Proceedings of the 1990 Winter Simulation Conference
Osman Balci, Randall P. Sadowski, Richard E. Nance (eds.)

SOME OPTIMAL SIMULATION DESIGNS FOR ESTIMATING QUADRATIC RESPONSE SURFACE FUNCTIONS

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ABSTRACT

This paper presents some experimental design strategies for simulation studies involving the estimation of quadratic response surfaces. Optimal design plans are developed in four common second-order design classes (central composite, Box-Behnken, three-level factorial, and small composite designs) using a criterion which incorporates both the bias and variance of the predicted response variable. Three alternative methods of assigning pseudorandom number streams to design points are considered: independent streams, common streams, and the simultaneous use of common and antithetic streams in an orthogonally blockable experimental design. Each method employs independent streams for replications of design points.

1. INTRODUCTION

Response surface methodology (RSM) offers a useful framework for the optimization of simulation models. Fundamental to RSM is the assumption that low-order polynomial models can be used to approximate the relationship between a set of controllable input variables and a simulated response within restricted regions of the operability space. Generally first-order experimental designs, in conjunction with the steepest ascent search procedure, are used to locate the region containing the optimal response. Then, in order to more accurately predict the system optimum, second-order experimental designs are used to fit a quadratic response function. Canonical and ridge analysis of the quadratic surface enable one to locate the optimum response within the current experimental region.

The experimental design plans used in a simulation study affect the accuracy of the results obtained in the RSM optimization procedures. This paper focuses on the choice of a design plan for fitting a quadratic response surface model. In each of four common second-order design classes, the levels of the input variables which minimize the bias error in the predicted response variable are determined. Then, the designs are augmented with the number of center runs needed to minimize the variance of the predicted response variable. In addition, three different strategies for the assignment of pseudorandom streams to design points are examined: independent streams, common streams, and the assignment rule blocking strategy [Schruben and Margolin 1978]. The assignment rule strategy requires the use of an orthogonally blockable experimental design and each of the design classes considered permit this type of blocking.

2. SECOND ORDER RESPONSE SURFACE DESIGNS

In the absence of theoretical models, RSM procedures seek to determine the optimum system response through a sequential exploration of the operability region. In the early stages of an RSM study, first-order designs are used to estimate the parameters of a linear response function. The model coefficients provide gradient information used to locate the region containing the optimum. In the later stages of an RSM study (after the optimum region has been tentatively located), second-order designs are used to estimate the parameters of a quadratic response function. The fitted second-order response model can be written as

$$\hat{y} = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{i=1}^{k} b_{ii} x_i^2 + \sum_{i<j}\sum b_{ij} x_i x_j \qquad (1)$$

where $\hat{y}$ denotes the fitted response variable, the *x's* denote the input variables of the simulation model, and the *b's* denote the ordinary least squares estimators of the model parameters. The abilities of canonical and ridge analysis to predict the optimum response depend on the accuracy of the estimated model parameters as well as the correctness of the assumed polynomial model. The accuracy of the model coefficients can be measured by their variances and the correctness of the assumed model can be measured by the bias in the model coefficients.

The variances of the coefficients in a second-order response function only depend on the experimental design plan, whereas the biases in the model coefficients also depend on the form of the true response function. It is reasonable to assume that any bias in the estimated model coefficients would largely be due to unfitted terms of order one degree higher than those in the fitted model. For example, if the fitted model is quadratic, then one would assume that unfitted third-order terms may be biasing the fitted model coefficients. The cubic response function which may be needed to adequately model the simulated response can be written as

$$\begin{aligned} y = \beta_0 &+ \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k} \beta_{iii} x_i^3 \\ &+ \sum_{i<j}\sum \beta_{ij} x_i x_j + \sum_{i<j}\sum \beta_{iij} x_i^2 x_j \\ &+ \sum_{i<j}\sum \beta_{ijj} x_i x_j^2 + \sum_{h<i<j}\sum\sum \beta_{hij} x_h x_i x_j + \varepsilon \end{aligned} \qquad (2)$$

where y denotes the simulated response variable, the β's are the unknown model parameters, and ε is the random error term.

