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MIXTURE DESIGNS FOR THREE FACTORS*

by
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MIXTURE DESIGNS FOR THREE FACTORS

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SUMMARY

Scheffé, in two recent papers (1953, 1963), has given designs for experimenting with mixtures. The basis of these designs is the choice of symmetrical arrangements of points in the factor space and the fitting of carefully chosen models which have exactly as many coefficients as there are data points. The designs are such that some of the experiments do not contain any of one or more ingredients of the mixture. This may or may not be a disadvantage depending on the problem involved.

Here an alternative form of design selection is made for the case of mixtures of three factors. (The method has also been extended to four factors.) This involves the premise that, in the absence of specialist knowledge about the form of the true response function, it is desired to fit a response surface equation of first or second order over the factor space of possible mixtures, and experimental runs are needed which, in a certain sense, ensure the best surface fit possible.

The principles used in the choice of appropriate designs will be those originally introduced by Box and Draper (1959).

1. INTRODUCTION

When three components \( z_1, z_2, z_3 \) form a mixture with total content \( m \leq 1 \), the possible mixtures are limited to a two-dimensional triangular area in the three-dimensional space \( (z_1, z_2, z_3) \). This triangular area lies on the plane \( z_1 + z_2 + z_3 = m \) and is bounded by the planes \( z_1 = z_2 = z_3 = 0 \). The region can thus be represented by an equilateral triangle in two dimensions. If we choose new axes \( (x_1, x_2) \) for the triangle so that one vertex passes through the line \( x_1 = 0 \), the other vertices are symmetrical about \( x_1 = 0 \), and the centroid.
is at \((0, 0)\) we can move between the two representations by

\[
x_1 = \frac{1}{2} (-z_1 + z_2)
\]
\[
x_2 = (-z_1 - z_2 + 2z_3) / 3 / 6
\]
\[
x_3 = z_1 + z_2 + z_3 = m
\]

or

\[
z_1 = (-3x_1 - x_2 \sqrt{3} + m) / 3
\]
\[
z_2 = (3x_1 - x_2 \sqrt{3} + m) / 3
\]
\[
z_3 = (2x_2 \sqrt{3} + m) / 3
\]

where \(m\) is the length of side of the triangle in the \(x_3 = m\) plane as well as the total to which the three ingredients add.

We now work in the coordinates \((x_1, x_2)\) and assume that a response surface either of first order \((d_1 = 1)\) or else of second order \((d_1 = 2)\), namely

\[
\hat{Y} = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_1^2 + b_4 x_2^2 + b_5 x_1 x_2 + b_6 x_1^2 x_2 + b_7 x_2^2
\]

will be fitted. Initially we shall assume that there is no variance error (this will later be considered) but that bias error will arise due to the possibility that the order \(d_1\) of the model is inadequate.

In particular we shall assume that when inadequacy is present, it arises due to an underestimate of order one of the degree \(d_2\) of the true model, i.e. if our model is linear \((d_1 = 1)\) there is a possibility of error due to presence of second degree terms \((d_2 = 2)\) in the true model, or if our model is quadratic \((d_1 = 2)\) there is a possibility of error due to
presence of third degree terms $d_2 = 3$. We shall determine in each of these cases the appropriate experimental designs which minimize the bias error.

Following the development of Box and Draper (1959) bias error will be defined as

$$B = N \Delta \sigma^2 \int_R \left[ E\hat{y}(x) - \eta(x) \right]^2 dx,$$

where $R$ is the 'region of interest' defined by the equilateral triangle, $N$ is the number of observations, $\eta(x)$ is the true response and $\hat{y}(x)$ is the estimated response at the point $x$, $\sigma^2$ is the experimental error variance, and $\Delta = \int_R dx$.

A theorem by Box and Draper (1959) states that if a polynomial of degree $d_1$ is to be fitted by the method of least squares over any region of interest $R$ in the space of the variables and if the true function is a polynomial of degree $d_2$, the average squared bias $B$ will be minimized for all values of the coefficients of neglected terms by choosing the experimental design in such a way that

$$\mu_{11}^{-1} M_{12} = \mu_{11}^{-1} \mu_{12}$$

(1.1)

where $M_{11}$ and $M_{12}$ are matrices of design moments and $\mu_{11}$ and $\mu_{12}$ are matrices of region moments up to order $d_1 + d_2$.

We shall search for experimental designs which satisfy these conditions for the case where $R$ is the equilateral triangle defined above. The value of the 'all-bias' designs, as we shall call them, lies in the fact that it appears, as has been shown elsewhere (Box and Draper, 1959, 1963; Draper and Lawrence, 1965) for spherical and cuboidal regions, and will be shown here for triangular regions, for the cases under consideration, that designs appropriate when both variance and bias errors
arise are not very different from all-bias designs. However, designs appropriate when only variance error exists (bias error is zero, i.e. the model is correct - a most unusual state of affairs) are quite unsuitable when both variance and bias errors occur.

In order to narrow the field of search for possible designs we shall make certain assumptions. These assumptions will restrict the class of possible designs by giving certain design moments specified values suggested by the values of the corresponding region moments. These assumptions will be stated as needed. We then examine the equations (1.1) (which, as we have noted, are necessary and sufficient for all-bias designs) and determine their implications under the restrictions placed on the designs.

2. Moment requirements for the all-bias designs. It is convenient to consider the case \( d_1 = 2, d_2 = 3 \); that is, the model to be fitted is a second degree polynomial and it is desired to guard against the possibility that the true response function is a third degree polynomial. The simpler case can then be derived easily. The region of interest \( R \) is an equilateral triangle of side \( m \) with centroid at the origin and base parallel to the \( x \)-axis. The coordinates of the vertices are \( (0,3^{1/3}m/3), (m/2,-3^{1/3}m/6), \) and \( (-m/2,-3^{1/3}m/6) \). When \( m = 1 \) the region \( R \) is the triangle obtained in the mixture problem with three factors adding to unity. The theory is applicable to any problem on mixtures or otherwise, which involves a triangular region of interest, whether equilateral or not. For by suitable transformation, any scalene triangle can be transformed to an equilateral triangle and it has been shown by Folks (1958) that the bias \( B \) as defined above is invariant under simple linear transformations of the kind needed.
The moments of the region are obtained from the moment generating function

