Another Look at Rotatability

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Rotatability is one of many desirable characteristics of a response-surface design. Recent work (Draper and Guttman 1988; Khuri 1988) has, for the first time, provided ways to measure "how rotatable" a design may be when it is not perfectly rotatable. This had previously been assessed by the viewing of tediously obtained contour diagrams. This article provides a criterion that is easy to compute and is invariant under design rotation. It also easily extends to higher degree models.

KEY WORDS: Composite designs; Measures of rotatability; Repairing rotatability; Response surface; Roquemore's designs.

1. INTRODUCTION

Rotatability was first defined by Box and Hunter (1957). Suppose we wish to fit a response-surface polynomial of degree d, $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ to k predictor variables, or factors, $x_1, x_2, \ldots, x_k$. Let $\mathbf{z}' = (1, x_1, \ldots, x_k, x_1^2, \ldots, x_k^2, x_1x_2, \ldots, x_{k-1}x_k, x_1^3, x_1x_2^2, \ldots)$ be a row vector of monomials up to and including order d, evaluated at a general point $\mathbf{x} = (x_1, x_2, \ldots, x_k)'$, with the form of $\mathbf{z}'$ being that of a row of $\mathbf{X}$. Then, if $\boldsymbol{\epsilon} \sim N(\mathbf{O}, \mathbf{I}\sigma^2)$ and we estimate $\boldsymbol{\beta}$ by ordinary least squares, $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ is the appropriate estimator, and the function

$$V\{\hat{y}(\mathbf{x})\} = \mathbf{z}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}\sigma^2 \qquad (1.1)$$

is the variance function of the predicted value $\hat{\mathbf{y}} = \mathbf{z}'\mathbf{b}$ at any point $(x_1, x_2, \ldots, x_k)$ in the predictor space (or x space). The $N \times k$ experimental design matrix $\mathbf{D}$, whose rows (or runs) $(x_{1u}, x_{2u}, \ldots, x_{ku})$ for $u = 1, 2, \ldots, N$ are part of $\mathbf{X}$, is said to be *rotatable* (of the order d of polynomial fitted) if (1.1) is a function only of $r^2 = x_1^2 + \cdots + x_k^2$. This important property is a desirable feature of any experimental design. Even if circumstances are such that exact rotatability is unattainable—because of more important restrictions such as orthogonal blocking, for example—it is still a good idea to make the design as "rotatable as possible." Thus it is important to know if a particular design is rotatable or, if it is not, to know "how rotatable" the design is.

In a first-order model ($d = 1$), we have $\mathbf{z}' = (1, x_1, x_2, \ldots, x_k)$, and rotatability is identical to orthogonality with equal scaling on the axes. The conditions for this are that

$$\lambda_2 N = \sum_{u=1}^{N} x_{iu}^2, \qquad i = 1, 2, \ldots, k, \qquad (1.2)$$

this equation serving to define the parameter λ_2, and, in addition, all sums of powers and products $\Sigma_u x_{iu}^a x_{ju}^b$ of odd first-order or second-order (namely, $a = 1, b = 0$; $a = 0, b = 1$; $a = b = 1$) are required to be 0. In a second-order model ($d = 2$), we have $\mathbf{z}' = (1, x_1, x_2, \ldots, x_k, x_1^2, \ldots, x_k^2, x_1x_2, \ldots, x_{k-1}x_k)$. For second-order rotatability (which is *not* equivalent to orthogonality), the conditions are

$$\lambda_2 N = \sum_u x_{iu}^2, \qquad i = 1, 2, \ldots, k$$
$$3\lambda_4 N = \sum_u x_{iu}^4 = 3 \sum_u x_{iu}^2 x_{ju}^2, \qquad i \neq j = 1, 2, \ldots, k, \qquad (1.3)$$

the latter defining λ_4, and, in addition, all other sums of powers and products of order up to and including 4 must be 0. See Box and Hunter (1957) or Box and Draper (1987, p. 489).

When a design is rotatable, we know exactly where we are, but how do we know when a design is "nearly rotatable"? In general, this has been hard to assess without actually drawing the variance contours—a tedious task, especially in dimensions $k \geq 3$. The assessment of rotatability has been the topic of two recent articles by Draper and Guttman (1988) and Khuri (1988). The thrust of the first article was to provide an m value such that, for symmetric designs, the contour

$$|x_1|^m + |x_2|^m + \cdots + |x_k|^m = 1 \qquad (1.4)$$

provided an excellent representation of a contour of the variance function (1.1). This contour was the one through all axial points one unit from the origin after the design had been scaled (i.e., shrunk or expanded) to bring all of its points inside or onto the unit circle. The m value was then compared with a standard set of m contours. Khuri (1988) compared the moments of a general design with the moments of a rotatable design and essentially obtained an R^2 statistic after regressing a vector of general design moments against vectors obtained from a rotatable design. This enabled him to say that a design was "R^2% rotatable."

