 x_j^2 d\Omega = (1/105) \int x_i^8 d\Omega = \rho^8 I_k/k(k+2)(k+4)(k+6)$ ($i \neq j \neq l \neq m$)

where i, j, l, m could be $1, 2, \dots, k$, and \int means $\int_0^{2\pi} \int_0^\pi \cdots \int_0^\pi$. The values of other integrals where at least one x_i has an odd exponent are all zeros.

In comparing designs, we have to consider the scaling of designs. The *traditional* way of scaling is to set $1/N \sum_{u=1}^N x_{iu}^2 = 1$. This was used by Box and Hunter (1957), and Khuri (1988). In this paper, as was adapted by Draper and Pukelsheim (1990), we scale designs so that all of the points lie inside or on the unit sphere. Therefore, if we have a set of points

$$\mathbf{x}'_i = (x_{1i}, x_{2i}, \dots, x_{ki}) \quad i = 1, 2, \dots, N,$$

then the scaled point, $g\mathbf{x}_i$, should satisfy

$$0 \leq g\sqrt{(x_{1i})^2 + (x_{2i})^2 + \cdots + (x_{ki})^2} \leq 1 \quad i = 1, 2, \dots, N.$$

One advantage of this is that, when we add center points, the remaining points do not have to be rescaled. For the 3^2 -factorial design, the scaling factor should be $g = 1/\sqrt{2} \doteq 0.7071$.

3. Illustration of the proposed measure

3.1 3^k factorial design

For the 3^k factorial design without replications, it can be shown that

$$\begin{aligned} v_0 &= \frac{2k + 1}{3^k} \sigma^2, \\ v_i &= \frac{1}{2 \times 3^{k-1}} \sigma^2 \quad (i = 1, 2, \dots, k), \\ v_{ii} &= \frac{1}{2 \times 3^{k-2}} \sigma^2 \quad (i = 1, 2, \dots, k), \\ v_{ij} &= \frac{1}{4 \times 3^{k-2}} \sigma^2 \quad (i \neq j), \\ c_{0,ii} &= -\frac{1}{3^{k-1}} \sigma^2 \quad (i = 1, 2, \dots, k) \end{aligned}$$

where v_0, v_i, v_{ii}, v_{ij} and $c_{0,ii}$ denote $\text{Var}(b_0), \text{Var}(b_i), \text{Var}(b_{ii}), \text{Var}(b_{ij})$ and $\text{Cov}(b_0, b_{ii})$, respectively, and $\mathbf{b}' = (b_0, b_1, \dots, b_k, b_{11}, \dots, b_{kk}, b_{12}, \dots, b_{k-1,k})$ which is explained in (1.2).

The other values of variances and covariances not mentioned above are all zeros. Thus, we can obtain the following results,

$$\begin{aligned} (3.1) \quad V(\mathbf{x}) &= \frac{N}{\sigma^2} \text{Var}(\hat{y}(\mathbf{x})) \\ &= \frac{N}{\sigma^2} [v_0 + (v_1 + 2c_{0,11})\rho^2 + v_{11}\rho^4 \\ &\quad + (v_{12} - 2v_{11})(x_1^2 x_2^2 + \dots + x_{k-1}^2 x_k^2)], \end{aligned}$$

and,

$$\begin{aligned} (3.2) \quad \bar{w}(\rho) &= \frac{1}{I_k} \int V(\mathbf{x}) d\Omega \\ &= \frac{N}{\sigma^2} \left[v_0 + (v_1 + 2c_{0,11})\rho^2 + v_{11}\rho^4 + (v_{12} - 2v_{11}) \binom{k}{2} \frac{\rho^4}{k(k+2)} \right]. \end{aligned}$$

