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KISS-PRECISE SEQUENTIAL ROTATABLE DESIGNS

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SUMMARY. A sequential procedure for the exploration of response surfaces is proposed. The procedure, which is for experiments with two factors, uses the kiss-precise configuration, i.e., the design points are on circles in mutual contact at each stage. Only three points need be added at each stage and the design points form a first-order rotatable design. A second-degree surface may be fitted when a near stationary region is reached.

1. **Introduction.** Several procedures have been proposed for the sequential exploration of response surfaces, to search the experimental region for a region of optimum response. Among these procedures are those of Kiefer & Wolfowitz [5], Spendley, Hext & Himsworth [7] and Springer [8]. Here a sequential procedure which makes use of rotatable designs at each stage is proposed. The procedure given is for experiments with two factors only, i.e., the two-dimensional case, as an exactly analogous procedure in higher dimensions is impossible although some variation may make a similar procedure applicable.

The configuration used at each stage is the 'kiss-precise' configuration of Sir Frederick Soddy [6]. It is shown how it is possible to proceed from one design to another always retaining the kiss-precise configuration.

The procedure makes use of only first-order designs; however, a second-degree surface may be fitted when a near-stationary region is reached. Although many first-order rotatable designs exist and are easy to construct, Soddy's configuration seems to give a neat way of proceeding from stage to stage. At each stage only three design points need be added; the minimum number of points required for a first order rotatable design is three.

2. **Spheres in mutual contact.** If k is the dimension of the space, there exists a configuration of $k+2$ spheres in mutual contact. If $r_1, \ldots, r_{k+2}$ are the radii of these spheres, then for $k \geq 2$,

$$k\left(\frac{1}{r_1^2}+\cdots+\frac{1}{r_{k+2}^2}\right) = \left(\frac{1}{r_1}+\cdots+\frac{1}{r_{k+2}}\right)^2. \tag{1}$$

For $k=2$, (1) becomes

$$2\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}+\frac{1}{r_3^2}+\frac{1}{r_4^2}\right) = \left(\frac{1}{r_1}+\frac{1}{r_2}+\frac{1}{r_3}+\frac{1}{r_4}\right)^2, \tag{2}$$

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or, as Soddy [6] states

Four circles to the kissing come,
The smaller are the benter.
The bend is just the inverse of
The distance from the centre.
Though their intrigue left Euclid dumb
There's now no need for rule of thumb.
Since zero bend's a dead straight line
And concave bends have minus sign,
The sum of the squares of all four bends
Is half the square of their sum.

In the procedure presented here, only the special two-dimensional case where three of the circles have the same radius $r=r_1=r_2=r_3$, and each circle is exterior to the other three, is used. Then from (2), $r=(3+2\sqrt{3})r_4$. Such a configuration is shown in Figure 1.

3. **Initial stage.** Suppose the response surface can be approximated by a polynomial of degree one, i.e., $\eta=\beta_0+\beta_1x_1+\beta_2x_2$, where η denotes the true response at (x_1, x_2), and that the experimenter is searching for the region of optimum response. Without loss of generality, it can be assumed that this is the region of maximum response.

Let $A(t)$ denote the circle with radius t centred at A. Then, as shown in Figure 1, $O_j(r)$ $(j=1, 2, 3)$ denote the three circles with equal radius r. Denote the points