We shall study designs through their $p \times p$ moment matrices

$$\mathbf{A} = N^{-1}\mathbf{X}'\mathbf{X} = N^{-1} \sum_{u=1}^{n} \mathbf{z}_u \mathbf{z}_u', \qquad (1.5)$$

where $\mathbf{z}_u$ contains the coordinate of the uth run, rather than through their design points. Because rotatability is defined in terms of moment relationships, this is entirely logical.

2. NOTATION

We shall be primarily concerned here with second-order rotatability. The traditional representation of a second-order model is such that a row of the $\mathbf{X}$ matrix consists of the terms

$$1; x_1, x_2, \ldots, x_k; x_1^2, x_2^2, \ldots, x_k^2; \quad x_1x_2, \ldots, x_{k-1}x_k. \qquad (2.1)$$

(These terms compose $\mathbf{z}'$.) There are certain theoretical disadvantages to this notation in terms of moving from second order to other orders. Box and Hunter (1957) were aware of these disadvantages and consequently introduced the Schläflian notation (see also Draper 1984) in which the terms used were

$$1; x_1, x_2, \ldots, x_k; \quad x_1^2, x_2^2, \ldots, x_k^2, 2^{1/2}x_1x_2, \ldots, 2^{1/2}x_{k-1}x_k. \qquad (2.2)$$

A disadvantage of this notation is that, as higher terms are added, the various proper constants must be introduced and carried through the computations.

A conceptually simpler notation, which we shall use here, is the following. Let $\mathbf{x} = (x_1, x_2, \ldots, x_k)'$. We shall denote the terms in the second-order model by $\mathbf{z}(\mathbf{x})'$ with elements

$$1; \mathbf{x}'; \mathbf{x}' \otimes \mathbf{x}', \qquad (2.3)$$

where the symbol $\otimes$ denotes the Kronecker product. Thus there are $(1 + k + k^2)$ terms,

$$1; x_1, x_2, \ldots, x_k; x_1^2, x_1x_2, \ldots, x_1x_k; \quad x_2x_1, x_2^2, \ldots, x_2x_k; \ldots; x_kx_1, x_kx_2, \ldots, x_k^2. \qquad (2.4)$$

An obvious disadvantage of (2.4) is that all cross-product terms occur twice, so the corresponding $\mathbf{X}'\mathbf{X}$ matrix is singular. A suitable generalized inverse is obvious, however, and this notation is very easily extended to higher orders. For example, third order is added via $\mathbf{x}' \otimes \mathbf{x}' \otimes \mathbf{x}'$, and so on.

3. MEASURING ROTATABILITY

Now consider any second-order rotatable design with second-order moments $\lambda_2 = N^{-1} \sum_u x_{iu}^2$ and $\lambda_4 = \sum_u x_{iu}^2 x_{ju}^2$. We can write its moment matrix $\mathbf{V}$ of order $(1 + k + k^2) \times (1 + k + k^2)$, in the form

$$\mathbf{V} = \mathbf{V}_0 + \lambda_2(3k)^{1/2}\mathbf{V}_2 + \lambda_4[3k(k + 2)]^{1/2}\mathbf{V}_4, \qquad (3.1)$$

where $\mathbf{V}_0$ consists of a one in the (1, 1) position and zeros elsewhere, where $\mathbf{V}_2$ consists of $(3k)^{-1/2}$ in each of the $3k$ positions corresponding to second-order moments in $\mathbf{V}$ and zeros elsewhere, and $\mathbf{V}_4$ consists of $3[3k(k + 2)]^{-1/2}$ in the k positions corresponding to pure fourth-order moments, $[3k(k + 2)]^{-1/2}$ in the $3k(k - 1)$ positions corresponding to mixed even fourth-order moments in $\mathbf{V}$, and zeros elsewhere. The values of $\mathbf{V}_2$ and $\mathbf{V}_4$ for $k = 3$ are given in the Appendix for illustration. Note that $\mathbf{V}_0$, $\mathbf{V}_2$, and $\mathbf{V}_4$ are symmetric and orthogonal so that $\mathbf{V}_i\mathbf{V}_j = \mathbf{0}$, and also the $\mathbf{V}_i$ have norms $\|\mathbf{V}_i\| = [\mathrm{tr}(\mathbf{V}_i\mathbf{V}_i)]^{1/2} = 1$.