The criterion used in developing the optimal second-order design plans incorporates possible third-order bias in the estimated model coefficients. Incorporation of bias into the criterion is particularly important in RSM studies because the fitted model represents an approximation to the unknown response function and, therefore, the fitted model coefficients are likely to be biased. A mean squared error criterion developed by Box and Draper [1963], which takes into account both the bias and the variance of the predicted response variable, is the basis for the design criterion used in this research. The variance error, unlike the bias error, does not depend on the order of the true response model; the variances of the model coefficients are determined by the experimental design plan. In this paper, four common second-order design classes (illustrated in Appendix A) are considered: central composite, Box-Behnken, three-level factorial, and small composite designs.

The central composite designs (CCDs) are the most widely used second-order response surface designs [Myers et al. 1989], consisting of two-level factorial designs augmented with a set of axial points. The CCDs permit orthogonal blocking with appropriate choices for the levels of the axial design points. Box-Behnken designs (BBDs) are a class of three-level, second-order designs formed by combining two-level factorial designs with incomplete block designs [1960]. These designs are less flexible than the CCDs but require the use of only three levels of each factor, as compared to five for the CCDs. The k=3 BBD does not block orthogonally and therefore is not examined. The class of three-level factorial designs (FACs) utilize k factors at each of three levels and can be partitioned into three orthogonal blocks. The FACs require a large number of experimental runs compared to other second-order design classes. The final class of second-order designs, the small composite designs (SCDs), are economical designs utilizing the minimum allowable number of experimental runs. Hartley's SCDs [1959] use fractional portions of the CCD designs and Draper's SCDs [1985] use incomplete Plackett-Burman designs in place of the factorial portion of the CCDs. Hartley's SCDs are examined for k=3,4,6 factors and Draper's SCDs are examined for k=5,7 factors.

3. THE DESIGN CRITERION

Protection against model inadequacy is particularly important in response surface exploration. Box and Draper [1963] have developed a mean squared error design criterion which provides protection against bias error due to model inadequacy. The criterion, termed the MSE of Response, calls for minimizing the average, normalized mean squared error of the predicted response variable. The MSE of Response, denoted by **J**, is the sum of the variance error and the squared bias error, defined as

$$\begin{aligned}\mathbf{J} &= \frac{N\Omega_r}{\sigma^2}\int_R \mathrm{MSE}[\hat{y}_{(\mathbf{x}_u)}]\,d\mathbf{x}\\ &= \frac{N\Omega_r}{\sigma^2}\int_R E\left\{\hat{y}_{(\mathbf{x}_u)} - E[y_{(\mathbf{x}_u)}]\right\}^2 d\mathbf{x}\\ &= \frac{N\Omega_r}{\sigma^2}\int_R \mathrm{Var}[\hat{y}_{(\mathbf{x}_u)}]\,d\mathbf{x} + \frac{N\Omega_r}{\sigma^2}\int_R \mathrm{Bias}^2[\hat{y}_{(\mathbf{x}_u)}]\,d\mathbf{x}\\ &= \mathbf{V} + \mathbf{B}\end{aligned} \tag{3}$$

where N is the number of experimental runs, Ω_r^{-1} is the volume of the region of experimentation, σ^2 is the experimental error variance, $\hat{y}_{(\mathbf{x}_u)}$ is the predicted response at the data location $\mathbf{x}_u$ (u=1,...,N), R is the centered and scaled region of experimentation, and **V** and **B** denote the variance and squared bias components of **J**.

The MSE of Response can be conveniently defined in terms of the region moments of the design when the response function is partitioned into two parts, as follows

$$\mathbf{y} = X_1\boldsymbol{\beta}_1 + X_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon} \tag{4}$$

where $X_1\boldsymbol{\beta}_1$ includes the first- and second-order terms in the fitted model and $X_2\boldsymbol{\beta}_2$ includes the unfitted third-order terms. Similarly, the fitted second-order model can be written as