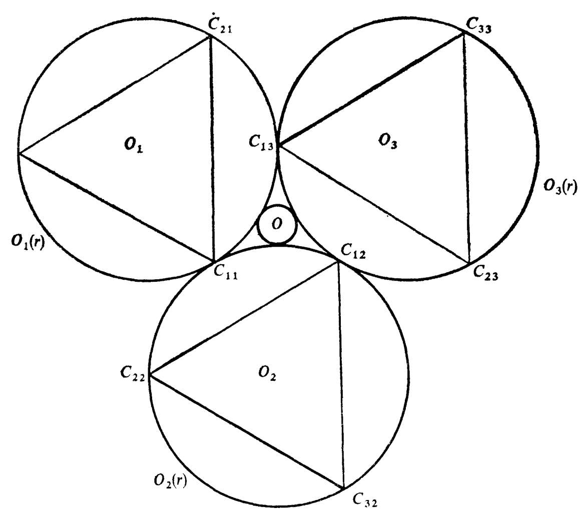

Figure 1
A particular case of the kiss-precise configuration

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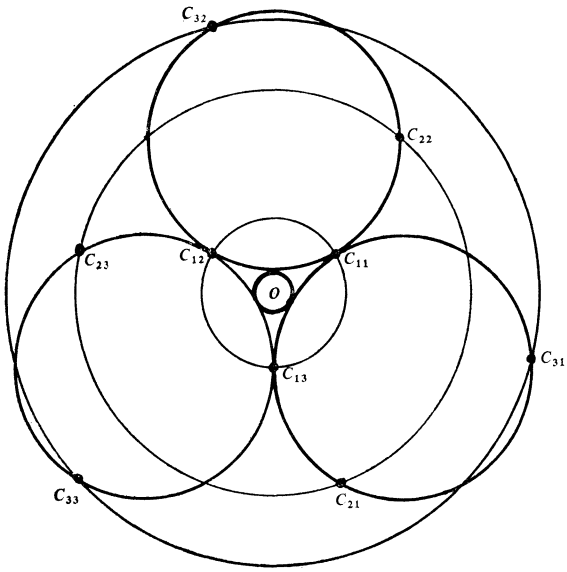

Figure 2
A first-order rotatable design showing points on circles $O(\rho_i)$ $(i=1, 2, 3)$

of contact of these three circles by C_{1j} $(j=1, 2, 3)$. Starting with C_{1j}, construct in $O_j(r)$ the unique inscribed equilateral triangle. Let its other vertices be C_{2j} and C_{3j} named in a counterclockwise direction.

If the points of the experimental design correspond to the points C_{ij} $(i, j=1, 2, 3)$, the design consists of 9 points partitioned into three sets of three points, the points of each set being equally spaced on a circle centred at O; see Figure 2. Box & Hunter [1] and Gardiner, Grandage & Hader [4] have shown that this configuration is sufficient for a first-order rotatable design in two dimensions. The radii of these concentric circles centred at O are

$$\rho_1 = \sqrt{\tfrac{1}{3}}r, \qquad \rho_2 = \sqrt{\tfrac{7}{3}}r, \qquad \rho_3 = \sqrt{\tfrac{13}{3}}r.$$

Rotatable designs, introduced by Box & Hunter [1] for the exploration of response surfaces, have the property that the variance of the estimated response at all points equidistant from the centre of the design is constant. It can easily be shown that the variance function of the estimated response for this 9 point design is

$$\operatorname{var}\{\hat{y}(\mathbf{x})\} = (\tfrac{1}{9} + \tfrac{2}{21}\rho^2)\sigma^2,$$

where $\hat{y}(\mathbf{x})$ denotes the estimated response at $\mathbf{x}=(x_1, x_2)$, σ^2 the experimental error variance, and $\rho=\|\mathbf{x}\|$. When nothing is known about the nature of the response surface it is reasonable to use a rotatable design at each stage since the variance of the estimated response is the same in all directions.

4. **Sequential procedure.** Let y_{ij} be the observed response at C_{ij} $(i, j=1, 2, 3)$. Let

$$\bar{y}_j = \tfrac{1}{3}\sum_{i=1}^{3} y_{ij} \qquad (j = 1, 2, 3),$$

i.e. $\bar{y}_i$ is the average of the responses on $O_i(r)$; see Figure 1. Once the responses have been found at each design point C_{ij}, the direction in which the experimenter should proceed in exploring the response surface is determined in the following way.

