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USING CENTRAL COMPOSITE DESIGNS IN SIMULATION EXPERIMENTS

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ABSTRACT

This paper identifies a strategy, jointly utilizing common random numbers and antithetic variates, for the assignment of random number streams in a simulation experiment which utilizes the central composite design for fitting second-order metamodels. Such designs are often used for the purpose of efficiently estimating a specific second-order metamodel of the relationship between the levels of the input factors and the mean of the univariate response variable of interest. In the past, correlation-based strategies for metamodel estimation in simulation experiments have focused on first-order metamodels. However, in many simulation experiments it is reasonable to expect that the relation between the levels of the input factors and the mean of the response of interest is better approximated by a second-order metamodel. Thus, second-order metamodels are, typically, of more interest to the simulation experimenter. The proposed strategy uses the variance reduction techniques of common random numbers to induce positive correlations between responses across design points and antithetic variates to induce negative correlations between responses across replicates within the simulation experiment. For the class of central composite designs and with respect to a variety of optimality criteria, this strategy is shown to give better estimates of the vector of unknown metamodel coefficients than the method of independent random number streams. Results of a numerical study on a two-factor experiment are presented to support these claims and to show that, in practice, the proposed strategy yields metamodel coefficient estimates that are superior to those obtained under the strategy of independent random number streams.

1 INTRODUCTION

In classical design of experiments, interest is often focused on fitting a second-order, linear regression model of the mean response of interest and the levels of the design variables. One of the most popular and usefull designs used for fitting such regression models is the central composite design (see Chapter 7 of Myers 1976). This popularity and usefullness should serve as a strong recommendation of the central composite design to the simulation analyst interested in performing designed second-order simulation experiments. Unfortunately, the central composite design has received little attention from the simulation community. We feel that the development of a strategy for assigning random number streams to design points in a simulation experiment which utilizes the central composite design, will greatly help this design gain broad acceptance within the simulation community. The development of such a strategy is the focus of this paper.

The variance reduction techniques of *common random numbers* and *antithetic variates* have been used successfully in simulation experiments that are designed to estimate an hypothesized first-order metamodel of the mean response of interest and levels of the design variables set by the simulation analyst. (Discussions of these two variance reduction techniques are given in Chapter 2 of Bratley, Fox, and Schrage 1987 and Chapter 11 of Law and Kelton 1991.) Schruben and Margolin (1978) showed that the strategy of applying common random numbers across all design points in the experiment yields superior estimates of the unknown metamodel coefficients to the strategy of assigning independent random number streams to all design points. Furthermore, they proposed an assignment rule that, for designs that are orthogonally blockable into *two* orthogonal blocks, assigns a combination of common and antithetic random number streams across the design points in the experiment. This assignment rule is shown to be superior to both the strategy of common random numbers alone and to the strategy of independently assigned random number streams. The requisite assumptions, as well as performance evaluations, for this assignment rule have been fully documented by Schruben (1979), Schruben and Margolin (1978), Tew (1986), and Tew and Wilson (1992a, b).

The major contribution of the Schruben-Margolin Assignment Rule was to show how common random numbers and antithetic variates could be successfully combined in one simulation experiment. However, their results are restricted to metamodels that admit orthogonal blocking into two blocks (see Section 4.2 of Schruben and Margolin 1978, Chapter 8 of Myers 1976, and Tew and Wilson 1992a). Often, second-order designs such as central composite designs, as well as others, require blocking into more than two orthogonal blocks (see Chapter 15 of Box and Draper 1987 and Chapter 8 of Myers 1976). Also, it is often desirable for a central composite design to have more than one *center point* (see Chapter 7 of Myers 1976). Such designs cannot accommodate the Schruben-Margolin Assignment Rule.

Our experience has suggested that for many simulation experiments, a second-order metamodel offers a better approximation to the true underlying relationship between the mean of the response of interest and the selected levels of the input factors, and that very often the designs are constructed sequentially in a manner that does not allow orthogonal blocking into two blocks. (This is especially true for response surface methodology (RSM) applications to simulation experiments.) In this paper we suggest a correlation-induction strategy for simulation experiments which utilize the central composite design in order to estimate a second-order metamodel without the restrictions of orthogonal blocking or a single center point. In keeping with the spirit of the Schruben-Margolin Assignment Rule, this strategy combines the use of common random numbers and antithetic variates in one experiment. This strategy is shown, under certain conditions, to be superior to the method of using independent, randomly selected random number streams across all design points for the central composite design.

This paper is organized as follows. Section 2 provides an introduction to the background results and notation that are utilized throughout the remainder of the paper. Section 3 gives an overview of the central composite design. The development of the proposed correlation-induction strategy is given in Section 4. An example of a simple job shop environment is given in Section 5 along with a discussion of how the correlation-induction strategy developed in this paper was implemented and the numerical results that were obtained. Concluding remarks and a summary are given in Section 6.

2 NOTATION AND BACKGROUND RESULTS

In this section we provide the statistical framework necessary to formally define a simulation experiment and its associated second-order metamodel. We also identify the second-order metamodel used to evaluate the correlation-induction strategy presented in Section 4.