\[
M_{x_1,x_2}(t_1,t_2) = A \int_{-a}^{b} \int_{-b}^{b} e^{x_1(t_1x_1 + t_2x_2)} \, dx_1 \, dx_2
\]

\[
= 1 + \frac{m^2}{2a} t_1^2 + \frac{m^2}{2i} t_2^2 + \frac{3}{360} \frac{1}{m} t_1 \frac{2}{2i} + \frac{3}{360} \frac{1}{m} t_2 \frac{3}{2i} + \frac{3}{240} \frac{1}{m} t_1 t_2 + \frac{1}{2i} \frac{1}{m} t_1
\]

\[
+ \frac{m}{720} \frac{1}{2a} + \frac{m}{240} \frac{1}{2i} + \frac{3}{7560} \frac{1}{m} t_1 \frac{2}{2i} + \frac{3}{2520} \frac{1}{m} t_2 \frac{2}{2i} + \frac{3}{1512} \frac{1}{m} t_1 t_2 + \ldots
\]

where \( A = 3^{1/2} m^2/4 \), \( a = 3^{1/2} m/6 \), \( b = (m-3^{1/2} x_2)/3 \).

When \( d_1 = 2 \) and \( d_2 = 3 \), the matrices \( \mu_{11} \) and \( \mu_{12} \) are given below. Borders indicate the arrangement of moments within the matrices; e.g., the moment at the intersection of the \( x_1 \) row and the \( x_2 \) column is

\[
A \int_{-a}^{b} \int_{-b}^{b} x_1 x_2 dx_1 dx_2.
\]

\[
\mu_{11} = \begin{bmatrix}
1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1 x_2
\end{bmatrix}
\]

\[
\mu_{11} = \begin{bmatrix}
1 & 0 & 0 & m^2/24 & m^2/24 & 0
0 & m^2/24 & 0 & 0 & 0 & -m^2/60
0 & 0 & m^2/24 & -m^2/60 & m^2/60 & 0
m^2/24 & 0 & -m^2/60 & m^4/240 & m^4/720 & 0
m^2/24 & 0 & m^2/60 & m^4/720 & m^4/240 & 0
0 & -m^2/60 & 0 & 0 & 0 & m^4/720
\end{bmatrix}
\]

(2.1)
\[
\begin{bmatrix}
x^3 & x x^2 & x^3 & x^2 x^2 \\
1 & 2 & 1 & 2 \\
\end{bmatrix}
\begin{bmatrix}
0 & 0 & am^2/60 & -am^2/60 \\
m^4/120 & m^4/720 & 0 & 0 \\
0 & 0 & -am^4/1260 & -am^4/420 \\
0 & 0 & 5am^4/1260 & -am^4/1260 \\
\end{bmatrix} =
\begin{bmatrix}
x^3 & x x^2 & x^3 & x^2 x^2 \\
1 & 2 & 1 & 2 \\
\end{bmatrix}
\begin{bmatrix}
0 & 0 & am^2/105 & 2am^2/105 \\
m^2/11 & m^2/11 & 0 & 0 \\
0 & 0 & m^2/11 & m^2/11 \\
0 & 0 & 0 & -4a/7 \\
\end{bmatrix}
\begin{bmatrix}
0 & 0 & 6a/7 & -2a/7 \\
-6a/7 & -2a/7 & 0 & 0 \\
\end{bmatrix}
\]

It can be shown that

\[
\begin{bmatrix}
0 & 0 & am^2/60 & -am^2/60 \\
m^4/120 & m^4/720 & 0 & 0 \\
0 & 0 & -am^4/1260 & -am^4/420 \\
0 & 0 & 5am^4/1260 & -am^4/1260 \\
\end{bmatrix}
\begin{bmatrix}
0 & 0 & am^2/105 & 2am^2/105 \\
m^2/11 & m^2/11 & 0 & 0 \\
0 & 0 & m^2/11 & m^2/11 \\
0 & 0 & 0 & -4a/7 \\
\end{bmatrix}
\begin{bmatrix}
0 & 0 & 6a/7 & -2a/7 \\
-6a/7 & -2a/7 & 0 & 0 \\
\end{bmatrix}
\]

We now restrict the class of possible designs by imposing the following conditions on the design moments

\[
[1] = [2] = [12] = [111] = [122] = [1112] = [1222] = \\
[11111] = [11122] = [1222] = 0;
\]

\[
[11] = [22]; [22] = [-112]; [1111] = [2222] = 3[1122]; \\
[11112] = 3[1122] = -0.6[2222]
\]

where, for example,

\[
[122] = N^{-1} \sum_{u=1}^{N} x_{1u} x_{2u}.
\]

These are the conditions implied as reasonable by a consideration of the moments of the region. Unless some such conditions are imposed.
the excessive number of moments that must be determined makes a search for a suitable design prohibitive. The matrices of design moments, after these assumptions, are then of the form given below; borders have been included as in the case of the matrices of the region moments.

\[
\begin{bmatrix}
1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1 x_2
\end{bmatrix}
\begin{bmatrix}
x_1^3 & x_1^2 x_2 & x_1 x_2^2 & x_2^3
\end{bmatrix}
\]

\[
\frac{M_{11}}{d} =
\begin{bmatrix}
1 & 0 & 0 & c & 0 & 0
c & 0 & 0 & 0 & d & x_1^1
c & d & -d & 0 & x_2^1
c & 0 & -d & f & 0 & x_2^1
c & 0 & 0 & 0 & f & x_1 x_2
\end{bmatrix}
\begin{bmatrix}
0 & 0 & -d & d & 0 & 1
3f & f & 0 & 0 & x_1
0 & 0 & 3f & f & x_2
0 & 0 & -5h & h & x_1
3h & h & 0 & 0 & x_2
\end{bmatrix}
\]

(2.3)

and therefore it follows that

\[
\begin{bmatrix}
0 & 0 & 8su & -8su
12rw & 4rw & 0 & 0
0 & 0 & 12rw & 4rw
0 & 0 & 2sv+6ru & -2sv+2ru
0 & 0 & 2sv-6ru & -2sv-2ru
12ru & 4ru & 0 & 0
\end{bmatrix}
\]

where

\[r = 2f - c^2, \ s = cf - d^2, \ u = ch - df, \ v = cd - 2h, \ \text{and} \ w = f^2 - dh.\]