Let the three points C_{ij} $(i=1, 2, 3)$ whose $\bar{y}_j$ is the minimum be removed. For example, if $\bar{y}_3$ is the minimum $\bar{y}_j$, C_{i3} is replaced by C_{i4} $(i=1, 2, 3)$, where C_{i4} is the image of C_{i3} by reflection in the line O_1O_2; see Figure 3. This procedure is continued until a region of maximum response is reached.

Referred to a co-ordinate system with origin at the centre of the small circle with radius r_4, the design points C_{ij} $(i, j=1, 2, 3)$ for the first configuration have co-ordinates

$$C_{11}\colon \left(-\frac{1}{2}r, -\frac{1}{2\sqrt{3}}r\right), \qquad C_{12}\colon \left(\frac{1}{2}r, -\frac{1}{2\sqrt{3}}r\right), \qquad C_{13}\colon \left(0, \frac{1}{\sqrt{3}}r\right),$$

$$C_{21}\colon \left(-\frac{1}{2}r, \frac{5}{2\sqrt{3}}r\right), \qquad C_{22}\colon \left(-r, -\frac{2}{\sqrt{3}}r\right), \qquad C_{23}\colon \left(\frac{3}{2}r, -\frac{1}{2\sqrt{3}}r\right),$$

$$C_{31}\colon \left(-2r, \frac{1}{\sqrt{3}}r\right), \qquad C_{32}\colon \left(\frac{1}{2}r, -\frac{7}{2\sqrt{3}}r\right), \qquad C_{33}\colon \left(\frac{3}{2}r, \frac{5}{2\sqrt{3}}r\right);$$

see Figure 4.

