The Use of Second Order "Spherical" and "Cuboidal" Designs in the Wrong Regions

by

Norman R. Draper and Willard E. Lawrence

University of Wisconsin and Marquette University

This research was partially supported by the United States Navy through the Office of Naval Research under Contract Nonr-1202 (17), Project NR 042 222.
The Use of Second Order "Spherical" and "Cuboidal" Designs in the Wrong Regions

Norman R. Draper and Willard E. Lawrence
University of Wisconsin and Marquette University

1. INTRODUCTION

Box and Draper (1963) discussed the selection of a suitable design for fitting a second order polynomial model when the region of interest $R$ was a unit sphere in the coded $k$-dimensional space of the $k$ factors being examined. A subsequent paper by Draper and Lawrence (1965) dealt with the selection of suitable second order designs when the region of interest $R$ was a $k$-dimensional cuboid with vertices $(±1, ±1, ..., ±1)$. In both papers, account was taken of averaged bias error (specifically error which arises when the second order model is inadequate and third order model is correct) as well as of averaged variance error (random error in the observed response). The averaging was performed over $R$ in both cases. In each case certain basic assumptions were made about the subset of designs from which particular designs could be selected. These assumptions were reasonable in the light of the relationships between the moments of the region under study (Box and Draper, 1959). Suppose

$$(x_{1u}, x_{2u}, ..., x_{ku}) \quad u = 1, 2, ..., N$$

are the $N$ design points and $y_u$ is the observed response at the $u$-th point; then we can define design moments $c$, $e$, and $f$ by

$$cN = \sum_{u=1}^{N} x_{iu}^2, \quad eN = \sum_{u=1}^{N} x_{iu}^4, \quad fN = \sum_{u=1}^{N} x_{iu}^2 x_{ju}^2.$$

This research was partially supported by the United States Navy through the Office of Naval Research under Contract Nonr-1202 (17), Project NR 042 222.
The basic design assumptions in both cases are that all other design moments up to and including order five are zero and, additionally,

(a) in the spherical case, \( e = 3f \), i.e., the design is rotatable (Box and Draper, 1963) while

(b) in the cuboidal case \( 5e = 9f \) (Draper and Lawrence, 1965).

In each case the procedure adopted was to find the all-bias designs (suitable when no variance error occurs) and to extend these to situations where there is some bias error also. If the bias coefficients are known exactly, exact calculations can be made as will be described in Section 2. However general conclusions can also be given when (as is usual) the exact bias is unknown. In fact it was found that designs for "average situations" were very like designs for situations where all the error arose from bias and not at all like designs suitable for situations where all the error arose from variance error. (Similar conclusions have been confirmed for triangular and tetrahedral regions which arise in mixture problems - see Draper and Lawrence (1965, 1966)).

In general design problems, there is some question as to what form the region of interest should take. (Note that this question does not arise in mixture problems where the sum of the ingredients' volumes or weights is fixed, unless the mixture is subject to additional restrictions.) Experimenters may define their region of interest in terms of pairs of limits on each variable (leading to a cuboidal region) or in terms of some radial restriction from a "known" central point or natural center of experimentation (leading to a spherical region). Two experimenters who disagree on their concept of a region of interest may perhaps wonder how crucially their region specification affects the design choice. More plainly, if we select a design on the basis of a (unit) spherical
region when we should be concerned with a cuboidal region (which, due to its corners, is somewhat larger) how disastrous will this be, and vice versa? We shall examine this question in this paper.

2. METHOD OF INVESTIGATION

Suppose we want a design suitable for obtaining a second order graduating function of the form

\[ \hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \cdots + b_k x_k + b_{11} x_1^2 + \cdots + b_{kk} x_k^2 + b_{12} x_1 x_2 + \cdots + b_{k-1,k} x_{k-1} x_k \]

or, in matrix notation,

\[ \hat{y} = x' \beta_1 \]

where

\[ b'_1 = (b_0, b_1, \ldots, b_k, b_{11}, \ldots, b_{kk}, b_{12}, \ldots, b_{k-1,k}) \]

\[ x'_1 = (1, x_1, \ldots, x_k, x_1^2, \ldots, x_k^2, x_1 x_2, \ldots, x_{k-1} x_k) \]