The necessary and sufficient conditions, \(M^{-1}_{11-12} = M^{-1}_{11/12}\), it can now be shown, imply that \(c = m^2 / 2h, \ d = -3^{1/2} m^3 / 360, \ f = m^4 / 720, \ \text{and} \ h = -3^{1/2} m^5 / 7560. \) Therefore, in this case and with the restrictions (2.2) the necessary and sufficient conditions for an all-bias design imply the sufficient conditions

\[
\begin{bmatrix}
M_{11} & M_{11/12} \nM_{12} & M_{12/12}
\end{bmatrix}
\]

(2.4)
We shall, below, search for designs which satisfy the restrictions (2.2) and the sufficient conditions (2.4). When \( d_1 = 1, d_2 = 2 \) the matrices \( \mu_{11} \) and \( \mu_{12} \) are given in the first three rows of the matrix (2.1), the first three columns forming \( \mu_{11} \) and the last three columns forming \( \mu_{12} \). The matrices \( \mu_{11} \) and \( \mu_{12} \) are obtained in similar fashion from the first matrix (2.3). The result in this case, also, is that the sufficient conditions are implied.

We now obtain designs which satisfy the restrictions assumed and the conditions derived above, for the two cases \( d_1 = 1, d_2 = 2 \). As mentioned above, we refer to them as the "all-bias designs" since they are obtained on the assumption that there is no variance error. The designs will be formed choosing various sets of points which satisfy some of the required conditions and combining them in such a way that all the conditions are satisfied. Table 1 shows a number of point sets which satisfy (2.2). The design moments are of the form \( N^{-1} \sum_{u=1}^{N} x_{1u}^{r} x_{ju}^{s} \). The contribution of each point set to the sum \( \sum_{u=1}^{N} x_{1u}^{r} x_{ju}^{s} \) is given for each moment. Region moments are included in Table 1 also.

3. Designs for the case \( d_1 = 1, d_2 = 2 \). The conditions to be satisfied in this case are the following, which are obtained by equating design moments and region moments up to and including moments of third order:

\[
\begin{align*}
\Sigma x_{1u} &= \Sigma x_{1u} x_{2u} = \Sigma x_{1u}^{3} = \Sigma x_{1u} x_{2u}^{2} = 0 \\
\Sigma x_{1u}^{2} &= \Sigma x_{2u}^{2} = Nm^{2}/2h \\
\Sigma x_{2u}^{3} &= -\Sigma x_{1u}^{2} x_{2u} = 3^{1/2} Nm^{3}/360
\end{align*}
\]

(3.1)

where all summations are over \( u \), from 1 to \( N \).
Table 1. Point sets in two dimensions.

<table>
<thead>
<tr>
<th>Set number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>Corresponding Region Moments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description of set (see below)</td>
<td>△</td>
<td>△</td>
<td>□</td>
<td>+</td>
<td>(◇)</td>
<td></td>
</tr>
<tr>
<td>No. of points in set</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>(\Sigma x_1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_1^2)</td>
<td>(p^2/2)</td>
<td>(q^2/2)</td>
<td>(u^2/2)</td>
<td>(2b^2)</td>
<td>(2(c^2+d^2))</td>
<td>(m^2/24)</td>
</tr>
<tr>
<td>(\Sigma x_2^2)</td>
<td>(p^2/2)</td>
<td>(q^2/2)</td>
<td>(u^2/2)</td>
<td>(2b^2)</td>
<td>(2(c^2+d^2))</td>
<td>(m^2/24)</td>
</tr>
<tr>
<td>(\Sigma x_1^3)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2^3)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_1^2 x_2)</td>
<td>(-3^{\frac{3}{4}} p^3/12)</td>
<td>(3^{\frac{3}{4}} q^3/12)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(-3^{\frac{3}{4}} m^3/360)</td>
</tr>
<tr>
<td>(\Sigma x_1 x_2^2)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2^3)</td>
<td>(3^{\frac{3}{4}} p^3/12)</td>
<td>(-3^{\frac{3}{4}} q^3/12)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(3^{\frac{3}{4}} m^3/360)</td>
</tr>
<tr>
<td>(\Sigma x_2 x_1^2)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_1 x_2)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2 x_1)</td>
<td>(p^4/24)</td>
<td>(q^4/24)</td>
<td>(u^4/24)</td>
<td>(2b^2)</td>
<td>(2(c^4+d^4))</td>
<td>(m^4/720)</td>
</tr>
<tr>
<td>(\Sigma x_1^5)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2^5)</td>
<td>(-3^{\frac{3}{5}} p^5/120)</td>
<td>(3^{\frac{3}{5}} q^5/120)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(-3^{\frac{3}{5}} m^5/2520)</td>
</tr>
<tr>
<td>(\Sigma x_1^3 x_2)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2^3)</td>
<td>(-3^{\frac{3}{5}} p^5/120)</td>
<td>(3^{\frac{3}{5}} q^5/120)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(-3^{\frac{3}{5}} m^5/7560)</td>
</tr>
<tr>
<td>(\Sigma x_1 x_2^3)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(\Sigma x_2^5)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Set number 1: vertices of an equilateral triangle, oriented as R, centroid at the origin, side p: \((0, 3^{1/2} p/3), (\pm p/2, -3^{1/2} p/6)\)

Set number 2: vertices of an equilateral triangle, similar to R, inverted with respect to R, centroid at the origin, side q: \((0, -3^{1/2} q/3), (\pm q/2, 3^{1/2} q/6)\)

Set number 3: vertices of a square, side a, centroid at the origin, sides parallel to coordinate axes: \((\pm a, \pm a)\)

Set number 4: points on the coordinate axes at distance b from the origin: \((\pm b, 0), (0, \pm b)\)

Set number 5: vertices of a rectangle: \((c, d), (d, c), (-c, -d), (d, -c)\).