2.1 Setup for Designed Simulation Experiments

Consider a simulation experiment consisting of m design points, where each design point is defined by the d-dimensional vector $\boldsymbol{\varphi}$ of factors that are deterministic inputs to the simulation model. Further, assume that the simulation experiment consists of r replicates at each design point. For $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, r$, let $\boldsymbol{\varphi}_i$ represent the settings of these d factors at the ith design point; and let y_{ij} denote the univariate response generated by the simulation run made at the ith design point and jth replicate. Moreover, let the design variables $\{x_h() : h = 1, 2, \ldots, p-1\}$ represent transformations (coding functions) of the original factors. Then, assuming that the relationship between the response y_{ij} and the coded design variables $\{x_h(\boldsymbol{\varphi}_i) : h = 1, 2, \ldots, p-1\}$ is linear in the unknown parameters and first-order, we can write

$$y_{ij} = \beta_0 + \sum_{h=1}^{p-1} \beta_h x_h(\boldsymbol{\varphi}_i) + \epsilon_{ij} \quad \text{for } i = 1, 2, \ldots, m \text{ and } j = 1, 2, \ldots, r \tag{1}$$

where $\beta_0, \beta_1, \ldots, \beta_{p-1}$ are the unknown parameters of the simulation metamodel (1); and the error ϵ_{ij} represents the inability of the linear function $\beta_0 + \sum_{h=1}^{p-1} \beta_h x_h(\boldsymbol{\varphi}_i)$ to determine the response y_{ij}.

The overall input-output structure of the simulation experiment is most conveniently expressed in terms of the following matrix notation. For each replication j ($j = 1, 2, \ldots, r$), the vector of responses from all m design points is represented by $\mathbf{y}_j = (y_{1j}, y_{2j}, \ldots, y_{mj})'$. In the $m \times p$ design matrix $\mathbf{X} = [\mathbf{1}_m \ \mathbf{T}]$, the first column is all ones, and the $(i, h+1)$ element is $x_h(\boldsymbol{\varphi}_i)$ for $i = 1, 2, \ldots, m$ and $h = 1, 2, \ldots, p-1$. Finally, let $\boldsymbol{\beta} \equiv (\beta_0, \beta_1, \ldots, \beta_{p-1})'$ and $\boldsymbol{\epsilon}_j \equiv (\epsilon_{1j}, \epsilon_{2j}, \ldots, \epsilon_{mj})'$ respectively denote the parameter vector and error vector for the simulation metamodel given in (1). Thus, for the jth replicate, the relationship between the response and the coded design variables across the entire experiment can be expressed as

$$\mathbf{y}_j = \mathbf{X}\beta + \epsilon_j, \quad \text{for } j = 1, 2, \ldots, r. \tag{2}$$

Much of the subsequent analysis of alternative strategies for estimating the coefficients of the metamodel in (2) will depend on the assumption that, for a given replicate, the simulation-generated outputs have the following nonsingular multivariate normal distribution

$$\mathbf{y}_j \sim \mathrm{N}_m(\mathbf{X}\beta, \Sigma) \text{ with } \det(\Sigma) \neq 0, \quad \text{for } j = 1, 2, \ldots, r. \tag{3}$$

A simulation model is usually driven by randomly chosen *streams* of (pseudo)random numbers. For example, in a queueing network simulation, different random number streams could be dedicated to sampling service times at different service centers. Each stream is a reproducible, deterministic sequence of real numbers that appears to constitute a random sample from the uniform distribution on the unit interval $[0,1]$. We suppose that the simulation model under discussion is driven by s such random number streams, and we use the following notation to indicate the random number input supplied to this model at different design points and replicates in the overall simulation experiment: (a) at the ith design point and jth replicate, the kth, potentially infinite, random number stream is

$$\mathbf{r}_{ijk} = (r_{ijk1}, r_{ijk2}, \ldots)' \quad \text{for } i = 1, 2, \ldots, m;\; j = 1, 2, \ldots, r; \text{ and } k = 1, 2, \ldots, s; \tag{4}$$

(b) the complete set of random number streams at the ith design point and j replicate is

$$\mathbf{R}_{ij} = (\mathbf{r}_{ij1}, \mathbf{r}_{ij2}, \ldots, \mathbf{r}_{ijs}) \quad \text{for } i = 1, 2, \ldots, m \text{ and } j = 1, 2, \ldots, r; \tag{5}$$

and (c) the aggregate random number input for the basic m-point experimental design at the jth replicate is

$$\mathbf{R}_j = \begin{bmatrix} \mathbf{R}_{1j} \\ \mathbf{R}_{2j} \\ \vdots \\ \mathbf{R}_{mj} \end{bmatrix}. \tag{6}$$

Now at the ith design point and jth replicate, $\mathbf{R}_{ij}$ completely determines the events of the associated simulation run so that we can rewrite equation (1) as

$$y_{ij}(\mathbf{R}_{ij}) = \beta_0 + \sum_{h=1}^{p-1} \beta_h x_h(\varphi_i) + \epsilon_{ij}(\mathbf{R}_{ij}) \quad \text{for } i = 1, 2, \ldots, m \text{ and } j = 1, 2, \ldots, r. \tag{7}$$

(On occassion throughout the remainder of the paper, we will use the notation $\bar{\mathbf{R}}$ to denote the set of random number streams that are *antithetic* to those in $\mathbf{R}$.)