$$\hat{\mathbf{y}} = X_1\mathbf{b}_1 \tag{5}$$

and the predicted value of the response at *uth* design point becomes

$$\hat{y}_{(\mathbf{x}_u)} = \mathbf{x}_{1u}'\,\mathbf{b}_1 \tag{6}$$

The region moment matrices of the response surface are defined as

$$\mu_{11} = \Omega_r \int_R \mathbf{x}_1'\,\mathbf{x}_1\,d\mathbf{x}$$

$$\mu_{21} = \Omega_r \int_R \mathbf{x}_2'\,\mathbf{x}_1\,d\mathbf{x}$$

$$\mu_{22} = \Omega_r \int_R \mathbf{x}_2'\,\mathbf{x}_2\,d\mathbf{x}$$

Utilizing the above region matrices, the MSE of Response criterion shown in equation (3) becomes the minimization of

$$\mathbf{J} = \frac{N}{\sigma_2}\,\mathrm{Trace}\,\{\mathrm{Var}[\mathbf{b}_1]\,\mu_{11}\} + \frac{N}{\sigma^2}\,\boldsymbol{\beta}_2'\,\{A'\mu_{11}A - 2\mu_{21}A + \mu_{22}\}\,\boldsymbol{\beta}_2 \tag{7}$$

where the variance-covariance matrix of the ordinary least squares estimators of the fitted model coefficients is

$$\mathrm{Var}[\mathbf{b}_1] = (X_1'X_1)^{-1}X_1'\,V\,X_1(X_1'X_1)^{-1}\sigma^2 \tag{8}$$

and **A** is the ordinary least squares alias matrix, defined as

$$A = (X_1'X_1)^{-1}X_1'X_2 \tag{9}$$

where

$$\begin{aligned}\mathrm{Bias}[\mathbf{b}_1] &= E[\mathbf{b}_1] - \boldsymbol{\beta}_1\\ &= A\,\boldsymbol{\beta}_2\end{aligned} \tag{10}$$

V is a matrix of the correlations between pairs of simulated responses, defined as

$$V = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1N}\\ \rho_{21} & 1 & 1 & \vdots\\ \vdots & & \cdot & \vdots\\ \vdots & & 1 & \rho_{ij}\\ \rho_{N1} & \cdots & \rho_{ij} & 1 \end{bmatrix} \tag{11}$$

and

$$\mathrm{Var}(\mathbf{y}) = \sigma^2 V \tag{12}$$

The form of V depends upon the pseudorandom number streams assigned to the experimental design points (discussed in the following section).

Under ordinary least squares parameter estimation, the bias component of **J** is independent of V and, therefore, does not depend upon the pseudorandom number stream assignments. The bias component can be minimized through the selection of an appropriate scaling factor and, subsequently, the minimum bias designs can be augmented with an appropriate number of center runs in order to minimize the variance error.

Exact minimization of the variance error is not possible, however, due to the integer restriction on the number of center runs. The variance error is a function of the random number stream assignments (through V) but, because the number of center runs must be an integer value, the optimal design plans are the same for each of the assignment strategies.

4. PSEUDORANDOM NUMBER STREAM ASSIGNMENTS

In addition to the choices of design class, number of center runs, and levels of the design points, experimentation on a stochastic simulation model involves the assignment of pseudorandom number streams to each design point. Three basic alternatives for assigning streams to design points are: different streams, identical streams, and antithetic streams. However, simultaneous use of the three alternatives results in a multitude of assignment strategies. Schruben and Margolin [1978] investigated 49 strategies using two-level factorial designs and found the following three strategies to be of particular importance:

- Independent streams (denoted IR),
- Common streams (denoted CR), and
- Assignment rule blocking strategy (denoted AR).

The IR strategy utilizes different streams of pseudorandom numbers for each stochastic model component on each simulation run, or $m \cdot N$ streams, where m represents the number of stochastic model components and N represents the number of simulation runs (design points). The CR strategy uses different streams for each stochastic model component, but uses a common set of streams on each simulation run, thereby requiring only m different streams. The AR strategy uses common streams within orthogonal blocks and antithetic streams for design points in opposite blocks. The antithetic streams are "one minus" the uniform (0,1) deviates generated by the m common streams. For the AR strategy, designs which partition into an odd number of orthogonal blocks utilize independent streams in the unpaired block. For the CR strategy, replicated design points utilize independent streams, and replicated design points within blocks utilize independent streams in the AR strategy.