It can be shown, first of all, that there are no designs consisting of only three or four points which satisfy the equations. There is an infinity of five-point designs which satisfy the equations, and these form a rather pretty pattern in two dimensions. The complete solution has been obtained by E. L. Albasiny (1964). The equations to be solved in this case are:

\[
\begin{align*}
   a + c + e + g + j &= 0 \\
   b + d + f + h + k &= 0 \\
   ab + cd + ef + gh + jk &= 0 \\
   a^2 + c^2 + e^2 + g^2 + j^2 &= Nm^2/24 \\
   b^2 + d^2 + f^2 + h^2 + k^2 &= Nm^2/24 \\
   a^3 + c^3 + e^3 + g^3 + j^3 &= 0 \\
   ab^2 + cd^2 + ef^2 + gh^2 + jk^2 &= 0 \\
   a^2b + c^2d + e^2f + g^2h + j^2k &= -3^{1/2} Nm^3/360 \\
   b^3 + a^3 + f^3 + h^3 + k^3 &= 3^{1/2} Nm^3/360
\end{align*}
\]
where \((a, b), (c, d), (e, f), (g, h), (j, k)\) are the design points away from the center, and \(N = 5 + n_0\), where \(n_0\) is the number of center points. Two cases of special interest arise when some of the points lie on the coordinate axes. The first has points \((0, 0.33\text{m}), (0, 0.128\text{m}), (0, -0.231\text{m}), (-0.323\text{m}, 0.115\text{m})\). The second has points \((0, 0.347\text{m}), (0.199\text{m}, 0.034\text{m}), (0.254\text{m}, -0.207\text{m})\). All other solutions are unsymmetrical with respect to the axes.

Since the equations (3.1) are not satisfied with four points or less, the individual point sets in Table 1 do not by themselves provide designs. Furthermore, in order to satisfy equations involving third order moments every combination must include at least one point set number 1. Let \((i, j, k, \ldots)\) indicate the combination of point sets \(i, j, k, \ldots\) from the table. The set combinations \((1, 2), (1, 3), (1, 4), (1, 5),\) and \((1, 1, 2)\) all provide designs with six or more points. For example consider the combination \((1, 2)\). The equations for this set are

\[
\begin{align*}
p^2 + q^2 &= \frac{N m^2}{12} \\
p^3 - q^3 &= \frac{N m^3}{30}
\end{align*}
\]

Let \(p - q = u\) and \(pq = v\). Then the equations become \(u^2 + 2v = \frac{N m^2}{12}\) and \(u^3 + 3uv = \frac{N m^3}{30}\), or \(v = (\frac{N m^2}{24}) - \frac{u^2}{2}\) and \(u^3 - \frac{N m^2 u^4}{14} + \frac{N m^3}{15} = 0\). For a given \(N\) this cubic equation in \(u\) is easily solved by the trigonometric method (Dickson, 1939) and \(p = .621\text{m}\) and \(q = .339\text{m}\) are obtained when, for example, \(N = 6\).

Although the intended models are different in the two cases, this six-point design may be compared with the simplex lattice design developed by Scheffé (1958) for experiments with mixtures of three components. Scheffé's design consists of the six points which correspond to mixture proportions \((1, 0, 0), (0, 1, 0), (0, 0, 1), (1/2, 1/2, 1/2), (1/2, 0, 1/2), (0, 1/2, 1/2),\) or in our notation the points \((0, 3^{1/2}m/3), (m/2, -3^{1/2}m/6),\)
\((m/4, 3^{1/2}m/12), (0, -3^{1/2}m/6)\). Note that all the design points are at
the vertices and mid-points of sides of the equilateral triangle which
forms the region \( R \), i.e. all design points lie on the boundary of the
region of interest. Since all design points must lie within or on the
triangle, due to the mixture restriction, Scheffe's design (it will be
shown) is actually the appropriate 'all-variance' design for our set-up
using the combination \((1,2)\) and thus as mentioned earlier is therefore
not appropriate for situations where both variance and bias errors exist
and a first order polynomial is to be fitted. In our design the point
sets form two equilateral triangles, one inverted, but they are entirely
inside the region \( R \), and the vertices of the smaller inverted triangle
are slightly outside the sides of the larger triangle. There is a possible
disadvantage to Scheffe's design worth mentioning. In some problems, the
characteristics of a mixture of three ingredients are not exhibited by
mixtures which do not contain all of the ingredients under study. Consider
for a two-factor example the gasoline-oil mixture used for two-stroke
motorcycle engines. Experiments on 'all gasoline, no oil!', or on
'no gasoline, all oil!' would not exhibit results typical of the mixture.
Scheffe's design would not be suitable for such problems while our design
does not encounter this difficulty. The simplex-centroid design of Scheffe
(1963) is, for three components, the same as the simplex-lattice design with
an added point representing a mixture \((1/3, 1/3, 1/3)\). This corresponds
in our notation to a point \((0,0)\), i.e. a center point.

Solutions of the systems of equations are quite easy to obtain for
the sets which provide designs and the results are summarized in Table 2.
Sets \((1,1), (2,2), (2,3), (2,4), (2,5), (3,4), (3,5),\) and \((4,5)\) do not
provide designs. Combinations containing more than nine points have not
been investigated.
<table>
<thead>
<tr>
<th>Point sets</th>
<th>N</th>
<th>Parameter values</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,2)</td>
<td>6</td>
<td>( p = .621m, q = .339m )</td>
</tr>
<tr>
<td>(1,2)</td>
<td>7</td>
<td>( p = .662m, q = .381m )</td>
</tr>
<tr>
<td>(1,2)</td>
<td>8</td>
<td>( p = .699m, q = .421m )</td>
</tr>
<tr>
<td>(1,2)</td>
<td>9</td>
<td>( p = .733m, q = .457m )</td>
</tr>
<tr>
<td>(1,3)</td>
<td>7</td>
<td>( p = .616m, a = .160m )</td>
</tr>
<tr>
<td>(1,4)</td>
<td>7</td>
<td>( p = .616m, b = .226m )</td>
</tr>
<tr>
<td>(1,5)</td>
<td>7</td>
<td>( p = .616m, c = (0.05lm^2-d^2)^{\frac{1}{2}}, d \text{ arbitrary} )</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>9</td>
<td>( p_2 \text{ arbitrary, } p_1 \text{ and } q \text{ satisfy equations:} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( p_1^2 + q_1^2 = .75m^2 - p_2^2 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( p_1^3 + q_1^3 = .3m^3 - p_2^3 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>e.g. ( p_1 = .606m, p_2 = .500m, q = .36lm )</td>
</tr>
<tr>
<td>(1,2,2)</td>
<td>9</td>
<td>( q_2 \text{ arbitrary, } p \text{ and } q_1 \text{ satisfy equations:} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( p^2 + q_1^2 = .75m^2 - q_2^2 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( p^3 - q_1^3 = .3m^2 + q_2^3 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>e.g. ( p = .727m, q_1 = .425m, q_2 = .200m )</td>
</tr>
</tbody>
</table>
H. Designs for the case \( d_1 = 2, \ d_2 = 3 \). As in the case \( d_1 = 1, \ d_2 = 2 \), we shall consider only those point sets which will provide designs under the conditions (2.2). The conditions to be satisfied now are obtained when design moments up to and including those of fifth order are equated to the corresponding region moments. This implies, for the non-zero moments