2.2 A Second-Order Metamodel

In this section we identify the general second-order metamodel which we will estimate via the central composite design described in the next section. Consider the following second-order, d-factor metamodel:

$$y_{ij} = \gamma_0 + \sum_{h=1}^{d} \gamma_h \varphi_{hi} + \sum_{h=1}^{d} \gamma_{hh} \varphi_{hi}^2 + \sum \sum\nolimits_{g<h} \gamma_{gh} \varphi_{gi} \varphi_{hi} + \epsilon_{ij} \quad \text{for } g = 1, 2, \ldots, d;\; h = 1, 2, \ldots, d;\; i = 1, 2, \ldots, m; \text{ and } j = 1, 2, \ldots, r; \tag{8}$$

where φ_{hi} is the level of the hth factor at the ith design point, γ_0 is the unknown constant coefficient, γ_h $(h = 1, 2, \ldots, d)$ are the unknown first-order coefficients, γ_{hh} $(h = 1, 2, \ldots, d)$ are the unknown pure second-order coefficients, γ_{gh} $(g = 1, 2, \ldots, d;\; h = 1, 2, \ldots, d;$ and $g < h)$ are the unknown mixed second-order coefficients, and y_{ij} and ϵ_{ij} are defined in Section 2.1. Since (8) is a second-order metamodel we must select at least 3 levels for each factor and have $m \geq (2d + \frac{1}{2}d(d-1) + 1)$ in order to obtain estimates of all parameters in the metamodel.

Typically, in estimating

$$\gamma = (\gamma_0, \ldots, \gamma_d, \gamma_{11}, \ldots, \gamma_{dd}, \gamma_{12}, \ldots, \gamma_{d-1,d}),$$

we select the levels of φ_h $(h = 1, 2, \ldots, d)$ so that they are evenly spaced and restate the model in (8) in terms of design variables determined by a suitable coding of φ_h. For example, if we code φ_h to x_h, where the x_h's $(h = 1, 2, \ldots, d)$ take on a 0 value in the *center* of the design and values of -1 and +1 at low and high levels, respectively, and the levels of φ_h's $(h = 1, 2, \ldots, d)$ are evenly spaced, then the model in (8) is rewritten as:

$$y_{ij} = \beta_0 + \sum_{h=1}^{d} \beta_h x_{hi} + \sum_{h=1}^{d} \beta_{hh} x_{hi}^2 + \sum \sum\nolimits_{g<h} \beta_{gh} x_{gi} x_{hi} + \epsilon_{ij} \quad \text{for } g = 1, 2, \ldots, d;\; h = 1, 2, \ldots, d;\; i = 1, 2, \ldots, m; \text{ and } j = 1, 2, \ldots, r. \tag{9}$$

Further, in order to obtained independent estimates of at least some of the second-order coefficients in (9), we use orthogonal polynomials to rewrite (9) as:

$$\begin{aligned} y_{ij} &= \beta'_0 + \sum_{h=1}^{d} \beta_h x_{hi} + \sum_{h=1}^{d} \beta_{hh}(x_{hi}^2 - \bar{x_h^2}) \\ &+ \sum\sum\nolimits_{g<h} \beta_{gh} x_{gi} x_{hi} + \epsilon_{ij} \\ &\text{for } g = 1,2,\ldots,d; \;\; h = 1,2,\ldots,d; \\ &i = 1,2,\ldots,m; \text{ and } j = 1,2,\ldots,r. \quad (10) \end{aligned}$$

where $\bar{x_h^2}$ is the average value of x_{hi}^2 $(h = 1,2,\ldots,d)$ taken over the m design points. (See Chapter 1 of Anderson and McLean 1974 and Chapter 3 of Myers 1976 for a more complete treatment of orthogonal polynomials for second-order designs.)

Throughout the remainder of this paper we will use, for the correlation-induction strategies considered, the following least squares estimate of β:

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\bar{\mathbf{y}}, \quad (11)$$

where the structure of $\mathbf{X}$ will be determined in the next section. This, in conjuction with (3), yields

$$\hat{\beta} \sim \mathrm{N}_p(\beta, (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\Sigma\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}). \quad (12)$$

In this paper, we can limit our discussion to *ordinary* least squares estimation of β given in (11) without loss of generality because the correlation-induction strategy developed in Section 4 results in a covariance structure for $\bar{\mathbf{y}}$ that satisfies the equivalency conditions for *weighted* and *ordinary* least squares given in Section 3 of Schruben and Margolin (1978). Thus, all results given in this paper are valid for both weighted and ordinary least squares estimation of β.

3 CENTRAL COMPOSITE DESIGNS

In this section we give a short review of central composite designs; more complete discussions of central composite designs are given by Box and Draper (1987) and Myers (1976). In particular, we will discuss the second-order central composite design used for fitting the second-order metamodel given in equation (10). Such a design consists of: (a) $m_f = 2^d$ *cubic* points comprising a two-level factorial component replicated r_c (≥ 1) times, (b) $m_a = 2d$ *axial* points arranged along the axes of the design variables and symmetrically positioned with respect to the factorial cube replicated r_a (≥ 1) times, and m_c (≥ 1) *center* points positioned at the center, $\mathbf{x}' = (0,0,\ldots,0)$, of the design replicated r_c times. Thus, $m = m_f + m_a + m_c$.