Suppose we now take an arbitrary design with moment matrix $\mathbf{A}$, say. Draper, Gaffke, and Pukelsheim (in press) showed that, by averaging $\mathbf{A}$ over all possible rotations in the x space, we obtain

$$\overline{\mathbf{A}} = \mathbf{V}_0 + \mathbf{V}_2\mathrm{tr}(\mathbf{A}\mathbf{V}_2) + \mathbf{V}_4\mathrm{tr}(\mathbf{A}\mathbf{V}_4). \qquad (3.2)$$

An alternative way to obtain (3.2) relies on a regression argument. Suppose that we regress $\mathbf{A}$ on $\mathbf{V}_0$, $\mathbf{V}_2$, $\mathbf{V}_4$ to give the fitted equation

$$\overline{\mathbf{A}} = \alpha\mathbf{V}_0 + \beta\mathbf{V}_2 + \gamma\mathbf{V}_4, \qquad (3.3)$$

with regression coefficients α, β, γ. These coefficients are determined by multiplying Equation (3.3) in turn by $\mathbf{V}_0$, $\mathbf{V}_2$, $\mathbf{V}_4$ and taking traces,

$$\begin{aligned}
\alpha &= \mathrm{tr}(\overline{\mathbf{A}}\mathbf{V}_0) = \mathrm{tr}(\mathbf{A}\overline{\mathbf{V}}_0) = \mathrm{tr}(\mathbf{A}\mathbf{V}_0) = 1 \\
\beta &= \mathrm{tr}(\overline{\mathbf{A}}\mathbf{V}_2) = \mathrm{tr}(\mathbf{A}\overline{\mathbf{V}}_2) = \mathrm{tr}(\mathbf{A}\mathbf{V}_2) \\
\gamma &= \mathrm{tr}(\overline{\mathbf{A}}\mathbf{V}_4) = \mathrm{tr}(\mathbf{A}\overline{\mathbf{V}}_4) = \mathrm{tr}(\mathbf{A}\mathbf{V}_4). \qquad (3.4)
\end{aligned}$$

Here we have profited from having the $\mathbf{V}_i$ scaled so as to have norms 1 and from their pairwise orthogonality. We call $\overline{\mathbf{A}}$ the *rotatable component* of $\mathbf{A}$. We shall be interested in two measures based on $\mathbf{A}$ and $\overline{\mathbf{A}}$. These will be defined as (a) the measure of rotatability,

$$\begin{aligned}
Q^* &= \|\overline{\mathbf{A}} - \mathbf{V}_0\|^2 / \|\mathbf{A} - \mathbf{V}_0\|^2 \\
&= \{\mathrm{tr}(\overline{\mathbf{A}} - \mathbf{V}_0)^2\} / \{\mathrm{tr}(\mathbf{A} - \mathbf{V}_0)^2\} \qquad (3.5)
\end{aligned}$$

($Q^* \leq 1$ with equality iff $\mathbf{A}$ is second-order rotatable), and (b) the distance between $\mathbf{A}$ and $\overline{\mathbf{A}}$,

$$\delta = \|\mathbf{A} - \overline{\mathbf{A}}\| = \{\mathrm{tr}(\mathbf{A} - \overline{\mathbf{A}})^2\}^{1/2}. \tag{3.6}$$

Our rotatability measure Q^* is, like Khuri's (1988, p. 98) Φ, essentially an R^2 statistic for the regression of the design moments of second and fourth order in $\mathbf{A}$ onto the "ideal" design moments represented by $\mathbf{V}$. There are, however, important differences. Because Khuri's regression is based on vectors selected from an upper triangular portion of a matrix similar to $\mathbf{V}$, his regression coefficients and R^2 value are weighted differently from ours. Because of this, his statistic is not invariant when the design is rotated in the x space, whereas ours is. For an example involving the 3^2 design, see Section 4. It is, of course, desirable that a measure of rotatability *not* be affected by how the design is oriented in the x space.

Scaling. An important issue that we have not yet discussed, which affects both Q^* and δ, is the scaling of the designs examined. In nearly all comparisons of two or more designs, a decision must be made on how far out from the origin to place a given set of design points. The "traditional" way, dating back to Box and Hunter (1957, p. 212), is to set $\lambda_2 = 1$. This was followed by Khuri (1988). We prefer, however, to think of the unit circle ($k = 2$) or unit sphere ($k \geq 3$) as the region of interest. Hence we scale designs so that all of the points lie inside or on the unit sphere. One consequence of this is that, when we add center points, the remaining points do not have to be rescaled and the values of Q^* and δ are unchanged. If λ_2 is to be fixed equal to 1, the addition of a (or another) center point will require the design to be rescaled; moreover, the "shape" of the original design-point setup will be axially distorted. It is of limited value to compare our numerical values with Khuri's, even if we ignore the rotational problem of the latter discussed earlier in this section. The values we provide are, however, internally consistent and invariant under design rotation.