\[
\begin{align*}
\sum x^2_{1u} &= \sum x^2_{2u} = N m^2/2h \\
\sum x^3_{2u} &= - \sum x^2_{1u} x_{2u} = 3^{1/2} N m^3/360 \\
\sum x^4_{1u} &= \sum x^4_{2u} = 3 \sum x^2_{1u} x^2_{2u} \\
\sum x^4_{1u} x_{2u} &= 3 \sum x^3_{1u} x^3_{2u} = -0.6 \sum x^5_{2u}
\end{align*}
\]  \( (4.1) \)

where all summations are over \( u \), from 1 to \( N \).

It is apparent that a combination of only two point sets is unlikely to provide a design because there are more equations than parameters. However, the combination \((1,2)\) provides approximate solutions to the equations when \( N = 7, 8, \) and 9, i.e., when there are 1, 2, or 3 center points. These solutions are approximate in the sense that when the parameters are given the tabulated values, the equations are not satisfied exactly but are almost satisfied. Combinations of three point sets which provide designs are \((1,3,4), (1,3,5), (1,1,5), (1,5,5), (1,1,2)\) and \((1,2,2)\). The first four provide designs only when \( N = 13; \) i.e., when there are two center points. The combinations \((1,1,2)\) and \((1,2,2)\) provide approximate solutions. For the approximate designs the difference between each design moment and the corresponding region moment has been calculated and this difference is
expressed as a percentage of the region moment. The maximum percentage
for each approximate design is indicated in Table 3 as "maximum discrepancy." Designs with maximum discrepancy greater than ten percent are not included.

If no maximum discrepancy is given, the design is exact.

Generally, combinations of four or more point sets will provide
designs, and some of these will be tabulated. Again, there must be at
least one point set number one in each combination in order that the equations
involving third and fifth order moments be satisfied. Combinations with more
than thirteen points have not been investigated, except for (1,1,2,5).

Solutions to the systems of equations (4.1) for certain set combina-
tions were obtained, in most cases, by use of electronic digital computer.

For combinations of two or three point sets elimination techniques may be
used first to reduce the system to a set of polynomials in one variable each;
in some instances these are easily solved and in others the IBM 1620 was used
to find solutions, using program 7.0.032 from the 1620 User's Group Library:
"Calculation of Roots (real and complex) of a Real Polynomial Equation."

Table 3 shows parameter values for designs when \( d_1 = 2, d_2 = 3. \)

Point sets are taken from Table 1.

To illustrate the cases which are most difficult to solve, consider
the combination (1,1,1,2) with \( N = 12. \) The equations to be satisfied are:

\[
\begin{align*}
    p_1^2 + p_2^2 + p_3^2 + q^2 &= m^2 \\
p_1^3 + p_2^3 + p_3^3 - q^3 &= 2m^3/5 \\
p_1^4 + p_2^4 + p_3^4 + q^4 &= 2m^4/5 \\
p_1^5 + p_2^5 + p_3^5 - q^5 &= 8m^5/35
\end{align*}
\]
Table 3. Designs for k=2, R Triangular, d_1=2, d_2=3.

<table>
<thead>
<tr>
<th>Point sets</th>
<th>N</th>
<th>Parameter values</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,2)</td>
<td>7</td>
<td>p = 0.670m, q = 0.385m (max. discrepancy: 5.0%)</td>
</tr>
<tr>
<td>(1,2)</td>
<td>8</td>
<td>p = 0.698m, q = 0.421m (max. discrepancy: 0.8%)</td>
</tr>
<tr>
<td>(1,2)</td>
<td>9</td>
<td>p = 0.723m, q = 0.450m (max. discrepancy: 4.7%)</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>9</td>
<td>p_1 = 0.715m, p_2 = 0.233m, q = 0.430m (max. disc.: 0.8%)</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>10</td>
<td>p_1 = 0.729m, p_2 = 0.323m, q = 0.455m (max. disc.: 0.6%)</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>11</td>
<td>p_1 = 0.738m, p_2 = 0.398m, q = 0.462m (max. disc.: 0.5%)</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>12</td>
<td>p_1 = 0.743m, p_2 = 0.465m, q = 0.450m (max. disc.: 1.5%)</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>13</td>
<td>p_1 = 0.742m, p_2 = 0.532m, q = 0.485m (max. disc.: 2.8%)</td>
</tr>
<tr>
<td>(1,2,2)</td>
<td>9</td>
<td>p = 0.716m, q_1 = 0.342m, q_2 = 0.342m (max. disc.: 4.3%)</td>
</tr>
<tr>
<td>(1,2,2)</td>
<td>10</td>
<td>p = 0.739m, q_1 = 0.367m, q_2 = 0.367m (max. disc.: 8.7%)</td>
</tr>
<tr>
<td>(1,1,1,2)</td>
<td>12</td>
<td>p_1 = 0.751m, p_2 = 0.422m, p_3 = 0.189m, q = 0.472m</td>
</tr>
<tr>
<td>(1,1,2,2)</td>
<td>12</td>
<td>p_1 = 0.748m, p_2 = 0.445m, q_1 = 0.468m, q_2 = 0.156m</td>
</tr>
<tr>
<td>(1,2,2,2)</td>
<td>12</td>
<td>p_1 = 0.782m, q_1 = 0.348m, q_2 = 0.348m, q_3 = 0.348m</td>
</tr>
<tr>
<td>(1,3,4)</td>
<td>13</td>
<td>p = 0.756m, a = 0.183m, b = 0.258m</td>
</tr>
<tr>
<td>(1,3,5)</td>
<td>13</td>
<td>p = 0.756m, a = 0.300m, o = 0.547m, d = 0.180m</td>
</tr>
<tr>
<td>(1,4,5)</td>
<td>13</td>
<td>p = 0.756m, b = 0.212m, c = 0.130m, d = 0.257m</td>
</tr>
<tr>
<td>(1,5,5)</td>
<td>13</td>
<td>p = 0.756m, a_1 = 0.094m, d_1 = 0.272m, c_2 = 0.172m, d_2 = 0.125m</td>
</tr>
<tr>
<td>(1,1,2,5)</td>
<td>13</td>
<td>p_1 = 0.297m, p_2 = 0.756m, q = 0.295m, c = 0.111m, d = 0.268m</td>
</tr>
<tr>
<td>(1,1,2,5)</td>
<td>13</td>
<td>p_1 = 0.478m, p_2 = 0.756m, q = 0.477m, c = 0.045m, d = 0.109m</td>
</tr>
<tr>
<td>(1,1,2,5)</td>
<td>14</td>
<td>p_1 = 0.369m, p_2 = 0.766m, q = 0.319m, c = 0.112m, d = 0.270m</td>
</tr>
<tr>
<td>(1,1,2,5)</td>
<td>14</td>
<td>p_1 = 0.514m, p_2 = 0.762m, q = 0.481m, c = 0.058m, d = 0.140m</td>
</tr>
<tr>
<td>(1,1,2,5)</td>
<td>15</td>
<td>p_1 = 0.545m, p_2 = 0.766m, q = 0.480m, c = 0.071m, d = 0.171m</td>
</tr>
</tbody>
</table>
This system was initially solved on the IBM 1620 computer by an iteration procedure using a program "Non-linear Estimation," developed at the University of Wisconsin by D. A. Meeter for the CDC 1604 computer and adapted for the IBM 1620 by G. D. Monroe at the Marquette University Computing Center. The general solution for this set of equations was provided by E. L. Albasy (1964, 1965).