The design matrix for the second-order central composite design where $m_c = 1$ is given on page 130 of Myers (1976) . The factorial portion of the design is chosen so as to allow the estimation of all first-order and two-factor interaction terms. The addition of the axial points allows for the estimation of the second-order terms in the model and the m_c observations taken at the center of the design allow for an estimate of *pure error* in the model, which, in turn, can be used to test for lack of fit in the hypothesized metamodel. From this form of $\mathbf{X}$ we get that

$$\mathbf{X}'\mathbf{X} = \mathbf{I}_{(m\times m)} \begin{bmatrix} m \\ m_f + 2\alpha^2 \\ \vdots \\ m_f + 2\alpha^2 \\ p-q \\ \vdots \\ p-q \\ m_f \\ \vdots \\ m_f \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ q^{\frac{1}{2}} \\ \vdots \\ q^{\frac{1}{2}} \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{(m\times 1)} [0\; 0\; \ldots\; 0\; q^{\frac{1}{2}}\; \ldots\; q^{\frac{1}{2}}\; 0\; \ldots\; 0]_{(1\times m)}, \quad (13)$$

where

$$p = m^{-1}[m_f(m_a+m_c) - 4m_f\alpha^2 - 4\alpha^4 + 2m\alpha^4], \quad (14)$$

and

$$q = m^{-1}[m_f(m_a+m_c) - 4m_f\alpha^2 - 4\alpha^4] \quad (15)$$

(see pp. 130-131 of Myers 1976). Although, in this paper, we only consider a central composite design with one center point, the choice of the number of center points to run (m_c) plays an important role in determining some of the properties of the second-order central composite design. As an example, the number of center points determines whether or not the design has uniform precision (see Chapter 7 of Myers 1976). Also, the number of center points affects the average mean squared error of the design and, consequently, must be considered when trying to determine an optimal design (see Chapter 9 of Myers 1976). We note here that the correlation induction strategy introduced in the next section easily accommodates central composite designs with multiple center points and, hence, is broadly applicable to *all* central composite designs.

4 CORRELATION INDUCTION STRATEGY

In this section, we develop a correlation induction strategy specifically designed for the central composite design. This strategy is based on the concept of correlated replicates introduced by Tew (1991 and 1992). First, we quickly review the independent random number streams strategy.

The method of independent random number streams involves randomly selecting a set of random number streams, $\mathbf{R}_{ij}$, for each design point, replicate combination in the experiment. That is, the independent random number streams strategy does not involve any variance reduction component in the experiment due to the assignment of the random number steams used. For this reason, it usually serves as the baseline strategy to which other variance reduction strategies are compared. In this study, inclusion of the independent random number streams strategy provides us the opportunity to obtain estimates of *absolute* variance reductions achieved by the other strategy developed later in this section.

In addition to the assumptions made in Section 1, we make two more assumptions regarding the behavior of the responses, y_{ij}, obtained from the independent random number streams strategy. First, we assume that the variance of the response is homogeneous across all design points *and* replicates in the experiment. Second, we assume that responses from any two simulation runs driven by different sets of random number streams (either at different design points and/or at different replicates) are uncorrelated. These two assumptions are summarized below ($i,k = 1,2,\ldots,m$; $j,l = 1,2,\ldots,r$; and $i \neq k$ and $j \neq l$):

$$\left.\begin{array}{l} \mathrm{var}(y_{ij}(\mathbf{R}_{ij})) = \sigma^2 \\ \text{(homogeneity of variances)}, \\ \mathrm{cov}(y_{ij}(\mathbf{R}_{ij}), y_{kl}(\mathbf{R}_{kl})) = 0 \\ \text{(otherwise)}. \end{array}\right\} \tag{16}$$

Under these assumptions it can be easily shown that for the central composite design discussed in the previous section with r replicates taken at each design point we get ($i,j = 1,2,\ldots,d$, and $i \neq j$):

$$\left[\begin{array}{l} \mathrm{var}(b_0{}') = \frac{\sigma^2}{rm}, \\ \mathrm{var}(b_i) = \frac{\sigma^2}{r(m_f+2\alpha^2)}, \\ \mathrm{var}(b_{ij}) = \frac{\sigma^2}{rm}, \\ \mathrm{var}(b_{ii}) = \frac{\sigma^2 e}{r}, \\ \mathrm{cov}(b_{ii}, b_{jj}) = \frac{\sigma^2 f}{r}, \end{array}\right]; \tag{17}$$

where

$$e = \frac{(p+(d-2)q)}{((p-q)(p+dq-q))} \tag{18}$$

and

$$f = \frac{q}{(q-p)(p+(d-1)q)}, \tag{19}$$

(see page 131 of Myers 1976). Next, we introduce the notation and assumptions needed to formally define the Correlated Replicates strategy.

The motivation behind the development of the Correlated Replicates strategy was to address the two major drawbacks associated with the Schruben-Margolin correlation-induction strategy (restricted experimental design application and failure to accomodate further variance reduction via correlated replicates) and retain the spirit of combining variance reduction techniques first introduced by Schruben and Margolin (1978). In this strategy a positive correlation via common random number streams is induced between design points within a given replicate as well as between pairs of antithetic replicates. Thus, the Correlated Replicates strategy attempts to utilize this additional measure of experimental control to further "explain away" variation in the response variable in a manner that is consistent with the experimental concept of blocking.