Suppose however we should (unknown to us) be fitting the third order polynomial

\[ \eta = x'_2 \beta_2 + x'_2 \beta_2 \]

where \( x_2 \) is as above, \( \beta_2 \) is defined like \( \beta_1 \) and

\[ \beta'_2 = (\beta_{111}, \beta_{122}, \ldots, \beta_{1kk}, \beta_{211}, \ldots, \beta_{2kk}, \ldots, \beta_{k-1,k}, \beta_{k2}, \ldots, \beta_{k-2,k-1,k}) \]

\[ x'_2 = (x_1, x_1^2, \ldots, x_k^2, x_1 x_2, x_1^2 x_2, \ldots, x_k x_2, \ldots, x_{k-1} x_k x_3, \ldots, x_{k-2} x_{k-1} x_k) \]

If the values of the elements of \( \beta_2 \) of \( N \) (the number of design points) and of \( V(y) = \sigma^2 \) were known, formulae provided by Box and Draper (1963) and Draper and Lawrence (1965) could be applied to obtain moments of suitable designs for spherical and cuboidal regions respectively. The details follow.

2.1 Spherical region.

We recall that \( e = 3f \) and define

\[ \sigma^2 p/N = (3\beta_{111} + \beta_{122} + \cdots + \beta_{1kk})^2 + \cdots + (3\beta_{kk} \beta_{k11} \cdots + \beta_{kk} \beta_{k-1,k})^2 \]
-4-

\[
\sigma^2 Q/N = 2(3 \beta^2_{111} + \beta^2_{122} + \ldots + \beta^2_{1kk}) + \ldots + 2(3 \beta^2_{kkk} + \beta^2_{k11} + \ldots + \beta^2_{k-k,k-1}) \\
+ (\beta^2_{123} + \ldots + \beta^2_{k-2,k-1,k}).
\]

It is shown in Box and Draper (1963), with slight changes in notation, that \( J = V + B \), the sum of the variance error and the bias error, is minimized for given \( k \) when \( c = e/c \) and \( P \) are related as follows:

\[
c = \theta \left\{ \frac{\left[ \frac{6}{2} (k+4) \theta^2 + 3(k+1) \right] \left[ (k+2) (k+4) \theta^2 - 6k(k+4) \theta + 9k \right]^{1/2} - 3k[2(k+4) \theta + 3(k+1)]}{3 \left[ 2 \theta^2 (k+2) (k+4) - 6k(k+4) \theta - 9k(k-1) \right]} \right\}
\]

\[
P = \frac{27(k + 2)}{2c[(k+4) \theta - 3]} \left\{ \frac{k-1}{(k+2) \theta^2} + \frac{k(k+2)(k+4)c^2 - 2k(k+4)c + (k+2)}{(k+2) \theta - 3k \theta^2} \right\}
\]

Thus for a given set of \( \beta_{ijk} \), \( N \), and \( \sigma^2 \), and for given \( k \), \( P \) is fixed and we can obtain the moments \( c, e, \) and \( f \) which provide minimum \( J = V + B \).

2.2. Cuboidal region.

We recall that \( 5e = 9f \) and define

\[
\sigma^2 R/N = (1.8 \beta_{111} + \beta_{122} + \ldots + \beta_{1kk})^2 + \ldots + (1.8 \beta_{kkk} + \beta_{k11} + \ldots + \beta_{k-k,k-1})^2
\]

\[
\sigma^2 S/N = [(27/35) \beta^2_{111} + \beta^2_{122} + \ldots + \beta^2_{1kk}] + \ldots + [(27/35) \beta^2_{kkk} + \beta^2_{k11} + \ldots + \beta^2_{k-k,k-1}] \\
+ (5/4) (\beta^2_{123} + \ldots + \beta^2_{k-2,k-1,k}).
\]

It is shown in Draper and Lawrence (1965) that \( J = V + B \) is minimized for given \( k \) when \( c, \theta, \) and \( R \) are related as follows:

\[
c = \frac{-3k \theta(4+5k)(10 \theta + 3k + 3) + 9(4+5k)}{9[10(4+5k) \theta^2 - 30k(2+k) \theta - 9k(k+2)(k-1)]} \left\{ 6(10 \theta + 3k + 3) \{ 5(4+5k) \theta^2 - 30k \theta + 9k \} \right\}^{1/2}
\]

\[
R = \frac{k(k+1)}{10c^2} - \frac{3k[27k \theta + (4+5k)(10 \theta - 15c \theta - 6)]}{50[(4+5k) \theta - 9kc]^2} \frac{243}{10(58 - 3)}
\]

(2.2.1)
Thus for a given set of $\beta_{ijk}$, $N$, $\sigma^2$, and for given $k$, $R$ is fixed and we can obtain the moments $c$, $e$, and $f$ which will provide minimum $J = V + B$.

