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HEURISTIC DIAGNOSTICS FOR THE PRESENCE OF PURE ERROR IN COMPUTER SIMULATION MODELS

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ABSTRACT

To facilitate the design and analysis of efficient simulation experiments, many authors have advocated the use of common random numbers and antithetic variates across the various runs that comprise the experiment. The objective of such *designed* experiments is often to estimate a general linear regression model on the basis of a quantitative response variable generated by the simulation model. This regression model is called the *metamodel* of the experiment. Along with methods of metamodel estimation under these various designed experiments, statistical methods have been developed to perform appropriate tests of hypothesis as well as confidence interval construction. The validity of these methods is contingent upon the presence of a pure error component (experimental error) in the response. The purpose of this paper is to examine the effect that the absence of a pure error component in the response has on these statistical analysis procedures and to provide recommendations for ensuring the presence of pure error in the response.

In particular, we investigate the effect that the absence of pure error in the response has on the Schruben-Margolin correlation-induction strategy and its recommended statistical analysis methods. We make recommendations for ensuring the presence of pure error in the response. We also provide an example that clearly illustrates these points.

1. INTRODUCTION AND BACKGROUND

To facilitate the design of efficient simulation experiments, Schruben and Margolin [1978] devised a correlation-induction strategy that effectively incorporates the variance reduction techniques of common random numbers and antithetic variates in the same designed simulation experiment. For a large class of experimental designs, their strategy was shown to give optimal results in terms of metamodel estimation. Nozari, Arnold, and Pegden [1987] developed a procedure for conducting statistical analysis under the Schruben-Margolin strategy. However, the validity of this statistical analysis procedure is contingent upon the presence of a pure error component in the observed responses. The purpose of this paper is to investigate the effect that the absence of pure error has on the Nozari, Arnold, and Pegden statistical analysis and to identify conditions under which the presence of the pure error component in the response is preserved. Next we give a brief overview of the Schruben-Margolin correlation-induction strategy and the statistical analysis given by Nozari, Arnold, and Pegden [1987]. In Section 2 we identify the effects that the absence of pure error in the response has on this statistical analysis. In Section 3 we given an example that illustrates how lack-of-fit variation in the response can be misinterpreted as pure error. Section 4 contains conclusions and suggests directions for future research.

1.1 Schruben-Margolin Strategy

In this section we give a brief review and summary of the Schruben-Margolin correlation induction strategy. For a more complete discussion of this strategy see [Schruben and Margolin, 1978; Schruben 1979; Tew and Wilson 1990].

The Schruben-Margolin correlation induction strategy is designed for the special case where $\mathbf{X}$ (the $m \times p$ design matrix) is orthogonally blockable into two blocks. The number of design points in each block represents the *block size*. Suppose that the design matrix $\mathbf{X} = (\mathbf{1}_m \mathbf{T})$ satisfies $\mathbf{T}'\mathbf{1}_m = \mathbf{0}_{p-1}$, a $(p - 1)$-dimensional column vector of zeros. This design is orthogonally blockable into two blocks if there exists an $(m \times 2)$ matrix $\mathbf{W}$ of zeros and ones such that $\mathbf{T}'\mathbf{W} = \mathbf{0}$ and $\mathbf{1}'_m\mathbf{W} = [m_1, m_2]$, where m_1 and m_2 are the respective block sizes. Schruben and Margolin [1978] proposed the following assignment rule which minimizes the determinant of the covariance matrix for the ordinary least squares and the weighted least squares estimators:

> If the m-point experimental design admits orthogonal blocking into two blocks of sizes m_1 and m_2, preferably chosen to be as nearly equal in size as possible, then for all m_1 design points in the first block, use a set of random numbers $\mathbf{R} = (\mathbf{r}_1\, \mathbf{r}_2, ..., \mathbf{r}_g)$ chosen randomly, and for all $\mathbf{r}_g$ design points in the second block, use $\overline{\mathbf{R}} = (1 - \mathbf{r}_1, 1 - \mathbf{r}_2, ..., 1 - \mathbf{r}_g)$.

