On Robustness of Response Surface Designs

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1. Introduction

This paper considers design aspects of response surface experiments in which emphasis is on robust estimation of the response variable, $\eta(x)$, to wild or 'aberrant' observations. It is assumed that the response relationship is to be approximated by a low order polynomial in one or more independent variables

$$\eta(x)=\beta_0+\sum\beta_i x_i+\sum\beta_i\beta_j x_i x_j+\sum\beta_i\beta_j\beta_k x_i x_j x_k+\cdots \quad (1)$$

As usual, the x's are transformations of the experimental variables, the origin of the x's coinciding with the center of some region of interest, R, over which the polynomial approximation is to be used. It is further convenient to scale so that the region R may be described as a unit cube, $-1\leqslant x_i\leqslant 1$, or as a unit sphere, $\sum x^2_i\leqslant 1$.

The polynomial (1) may be written in matrix form

$$\eta(x)=x'\beta$$

in which x' is a row vector whose elements are the values of the independent variables, their squares, products, etc., and β is a column vector of the coefficients associated with the elements of x'. Observations, $y_i(x)=\eta(x)+e_i$, are taken at n selected combinations of the x variables, the set of such combinations being called the experimental design. The e_i are assumed to be uncorrelated random errors with zero means and constant variance, σ^2. Based on some design in the space of the independent variables, the β's are estimated by least squares

$$b=(X'X)^{-1}X'Y$$

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where X is the matrix of values of the elements of x' at the design points, and Y is the $n\times 1$ matrix of y observations.

Suppose that the ith observation has added to it an 'aberration' d_i, making it an outlier. For generality, consider a discrepancy vector, $d=(d_1,d_2,\cdots,d_n)$, of non-random aberrations added to the Y vector. It is easily shown that, by assuming $T=(X'X)^{-1}X'$,

$$\begin{aligned}E(b)&=(X'X)^{-1}XE(Y)\\&=(X'X)^{-1}X'(X\beta+d)\\&=\beta+Td\end{aligned}$$

and, for any arbitrary point x, the estimated response, $\hat{y}(x)$, has

$$\begin{aligned}E(\hat{y}(x))&=E(x'b)\\&=x'(\beta+Td)\\&=\eta(x)+x'Td.\end{aligned}$$

Therefore, the mean squared error, MSE, is

$$\begin{aligned}\mathrm{MSE}(\hat{y}(x))&=E[\hat{y}(x)-\eta(x)]^2\\&=E[\hat{y}(x)-E(\hat{y}(x))]^2+[E(\hat{y}(x))-\eta(x))]^2\\&=V(x)+B(x)\\&=x'\mathrm{Var}(b)x+d'T'xx'Td\end{aligned}$$

where $V(x)=x'\,\mathrm{Var}(b)x$ is the variance and $B(x)=d'T'xx'Td$ is the squared bias of $\hat{y}(x)$.

Since we are interested in using $\hat{y}(x)$ over the entire region of interest, R, we will consider the integrated mean squared error, IMSE, under, a weighting function $W(x)$. Then

$$\begin{aligned}\mathrm{IMSE}&=\int_R \mathrm{MSE}(\hat{y}(x))\,dW(x)\\&=\int_R V(x)\,dW(x)+\int_R B(x)\,dW(x)\\&=\sigma^2\mathrm{Tr}[(X'X)^{-1}M]+d'T'MTd\end{aligned}\qquad(2)$$

where $M=\int_R xx'\,dW(x)$ and Tr indicates trace. The weight function $W(x)$ can be treated as a probability distribution function on R. It allows for differential importance of estimates of $\eta(x)$ at different points in the region

and can even be specialized to a discrete set of points if desired.

In equation (2) it is clear that IMSE is the sum of the integrated variance and the integrated squared bias $\boldsymbol{d}'\boldsymbol{T}'\boldsymbol{M}\boldsymbol{T}\boldsymbol{d}$ with the latter term being the effect of the non-random discrepancies. Sensitivity of IMSE to a given discrepancy vector $\boldsymbol{d}$ depends on the experimental design through the matrix $\boldsymbol{T}'\boldsymbol{M}\boldsymbol{T}$. Hence, robustness to wild observations can be achieved if $\boldsymbol{d}'\boldsymbol{T}'\boldsymbol{M}\boldsymbol{T}\boldsymbol{d}$ is made as small as possible for any given vector $\boldsymbol{d}$.