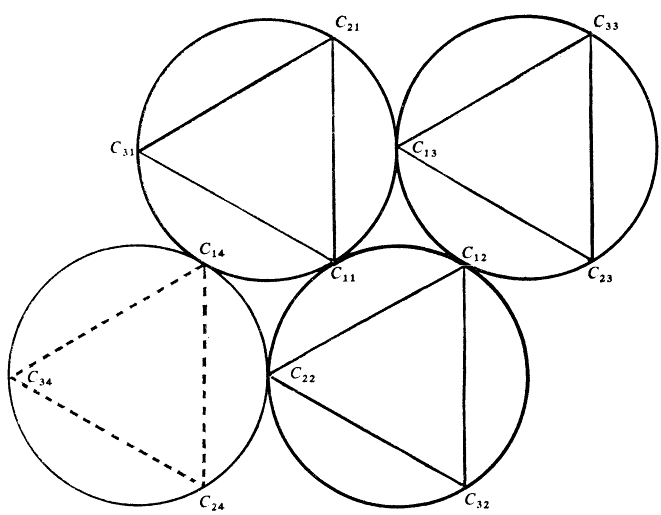

Figure 3
Sample step in the sequential procedure

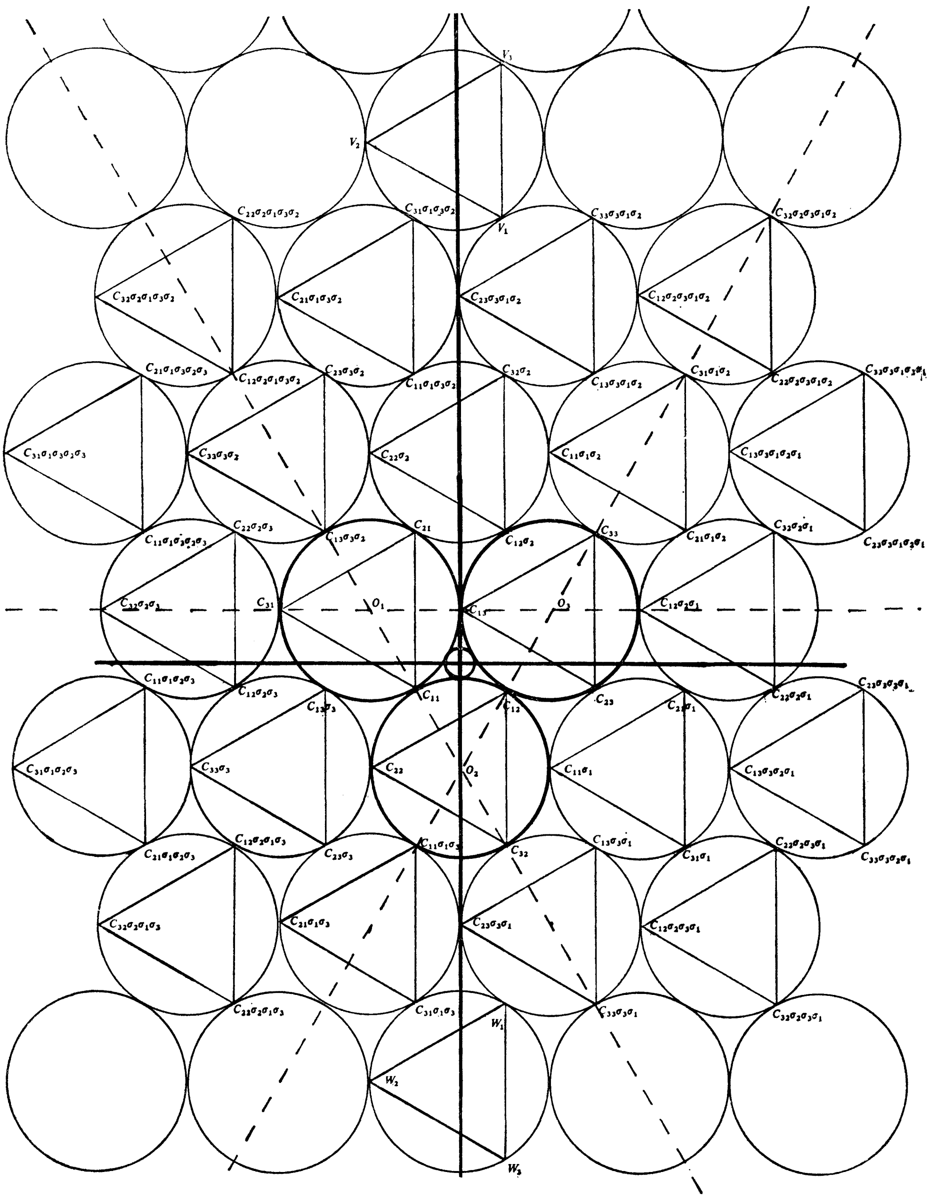

Figure 4
A finite number of design points

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The points C_{i4} are the images of the points C_{i3} by reflection in the line O_1O_2. If $(x, y, 1)$ represents the point (x, y) of the plane, then its image under the reflection σ_3 in this line is represented by $(x', y', 1)$, where

$$(x', y', 1) = (x, y, 1)\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -r & -\frac{r}{\sqrt{3}} & 1 \end{pmatrix}.$$

Thus the points C_{i4} can be labelled $C_{i3}\sigma_3$.

Similarly it might be necessary to replace the points C_{i2} by the points $C_{i2}\sigma_2$, where σ_2 represents the reflection in the line O_3O_1:

$$(x, y, 1)\sigma_2 = (x, y, 1)\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & \frac{2}{\sqrt{3}}r & 1 \end{pmatrix}.$$

The points C_{i1} would be replaced by the points $C_{i1}\sigma_1$, where σ_1 represents the reflection in the line O_2O_3:

$$(x, y, 1)\sigma_1 = (x, y, 1)\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ r & -\frac{r}{\sqrt{3}} & 1 \end{pmatrix}.$$

With products of these reflections, any set $\{C_{ij}: i=1, 2, 3\}$ of design points can be replaced by another such set of design points at any stage in the sequential procedure, but the original configuration is still preserved. Figure 4 gives the co-ordinates of a finite number of design points.