Here, $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_g)$ represents the set of g random number streams used to drive the simulation model. Further, they suggest that the set of random number streams that drive the simulation model produces random controllable block effects that need to be incorporated in the model. Blocking theory is utilized to assign random number streams to the design points.

Schruben and Margolin [1978] decomposed the error term at the ith design point, ε_i, into a random block effect b_i and a residual ε_i^o, both of which are functions of $\mathbf{R}_i$. Thus, the first-order model of the relationship between the response and the design variables, x_k, of interest can be written as:

$$y_i(\mathbf{R}_i) = \beta_0 + \sum_{k=1}^{p-1} \beta_k x_k + b_i(\mathbf{R}_i) + \varepsilon_i^o(\mathbf{R}_i) \text{ for } i = 1, 2, ..., m, \quad (1)$$

or in terms of the matrix notation:

$$\mathbf{y}(\mathbf{R}) = \mathbf{X}\beta + \mathbf{W}\mathbf{B}(\mathbf{R}) + \varepsilon^o(\mathbf{R}) \quad (2)$$

where $\mathbf{y} = (y_1, y_2, ..., y_m)'$, $\mathbf{R} = (\mathbf{R}'_1, \mathbf{R}'_2, ..., \mathbf{R}'_m)'$,

$$\mathbf{B} = \begin{bmatrix} b(\mathbf{R}) \\ b(\overline{\mathbf{R}}) \end{bmatrix} \tag{3}$$

is the (2×1) vector of random block effects for the two sets of streams, $\mathbf{R}$ and $\overline{\mathbf{R}}$, used in the experiment, and $\overset{o}{\varepsilon}$ is the $(m \times 1)$ vector of residual errors.

Schruben and Margolin [1978] made the following assumptions about the assigned inputs:

1. The response variance is constant across all points in the design.
2. If y_i and y_j (for $i \neq j$) are realized from the same random number stream, then

$$\mathrm{Corr}[y_i(\mathbf{R}_i), y_j(\mathbf{R}_i)] = \rho_+, \quad 0 \le \rho_+ \le 1. \tag{4}$$

3. If y_i and y_j (for $i \neq j$) are realized from antithetic (complementary) random number streams, $\mathbf{R}_i$ and $\overline{\mathbf{R}}_i$ respectively, then

$$\mathrm{Corr}[y_i(\mathbf{R}_i), y_j(\overline{\mathbf{R}}_i)] = -\rho_-, \quad -1 \le -\rho_- \le 0. \tag{5}$$

Let $\mathbf{X}_i$ represent the design matrix for the ith block ($i = 1, 2$). If the design points are arranged such that

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{1}_{m_1} T_1 \\ \mathbf{1}_{m_2} T_2 \end{bmatrix}, \tag{6}$$

then these assumptions lead to the following structure for the covariance matrix of $\mathbf{y}$:

$$\Sigma_1 = \sigma^2 \begin{bmatrix} 1 & \rho_+ & \cdot & \rho_+ & -\rho_- & \cdot & \cdot & -\rho_- \\ \rho_+ & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \rho_+ & \cdot & \cdot & 1 & -\rho_- & \cdot & \cdot & -\rho_- \\ -\rho_- & \cdot & \cdot & -\rho_- & 1 & \rho_+ & \cdot & \rho_+ \\ \cdot & \cdot & \cdot & \cdot & \rho_+ & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -\rho_- & \cdot & \cdot & -\rho_- & \rho_+ & \cdot & \cdot & 1 \end{bmatrix} = \sigma^2 \begin{bmatrix} \Sigma_{11} \Sigma_{12} \\ \Sigma_{21} \Sigma_{22} \end{bmatrix} \tag{7}$$

where Σ_{11} is $(m_1 \times m_1)$, Σ_{12} is $(m_1 \times m_2)$, Σ_{21} is $(m_2 \times m_1)$, and Σ_{22} is $(m_2 \times m_2)$. Thus, under the assumption that