Schruben and Margolin [1978] note that the use of independent, common, and antithetic pseudorandom number streams, respectively, for pairs of simulation runs, tends to result in simulated responses that are independent, positively correlated, and negatively correlated. Further, in the development of the IR, CR, and AR strategies, these authors assume that the positive correlations between responses generated with common streams is equal to ρ_+, and the negative correlation between responses generated with antithetic streams is equal to $-\rho_-$. The relationship between the magnitudes of the correlations, which is consistent with empirical findings, is

$$0 \le \rho_- \le \rho_+ < 1 .$$

Under these assumptions, the correlation matrix shown in equation (11) can be written as follows (for the IR, CR, and AR strategies):

$$V_{IR} = I_N \qquad (13)$$

$$V_{CR} = I_N + \rho_+ \underline{u}\,\underline{u}' - \rho_+ U \qquad (14)$$

$$V_{AR} = I_N + \tfrac{1}{2}(\rho_+ - \rho_-)\underline{u}\,\underline{u}' + \tfrac{1}{2}(\rho_+ + \rho_-)\underline{v}\,\underline{v}' - \rho_+ U \qquad (15)$$

where $\mathbf{I}_N$ is an NxN identity matrix and $\mathbf{U}$ is an NxN diagonal matrix of the vector $\underline{u}$, whose ith element is

u_i = 0 if independent random number streams are used for the ith design point,
= 1 if a common or antithetic random number streams are used for the ith design point,

and $\underline{v}$ is an $Nx1$ vector whose ith element is

v_i = 1 if a common random number streams are used for the ith design point,
= 0 if independent random number streams are used for the ith design point,
= -1 if antithetic random number streams are used for the ith design point.

Incorporation of these three correlation matrices (also shown in Appendix B) into the equation for the MSE of Response enables a comparison of the optimal design plans. Since the bias error is not a function of the correlation matrix, the optimal designs are compared in terms of the variance error alone.

5. OPTIMAL EXPERIMENTAL DESIGNS

Second-order designs which minimize the variance component of the MSE of Response, given minimum bias components, are developed in four design classes for models with two through seven factors, as follows:

1. Central Composite Designs (CCDs)
   a) Full factorial replications k = 2, 3, 4, 5
   b) One-half fractional factorials k = 6, 7
2. Box-Behnken Designs (BBDs) k = 4, 5, 7
3. Three-level Factorials (FACs)
   a) Full factorial replications k = 3, 4, 5
   b) One-third fractional factorials k = 6, 7
4. Small Composite Designs (FACs)
   a) Hartley designs (SCD-H) k = 3, 4, 6
   b) Draper designs (SCD-D) k = 5, 7.

The BBDs and FACs can be partitioned into orthogonal blocks regardless of the levels of the design points, but the CCDs and SCDs require specific levels of the axial design points, relative to the factorial design points (assumed scaled to ±1), in order to block orthogonally. The required axial levels are shown in Table 1.

Table 1. Levels of the Axial Design Points Required for Orthogonal Blocking in the CCDs and SCDs

DESIGN CLASS	Values of α in the CCDs					
	k = 2	k = 3	k = 4	k = 5	k = 6	k = 7
CCD	1.414	1.764	2.058	2.309	2.511	2.717
SCD	-	1.673	2.000	2.253	2.473	2.691

The bias component of the MSE of Response can be minimized through the use of an appropriate scaling factor, denoted g. For each region of experimentation, the design points are generally scaled such that +1 and -1 represent the high and low levels of each factor. In order to protect against bias due to model inadequacy, these ±1 levels need to be scaled by a factor of g, which requires moving the design points closer to the center of the experimental region. The optimal values of the scaling factor, for both spherical and cuboidal regions of interest are shown in Tables 2 and 3.