This method of obtaining co-ordinates of the design points can be continued indefinitely. As an example, suppose one wishes to examine the three triangles specified by the points

$$C_{i3}\sigma_3\sigma_1\sigma_2, \qquad C_{i1}\sigma_1\sigma_3\sigma_2, \qquad C_{i2}\sigma_2 \qquad (i = 1, 2, 3)$$

and wishes to replace the triangle $C_{i2}\sigma_2$ $(i=1, 2, 3)$ by the triangle $V_3V_2V_1$ as marked at the top of Figure 4. This triangle is the image of triangle $W_3W_2W_1$ shown at the bottom of the figure under the reflection σ_2, so that $V_i = W_i\sigma_2$ $(i=1, 2, 3)$. But the triangle $W_1W_2W_3$ is clearly the image, under σ_3, of the triangle $C_{12}\sigma_2\sigma_3\sigma_1$, $C_{22}\sigma_2\sigma_3\sigma_1$, $C_{32}\sigma_2\sigma_3\sigma_1$. Thus,

$$W_i = C_{i2}\sigma_2\sigma_3\sigma_1\sigma_3.$$

Therefore,

$$V_i = W_i\sigma_2 = C_{i2}\sigma_2\sigma_3\sigma_1\sigma_3\sigma_2.$$

Thus the point V_1, for example, has co-ordinates

$$(\bar{x}, \bar{y}, 1) = \left(\frac{1}{2}r, -\frac{1}{2\sqrt{3}}r, 1\right)\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & \frac{2}{\sqrt{3}}r & 1 \end{pmatrix}\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -r & -\frac{r}{\sqrt{3}} & 1 \end{pmatrix}$$

$$\times\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ r & -\frac{r}{\sqrt{3}} & 1 \end{pmatrix}\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -r & -\frac{r}{\sqrt{3}} & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & \frac{2}{\sqrt{3}}r & 1 \end{pmatrix}.$$

Since Figure 4 is a fragment of an infinite tessellation, any desired triangle can be expressed as

$$C_{1j}\sigma_{l_1}\sigma_{l_2}\cdots\sigma_{l_n}, \qquad C_{2j}\sigma_{l_1}\sigma_{l_2}\cdots\sigma_{l_n}, \qquad C_{3j}\sigma_{l_1}\sigma_{l_2}\cdots\sigma_{l_n}$$
$$(j = 1, 2, \text{ or } 3; \qquad l_1, l_2, \ldots, l_3 = 1, 2, 3)$$

for some finite n. In fact, all triangles could be expressed as images of just one of the original triangles, say $C_{13}C_{23}C_{33}$ (Coxeter [2, p. 62]), but for present purposes this has no practical advantage.

5. **A stopping rule.** Various possibilities may occur during the sequential procedure. A 'stalemate' may be reached when the three new design points must be discarded in favour of the three design points just discarded. Such a situation suggests that some sort of extremal region has been reached and the region should be analyzed carefully.

If the experimental points on a particular $O(r)$ remain in the design five times, it is highly probable that a near-stationary region has been reached. For example consider Figure 5 where it is assumed that the points 2, 3 and 4 have been in the sequential design in five consecutive stages.