$$\overset{o}{\varepsilon} = (\overset{o}{\varepsilon}_1, \overset{o}{\varepsilon}_2, \ldots, \overset{o}{\varepsilon}_m)' \sim N_m(\mathbf{O}_m, \sigma^2(1 - \rho_+)\mathbf{I}_m) \tag{8}$$

we have that

$$\mathbf{y} \sim N_m(\mathbf{X}\beta, \Sigma_1). \tag{9}$$

Based on experimental designs that admit orthogonal blocking, Schruben and Margolin prove the following theorem:

Theorem 1: If an experimental design admits orthogonal blocking, and if the assumptions given above hold, then under the assignment rule the ordinary least squares estimator of β has a smaller generalized variance than it has under the following strategies: (1) the assignment of one common set of random numbers to all design points, or (2) the assignment of a different set of random numbers to each design point, provided

$$[1 + (m - 1)\rho_+ - (\tfrac{2}{m})(m_1)(m_2)(\rho_+ + \rho_-)]\,(1 - \rho_+)^p < 1 \tag{10}$$

in the latter case.

Corollary 1: Under the assumptions of Theorem 1, the assignment rule is superior to the use of common random numbers in estimation β_o; the two are equivalent in terms of dispersion for estimating $(\beta_1, \beta_2, \ldots, \beta_{p-1})$. When compared to the use of a different random number stream at each point, both the assignment rule and common random numbers are superior in terms of dispersion for estimating $(\beta_1, \beta_2, \ldots, \beta_{p-1})$.

Corollary 2: For the assignment rule, the variance is minimized when the two block sizes are equal; i.e., when $m_1 = m_2 = \frac{m}{2} = q$.

Thus, Schruben and Margolin [1978] showed that their alternative strategy based upon blocking concepts is a successful means of combining the two correlation methods of common random numbers and antithetic variates for a large class of experimental designs.

1.2 The Nozari, Arnold, and Pegden Statistical Analysis Procedure

In this section we give a brief review and summary of the statistical analysis procedure of Nozari, Arnold, and Pegden [1987]. Nozari, Arnold, and Pegden devised a procedure for conducting statistical analysis under the Schruben-Margolin strategy. They assumed that r independent replications are taken at each experimental point such that:

$$\mathbf{Y} \sim N_{mr}(\mathbf{G}\beta, \Theta_1), \tag{11}$$

where $\mathbf{Y} = (\mathbf{y}'_1, \mathbf{y}'_2, \ldots, \mathbf{y}'_r)'$ is the $(mr \times 1)$ vector of responses across all design points and replicates;

$$\mathbf{G} = \mathbf{X} \otimes \mathbf{1}_r, \tag{12}$$

is the overall $(mr \times p)$ design matrix; $\mathbf{X} = [\mathbf{1}_m \mathbf{T}]$ is the original m-point design matrix for one replication given by (6); β is the $(p \times 1)$ vector of model parameters; and $\Theta_1 = \Sigma_1 \otimes \mathbf{I}_r$ is the $(mr \times mr)$ covariance matrix with Σ_1 given by (7); and $\otimes$ defined to be the *right Kronecker product* such that, for any matrices $\mathbf{A}$ and $\mathbf{B}$ with dimensions $(h \times i)$ and $(j \times k)$, respectively:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} Ab_{11} & Ab_{12} & \ldots & Ab_{1k} \\ Ab_{21} & Ab_{22} & \ldots & Ab_{2k} \\ \cdot & \cdot & \ldots & \cdot \\ \cdot & \cdot & \ldots & \cdot \\ Ab_{j1} & Ab_{j2} & \ldots & Ab_{jk} \end{bmatrix}_{(hj \times ik)} \tag{13}$$

They also assume that the responses on each replication are jointly normal. The assumptions underlying the follow-up analysis of Nozari, Arnold, and Pegden can be summarized as follows:

$$\{y_i\!: i = 1, 2, \ldots, r\} \text{ IID} \sim N_m(\mathbf{X}\beta, \Sigma_1). \tag{14}$$

Nozari, Arnold, and Pegden's method focused on finding ways to effectively:

1. estimate β,
2. test H_0: $K\beta = 0$ versus H_1: $K\beta \neq 0$ for some $(k \times p)$ known matrix K of rank $k \leq p$, and
3. construct simultaneous confidence intervals for $l'K\beta$ for all $l \in R^k$.