Table 2. Min B Values of the scaling factor in a Spherical Region

DESIGN CLASS	Min-B Values of g					
	k=2	k=3	k=4	k=5	k=6	k=7
CCD	.58	.48	.42	.39	.36	.34
BBD	-	-	.61	.62	-	.52
FAC	-	.55	.50	.46	.43	.40
SCD	-	.52	.42	.39	.36	.34

Table 3. Min B Values of the scaling factor in a Cuboidal Region

DESIGN CLASS	Min-B Values of g					
	k=2	k=3	k=4	k=5	k=6	k=7
CCD	.68	.64	.63	.62	.61	.61
BBD	-	-	.89	.98	-	.93
FAC	-	.74	.73	.73	.72	.72
SCD	-	.66	.63	.62	.61	.61

After minimizing the bias component of the MSE of Response, the variance component can then be minimized by augmenting the design with an appropriate number of center runs, Nc. The optimal number of center runs (which have been rounded to the nearest integer) for a Min-V | Min-B design are shown in Tables 4 and 5.

Table 4. Min-V | Min-B Number of Center Runs in a Spherical Region

DESIGN CLASS	Min-V | Min-B Values of Nc					
	k=2	k=3	k=4	k=5	k=6	k=7
CCD	2	2	2	3	2	3
BBD	-	-	2	3	-	2
FAC	-	0	0	0	0	0
SCD	-	1	1	1	1	2

Table 5. Min-V | Min-B Number of Center Runs in a Cuboidal Region

DESIGN CLASS	Min-V | Min-B Values of Nc					
	k=2	k=3	k=4	k=5	k=6	k=7
CCD	2	2	3	4	3	4
BBD	-	-	3	3	-	3
FAC	-	0	0	0	0	0
SCD	-	2	2	2	2	2

6. PERFORMANCE RESULTS

In order to compare the performance of the four design classes, the variance component of the MSE of Response is computed for the three assignment strategies. The bias component of the MSE of Response is independent of the assignment strategy, as indicated in equation (7), and therefore the performance of the optimal design plans are evaluated in terms of the variance component of the MSE of Response.

Figure 1 illustrates the relative performance of the four design classes using the CR strategy (common streams) for k=5 factors. (Similar results are obtained for k=2,3,4,6,7.) The results indicate that the CCDs and BBDs tend to perform the best of the four design classes. However, when the magnitude of the induced correlation between pairs of simulated responses is greater than 0.6, the SCDs perform better than the CCDs and BBDs. Figure 1 also indicates that the CR strategy is inferior to the IR strategy (independent streams) for the CCDs, BBDs, and FACs. (The IR strategy is illustrated when the induced correlation is equal to zero.)

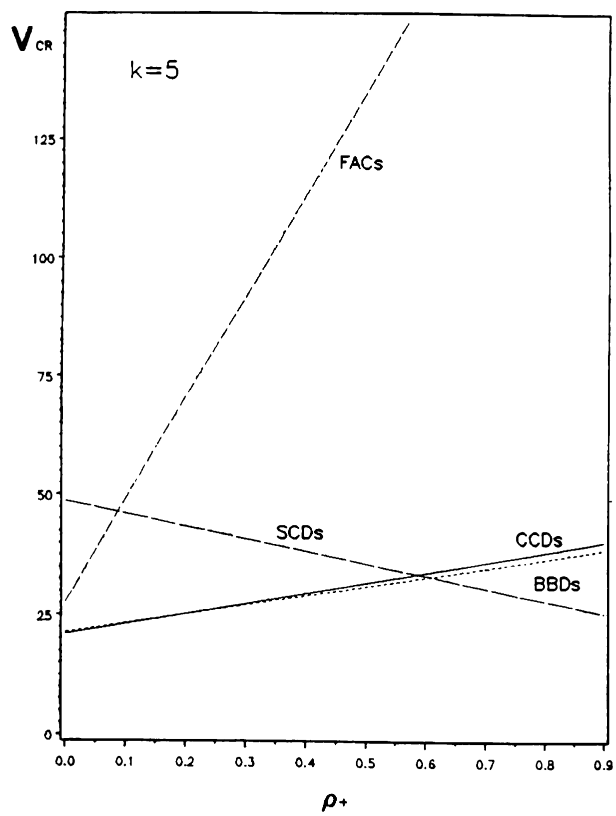

Figure 1. Optimal Values of V for k=5 Min-V | Min-B Designs Using the CR Strategy in a Spherical Region