2. Robustness of Design to Wild Observations

Let $S=\boldsymbol{T}'\boldsymbol{M}\boldsymbol{T}$. Clearly, S is positive semi-definite since $\boldsymbol{d}'\boldsymbol{S}\boldsymbol{d}$ is the integrated bias. Robustness of IMSE to aberrant observations is achieved by minimizing $\boldsymbol{d}'\boldsymbol{S}\boldsymbol{d}$. For a single discrepancy of magnitude g in the ith observation,

$$\boldsymbol{d}'\boldsymbol{S}\boldsymbol{d}=s_{ii}g^2$$

where s_{ii} is the ith diagonal element of S. If we assume that the single discrepancy of magnitude g, $\boldsymbol{d}'=(0, 0, \cdots, 0, g, 0, \cdots, 0)$, has equal probability of occurring with any of the n observations, than the average value of $\boldsymbol{d}'\boldsymbol{S}\boldsymbol{d}$ is

$$\begin{aligned}\mathrm{Avg}(\boldsymbol{d}'\boldsymbol{S}\boldsymbol{d}) &= \mathrm{Avg}[\mathrm{Tr}(\boldsymbol{d}'\boldsymbol{S}\boldsymbol{d})] \\ &= \mathrm{Avg}[\mathrm{Tr}(\boldsymbol{S}\boldsymbol{d}\boldsymbol{d}')] \\ &= \mathrm{Tr}[\boldsymbol{S}\,\mathrm{Avg}(\boldsymbol{d}\boldsymbol{d}')] \\ &= \mathrm{Tr}[\boldsymbol{S}(g^2/n)\boldsymbol{I}] \\ &= (g^2/n)\,\mathrm{Tr}(\boldsymbol{S}).\end{aligned}$$

Thus $\mathrm{Tr}(\boldsymbol{S})$ should be minimized to achieve robustness of IMSE to an aberrant observation. It is interesting to note that

$$\mathrm{Tr}(\boldsymbol{S})=\mathrm{Tr}(\boldsymbol{T}'\boldsymbol{M}\boldsymbol{T})=\mathrm{Tr}[(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{M}]$$

which is the integrated variance (apart from σ^2). Thus it appears that to ensure insensitivity to an aberrant observation, the integrated variance should be made small.

If there are two or more aberrant observations a similar conclusion can be

deduced. Consider a general discrepancy vector, $d'=(d_1, d_2, \cdots, d_n)$. Then

$$d'Sd=\sum_{i=1}^{n}\sum_{j=1}^{n} s_{ij}d_id_j.$$

A convenient measure of robustness might be

$$Q=\sum_{i=1}^{n}\sum_{j=1}^{n} s^2_{ij}.$$

Since S is positive semi-definite, $s^2_{ij}\leq s_{ii}s_{jj}$, and therefore,

$$Q\leq\sum_{i=1}^{n} s^2_{ii}+2\sum_{i=1}^{n}\sum_{j>i}^{n} s_{ii}s_{jj}=\left(\sum_{i=1}^{n} s_{ii}\right)^2$$

$$=[\mathrm{Tr}(S)]^2.$$

Thus Q is made small by making $\mathrm{Tr}(S)$ small, that is, by making the integrated variance of $\hat{y}(x)$ small.

3. Discussion

The approach taken in this paper differs from that of Box and Draper [1] primarily in that we consider integrated bias of $\hat{y}(x)$ over some region of interest, R, as the basic quantity to be made insensitive to non-random discrepancies. Box and Draper [1] concentrate on bias in $\hat{y}(x)$ at the design points only. They propose that the sum of squares of diagonal elements of the matrix $X(X'X)^{-1}X'$ should be made small. The basis of their criterion is that $\mathrm{Var}(y(x))$ at the design points can be made as uniform as possible if the sum of squares of diagonal elements of $X(X'X)^{-1}$ is made small.

In general, the fitted equation $\hat{y}(x)$ in response surface experiments is intended to be used not only at the design points but within some region of the x space of interest to the experimenter. For enlightening references of response surface experiments, the readers may refer to Box and Hunter [2], Box and Willson [3], and Myers [4].

If a criterion is to be developed based on insensitivity of the $\hat{y}(x)$ to aberrant observations, it seems more satisfactory to evaluate its performance over the whole region than just over the design points only. From this

viewpoint, the proposed criterion possesses a clear advantage over the Box and Draper's criterion.