Therefore,

$$\begin{aligned} &[w(\rho, \phi_1, \phi_2, \dots, \phi_{k-2}, \theta) - \bar{w}(\rho)]^2 \\ &= \left(\frac{N}{\sigma^2} \right)^2 (v_{12} - 2v_{11})^2 \left[(x_1^2 x_2^2 + \dots + x_{k-1}^2 x_k^2)^2 + \frac{(k-1)^2}{4(k+2)^2} \rho^8 \right. \\ &\quad \left. - \frac{(k-1)}{(k+2)} (x_1^2 x_2^2 + \dots + x_{k-1}^2 x_k^2) \rho^4 \right]. \end{aligned}$$

From this, for (2.4) we can obtain

$$(3.3) \quad h(\rho) = \left(\frac{N}{\sigma^2} \right)^2 \frac{6(v_{12} - 2v_{11})^2 (k-1) \rho^8 I_k}{(k+2)^2 (k+4)(k+6)}.$$

Thus, from (2.6)

$$(3.4) \quad R_k(D) = \frac{k}{I_k} \left(\frac{N}{\sigma^2} \right)^2 \frac{6(v_{12} - 2v_{11})^2(k-1)I_k}{(k+2)^2(k+4)(k+6)(k+8)}.$$

If we take the scaling factor $g = 1/\sqrt{k}$ in the 3^k -factorial design, the variances v_{12} and v_{11} become $(1/g^4)v_{12}$ and $(1/g^4)v_{11}$, respectively, after scaling. So

$$(3.5) \quad R_k(D) = \left(\frac{N}{\sigma^2} \right)^2 \frac{6k(v_{12} - 2v_{11})^2(k-1)}{(k+2)^2(k+4)(k+6)(k+8)g^8}.$$

Table 1 gives the values of $P_k(D) = 1/[1 + R_k(D)]$ for various k , which indicates that as k increases 3^k -factorial designs deviate more from rotatability.

Table 1. Values of $P_k(D)$ for 3^k -factorial designs.

k	2	3	4	5	6
$P_k(D)$	0.468	0.115	0.040	0.018	0.010

3.2 Central composition designs

In general, the Central Composition Design (CCD) consists of 2^k or a fraction of 2^k factorial points $(\pm 1, \pm 1, \dots, \pm 1)$, $2k$ axial points of the form $(\pm \alpha, 0, \dots, 0)$, etc., and a center point $(0, 0, \dots, 0)$. The center point may be replicated n_0 times. Thus the total number N of experimental points can be written as

$$N = F + 2k + n_0 = F + T$$

where F is the number of factorial points ($F = 2^k$ if a full factorial is used and $F = 2^{k-p}$ ($p \geq 1$) if a fractional factorial is used), and $T = 2k + n_0$. For the CCD, it can be shown that for any fractional factorial configurations,

$$v_0 = \frac{kF + 2\alpha^4}{2\alpha^4(F + T - 2k) - 4\alpha^2kF + kFT} \sigma^2,$$

$$v_i = \frac{1}{F + 2\alpha^2} \sigma^2 \quad (i = 1, 2, \dots, k),$$

$$v_{ij} = \frac{1}{F} \sigma^2 \quad (i \neq j),$$

$$v_{ii} = \frac{\{2\alpha^4 + 4(1-k)\alpha^2 + (k-1)T\}F + 2\alpha^4(T - 2k + 2)}{2\alpha^4\{(2\alpha^4 + kT - 4k\alpha^2)F + 2\alpha^4(T - 2k)\}} \sigma^2$$

$$(i = 1, 2, \dots, k),$$

$$c_{ii,jj} = \frac{4\alpha^4 + 4\alpha^2F - TF}{2\alpha^4\{(2\alpha^4 + kT - 4k\alpha^2)F + 2\alpha^4(T - 2k)\}} \sigma^2 \quad (i \neq j),$$

$$c_{0,ii} = \frac{-(F + 2\alpha^2)}{2\alpha^4(F + T - 2k) - 4\alpha^2kF + kFT} \sigma^2 \quad (i = 1, 2, \dots, k)$$