The design obtained by using the combination (1, 3, 4) is shown in Figure 1. The region \( R \) is the equilateral triangle with side \( m \). Three points are at the vertices of an equilateral triangle with side 0.756\( m \), two points are on the \( x_1 \)-axis at \((\pm 0.258 m, 0)\), two points are on the \( x_2 \)-axis at \((0, \pm 0.258 m)\), four points are at \((\pm 0.183 m, \pm 0.183 m)\), and two points are at the origin. The eight points from sets 3 and 4 are vertices of an octahedron inscribed in a circle of radius 0.258\( m \).

![Figure 1. Design points in triangular region.](image)

Note that if the region \( R \) is not originally an equilateral triangle it may be transformed to an equilateral triangle, the chosen design used in the experiment, and the equation of the fitted response surface calculated. The inverse transformation then gives the equation of the response surface for the original region.
5. Designs for minimizing variance plus bias.

We assume that the model

\[ \hat{y}(x) = \beta_1 x_1 \]

is to be fitted when the true response may be of the form

\[ y(x) = \beta_1 x_1 + \beta_2 x_2 \]

where \( x_1, x_2, \beta_1, \) and \( \beta_2 \) are defined as in Box and Draper (1965).

We saw earlier that when possible designs were restricted to those of the class satisfying the conditions \((2.2)\) bias was minimized when \( N_{11} = \mu_{11} \) and \( N_{12} = \mu_{12} \). We shall now see how designs of this class should be modified when both variance and bias errors arise.

5.1 Case \( d_1 = 1, d_2 = 2 \).

Following the development of Box and Draper (1969, 1963) we find variance

\[ V = \text{tr} \left[ \Omega_1 \Omega_1^{-1} \right] = 1 + m^2/12c \]

and bias

\[ B = \frac{N}{\sigma^2} \left[ \beta_2^2 \mu_{22} - \beta_1 \mu_{12} \mu_{12}^{-1} \beta_2 \right] \]

When \( B \) is evaluated, this leads to \( J = V + B \) given by

\[ J = \left( 1 + m^2/12c \right) \left\{ 4 \left( \sigma_{11}^2 + 2\sigma_{12} \sigma_{22} + \sigma_{22}^2 + 4\sigma_{12}^2 \right)/4800 + \left( \sigma_{11} - \sigma_{22} \right)^2 \left( c - m^2/24 \right)^2 \right\} + m^2 \left( \sigma_{11}^2 - \sigma_{22}^2 \right) \left( d/c + 3/8m/15 \right)^2 /24 \]  \hspace{1cm} (5.1)

where \( \sigma_{ij}^2 = N\beta_{ij}^2/\sigma^2 \).

For the all-bias situation, the variance terms in \((5.1)\) are missing and \( J \) is minimized, as we have seen earlier, when \( c = m^2/24 \) and \( d/c = -\frac{1}{3}m/15 \)
For the all-variance situation the bias terms in (5.1) are missing and the best design is obtained when we take c as large as possible. For intermediate situations when both variance and bias are present we see that if \( d/c = -3^3_m/15 \), the final term is zero irrespective of the value of c. The optimum value for c can then be determined by setting \( \partial J/\partial c = 0 \), which implies that

\[
24(\alpha_{11} + \alpha_{22})^2 c^3 - (\alpha_{11} + \alpha_{22})^2 m c^2 - m^2 = 0.
\]

The optimum c for various values of \((\alpha_{11} + \alpha_{22})^2\) is shown in Figure 2 for \( m = 1 \). (For other values of \( m \), the graph has the same general shape.) Note that the quantity \( c^3 \), the root mean square deviation of the design points from the origin, is used as ordinate. It is seen that the optimum value of \( c^3 \) varies little over a large range of possible values of the quantity \((\alpha_{11} + \alpha_{22})^2\), and stays close to the value of \( c^3 \) appropriate for the all-bias situation. It is only when the bias quantity \((\alpha_{11} + \alpha_{22})^2\) becomes very small compared with the experimental error that the optimum value of \( c^3 \) is much different from the all-bias value.