4. Some Robust Two-Variable Designs

Suppose that for a response surface experiment of two variables the second order polynomial model is adequate over the region of interest, R. To illustrate the application of the $\mathrm{Tr}(S)$ criterion, we consider a useful class of two-variable designs with points equally spaced on one or two circles, and center points. This class includes the 3^2 factorial, the central composite, the hexagon and many other commonly known designs. We take the weight function, $W(\boldsymbol{x})$, to be constant and minimize $\mathrm{Tr}(S)$ either over a square region of interest, i.e., $R_1=\{(x_1,x_2):-1\leq x_1\leq 1,\ -1\leq x_2\leq 1\}$, or a unit circle region of interest, i.e., $R_2=\{(x_1,x_2):x^2{}_1+x^2{}_2\leq 1\}$. Recall that $M=\int_R \boldsymbol{x}\boldsymbol{x}'\,dW(\boldsymbol{x})$ and if we take $W(\boldsymbol{x})$ to be constant over the region, then

$$M=(1/4)\int_{R_1}\boldsymbol{x}\boldsymbol{x}'dx_1dx_2 \quad \text{if } R=R_1$$

$$=(1/\pi)\int_{R_2}\boldsymbol{x}\boldsymbol{x}'dx_1dx_2 \quad \text{if } R=R_2.$$

We assume the experimental points are to be restricted to the region of interest, R.

For a fixed n, the design parameters which can be varied in the minimization are the number of points on each circle, the orientation angle of the points on each circle with respect to the positive direction of the x_1-axis, the radii of the circles and the number of center points, n_0. In the tables the notation $(n_1,\alpha_1)+(n_2,\alpha_2)$ is used to indicate the numbers of points and orientation angles for the two circles with n_1 and α_1 always referring to the larger circle. For example, from Table 1, with $n=8$ the optimum design has $n_1=4$ points on an outer circle of radius $r_1=\sqrt{2}$. These points are in the corners of the square region ($\alpha_1=\pi/4$). The design has $n_2=4$ points on a second circle of radius $r_2=0.794$. These points are on the x_1-axis and x_2-axis with

distance 0.794 from the origin. The design does not have center points ($n_0=0$). The design is illustrated in Figure 1.

Figure 1. The Design $(4,\pi/4)+(4,0)$ with $r_1=\sqrt{2}$ and $r_2=0.794$

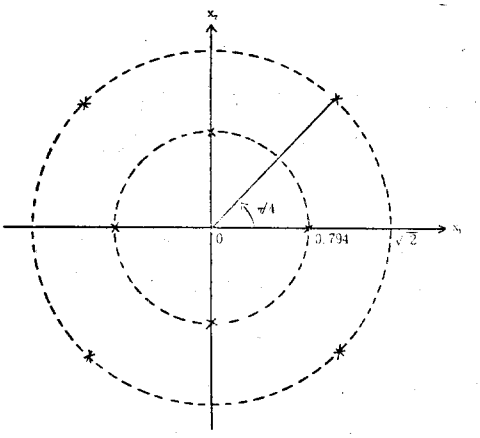

Table 1. Designs with $T(S)$ Minimized over Square Region R_1

n	Design	n_0	r_1	r_2
6	$(5,\pi/20)$	1	1.012	
7	$(4,\pi/4)+(2,0)$	1	$\sqrt{2}$	1
8	$(4,\pi/4)+(4,0)$	0	$\sqrt{2}$	0.794
9	$(4,\pi/4)+(4,0)$	1	$\sqrt{2}$	0.906
10	$(4,\pi/4)+(4,0)$	2	$\sqrt{2}$	1
11	$(4,\pi/4)+(4,0)$	3	$\sqrt{2}$	1

Table 2. Designs with $T(S)$ Minimized over Circular Region R_2

n	Design	n_0	r_1
6	(5, 0)	1	1
7	(5, 0)	2	1
8	(6, 0)	2	1
9	(6, 0)	3	1
10	(7, 0)	3	1
11	(8, 0)	3	1

Inspection of Tables 1 and 2 indicates that the experimental points tend to be located on the boundary of the experimental region though center points seem to be necessary for most cases. By way of comparison with Box

and Draper [1], their two-variable central composite design had 8 points equally spaced on a circle and had $n_0=2$. The $n=10$ design of Table 2 has 7 points on a circle and $n_0=3$. The $n=11$ design is a rotatable central composite with $n_0=3$. For the square region of interest, however, the designs of Table 1 for $n=10$ and 11 are the traditional 3^2 factorials with added center points.

SUMMARY

One of the important properties of a 'good' response surface design is that the design should be insensitive to wild observations. In this note, a measure of sensitivity to wild observations is studied. It is shown that designs are made robust to wild observations by making $\mathrm{Tr}[(X'X)^{-1}M]$ small where M is a moment matrix over some region of interest. The proposed criterion is compared with that suggested by Box and Draper [1]. Some robust two-variable response surface designs are given.

REFERENCES

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