The performance of the four design classes under the AR strategy (assignment rule) is shown in Figures 2 and 3. The horizontal axis represents the magnitude of the induced positive correlation between responses within orthogonal blocks. The upper lines of the triangular regions correspond to induced negative correlations of zero, and the lower lines of the triangular regions correspond to equal positive and negative correlations. Similar to the results for the CR strategy, the CCDs and BBDs perform the best when $\rho_+ < 0.6$ and SCDs perform the best when $\rho_+ > 0.6$. However, with the exception of the FACs, the AR strategy tends to perform better than the IR strategy.

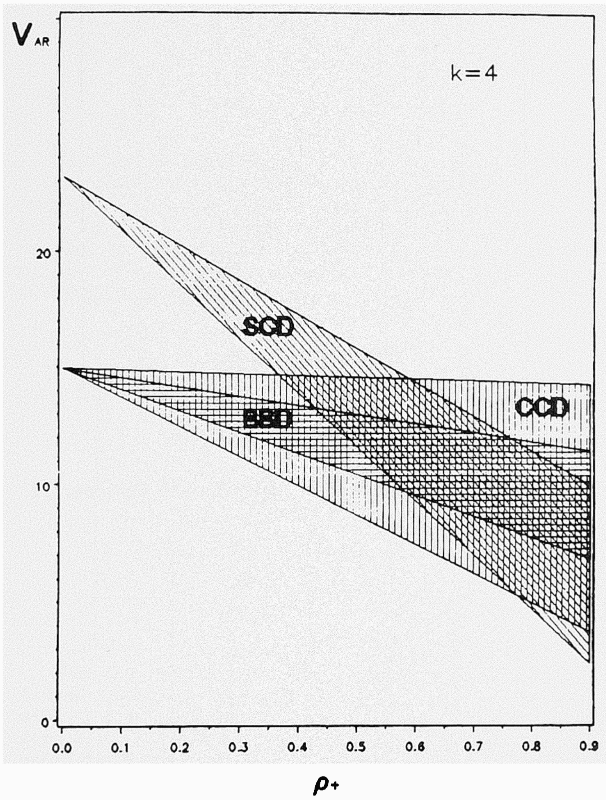

Figure 2. Optimal Values of V for k=4 Min-V | Min-B Designs Using the AR Strategy in a Spherical Region

The results indicate that medium-size designs (CCDs and BBDs) tend to be preferred to the large FACs for all three assignment strategies. The smaller SCDs are preferred to the CCDs and BBDs only if the assignment strategy results in correlations of at least 0.6 between simulated response pairs. In comparing the use of the three assignment strategies on the optimal Min-V | Min-B designs, the CR strategy tends to perform the poorest and the AR strategy tends to perform the best in terms of the variance component of the MSE of Response. In addition, the performance of the AR strategy improves as the magnitudes of the induced correlations increase.

7. DISCUSSION

Previous research on quadratic response surface estimation by Hussey et al. [1987] reached similar conclusions concerning the relative performance of the assignment strategies. These authors compared the IR, CR, and AR strategies using designs which minimized the variance component of the MSE of Response. This current research indicates that there should be even greater emphasis placed on the importance of the AR strategy when bias is incorporated into the development of an optimal design plan; the AR strategy was found to be superior over a wider range of induced correlation magnitudes than was found in the Hussey et al. study.