Their statistical analysis procedure is based on the following four results:

Result 1:

$$\hat{\beta} = (G'G)^{-1}G'Y \tag{15}$$

is the optimal (minimum variance, unbiased) estimator for the model of (11). This result yields the formula to estimate β.

Result 2:

$$\frac{(mr)^{1/2}(\hat{\beta}_0 - \beta_0)}{\hat{\tau}_1} \sim t_{(r-1)}, \tag{16}$$

where

$$\hat{\tau}_1^2 = \frac{m \sum_{i=1}^{r} (\overline{y}_{i..} - \overline{y}_{...})^2}{(r-1)}, \tag{17}$$

y_{ijk} is the response for the ith replication of the kth design point in the jth block, $\overline{y}_{i..}$ is the average on the ith replication, and $\overline{y}_{...}$ is the overall average response. Equation (16) can be used in the obvious way to construct a $100(1-\alpha)\%$ confidence interval for β_o and to give an optimal (minimum variance, unbiased) test for β_o.

Result 3: The optimal (minimum variance, unbiased) size α test for

$$H_0\text{: } H\beta_1 = 0 \text{ versus } H_1\text{: } H\beta_1 \neq 0 \tag{18}$$

where H is a known $(h \times (p-1))$ matrix of rank $h < p$, rejects, H_0 if

$$f^* = \frac{(f\hat{\sigma}^2)}{\hat{\tau}_3^2} > F_{1-\alpha}(h, mr - p - 2r + 1), \tag{19}$$

where

$$f = \frac{r(H\hat{\beta}_1)'[H(T'T)^{-1}H']^{-1}(H\hat{\beta}_1)}{(h\hat{\sigma}^2)} \tag{20}$$

$$\hat{\tau}_3^2 = \frac{(mr-p)\hat{\sigma}^2 - \frac{m}{2}\sum_{i=1}^{r}\sum_{j=1}^{2}(\overline{y}_{ij.} - \overline{y}_{...})^2}{(mr - p - 2r + 1)}, \tag{21}$$

and

$$\hat{\sigma}^2 = \frac{\|Y - G\hat{\beta}\|^2}{(mr - p)}. \tag{22}$$

For simplicity purposes, $\hat{\tau}_3^2$ can be conveniently expressed as:

$$\hat{\tau}_3^2 = \frac{[m(r-1)]\hat{\sigma}^2 - r(\hat{\tau}_1 + \hat{\tau}_2)}{r(m-2)}, \tag{23}$$

where $\hat{\tau}_1^2$ is given in Result 2, and

$$\hat{\sigma}^2 = [m(r-1)]^{-1}\sum_{i=1}^{r}\sum_{j=1}^{2}\sum_{k=1}^{q})y_{ijk} - \overline{y}_{jk})^2, \tag{24}$$

$$\hat{\tau}_2^2 = (2r)^{-1} q \sum_{i=1}^{r}[\overline{y}_{i1.} - \overline{y}_{i2.}) - (\overline{y}_{.1.} - \overline{y}_{.2.})]^2, \tag{25}$$

such that

$$\overline{y}_{ij.} = q^{-1}\sum_{i=1}^{r} y_{ijk}, \quad \overline{y}_{i..} = 1/2\sum_{j=1}^{2} y_{ij}, \quad \overline{y}_{...} = r^{-1}\sum_{i=1}^{r}\overline{y}_{i..}. \tag{26}$$

Together Results 2 and 3 comprise the formula for testing H_0: $K\beta = 0$ versus H_1: $K\beta \neq 0$ for some $(k \times p)$ known matrix K of rank $\leq p$.