where $c_{ii,jj} = \text{Cov}(b_{ii}, b_{jj})$ and $c_{0,ii} = \text{Cov}(b_0, b_{ii})$. Thus, we can obtain the following results:

$$(3.6) \quad V(\mathbf{x}) = \frac{N}{\sigma^2} [v_0 + (v_1 + 2c_{0,11})\rho^2 + v_{11}\rho^4 + (v_{12} + 2c_{11,22} - 2v_{11})(x_1^2x_2^2 + \dots + x_{k-1}^2x_k^2)],$$

$$(3.7) \quad \bar{w}(\rho) = \frac{N}{\sigma^2} \left[v_0 + (v_1 + 2c_{0,11})\rho^2 + v_{11}\rho^4 + (v_{12} + 2c_{11,22} - 2v_{11}) \frac{(k-1)}{2(k+2)} \rho^4 \right]$$

and

$$(3.8) \quad h(\rho) = \left(\frac{N}{\sigma^2} \right)^2 \frac{6(v_{12} + 2c_{11,22} - 2v_{11})^2(k-1)I_k\rho^8}{(k+2)^2(k+4)(k+6)}.$$

In the CCDs, the scaling factor, g , should be

$$g = \begin{cases} 1/\alpha, & \text{if } \alpha \geq \sqrt{k} \\ 1/\sqrt{k}, & \text{if } \alpha < k. \end{cases}$$

Then

$$(3.9) \quad R_k(D) = \left(\frac{N}{\sigma^2} \right)^2 \frac{6k(v_{12} + 2c_{11,22} - 2v_{11})^2(k-1)}{(k+2)^2(k+4)(k+6)(k+8)g^8}.$$

Table 2 gives the values of $P_k(D)$ for various k, p and α .

Figures 1 through 3 give the contour plot of $V(\mathbf{x})$ for the CCDs ($k = 2, p = 0, n_0 = 1$) with $\alpha = 1.00, 2.00$ and 3.00 . Note that when $\alpha = 1.00$, the CCD is the 3^2 factorial design.

Table 2. Values of $P_k(D)$ for CCDs for various k, p and α ($n_0 = 1$).

α	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 5$	$k = 6$	$k = 6$
	$p = 0$	$p = 0$	$p = 0$	$p = 0$	$p = 1$	$p = 1$	$p = 2$
1.00	0.4675	0.0333	0.0034	0.0005	0.0013	0.0002	0.0006
1.50	0.9911	0.8339	0.1413	0.0162	0.0595	0.0082	0.0292
2.00	0.4675	0.6814	1.0000	0.3177	1.0000	0.1890	1.0000
2.50	0.0932	0.1242	0.2699	0.8537	0.2576	0.8583	0.2548
3.00	0.0209	0.0250	0.0445	0.1081	0.0419	0.1117	0.0413
3.50	0.0059	0.0067	0.0108	0.0205	0.0102	0.0212	0.0100
Rotatable α	1.41	1.68	2.00	2.38	2.00	2.38	2.00

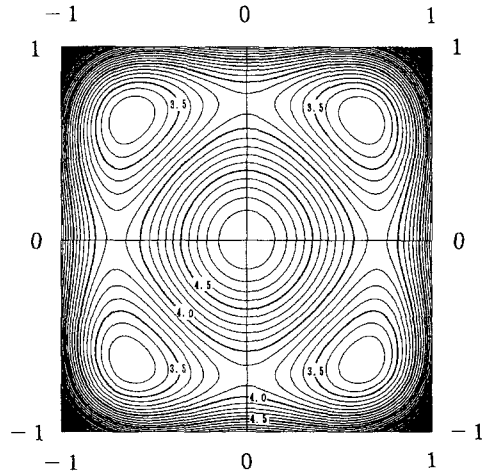


Fig. 1. Contour plot of $V(\boldsymbol{x})$ for CCD ($k = 2$, $p = 0$, $n_0 = 1$, $\alpha = 1.00$).