3. COMPARISON OF DESIGNS

To determine the effects of using a cuboidal design in a spherical region or a spherical design in a cuboidal region we will proceed as follows. Four values of $k$: 2, 3, 4, 5 will be considered. First we will select sets of bias coefficients of the form $\alpha_{ijk} = (N/\sigma^2)\beta_{ijk}$ using an internal random selection procedure in a computer.

For a given $k$ we can compute values $P$, and $Q$ (and also $R$ and $S$, required below). The formulae (2.1.1) provide the moments $c$, $e$ (=3f) and $f$ for minimum $V + B$ and the minimum values of $V$, $B_1$ (the variable part of the bias $B = B_1 + B_2$ which depends on the moments $c$, $e$, and $f$) and $B_2$ (the constant part of the bias) are evaluated for the spherical design in the spherical region. The same moment values $c$, $e$, and $f$ are then used to obtain values $V$, $B_1$ and $B_2$ for the cuboidal region. The appropriate formulae for this latter calculation are more general than those in Draper and Lawrence (1965) (where it is assumed that $5e = 9f$) and are unpublished. This permits a direct comparison of the effect of using a spherical design in both (the correct) spherical region and in (the incorrect) cuboidal region. Similar calculations beginning with $R$ and $S$ and using (2.2.1) can be performed to examine cuboidal designs.

The above comparisons were made for $k = 2, 3, 4$ and 5 and for many sets of bias coefficients. We present here however only a selection of results for $k = 3$, shown as Table 1. The Table is arranged in order of increasing $R$ but since sets of coefficients which give rise to increasing values of $R$ do not necessarily give increasing values of $P$ the values of $P$ are in an irregular order. This is of no particular consequence.
Table 1.
Values of variance and bias for spherical and cuboidal designs in two regions.