The numerical value of Q^* is completely unaffected by the choice of notation used to represent the second-order terms discussed in Section 2. Our selected notation makes the proof that Q^* is not dependent on orientation very straightforward, for, if we rotate any $\mathbf{x}$-vector into $\mathbf{Rx}$, where $\mathbf{R}$ is a $k \times k$ orthogonal matrix, we obtain the transformation $\mathbf{Q}$ in the $\mathbf{z}(\mathbf{x})$ space from (2.3) as

$$\mathbf{Q} = \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{R} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{R} \otimes \mathbf{R} \end{pmatrix}, \text{ since } \mathbf{z}(\mathbf{x}) = \begin{pmatrix} 1 \\ \mathbf{x} \\ \mathbf{x} \otimes \mathbf{x} \end{pmatrix}. \tag{3.7}$$

Hence the matrix $\mathbf{Q}$, of order $(1 + k + k^2) \times (1 + k + k^2)$, is also orthogonal. But the norms and distances used in the definition of Q^* and δ are orthogonally invariant. Hence Q^* and δ stay the same under design rotation.

Note that if two moment matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ have the same $\overline{\mathbf{A}} = \overline{\mathbf{A}}_1 = \overline{\mathbf{A}}_2$, then they can be directly compared via the distance measure, the one with smaller δ being more rotatable. This follows from

$$Q^* = \frac{\|\overline{\mathbf{A}} - \mathbf{V}_0\|^2}{\delta^2 + \|\overline{\mathbf{A}} - \mathbf{V}_0\|^2}. \tag{3.8}$$

If $\overline{\mathbf{A}}_1 \neq \overline{\mathbf{A}}_2$, however, a simple comparison of Q^* and δ is not available. When $\mathbf{A}_1 - \mathbf{A}_2$ is positive semidefinite, we may have $\delta(\mathbf{A}_1) > \delta(\mathbf{A}_2)$ and $Q^*(\mathbf{A}_1) = Q^*(\mathbf{A}_2)$. Since we shall not consider this type of behavior in the present article, we henceforth concentrate on Q^*.

Equation (3.2) is appropriate for second-order rotatability. For additional theoretical discussion, see Draper et al. (in press). This concept can be extended straightforwardly to higher-order rotatability, which will be discussed in a subsequent article.

4. COMPOSITE DESIGNS

Composite designs consist of a combination of a *cube*—that is, a two-level factorial or fractional factorial 2^{k-p} design with coordinates $(\pm 1, \pm 1, \ldots, \pm 1)$—plus a *star* of $2k$ points $(\pm\alpha, 0, \ldots, 0)$, $(0, \pm\alpha, 0, \ldots, 0)$, $\ldots$, $(0, 0, \ldots, 0, \pm\alpha)$, plus n_o center points. Table 1 shows the values of the rotatability measure Q^* for a selection of such designs with the cube portion of resolution V or higher when the design is rescaled so that all of the points lie inside or on the unit ball. This table is designed to be visually comparable to table 1 of Draper and Guttman (1988, p. 109), which showed the shape of a variance contour through the point $(1, 0, \ldots, 0)$ *after* rescaling the design so that all points were inside or on the unit sphere, the same rescaling as that done for Q^*. A comparison of these two tables shows that Q^* is a sensible criterion and that the two tables are entirely consistent. Moreover, any rotation of these designs will leave Q^* unaltered.

We can compare the three criteria mentioned in this article via an example. Consider the 3^2 design, which is a composite design with $\alpha = 1$ and one center point. Figure 1 shows how Khuri's Φ changes as the 3^2 design is rotated through an angle θ, $0 \leq \theta \leq 90°$. Our $Q^* = .9826$, from Table 1, remains constant throughout. The Draper and Guttman (1988, pp. 110–111) m criterion can be evaluated only for the symmetric cases $\theta = 0$ or $90°$ (when $m = 3.73$) and $\theta = 45°$ (when $m = 1.29$). Note that these m values apply to different variance contours; if the same contour is used (as in Draper and Guttman

Table 1. Values of Rotatability Measure Q^* for Standard Composite Designs, With 2^{k-p} Cube at ($\pm 1, \pm, \ldots, \pm 1$) and Axial Points at Distance α, Rescaled to the Unit Sphere