The remaining points excluding 1 have entered the design at some stage while the points 2, 3 and 4 have been in the design. For example, 2, 3, 4, 5, 6, 7, 8, 9 and 10 were in the design, then points 5, 6 and 7 were replaced by 11, 12 and 13, etc. It is then possible to analyze the results corresponding to the 21 experiments together. The co-ordinates of these 21 experimental points are listed in Table 1. Note that the co-ordinate system in Figure 5 differs from that of Figure 4; the point 1 is the origin and the axes are indicated. The points numbered 2 to 22 form

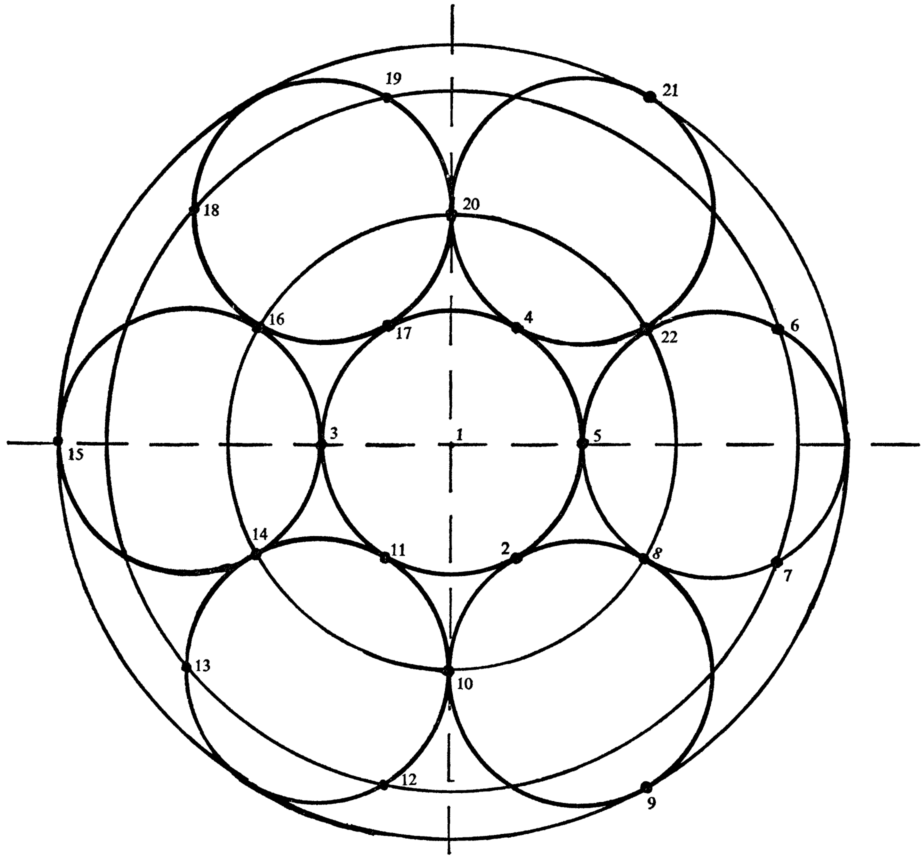

Figure 5
The stopping rule configuration

a second-order rotatable design since

$$(3) \qquad \begin{aligned} &\sum_u x_{iu}^2 = A && (i = 1, 2), \\ &\sum_u x_{iu}^4 = 3 \sum_u x_{iu}^2 x_{ju}^2 = B && (i, j = 1, 2;\ i \neq j), \end{aligned}$$

where A and B are constants, all other moments of the design of order four or less are zero and the points lie on at least two distinct concentric circles with centre (0, 0), point 1 (Draper [3, p. 867]). A second degree surface may, therefore, be fitted in this region.

If the fit of the estimated surface proves to be 'inadequate', the responses at the points 9, 15 and 21 may be removed from the analysis and the surface estimated from the remaining points, thus giving a smaller region over which the second degree surface should fit. These 18 points also form a second order design since the co-ordinates of the points satisfy (3). Similarly, at the next stage, points 6, 7,

TABLE 1. The co-ordinates of the experimental points shown in Figure 5.