The experimental concept behind common random number streams is to apply the *same* random experimental conditions to different simulation runs so as to more effectively compare their outputs (see Chapter 11 of Law and Kelton 1991, Section 3 of Schruben and Margolin 1978, and Joshi and Tew 1991). That is, under common random number streams, if in comparing outputs from two simulation runs, differences are observed, then they must be the result of differences in the input factors between the two runs and *not* due to the differences in the random number streams used to drive the simulation since both runs utilized the same set of random number streams. This, of course, is why using common random number streams is viewed as a form of experimental blocking (see Chapter 5 of Anderson and McLean 1974, Mihram 1974, Joshi and Tew 1991, and Crenshaw and Tew 1992).

However, implementation of common random number streams requires some careful thought if the assumptions on the *experimental error* given in Section 2 are to be met. Crenshaw and Tew (1992) and Mihram (1974) both recognized that at least one of the s random number streams used to drive the simulation model should be randomly selected in order to insure that an experimental component, ϵ_{ij}, is properly included in the response y_{ij} (for a detailed treatment of this topic along with some illustrative examples, see Crenshaw and Tew 1992).

Thus, if we separate $\mathbf{R}_{ij}$ ($i = 1,2,\ldots,m$ and $j = 1,2,\ldots,r$) into two mutually exclusive sets of random number streams, $(\mathbf{R}_{1ij}, \mathbf{R}_{2ij})$, such that $\mathbf{R}_{2ij}$ ($i = 1,2,\ldots,m$ and $j = 1,2,\ldots,r$) is *randomly* selected across all design points and replicates, then we are assured of the presence of ϵ_{ij} ($i = 1,2,\ldots,m$ and $j =$

$1,2,\ldots,r$) in (10). Hence, in inducing correlations we use only $\mathbf{R}_{1ij}$ ($i=1,2,\ldots,m$ and $j=1,2,\ldots,r$). (Note, in this section and in the remainder of the paper, we assume that r is an even number.)

In this section, as well as the example, the additional measure of control brought about by the Correlated Replicates strategy is shown to yield superior variance reduction under certain assumptions.

This stategy involves using common random number streams across all m design points within a replicate and using antithetic variates between replicates, which are grouped into pairs and then using the same set of random number streams (except for the $\mathbf{R}_{2ij}$ components) in order to construct positively correlated pairs of replicates. That is, from an experimental design point of view, we are using $\mathbf{R}_{111}$ and $\bar{\mathbf{R}}_{111}$ to construct *two* blocks of r internal replicates each (see Chapter 5 of Anderson and McLean 1974 for a discussion on the concept of experimental blocking).

From Table III of Tew (1992) we see that we separate $\mathbf{R}_{ij}$ ($i=1,2,\ldots,m$ and $j=1,2,\ldots,r$) into two mutually exclusive sets of random number streams, $(\mathbf{R}_{1ij},\mathbf{R}_{2ij})$, such that $\mathbf{R}_{2ij}$ ($i=1,2,\ldots,m$ and $j=1,2,\ldots,r$) is randomly selected across all design points and replicates so as to insure the presence of ϵ_{ij} ($i=1,2,\ldots,m$ and $j=1,2,\ldots,r$) in (10). Also, the number of replicates, r, is assumed to be even. We assume that ($i,k=1,2,\ldots,m$ and $j,l=1,2,\ldots,r$):

$$\left.\begin{array}{l}
\mathrm{var}(y_{ij}(\mathbf{R}_{ij}))=\sigma^2\\
\text{(homogeneity of variances)},\\
\mathrm{cov}(y_{ij}(\mathbf{R}_{ij}),y_{kj}(\mathbf{R}_{kj}))=\sigma^2\rho_+\\
\quad\text{where } 0\le\rho_+\le 1 \text{ and } i\ne k\\
\text{(homogeneity of } \rho_+ \text{ correlations}\\
\text{across design points)},\\
\mathrm{cov}(y_{ij}(\mathbf{R}_{ij}),y_{kl}(\mathbf{R}_{kl}))=\sigma^2\rho_+\\
\quad\text{where } 0\le\rho_+\le 1 \text{ and}\\
\quad |l-j|=2,4,\ldots,r-2\\
\text{(homogeneity of } \rho_+ \text{ correlations}\\
\text{across replicates)},\\
\mathrm{cov}(y_{ij}(\mathbf{R}_{ij}),y_{kl}(\mathbf{R}_{kl}))=\sigma^2\rho_-\\
\quad\text{where } -1\le\rho_-\le 0, \text{ and}\\
\quad |l-j|=r-1\\
\text{(homogeneity of } \rho_- \text{ correlations}\\
\text{across replicates)},
\end{array}\right\}\qquad(20)$$

where $\mathbf{R}_{ij}=(\mathbf{R}_{1ij},\mathbf{R}_{2ij})$ as described earlier. These assumptions along with the assignment procedure given in Table III of Tew (1992) yield:

$$\begin{aligned}
\Sigma_{\bar{\mathbf{y}}}^{(cr)} &= \mathrm{Cov}(\bar{\mathbf{y}})\\
&= \frac{\sigma^2}{r}(1-\rho_+)\mathbf{I}_{(m\times m)}\\
&\quad+\frac{\sigma^2}{r}(\rho_++\rho_-)\mathbf{E}_{(m\times m)},
\end{aligned}\qquad(21)$$

where $\mathbf{E}_{(m\times m)}$ is the $m\times m$ matix of ones. A proof of (21) is given in Appendix II of Tew (1992).