Result 4: A size α procedure for testing

$$H_0\text{: } K\beta = 0 \text{ versus } H_1\text{: } K\beta \neq 0 \tag{27}$$

where K is a $(k \times p)$ known matrix of rank $k \leq p$, is to reject H_0 if

$$\frac{r(r-k)}{k(r-1)}\hat{\beta}'K'(K\hat{\Delta}K')^{-1}K\hat{\beta} > F_{1-\alpha}(k, r-k), \tag{28}$$

where $\hat{\Delta} = (X'X)^{-1}X'SX(X'X)^{-1}$ with

$$S = \frac{1}{(r-1)}\sum_{i=1}^{r}(y_i - \overline{y})(y_i - \overline{y})'. \tag{29}$$

This final result gives us a method for constructing the simultaneous confidence intervals for $l'K\beta$ for all $l \in R^k$.

The validity of this statistical analysis procedure depends upon the validity of the Schruben-Margolin correlation induction strategy. It requires that the correlation structure along with all other assumptions prescribed by Schruben and Margolin [1978] are true. If all of the assumptions given have been satisfied, then results for drawing inferences about β_o and β_1 can be derived by transforming the model to one with independent observations. Nozari, Arnold, and Pegden [1987] present an invertible transformation that does not involve any unknown parameters. Thus, any inferences drawn about the transformed variables can also be applied to the original variables. The authors employ this transformation to derive the 4 results given above. This same transformation will be discussed and utilized in Section 2 to investigate the effects on this statistical analysis procedure when no pure error component is present in the response.

2. THE PURE ERROR COMPONENT IN DESIGNED SIMULATION EXPERIMENTS

In this section we first give a discussion on how pure error components arise in designed simulation experiments. This discussion is based on the concepts first presented by Mihram [1972 and 1974]. Second, we identify the effect that the absence of a pure error component in the response has on the Nozari, Arnold, and Pegden statistical analysis.

2.1 Presence of Pure Error

Mihram [1972] asserts that a simulation model may be classified as either static or dynamic. The static effect of a model's performance is denoted by y_t, the value of the response variable at simulation time t. This response may be represented by:

$$y_t(\mathbf{R}) = \mu(x_1, x_2, ..., x_{p-1}) + \varepsilon_t(\mathbf{R}), \quad (30)$$

where $\mu(x_1, x_2, ..., x_{p-1})$ is the mean response at the design point defined by the levels of the design variables $x_1, x_2, ..., x_{p-1}$; and ε_t $(\mathbf{R})$ is the value of the random error at simulation time t.

Mihram [1974], offers an explanation of the variation in the response variable, y_t, from a computer simulation experiment when common random numbers are employed. He identifies two separate components that contribute to this variation: (1) block effects and (2) pure error. The block effects arise from using generated random number streams repetitively across design points. Mihram contends that this technique is compatible with the experimental statistician's concept of blocking. However, he cautions that the resulting block effect should be interpreted as a variance component or random block effect in that the streams used for blocking are randomly selected. The pure error arises from randomly selecting different generated random number streams across design points.

Since the randomness in a stochastic simulation model arises from the sequences of random numbers used in the simulation code, simulation analysts have long debated the merits of using the same random number streams in simulating different systems (Heikes, Montgomery, and Rardin [1976]). The idea of comparing alternative systems under the same statistical conditions is *similar* to the use of the variance-reduction technique known as common random numbers and the use of "blocking" in statistical design. Blocking is evoked to reduce the experimental error across the design points. Mihram was the first to propose considering the effects of pseudo-random number streams as random block effects. He states that "in order to obtain a true measure of experimental error, one should select at least one (and typically all save one) seed value randomly and nonrepetitively among the encounters defined in a similar experimental design."