Point number	*Co-ordinates*
1	$0, 0$
2	$\frac{1}{2}r, -\frac{\sqrt{3}}{2}r$
3	$-r, 0$
4	$\frac{1}{2}r, \frac{\sqrt{3}}{2}r$
5	$r, 0$
6	$\frac{5}{2}r, \frac{\sqrt{3}}{2}r$
7	$\frac{5}{2}r, -\frac{\sqrt{3}}{2}r$
8	$\frac{3}{2}r, -\frac{\sqrt{3}}{2}r$
9	$\frac{3}{2}r, -\frac{3\sqrt{3}}{2}r$
10	$0, -\sqrt{3}r$
11	$-\frac{1}{2}r, \frac{\sqrt{3}}{2}r$
12	$-\frac{1}{2}r, -\frac{3\sqrt{3}}{2}r$
13	$-2r, -\sqrt{3}r$
14	$-\frac{3}{2}r, -\frac{\sqrt{3}}{2}r$
15	$-3r, 0$
16	$-\frac{3}{2}r, \frac{\sqrt{3}}{2}r$
17	$-\frac{1}{2}r, \frac{\sqrt{3}}{2}r$
18	$-2r, \sqrt{3}r$
19	$-\frac{1}{2}r, \frac{3\sqrt{3}}{2}r$
20	$0, \sqrt{3}r$
21	$\frac{3}{2}r, \frac{3\sqrt{3}}{2}r$
22	$\frac{3}{2}r, \frac{\sqrt{3}}{2}r$

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12, 13, 18 and 19 can be removed and the properties of a second-order rotatable design are still retained. If necessary, points 8, 10, 14, 16, 20 and 22 can be removed; the remaining points form a singular design. In this case an experiment must be performed at point 1 (Draper [3, p. 867]). In this way the near-stationary region may be explored for a maximum.

6. **Extension to higher dimensions.** In three dimensions, the kiss-precise configuration consists of five spheres in mutual contact. The particular case of interest has four spheres of equal radius surrounding a smaller sphere. These four spheres touch each other in six points, the vertices of a regular octahedron. In strict analogy with the two-dimensional case, it would be necessary to choose four of these points, one on each sphere; starting with each point, a regular tetrahedron would have to be constructed in each sphere. In order to have a rotatable design, these four points must be equally spaced on a sphere and so form a regular tetrahedron. But it is impossible to pick the four vertices of a regular tetrahedron from the six vertices of a regular octahedron (Coxeter [2, §3.6]). Thus an extension to three dimensions of the procedure described in §4 is impossible.

In k dimensions, this particular case of the kiss-precise configuration involves $k+1$ mutually tangent hyperspheres with equal radii surrounding a smaller hypersphere. These $k+1$ hyperspheres touch each other in $\binom{k+1}{2}$ points forming a k-dimensional polytope $\left\{\begin{matrix}3\\3, 3, \ldots, 3\end{matrix}\right\}$ (Coxeter [2, §8.1]). One point must be chosen on each sphere, and these $k+1$ points must be equally spaced on a hypersphere thus forming a k-dimensional regular simplex $\{3, 3, \ldots, 3\}$. But it is impossible to pick the vertices of a regular simplex from those of $\left\{\begin{matrix}3\\3, 3, \ldots, 3\end{matrix}\right\}$ (see the co-ordinates in Coxeter [2, p. 157]). Hence the procedure cannot be extended to higher dimensions.

Another possible extension to three dimensions of the procedure of §4 would be to arbitrarily inscribe regular tetrahedra in each of the four equal spheres of the kiss-precise configuration. A sequential rotatable design would be obtained if these tetrahedra were 'similarly placed' in each sphere, i.e. corresponding vertices are equidistant from the centre of the configuration, and if each tetrahedron could be replaced by its image under reflection in the plane determined by the centres of the other three tetrahedra, so that the resulting configuration is the same as the original one (as in the 2-dimensional case; Figure 2). But tedious algebraic manipulations show that four regular tetrahedra satisfying these conditions cannot be found.

Perhaps, in higher dimensions a sequential procedure may be obtained which has the property described here in two of the dimensions and some other property in the remaining dimensions.

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