Substitution of $\Sigma_{\bar{\mathbf{y}}}^{cr}$ into the expression for the dispersion of $\hat{\boldsymbol{\beta}}$ in (12):

$$\begin{aligned}
\mathrm{Cov}(\hat{\boldsymbol{\beta}}^{(cr)}) &= \Sigma_{\boldsymbol{\beta}}^{(cr)}\\
&= \frac{\sigma^2}{r}(1-\rho_+)(\mathbf{X}'\mathbf{X})^{-1}\\
&\quad+\frac{\sigma^2}{r}(\rho_++\rho_-)\begin{bmatrix}1 & \mathbf{0}'\\ \mathbf{0} & \mathbf{O}\end{bmatrix},
\end{aligned}\qquad(22)$$

where $\mathbf{0}$ is a $(p-1)\times 1$ column vector or zeros and $\mathbf{O}$ is a $(p-1)\times(p-1)$ matrix of zeros. Inspection of equations (17) and (22) clearly indicates that $\mathrm{Cov}(\hat{\boldsymbol{\beta}}^{(cr)})$ is superior to $\mathrm{Cov}(\hat{\boldsymbol{\beta}}^{(is)})=\mathrm{Cov}(\bar{\mathbf{y}})$ provided that the assumptions in (20) are not violated.

Note that a direct comparison of the entries in these matrices may not always be appropriate due to violations of the assumptions needed for each strategy. We recommend that, as a first step in the analysis, the simulation analyst conduct a relatively small pilot study to test for these assumptions before conducting the full experiment with its associated assignment strategy. Presently, such a pilot study has not been developed for this strategy. This subject is to be addressed in a future paper (see Tew and Wilson 1992a for the development of such a pilot study for the Schruben-Margolin correlation induction strategy).

5 EXAMPLE

In this section we illustrate the implementation of the correlation induction strategy presented in Section 4. We also present and summarize the results of a large-scale Monte Carlo experiment conducted with this strategy in order to assess its performance in estimating $\boldsymbol{\beta}$ for the metamodel given in equation (10).

5.1 A Job Shop Network

We consider the job shop example introduced by Nozari, Arnold, and Pegden (1987) and Tew and Wilson (1987) which is given in Figure 1 of Tew (1992). This job shop network operates as follows. Jobs arrive to the shop according to a Poisson process with an arrival rate of 10 jobs per hour. All jobs enter the network through Station 1. The processing of jobs at Station 1 constitutes a single server, single queue operation with a FIFO queue discipline. Upon completing service at Station 1, 80% of the jobs go to

Station 2, 5% go to Station 3, and 15% leave the network. The processing of jobs at each of stations 2 and 3 constitutes a single server, single queue operation with a FIFO queue discipline. A job at either Station 2 or Station 3 leaves the network upon completion of service. The shop admits jobs from 8:00 A.M. to 4:00 P.M. daily. However, service at each station continues until *all* jobs admitted on one day depart the network. The service time distribution (in minutes) at Station 3 is $U(21.0, 33.0)$. The service time distribution at Station 1 is a constant and at Station 2 is uniformly distributed. The specific distributions of the service times for both Station 1 and Station 2 are given in Table II. The purpose of this example is to estimate the effects that different service time distributions at Station 1 and Station 2 have on the expected time in system for a job. Thus, the performance measure of interest is the daily average system sojourn time for all jobs entering the system. In the next section, we discuss the metamodel used to relate the effects that the service time distributions used at Station 1 and Station 2 have on this performance measure.

5.2 The Metamodel

In order to study this network, we employed the a two-factor second-order central composite design with one center point and the following independent variables (factors): (a) service time distribution at Station 1 (φ_1) and service time distribution at Station 2 (φ_2) (past computational experience has indicated that a first-order metamodel is inappropriate for this system). That is, we used the following metamodel (given in equation (10)) to study the effects that these independent variables have on the mean response (y) over the design region of interest

$$\begin{aligned} y_{ij} &= \beta_0' + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_{11}(x_{1i}^2 - \bar{x}_1^2) \\ &\quad + \beta_{22}(x_{2i}^2 - \bar{x}_2^2) + \beta_{12} x_{1i} x_{2i} + \epsilon_{ij} \\ &\quad \text{for } i = 1, 2, \ldots, m \text{ and} \\ &\quad j = 1, 2, \ldots, r, \end{aligned} \tag{23}$$

where:

- y_{ij} is the sample daily average job sojourn time at the ith design point and jth replicate;
- β_0' is the long-run daily average job sojourn time across all design points;
- β_1, β_2, β_{11}, β_{22}, and β_{12} are the metamodel coefficients;
- $x_{1i}(\varphi_{1i}) = \left\{\frac{\varphi_{1i}-9}{8}\right\}$ is the first coded design variable at the ith design point;
- $x_{2i}(\varphi_{2i}) = \left\{\begin{array}{l} -1 \text{ if } \varphi_{2i} = U(0.5, 1.5), \\ 0 \text{ if } \varphi_{2i} = U(8.5, 9.5), \\ 1 \text{ if } \varphi_{2i} = U(16.5, 17.5), \end{array}\right\}$ is the second coded design variable at the ith design point; and
- ϵ_{ij} is the experimental error at the ith design point and jth replicate.