Another question of interest can be investigated through examination of J. The all-bias designs have \( c = m^2/24 \) and \( d = -3^3_m/360 \). Suppose we decided to maintain the basic shape of the design and merely inflate or deflate it to accommodate various amounts of variance and bias error, i.e. replace each design point \((x_1, x_2)\) by \((\theta x_1, \theta x_2)\) where \( \theta > 1 \) is a scale factor. (Actually negative values of \( \theta \) could also be considered.) What values of \( \theta \) would be appropriate for various values of the bias coefficients? For the inflated design, \( c = m^2 \theta^2/24 \) and \( d/c = -3^3_m \theta/15 \), so that

\[
J(\theta) = 1 + 2\theta + m^4(9\alpha_{11}^2 + 2\alpha_{11} \alpha_{22} + 9\alpha_{22}^2 + 4\alpha_{12}^2)/4800
+ m^4(\theta - 1)^2 \left\{ 25(\alpha_{11} + \alpha_{22})^2 (\theta + 1)^2 + 8 \left[ (\alpha_{11} - \alpha_{22})^2 + \alpha_{12}^2 \right] \right\}/14400.
\]
As expected, the all-variance design requires $\theta = \infty$ and the all-bias design, $\theta = 1$. When both variance error and bias error occur the optimum $\theta$ can be determined from $\partial J / \partial \theta = 0$, namely

$$e^3(\theta - 1)[\theta(\theta + 1)T_1 + T_2] - 4 = 0,$$

where

$$T_1 = m^4(\alpha_{11}^2 + \alpha_{22}^2) / 144,$$

$$T_2 = m^4[(\alpha_{11}^2 - \alpha_{22}^2)^2 + \alpha_{12}^2] / 900,$$

are both functions of the unknown coefficients $\beta_{11}, \beta_{22}, \beta_{12}$. The optimum $\theta$ can be evaluated for given values of $T_1$ and $T_2$. Selected values are shown in Table 4.

Table 4. Optimum values of $\theta$ for selected values of $T_1$ and $T_2$.

<table>
<thead>
<tr>
<th>$T_1$</th>
<th>0</th>
<th>.01</th>
<th>.1</th>
<th>1</th>
<th>10</th>
<th>100</th>
<th>$\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>$\infty$</td>
<td>2.78</td>
<td>1.96</td>
<td>1.41</td>
<td>1.12</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>.01</td>
<td>4.74</td>
<td>2.74</td>
<td>1.94</td>
<td>1.41</td>
<td>1.12</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>.1</td>
<td>2.81</td>
<td>2.46</td>
<td>1.90</td>
<td>1.41</td>
<td>1.12</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>1</td>
<td>1.75</td>
<td>1.73</td>
<td>1.64</td>
<td>1.37</td>
<td>1.12</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>10</td>
<td>1.22</td>
<td>1.22</td>
<td>1.22</td>
<td>1.19</td>
<td>1.09</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>100</td>
<td>1.04</td>
<td>1.04</td>
<td>1.04</td>
<td>1.04</td>
<td>1.03</td>
<td>1.01</td>
<td>1.00</td>
</tr>
<tr>
<td>$\infty$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Consideration of values for $T_1$ and $T_2$ which might arise from reasonable discrepancies between the fitted and true models over the region $R$ indicates that $\theta$ should be chosen close to unity except when variance error predominates. As a rough rule of thumb, $\theta = 1.1$ is suggested when no knowledge whatever is available on the possible sizes of the $\beta_{ij}$. (Such a value would be suitable, for example, if $T_1 = 10$, $m = 1$, $N = 9$, $\alpha_{11} = \alpha_{22} = \beta \sqrt{N}/\sigma$ and $\alpha_{12} = 0$, so that $T_2$ is zero; then $\beta = 6.325 \sigma$. The discrepancy $\beta(x_1^2 + x_2^2)$ would be about $2.1 \sigma$ at $(0, 1/\sqrt{3})$, the extreme point of the region, less at points nearer the origin.)
One way of thinking about the design determined by the above procedure is that the expanded 'minimum variance plus bias' design for a triangle of side $m$ will be the 'minimum bias' design for the triangle of side $\delta m$.

5.2 Case $d_1 = 2, \ d_2 = 3$.

Performing the necessary substitutions for this case we can write

$$V = \frac{(720f - 30cm^2 + m^4)/360(2f - c^2) + m^2[30f + 4(3)^{\frac{3}{2}}dm + cm^2]}{360(cf - d^2)}$$

and

$$B = m^6\left(85d^2_{111} + 10d^2_{111}d^2_{122} + 25d^2_{122} + 81d^2_{222} + 18d^2_{112}d^2_{222} + 21d^2_{112}\right)/940800$$

$$+ \left[(3d^2_{111} + d^2_{122})^2 + (3d^2_{222} + d^2_{112})^2\right]P + (d^2_{222} - d^2_{112})^2Q,$$

where

$$P = m^2\left[(f^2 - dh)/(cf - d^2) - m^2/42 - 3\delta^2((ch - df)/(cf - d^2) + 3m^3/21)]/15\right]^2/24$$

$$+ [(ch - df)/(cf - d^2) + 3m^3/21]^2/50$$

$$Q = 4\left[(ch - df)/(2f - c^2) + \frac{3m^3}{630} + m^2\{(ch - df)/(2f - c^2) - \frac{3m^3}{7!}\}/48\right]^2$$

$$+ m^4\{(ch - df)/(2f - c^2) - \frac{3m^3}{7!}\}/3840$$

In a situation where both variance and bias errors occur we should choose the design to minimize $J$ above. The values of the $\sigma^2_{ijk} = N\beta^2_{ijk}/\sigma^2$ would of course be unknown in general. The expression for $J$ is a rather complicated function of the design moments $c$, $d$, $f$, and $h$ and direct minimization of $J$ appears difficult. We shall, instead, investigate the best design of a certain form as follows.