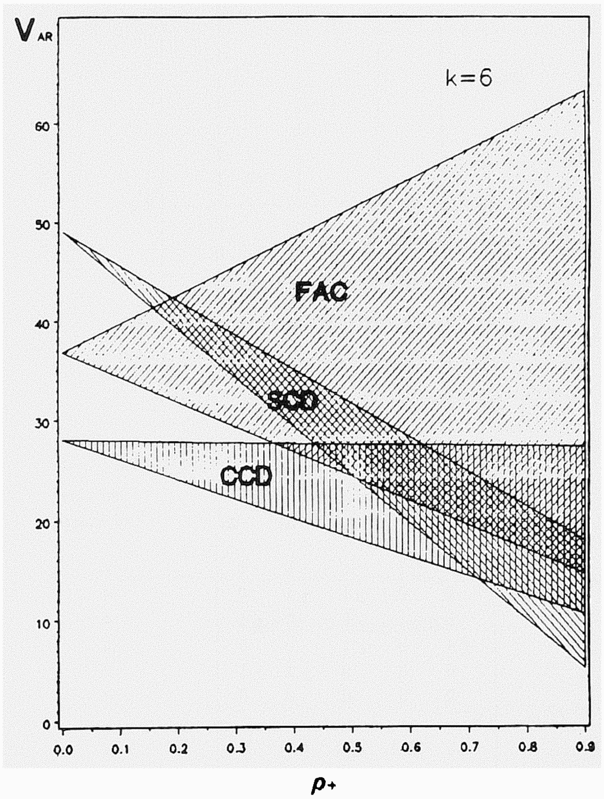

Figure 3. Optimal Values of V for k=6 Min-V | Min-B Designs Using the AR Strategy in a Spherical Region

The findings presented here clearly indicate that carefully planned experimental designs can substantially improve the estimation of quadratic response surface models. Such improvements in the prediction of response should inevitably lead to improved efficiency in the estimation of the optimum operating conditions of the simulated system.

APPENDIX A. EXPERIMENTAL DESIGN PLANS

Central Composite Design with k=3 Factors

D =

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
1	1	1
- - -	- - -	- - -
α	0	0
$-\alpha$	0	0
0	α	0
0	$-\alpha$	0
0	0	α
0	0	$-\alpha$
0	0	0

$\times g$

Box-Behnken Design with k=5 Factors

D =

x_1	x_2	x_3	x_4	x_5	Number of Points
± 1	± 1	0	0	0	4
0	0	± 1	± 1	0	4
0	± 1	0	0	± 1	4
± 1	0	± 1	0	0	4
0	0	0	± 1	± 1	4
0	0	0	0	0	3
- - -	- - -	- - -	- - -	- - -	
0	± 1	± 1	0	0	4
± 1	0	0	± 1	0	4
0	0	± 1	0	± 1	4
± 1	0	0	0	± 1	4
0	± 1	0	± 1	0	4
0	0	0	0	0	3

$\times g$

N = 46

Hartley's Small Composite Design with k=3 Factors

D =

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
1	1	1
- - -	- - -	- - -
α	0	0
$-\alpha$	0	0
0	α	0
0	$-\alpha$	0
0	0	α
0	0	$-\alpha$
0	0	0

$\times g$

Draper's Small Composite Design with k=5 Factors

D =

x_1	x_2	x_3	x_4	x_5
-1	-1	-1	-1	-1
1	1	1	1	1
-1	-1	1	1	1
-1	1	1	-1	1
1	-1	-1	1	1
1	1	-1	1	-1
1	1	1	-1	-1
1	-1	1	-1	-1
1	-1	-1	-1	1
-1	1	-1	1	-1
-1	1	-1	-1	1
-1	-1	1	1	-1
- - -	- - -	- - -	- - -	- - -
$\pm\alpha$	0	0	0	0
0	$\pm\alpha$	0	0	0
0	0	$\pm\alpha$	0	0
0	0	0	$\pm\alpha$	0
0	0	0	0	$\pm\alpha$

$\times g$

Three-level Factorial Design with k=3 Factors

D =

x_1	x_2	x_3
-1	-1	1
-1	0	0
-1	1	-1
0	-1	1
0	0	0
0	1	-1
1	-1	1
1	0	0
1	1	-1
- - -	- - -	- - -
-1	-1	0
-1	0	-1
-1	1	1
0	-1	-1
0	0	1
0	1	0
1	-1	1
1	0	0
1	-1	-1
0	0	0
- - -	- - -	- - -
-1	-1	-1
-1	0	1
-1	1	0
0	-1	1
0	0	0
0	1	-1
1	-1	0
1	0	-1
1	1	1