<table>
<thead>
<tr>
<th>Cuboidal Region</th>
<th>Spherical Design</th>
<th>C</th>
<th>B</th>
<th>B_2</th>
<th>V + B</th>
<th>P</th>
<th>V</th>
<th>B</th>
<th>B_2</th>
<th>V + B</th>
</tr>
</thead>
<tbody>
<tr>
<td>R 2.29 V 3.21 B_1 0.606 B_2 0.047 V + B 3.38</td>
<td>3.12 B_1 0.413 B_2 0.047 V + B 3.58</td>
<td>2.29 V 2.67 B_1 0.536 B_2 0.0067 V + B 2.78</td>
<td>2.38 B_1 0.393 B_2 0.0067 V + B 2.78</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8.16 V 3.92 B_1 0.788 B_2 0.0710 V + B 4.78</td>
<td>4.47 B_1 0.549 B_2 0.0710 V + B 5.09</td>
<td>4.47 B_1 0.549 B_2 0.0710 V + B 5.09</td>
<td>4.47 B_1 0.549 B_2 0.0710 V + B 5.09</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21.1 V 4.61 B_1 0.902 B_2 0.123 V + B 5.63</td>
<td>5.69 B_1 0.541 B_2 0.123 V + B 6.36</td>
<td>5.69 B_1 0.541 B_2 0.123 V + B 6.36</td>
<td>5.69 B_1 0.541 B_2 0.123 V + B 6.36</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>46.6 V 5.29 B_1 0.970 B_2 0.226 V + B 233.</td>
<td>18.6 B_1 0.39 0.226 V + B 284.</td>
<td>18.6 B_1 0.39 0.226 V + B 284.</td>
<td>18.6 B_1 0.39 0.226 V + B 284.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>140. V 6.39 B_1 0.946 B_2 0.856 V + B 563.</td>
<td>22.7 B_1 0.102 B_2 0.856 V + B 931.</td>
<td>22.7 B_1 0.102 B_2 0.856 V + B 931.</td>
<td>22.7 B_1 0.102 B_2 0.856 V + B 931.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>267. V 7.04 B_1 0.893 B_2 0.816 V + B 824.</td>
<td>20.6 B_1 0.846 B_2 0.816 V + B 921.</td>
<td>20.6 B_1 0.846 B_2 0.816 V + B 921.</td>
<td>20.6 B_1 0.846 B_2 0.816 V + B 921.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>504. V 7.69 B_1 0.764 B_2 0.123 V + B 20.8</td>
<td>11.3 B_1 0.270 B_2 0.123 V + B 26.3</td>
<td>11.3 B_1 0.270 B_2 0.123 V + B 26.3</td>
<td>11.3 B_1 0.270 B_2 0.123 V + B 26.3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1003. V 8.34 B_1 0.582 B_2 0.872 V + B 17.6</td>
<td>16.3 B_1 0.742 B_2 0.872 V + B 25.7</td>
<td>16.3 B_1 0.742 B_2 0.872 V + B 25.7</td>
<td>16.3 B_1 0.742 B_2 0.872 V + B 25.7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2294. V 8.94 B_1 0.367 B_2 0.419 V + B 429.</td>
<td>10.1 B_1 0.434 B_2 0.419 V + B 473.</td>
<td>10.1 B_1 0.434 B_2 0.419 V + B 473.</td>
<td>10.1 B_1 0.434 B_2 0.419 V + B 473.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4000. V 9.23 B_1 0.247 B_2 0.160 V + B 170.</td>
<td>18.1 B_1 0.374 B_2 0.160 V + B 216.</td>
<td>18.1 B_1 0.374 B_2 0.160 V + B 216.</td>
<td>18.1 B_1 0.374 B_2 0.160 V + B 216.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Examination of the entries in Table 1 shows that in every case but one, the appropriate cuboidal design performs better than the appropriate spherical design in the cuboidal region, while the spherical design performs better than the cuboidal design in the spherical region. The comparisons are here made for the separate regions (rather than the separate designs) because, in a given region, and for given coefficients, $B_2$ is fixed, and the choice of design will affect only $V$ and $B_1$. The atypical case occurs when $R=2.29$ when the spherical design is slightly better. The reason this can happen is as follows. Since cuboidal designs are restricted by $3e=9f$, and spherical designs by $e=3f$, it is possible, in a particular case, that the spherical design may produce a smaller overall bias in the cuboidal region than does the cuboidal design. However in general this is not so. Note also that the atypical case occurs when $R$ is small, so that bias error is small and most of the error present is due to variance.

The results of a series of calculations with randomly chosen bias coefficients completely covering the possible ranges are summarised in Table 2.

<table>
<thead>
<tr>
<th>Spherical Region</th>
<th>Cuboidal Region</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cases</td>
</tr>
<tr>
<td>$k$</td>
<td>Examined</td>
</tr>
<tr>
<td>2</td>
<td>42</td>
</tr>
<tr>
<td>3</td>
<td>57</td>
</tr>
<tr>
<td>4</td>
<td>69</td>
</tr>
<tr>
<td>5</td>
<td>61</td>
</tr>
</tbody>
</table>
We see from Table 2 that in a minority of cases the "wrong" design produces smaller total variance plus bias than the "correct" design. A detailed examination of the computer printouts reveals that in all the exceptional cases the actual numerical improvement is small and the value of $R$ obtained from the coefficients is also small, which implies that variance is almost completely dominant and the appropriate cuboidal design is well spread out. In such cases the exact positioning of the design points does not much matter and a spherical design may produce slightly smaller, or slightly larger, variance plus bias according to the region under study and the value of $P$. The following general conclusion can be made however. When bias error is not an important factor the correct design is, in most cases, better. When bias error is an important factor—as would usually happen in practical circumstances—-the correct design is always better.

4. ACKNOWLEDGEMENTS

We are grateful to a referee of Draper and Lawrence (1965) whose remarks led to this investigation, and to Eunice Stefanowski of the Marquette University Computing Center who performed the calculations.

This work was partially supported by the United States Navy through the Office of Naval Research under Contract Nonr-1202(17), Project NR 042 222.
REFERENCES