Table I
Second-Order Central Composite Design

Design Point i	Factor Combination (uncoded) $\varphi_i = (\varphi_{1i}, \varphi_{2i})$ φ_{1i}	φ_{2i}
1	1	$U(0.5, 1.5)$
2	17	$U(0.5, 1.5)$
3	1	$U(16.5, 17.5)$
4	17	$U(16.5, 17.5)$
5	17	$U(8.5, 9.5)$
6	1	$U(8.5, 9.5)$
7	9	$U(16.5, 17.5)$
8	9	$U(0.5, 1.5)$
9	9	$U(8.5, 9.5)$

Table II
Second-Order Central Composite Design

Design Point i	Factor Combination (coded) $\mathbf{x}_i = (x_{1i}, x_{2i})$ x_{1i}	x_{2i}
1	-1	-1
2	1	-1
3	-1	1
4	1	1
5	1	0
6	-1	0
7	0	1
8	0	-1
9	0	0

The design variable level assignments used for this experiment are given in Tables I and II. In the next section we describe how the Monte Carlo study was conducted in order to make valid comparisons of the correlation induction strategy presented in Section 3 to the method of independent random number streams.

5.3 The Monte Carlo Study

We used the SLAM II simulation language (Pritsker 1986) to implement a model of the job shop network described above. (The SLAM II code used by the author as well as tables of the random number seeds used and of the observed responses are available from the author upon request.) In simulating this network we dedicated a *separate* random number stream to each of the following four random components in the model: (a) interarrival times at Station 1 ($\mathbf{r}_1$), (b) probabilistic branching upon completion of service at Station 1 ($\mathbf{r}_2$), (c) service times at Station 2 ($\mathbf{r}_3$), and (d) service times at Station 3 ($\mathbf{r}_4$). Under the correlated replicates strategy, we randomly selected $\mathbf{r}_3$ across all design points and replicates in order to ensure the presence of ϵ_{ij} in (10) (see Crenshaw and Tew 1992, and Mihram 1974). That is, we set $\mathbf{R}_1 = (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ and $\mathbf{R}_2 = (\mathbf{r}_4)$.

The Monte Carlo study consisted of performing 50 independent *metareplications*, where the basic metareplication consisted of making 18 replications at each of the 9 design points given in Table II. That is, for this study, the full implementation for each correlation-induction strategy was comprised of 8,100 simulation runs of the job shop network model discussed above, where a run consisted of simulating the network for one 10-hour (simulation time) workday. Thus, 16,200 simulation runs were required to perform the Monte Carlo study. Next, we discuss the numerical results that we obtained.

5.4 Numerical Results

In order to give a concise and meaningful presentation of the numerical results, we have condensed them into the following components: (a) $\hat{\text{Cov}}(\hat{\boldsymbol{\beta}})$, (b) $\hat{\boldsymbol{\beta}}$, (c) $\det(\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}))$, (d) $\text{trace}(\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}))$, (e) observed estimated bias for all six metamodel coefficients (OEB), (f) average-estimated-absolute bias across all six coefficients (AEAB), (g) observed relative-estimated bias for all six metamodel coefficients (OREB), (h) average-relative-estimated-absolute bias across all six coefficients (AREAB) and (i) total-estimated-mean square-error for all six metamodel coefficients (TEMSE). The last three items are calculated using the independent random number streams case as the norm. That is, bias is estimated in terms of the deviation from that observed for the independent random number streams case. In all cases we used four decimal-place accuracy. Though, the matrices in (24) and (30) don't indicate so because of space limitations. The estimation of $\boldsymbol{\beta}$, and $\text{Cov}(\hat{\boldsymbol{\beta}})$ was performed as follows: independent estimates obtained for *each* metareplication were averaged over all 50 metareplications.

First, we consider the numerical results obtained under the independent random number streams strategy. For this strategy, we obtained:

$$\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}^{(is)}) = \begin{bmatrix} 44 & 5 & 6 & -31 & -13 & -10 \\ 5 & 51 & -10 & 15 & 17 & 11 \\ 6 & -10 & 67 & 15 & 9 & 16 \\ -31 & 15 & 15 & 261 & 0 & -8 \\ -13 & 17 & 9 & 0 & 221 & -12 \\ -10 & 11 & 16 & -7.9 & -12 & 66 \end{bmatrix}, \quad (24)$$

$$\hat{\boldsymbol{\beta}}^{(is)} = \begin{bmatrix} \hat{\beta}_0' \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \\ \hat{\beta}_4 \\ \hat{\beta}_5 \end{bmatrix} = \begin{bmatrix} 136.638 \\ 70.181 \\ 31.433 \\ 5.832 \\ 10.544 \\ -28.767 \end{bmatrix}, \quad (25)$$

$$\det(\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}^{(is)})) = 3.2307 \times 10^{11.0}, \quad (26)$$

$$\text{trace}(\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}^{(is)})) = 710.9968, \quad (27)$$

and

$$TEMSE = 710.9968. \quad (28)$$

(Note that OEB, AEAB, OREB, and AREAB all are equal to 0 in this case since the independent random number streams is taken as the norm.)