α	$k = 2$, $p = 0$	$k = 3$, $p = 0$	$k = 4$, $p = 0$	$k = 5$, $p = 0$	$k = 5$, $p = 1$	$k = 6$, $p = 1$	$k = 7$, $p = 1$	$k = 8$, $p = 1$	$k = 8$, $p = 2$	$k = 9$, $p = 2$
1.00	.9826	.9754	.9752	.9781	.9814	.9830	.9853	.9875	.9880	.9896
1.25	.9967	.9873	.9819	.9812	.9864	.9854	.9864	.9879	.9889	.9900
1.41	1.0000									
1.50	.9992	.9972	.9897	.9854	.9922	.9887	.9880	.9887	.9902	.9906
1.68		1.0000								
1.75	.9916	.9995	.9968	.9906	.9976	.9927	.9901	.9897	.9919	.9914
2.00	.9826	.9928	1.000	.9957	1.0000	.9967	.9927	.9910	.9941	.9926
2.25	.9746	.9829	.9969	.9994	.9965	.9995	.9956	.9927	.9964	.0040
2.38				1.0000		1.0000				
2.50	.9682	.9729	.9900	.9996	.9887	.9995	.9983	.9947	.9986	.9956
2.75	.9632	.9639	.9817	.9965	.9792	.9962	.9999	.9968	.9999	.9973
2.83							1.0000		1.0000	
3.00	.9592	.9559	.9732	.9917	.9694	.9909	.9996	.9989	.9995	.9989
3.25	.9560	.9492	.9649	.9858	.9600	.9846	.9977	.9999	.9976	.9999
3.36								1.0000		1.0000
3.50	.9534	.9434	.9572	.9796	.9512	.9777	.9947	.9999	.9945	.9999
4.00	.9497	.9344	.9438	.9668	.9358	.9637	.9869	.9978	.9862	.9977
4.50	.9471	.9277	.9329	.9547	.9233	.9504	.9777	.9938	.9766	.9936
5.00	.9452	.9228	.9241	.9436	.9133	.9384	.9679	.9888	.9663	.9884

NOTE: When $Q^* = 1$, the design is fully rotatable. The α values $2^{(k-p)/4}$ that achieve rotatability are also given.

1988, p. 111) the corresponding m values become 4.44 and 1.29. These values are conjugates of each other in the sense that $(4.44)^{-1} + (1.29)^{-1} = 1$. This conjugacy relationship shows a pattern balanced around the circle ($m = 2$), which is self-conjugate in that $\frac{1}{2} + \frac{1}{2} = 1$.

5. ROQUEMORE'S DESIGNS

Three designs given by Roquemore (1976, p. 420) were examined by both Khuri (1988, p. 100) and Draper and Guttman (1988, p. 110, with rescaled coordinates). The values of the rotatability measures for the designs are shown in Table 2. Obviously the values are sensibly consistent. As other authors have remarked, 311A is the "most rotatable" of the three designs.

6. REPAIRING DESIGN ROTATABILITY

The idea of adding one or more points to a design to make it conform better to a desirable criterion is long established, and Khuri used this idea to make designs more rotatable as measured by his criterion Φ. We now reconsider Khuri's (1988, p. 100) example 4.3, due originally to Hebble and Mitchell (1972, ex. 1, p. 769). The initial nonrotatable design with 10 design points is given in Table 3, in which $Q^* = .9496$. New points are restricted to a circle of radius 2 in the original coordinate system. The best 11th, 12th, 13th, and 14th points to add to the design to provide a maximum increase in rotatability are as shown in Table 4. We have searched only to one decimal place, which is all that is justified by the stability of Q^* in this example. Figure 2 shows the progressive changes in the variance contours as points are added to make the design more rotatable.

Note that, if we repair design rotatability using the traditional $\lambda_2 = 1$ scaling, we immediately distort our initial design space. For repair of designs, choosing a scaling that merely shrinks or expands equally in all directions seems more sensible.

As a second example, we reconsider Khuri's (1988, p. 100) example 4.4, provided by John Cornell. The initial design is given in Table 5. This was a modification of a central composite design with axial dis-

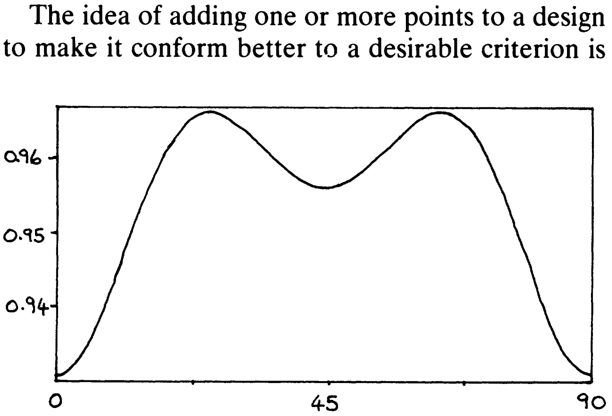

Figure 1. Plot of Khuri's Φ for a 3^2 Design Rotated Through an Angle θ ($0 \le \theta \le 90°$).