Mihram [1974] provides a procedure for appropriately selecting the random number seeds across design points for a dynamic, stochastic simulation model. To employ his procedure, the dynamic, stochastic simulation model must be viewed as a generator of the set of sample paths from a stochastic process $\{y_t\}$, such that:

$$y_t = y_{\mathbf{x},t}(\mathbf{R}) \quad (31)$$

where y_t is the simulation response, $\mathbf{x} = (x_1, x_2, ..., x_{p-1})$ is the set of p-1 factors, and $\mathbf{R}$ is the set of random number streams. In the above equation, the variables t and x are fixed. The response, y_t, can be separated into two components as follows:

$$y_{\mathbf{x},t}(\mathbf{R}) = \mu(\mathbf{x}) + e_t(\mathbf{x}; \mathbf{R}) \quad (32)$$

where $\mu(\mathbf{x}) = E(y_{\mathbf{x},t}(\mathbf{R}))$ is the mean response and $\varepsilon_t(\mathbf{x}; \mathbf{R})$ represents the experimental error due to the random selection of $\mathbf{R}$.

By repeatedly employing the same seed values $\mathbf{R}_0$ for different values of $\mathbf{x}$, the simulation analyst can form a block of experimental units. When the same seed values, $\mathbf{R}_0$, are used repeatedly across design points, $\varepsilon_t(\mathbf{x}; \mathbf{R})_0$ is no longer a representation of pure error, but a representation of random block effect. This interpretation of a block effect is consistent with that given in the experimental design literature. That is, using the same random number streams at different design points is analogous to subjecting different experimental units to the same experimental conditions. For example, consider the case where g streams denoted by $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_g)$, are used for each simulation run. This allows the response to be represented as

$$y_{\mathbf{x},t}(\mathbf{R}) = \mu(\mathbf{x}) + b_t(\mathbf{R}^*) + \varepsilon_t(\mathbf{x}; \mathbf{R} - \mathbf{R}^*) \quad (33)$$

where $\mathbf{R}^*$ is the vector of fixed seed values, $\mathbf{R} - \mathbf{R}^*$ is the non-empty vector of seed values that are randomly selected across design points, and $b_t(\mathbf{R})$ is a random block effect. An appropriate measure of experimental error is obtained by randomly and non-repetitively specifying across design points the streams in $\mathbf{R} - \mathbf{R}^*$

Mihram [1974] concludes that the proper interpretation of the block effect obtained from the repetitious use of random number streams across design points is in the form of a *random* block effect. This constitutes a variance component of the dispersion inherent in the responses from dynamic, stochastic simulation models. In simulation, the analyst must not only be concerned with interpreting the resulting block effect, but also with retaining an appropriate measure of experimental error. Mihram [1974] asserts that in order to obtain a true measure of experimental error, one should select at least one seed value randomly and non-repetitively among the encounters defined in a simulation experiment. In the next section we discuss the effect that using all available streams for blocking has on the Nozari, Arnold, and Pegden statistical analysis.

2.2 Statistical Analysis in the Absence of Pure Error

In order to construct valid inferences about the performance of a stochastic simulation model, the technique used to execute the simulation experiment must be properly identified. For purposes of this research, the problem of proper identification takes the form of ensuring that the hypothesized model is appropriate for the number of random number streams used to induce correlations. This section identifies an appropriate model for simulation experiments designed under the Schruben-Margolin correlation induction strategy in the absence of pure error.

As discussed in Section 1.1, under the Schruben-Margolin correlation induction strategy, sets of random number streams are assigned to design points in order to induce correlations across the design points in the experiment. The number of random number streams that the simulation analyst employs at each design point determines whether a pure error component is present in the generated responses. In particular, if all random number streams are used to induce correlations across the design points, then no pure error component is present in the response.