Next, we consider the numerical results obtained under the correlated replicates strategy. For this strategy, we obtained:

$$\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}^{(cr)}) = \begin{bmatrix} .04 & .02 & .01 & .02 & .00 & -.01 \\ .02 & .06 & -.00 & .02 & -.00 & .02 \\ .01 & -.00 & .04 & .01 & -.01 & .01 \\ .02 & .02 & .01 & .08 & .01 & .01 \\ .00 & -.00 & -.01 & .01 & .09 & -.02 \\ -.01 & .02 & .01 & .01 & -.02 & .08 \end{bmatrix}, \quad (29)$$

$$\hat{\boldsymbol{\beta}}^{(cr)} = \begin{bmatrix} \hat{\beta}_0' \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \\ \hat{\beta}_4 \\ \hat{\beta}_5 \end{bmatrix} = \begin{bmatrix} 135.362 \\ 69.656 \\ 31.345 \\ 5.524 \\ 10.251 \\ -28.568 \end{bmatrix}, \quad (30)$$

$$\det(\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}^{(cr)})) = 29907 \times 10^{-8.0}, \quad (31)$$

$$\text{trace}(\hat{\text{Cov}}(\hat{\boldsymbol{\beta}}^{(cr)})) = 0.3900, \quad (32)$$

$$\text{OEB}(\hat{\boldsymbol{\beta}}^{(cr)}) = \begin{bmatrix} 1.2760 \\ 0.5250 \\ 0.0880 \\ 0.3080 \\ 0.2930 \\ -0.1990 \end{bmatrix}, \quad (33)$$

$$AEAB = 0.4482, \quad (34)$$

$$\text{OREB}(\hat{\beta}^{(cr)}) = \begin{bmatrix} 0.9338\% \\ 0.7480\% \\ 0.2799\% \\ 5.2812\% \\ 2.7788\% \\ 0.6918\% \end{bmatrix}, \quad (35)$$

$$AREAB = 1.7856\%, \quad (36)$$

and

$$TEMSE = 2.5218. \quad (37)$$

Upon first view, some might think that with the restricted number of *blocks* used in the Correlated Replicates strategy, that an increase in bias would occur due to the seemingly restricted sampling of the blocking factor subspace (see Chapter 5 of Anderson and McLean 1974 for a discussion of this concept). However, this is not the case, in that in computer simulation experiments the blocking factor is *not* the seed selected, rather it is the resulting *stream* of random numbers generated from that seed. Bias in the response would arise if an *inadequate sampling* from the selected random number stream occurred during the simulation run, or if the generated stream itself had bad properties (e.g., dependent elements, nonuniform elements, etc.). Thus, as long as the random number generators used to drive a simulation model arevalid and an adequate sampling of the random number streams selectedis done during the simulation run, then bias will not be significantly affected under the Correlated Replicates strategy.

Inspection of the numerical results also clearly indicates that the Correlated replicates strategy can yield a greater than 99% improvement in performance over the independent random number streams strategy. These results are summarized in Table III below. We also note, that this improvement in performance has not resulted in any degredation in the diagonal structure of $\hat{\text{Cov}}(\beta)$. In summary, we recommend the Correlated Replicates strategy for the estimation of the second-order metamodel coefficients in (10).

Table III

Observed Variance Reductions

Performance Measure	Variance Reduction (percent)
var($\hat{\beta}_0$)	99.9081
var($\hat{\beta}_1$)	99.8783
var($\hat{\beta}_2$)	99.9416
var($\hat{\beta}_{11}$)	99.9689
var($\hat{\beta}_{22}$)	99.9615
var($\hat{\beta}_{12}$)	99.8755
det$\hat{\text{Cov}}$(β))	$\geq$ 99.9999
trace$\hat{\text{Cov}}$(β))	99.9451
TEMSE	99.6453

6 SUMMARY AND CONCLUSIONS

In this paper, we have proposed a correlated replicates strategy for computer simulation experiments which utilize the central composite design that allow effective estimation of the unknown coefficients in a second-order metamodel by *blocking* on the random number streams used to drive the simulation model. Under certain mild restrictions, this strategy is shown to be superior to the independent random number streams strategy. A Monte Carlo study was performed in order to empirically compare this strategy to the independent random number streams strategy. This study clearly shows that the superior performance of the Correlated Replicates strategy. In summary, we conclude that the Correlated Replicates strategy is a preferred strategy for performing simulation experiments that utilize the cental composite design.

Although the results presented in this paper are conclusive within the context of the simulation experiment given in Sections 4 and 5, we point out that we have considered only one type of second-order metamodel. Much work remains to be done in the areas of: (a) developing similar strategies to other classes of second, and higher, order metamodels, (b) integrating the correlated replicates concept with other productive variance reduction techniques (e.g., control variates, batch means, etc.), (c) developing tests of validation for the required assumptions for the Correlated Replicates strategy, and (d) extending these strategies to multiple-response simulation experiments. Many elements of these research topics are currently being undertaken by the author.

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