Table 2. The Values of Rotatability Measures for Roquemore's Designs

Rotatability measures	Design number 310	311A	311B
Khuri's Φ	.9489	.9940	.9899
Our Q^*	.9903	.9993	.9969

Table 3. First Example: The Design to Be Repaired (Q^* = .9496)

u	x_1	x_2
1	−1	1.35
2	1	−1.25
3	−1.6	−.85
4	1	1
5	−1.5	0
6	1.55	0
7	0	−1
8	0	1.55
9	.55	.30
10	0	0

tance 1.682. The codings from the original variables P (a polymer), CA (a coupling agent), and L (a lubricant) were

$$x_1 = (P - 250)/25, \quad x_2 = (CA - 22.5)/2.5, \quad x_3 = (L - 7.5)/2.5, \tag{6.1}$$

and the design modification resulted from a requirement that $P + CA + L \leq 305$—namely,

$$10x_1 + x_2 + x_3 \leq 10. \tag{6.2}$$

In adding new points to the design, we shall observe both this restriction and the one that $x_1^2 + x_2^2 + x_3^2 \leq 3$, as observed by Khuri (1988), which keeps new points within the maximum radial distance of the old points. Because of the (x_2, x_3) symmetry of the initial design in Table 5, there is no need to search in three dimensions, so we seek points of form (x_1, x_2, x_2) such that

$$10x_1 + 2x_2 \leq 10 \tag{6.3}$$

and

$$x_1^2 + 2x_2^2 \leq 3. \tag{6.4}$$

Thus we search within the left portion of the ellipse (6.4) cut off by the line (6.3) in the (x_1, x_2) subspace. Table 6 shows the points 17–19 that, added singly, make the design the most rotatable at each stage of addition. For the 17th point, we searched on a .05 unit grid, but the stability of Q^* again showed that one decimal place was perfectly adequate here, and this was used for the subsequent points. Note that (1, 0, 0) was used as the 18th point giving Q^* = .9899. In fact, (.98, .1, .1) provided Q^* = .9900, so slight an improvement that we continued with the neater (1, 0, 0). Figure 3 shows the progressive changes in the variance contours. Remember that, because of the dimensional reduction from (x_1, x_2, x_3) to $(x_1, x_2 = x_3)$, rotatable contours would be elliptical, like (6.4). We see that the variance contours of the original design were already quite satisfactory and the addition of the new points provides only a marginal improvement.

Table 4. First Example: Points That Most Improve Q^*

u	x_1	x_2	Q^*
11	−.1	−1.5	.9861
12	.2	.4	.9875
13	−.1	0	.9876
14	0	0	.9876

Table 5. Second Example: The Design to Be Repaired (Q^* = .9710)

x_1	x_2	x_3
−1	−1	−1
1	−1	−1
−1	1	−1
1	1	−1
−1	−1	1
1	−1	1
−1	1	1
.48	1	1
−1.682	0	0
1	0	0
0	−1.682	0
0	1.682	0
0	0	−1.682
0	0	1.682
0	0	0
0	0	0

We note that, for this second example, our calculations contradict Khuri's, whose 17th point was at (−.828, −.506, −.506). When we inserted that point as number 17, Q^* fell to .9626. This seems logical. The design moment $\Sigma_u x_{1u}/N = -.075125$ initially, and it would thus seem appropriate to add a 17th design point with a positive x_1 coordinate, as we have done, rather than a negative one. Khuri's 18th and last point, (.966, .151, .151), is much like our 17th and 18th points.

7. SUMMARY

A new criterion for rotatability is suggested. The criterion is invariant under design rotation and, because of the use of Kronecker product formation of the terms of a polynomial model, is extendable to models of any order. Detailed calculations are provided for composite designs, and the criterion is used