$\times g$

APPENDIX B. CORRELATION MATRICES

The matrix form of equation (13), the correlation matrix for the IR strategy, can be written as

$$\mathbf{V}_{IR} = \begin{bmatrix} 1 & 0 & \cdots & & 0 \\ 0 & 1_1 & & & \vdots \\ \vdots & & \cdot & & \vdots \\ \vdots & & & 1 & 0 \\ 0 & \cdots & & 0 & 1 \end{bmatrix}$$

For the CR strategy, the response vector has been partitioned into two parts; the first part contains responses generated with common streams and the second part contains responses generated with independent streams (replicated design points). The matrix form of equation (14), the correlation matrix for the CR strategy, can be written as

$$V_{CR} = \left[\begin{array}{ccccc|c} 1 & \rho_+ & \rho_+ & \cdots & \rho_+ & \\ \rho_+ & 1 & & \rho_+ & \vdots & \\ \vdots & \rho_+ & 1 & \cdot & \vdots & \mathbf{0} \\ \vdots & & & \cdot & \rho_+ & \\ \rho_+ & & \cdots & \rho_+ & 1 & \\ \hline & & \mathbf{0} & & & \mathbf{I} \end{array}\right]$$

For the AR strategy, the response vector is partitioned into three parts; the first contains responses within one orthogonal block (generated with common streams), the second contains responses within the opposite block (generated with antithetic streams), and the third contains responses generated with independent streams (replicated design points and any responses in a third block). The matrix form of equation (15), the correlation matrix for the AR strategy, can be written as

$$V_{AR} = \left[\begin{array}{ccccc|ccccc|c} 1 & \rho_+ & & \cdots & \rho_+ & & & & & & \\ \rho_+ & 1 & & & \vdots & & & & & & \\ \vdots & & 1 & & \vdots & & & -\boldsymbol{\rho}\_ & & & \mathbf{0} \\ \vdots & & & \cdot & \rho_+ & & & & & & \\ \rho_+ & \rho_+ & \cdots & \rho_+ & 1 & & & & & & \\ \hline & & & & & 1 & \rho_+ & \cdots & & \rho_+ & \\ & & -\boldsymbol{\rho}\_ & & & \rho_+ & 1 & & & \vdots & \mathbf{0} \\ & & & & & \vdots & & & \cdot & \rho_+ & \\ & & & & & \rho_+ & \cdots & & \rho_+ & 1 & \\ \hline & & \mathbf{0} & & & & & \mathbf{0} & & & \mathbf{I} \end{array}\right]$$

where $-\boldsymbol{\rho}\_$ is a matrix in which each element is equal to $-\rho\_$.

APPENDIX C. SCALING FACTORS

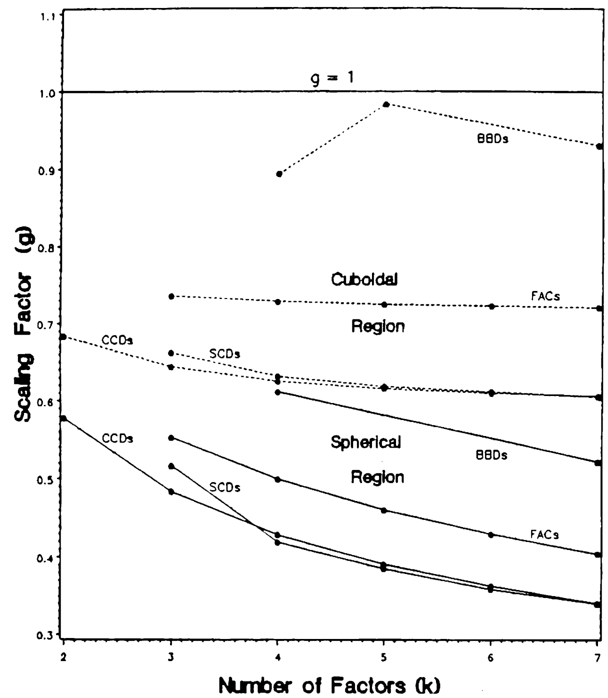

Figure C.1. Optimal Values of the Scaling Factor for Min-B Designs

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