If there were no variance error, i.e. $V = 0$, the best design would be such that $P = Q = 0$. This would imply, as we have shown by other means, that $c = m^2/24$; $d = -3m^3/360$; $f = m^4/720$; and $h = -3m^5/7560$. We shall
consider deformations of this design such that any point \((x_1, x_2)\) is transformed to the point \((\theta x_1, \theta x_2)\). This will enable us to expand or contract the all-bias design while preserving the shape of the point arrangements to take account of varying amounts of variance and bias errors. The moments of the deformed design up to and including fifth order are then zero except for

\[
c = m^2 \theta^2/24; \quad d = -3m^3 \theta^3/360; \quad f = m^4 \theta^4/720; \quad h = -3m^5 \theta^5/7560.
\]

Substituting these values into \(J = V + B\) gives

\[
V = 8/3 + 2(9-46)/306,
\]

\[
m^{-6}B = (85 \theta^2_{111} + 10 \theta^2_{112} + 25 \theta^2_{12} + 67 \theta^2_{222} + 18 \theta^2_{222} \theta^2_{112} + 21 \theta^2_{112})/940800 + (\theta-1)^2 \left[ (5(5 \theta^2_{111} + 14 \theta + 1)) + (3 \theta^2_{111} + \theta_{112}^2)^2 \right] + 4(9 \theta^4 + 16 \theta^3 - 6 \theta^2 + 23)(\theta^2_{222} - \theta_{112}^2)^2/1058400.
\]

Variance alone is minimized when \(\theta = 3\). This does not conform with the conclusion in the \(d_1 = 1, d_2 = 2\) case when we obtained \(\theta = \infty\), and is due to the fact that we are restricting the design in a rather definite way allowing only a scale-up of points. This links the four moments \(c, d, f,\) and \(h\) and allows choice only from designs so linked. However, if variance is plotted as a function of \(\theta\) we find

- \(V\) is a maximum at \(\theta = 0\), where \(V = \infty\).
- \(V\) decreases monotonically for \(0 \leq \theta \leq 3\).
- \(V\) is a minimum at \(\theta = 3\), where \(V = 8/3 = 2/81\).
- \(V\) increases monotonically to a value of \(8/3\) at \(\theta = \infty\).

In other words, although the minimum of \(V\) is achieved at \(\theta = 3\), and not as we might hope (to conform to other work, e.g. Box and Draper (1969, 1963), Draper and Lawrence (1965), and earlier in this paper) \(\theta = \infty\), the actual
numerical change in $V$ when $3 \leq \Theta < \infty$ is only $2/\theta_1$, i.e. less than 1% of the minimum value. In any case, a multiple as great as $\theta = 3$ applied to any of the designs we have found would take some or all of the design points outside the region. While this might be permissible in some investigations, it would not be in mixture problems, in which case the design would be expanded until some points fell on the boundary.

Bias alone is minimized when $\Theta = 1$, of course, since this simply gives the all-bias design.

When both variance and bias errors occur, the optimum $\Theta$ is given by $\partial J / \partial \Theta = 0$, which leads to

$$8(\Theta-3) + \Theta^2(\Theta-1) \left\{ 5(5\Theta^2 + 8\Theta + 2) W_1 + 6(8\Theta^4 + 8\Theta^3 - 12\Theta^2 - 5\Theta + 10) W_2 \right\}$$

(5.2)

where

$$W_1 = \{(3a_{111} + a_{122})^2 + (3a_{222} + \beta_{112})^2\} m^6 / 264600$$

$$W_2 = (a_{222} - a_{112})^2 m^6 / 264600$$

are both functions of the unknown coefficients $\beta_{111}$, $\beta_{122}$, $\beta_{222}$, and $\beta_{112}$. The optimum $\Theta$ can be evaluated for given values of $W_1$ and $W_2$. Selected values are shown in Table 5.
Table 5. Optimum values of $\theta$ for selected values of $W_1$ and $W_2$.

<table>
<thead>
<tr>
<th>$W_2$</th>
<th>(0)</th>
<th>(0.0001)</th>
<th>(0.01)</th>
<th>(0.01)</th>
<th>(0.1)</th>
<th>(1)</th>
<th>(10)</th>
<th>$\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0)</td>
<td>3.00</td>
<td>2.50</td>
<td>2.05</td>
<td>1.64</td>
<td>1.32</td>
<td>1.11</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>(0.0001)</td>
<td>2.17</td>
<td>2.14</td>
<td>1.98</td>
<td>1.64</td>
<td>1.32</td>
<td>1.11</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>(0.001)</td>
<td>1.82</td>
<td>1.81</td>
<td>1.78</td>
<td>1.61</td>
<td>1.32</td>
<td>1.11</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>(0.01)</td>
<td>1.52</td>
<td>1.52</td>
<td>1.52</td>
<td>1.48</td>
<td>1.30</td>
<td>1.11</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>(0.1)</td>
<td>1.29</td>
<td>1.29</td>
<td>1.29</td>
<td>1.28</td>
<td>1.23</td>
<td>1.10</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>(1)</td>
<td>1.11</td>
<td>1.11</td>
<td>1.11</td>
<td>1.11</td>
<td>1.11</td>
<td>1.07</td>
<td>1.02</td>
<td>1.00</td>
</tr>
<tr>
<td>(10)</td>
<td>1.02</td>
<td>1.02</td>
<td>1.02</td>
<td>1.02</td>
<td>1.02</td>
<td>1.02</td>
<td>1.01</td>
<td>1.00</td>
</tr>
<tr>
<td>$\infty$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Consideration of values of $W_1$ and $W_2$ which might arise from reasonable discrepancies between the fitted and true models over the region $R$ indicates that $\theta$ should be close to unity except when variance error predominates. When nothing is known about the $\beta_{ijk}$ a value of $\theta = 1.2$ approximately is suggested as a rough rule of thumb. (Such a value does not appear in the table but would be reasonable, for example, for situations somewhere between the two cases which follow. If $T_1 = 0.1$, $m = 1$, $N = 12$, $\alpha_{111} = \alpha_{122} = 0$, and $\alpha_{222} = \alpha_{112} = \beta \sqrt{N/\sigma}$ so that $T_2 = 0$, then $\beta = 11.74 \sigma$. The discrepancy $\beta(x_1^3 + x_2^3 x_3)$ would be about $2.25 \sigma$ at the extreme point $(0, 1/\sqrt{3})$, considerably less at points nearer the origin; the appropriate value of $\theta$ is 1.32. A similar calculation with $T_1 = 1$, but all other figures the same, would imply a discrepancy of about
7. In the extreme point, considerably less at points nearer the origin; the appropriate value of $\theta$ is $1.11$. If, in a mixture problem, a design cannot be expanded to this extent without some of the points going outside the region, a slightly smaller value of $\theta$ can be used.

6. ACKNOWLEDGEMENTS

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REFERENCES