Table 6. Second Example: Points That Most Improve Q^*

u	x_1	x_2	x_3	Q^*
17	.95	.25	.25	.9855
18	1	0		.9888
19	−.6	−.2	−.2	.9918

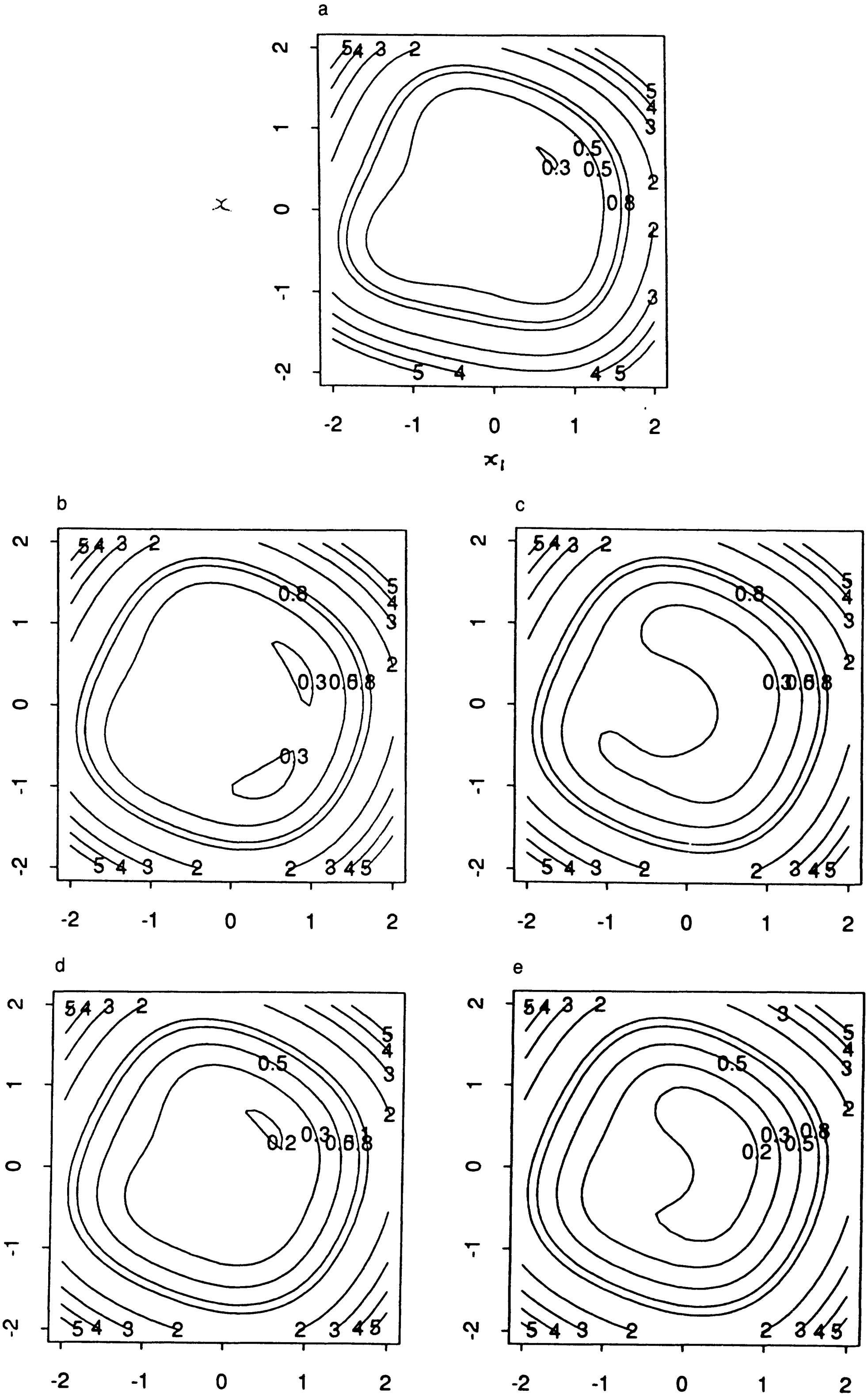

Figure 2. Successive Variance Contours as Points Are Added Sequentially to the Design of Table 2: (a) Original Design, N = 10, Q* = .9496; (b) Points 1–11, N = 11, Q* = .9861; (c) N = 12, Q* = .9875; (d) N = 13, Q* = .9876; (e) N = 14, Q* = .9876.