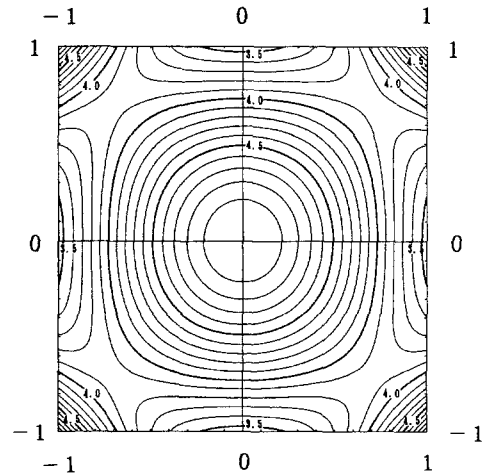


Fig. 2. Contour plot of $V(\boldsymbol{x})$ for CCD ($k = 2$, $p = 0$, $n_0 = 1$, $\alpha = 2.00$).

4. Comparison of rotatability measures

It is of interest to compare the proposed measure $P_k(D)$ with the measures of Khuri (1988), Draper and Guttman (1988) and Draper and Pukelsheim (1990). Both Khuri's measure and Draper and Pukelsheim's measure compare the form of $X'X$ matrix from regression model with that of rotatable design, and can be used with any model of order d (≥ 1). However, both measures do not provide information about variance contour shape. On the other hand, Draper and Guttman provide an index that characterizes the general overall shape of variance contours. But it is difficult to apply this index to general nonsymmetric designs.

For the usefulness of our proposed measure, we want to mention the following facts.

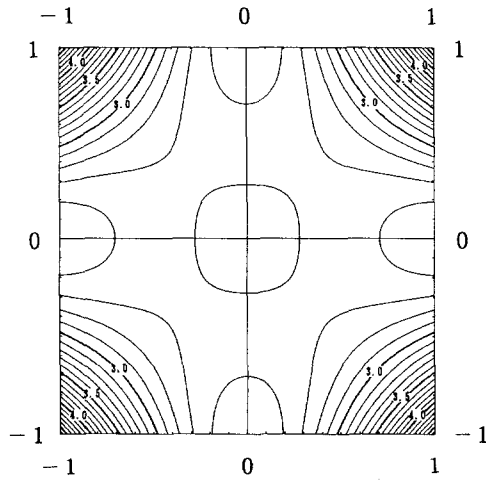


Fig. 3. Contour plot of $V(\mathbf{x})$ for CCD ($k = 2, p = 0, n_0 = 1, \alpha = 3.00$).

Table 3. Comparison of the four measures of rotatability.

Criteria	Khuri	Draper & Guttman	Draper & Pukelsheim	$P_k(D)$
Applicability to asymmetric design	Yes	No	Yes	Yes
Invariance w.r.t the design rotation	No	No	Yes	Yes
Information about variance contour shape	No	Yes	No	No
Range	$0 \sim 100$	$0 \sim +\infty$	$0 \sim 1$	$0 \sim 1$
Order of the model to which the measure applies	$d \geq 1$	2	$d \geq 1$	2

First of all, we can easily obtain the variance contour $V(\mathbf{x})$ like Figs. 1–3 from the equations (3.1) and (3.6), since $V(\mathbf{x})$ is expressed in terms of spherical coordinates. Next, it is true that the proposed measure is only applied to second order designs. However, rotatability is mainly discussed for second order response surface designs, and this limitation does not pose any practical problems for the usefulness of this measure in response surface methodology. Last of all, we have a computer program, named SROTA, which computes $P_k(D)$ for any second-order design. This program can be obtained from the authors upon request. For a given

design, this program obtains $V(\mathbf{x})$, compute $\bar{w}(\rho)$ and $h(\rho)$, and then calculate $R_k(D)$.

In Table 3, we make a comparison of the four measures of rotatability on the basis of five criteria.

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