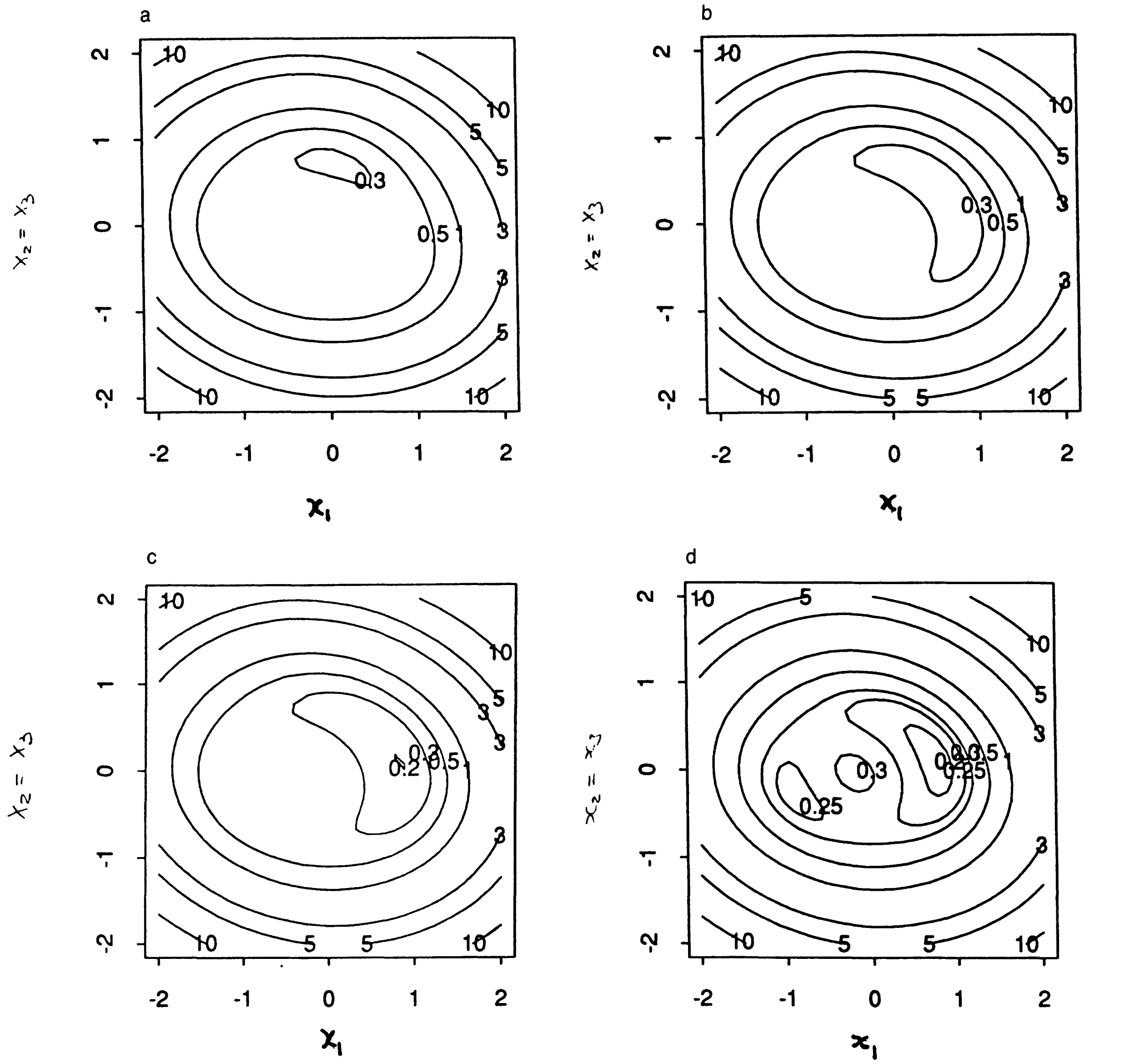

Figure 3. Successive Variance Contours as Points Are Added Sequentially to the Design of Table 4: (a) Original Design, N = 16, Q = .9710; (b) Points 1–17, N = 17, Q* = .9855; (c) N = 18, Q* = .9899; (d) N = 19, Q* = .9918.*

to repair two specific designs already considered by previous authors.

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APPENDIX: THE VALUES OF $\mathbf{V}_2$ AND $\mathbf{V}_4$ FOR $k = 3$

The matrices $\mathbf{V}_2$ and $\mathbf{V}_4$ for the $k = 3$ second-order case are both of sizes 13×13. [In general, the dimensions are $(k^2 + k + 1) \times (k^2 + k + 1)$.] With columns and rows designated by the elements in (2.4), we have

$$\mathbf{V}_2 = \left[\begin{array}{ccccccccccccc}
0 & 0 & 0 & 0 & a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\
0 & a & & & & & & & & & & & \\
0 & & a & & & & & & & & & & \\
0 & & & a & & & & & & & & & \\
a & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
a & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
a & & & & & & & & & & & &
\end{array}\right]$$

and

$$
\mathbf{V}_4 = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
0 & & & & & & & & & & & & \\
0 & & & & 3b & & & & b & & & & b \\
0 & & & & & b & & b & & & & & \\
0 & & & & & & b & & & & b & & \\
0 & & & & & b & & b & & & & & \\
0 & & & & b & & & & 3b & & & & b \\
0 & & & & & & & & & b & & b & \\
0 & & & & & & b & & & & b & & \\
0 & & & & & & & & & b & & b & \\
0 & & & & b & & & & b & & & & 3b
\end{bmatrix}
$$

In $\mathbf{V}_2$, $a = \frac{1}{3}$ and all unfilled positions are zeros; in $\mathbf{V}_4$, $b = (45)^{-1/2}$ and all unfilled positions are zeros.

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