Under the assumptions of the Schruben-Margolin correlation induction strategy given in Section 1.1, when all random number streams are used to induce correlations at each design point, the response z_i, which has mean μ and variance σ^2, will reduce the model of (1) to:

$$z_i(\mathbf{R}) = \beta_0 + \sum_{k=1}^{p-1} \beta_k x_k + b_i(\mathbf{R}) \quad \text{for } i = 1, 2, ..., m. \quad (34)$$

(Note: the response variable z, which has similar properties to the response variable y, will be used to distinguish responses generated by model (34) from those discussed earlier). Model (34) can be written in matrix notation as:

$$\mathbf{Z} = \mathbf{G}\beta + (\mathbf{WB}) \otimes \mathbf{1}_r, \tag{35}$$

where $\mathbf{G}$, β, $\mathbf{W}$, and $\mathbf{B}$ are defined in Section 1, and $\mathbf{Z} = (z_1', z_2', ..., z_r')'$ is the column vector of responses for all r independent replications across all m design points generated by (34). Now, it can be shown that under (35):

$$\mathbf{Z} \sim N_{mr}(\mathbf{G}\beta, \text{Cov}(\mathbf{Z})), \tag{36}$$

where:

$$\text{Cov}(\mathbf{z}) = \Sigma_2 \otimes \mathbf{I}_r = \Theta_2, \tag{37}$$

$$\Sigma_2 = \text{Cov}(\mathbf{z}_i) = \sigma^2 \begin{bmatrix} \rho_+ \mathbf{E}_{(m_1 \times m_1)} & -\rho_- \mathbf{E}_{(m_1 \times m_2)} \\ -\rho_- \mathbf{E}_{(m_2 \times m_1)} & \rho_+ \mathbf{E}_{(m_2 \times m_2)} \end{bmatrix}, \tag{38}$$

and $\mathbf{E}_{(i \times j)}$ is the $(i \times j)$ matrix of ones.

Applying the orthogonal transformation Γ (see Nozari, Arnold, and Pegden (1987)) to (35) yields:

$$\mathbf{Z}^* = (\Gamma \otimes \mathbf{I}_r)\mathbf{Z} = (\Gamma \otimes \mathbf{I}_r)\mathbf{G}\beta + (\Gamma \otimes \mathbf{I}_r)((\mathbf{WB}) \otimes \mathbf{1}_r), \tag{39}$$

which by (36), (37), and (38) yields:

$$\mathbf{Z}^* \sim N_{mr}(\mathbf{G}^* \beta, \Theta_2^*), \tag{40}$$

with

$$\Theta_2^* = (\Gamma \otimes \mathbf{I}_r)\, \Theta_2 (\Gamma \otimes \mathbf{I}_r)' = \begin{bmatrix} \lambda_1^2 & 0 & \mathbf{0}' \\ 0 & \lambda_2^2 & \mathbf{0}' \\ \mathbf{0} & \mathbf{0} & \lambda_3^2 \mathbf{I}_{2r(q-1)} \end{bmatrix}, \tag{41}$$

such that $\lambda_1^2 = \sigma^2 q(\rho_+ - \rho_-)$, $\lambda_2^2 = \sigma^2 q(\rho_+ + \rho_-)$, and $\lambda_3^2 = 0$. A proof of (41) is given in Appendix IV of Crenshaw [1989].

Theorems analogous to the ones given by Nozari, Arnold, and Pegden [1987] can be established from conditions (39), (40), and (41), such that:

Theorem 5. $\mathbf{Z}_1^*$, $\mathbf{Z}_2^*$, and $\mathbf{Z}_3^*$ are independent,
Theorem 6. $\mathbf{Z}_1^* \sim N_r((2q)^{1/2} \mathbf{1}_r \beta_0, \lambda_1^2 \mathbf{I}_r)$,
Theorem 7. $\mathbf{Z}_2^* \sim N_r(0, \lambda_2^2 \mathbf{I}_r)$,
Theorem 8. $\mathbf{Z}_3^* \sim N_{2r(q-1)}(\mathbf{T}^* \beta_1, \lambda_3^2 \mathbf{I}_{2r(q-1)})$.

The invertible transformation given by Nozari, Arnold, and Pegden [1987] does not involve any unknown parameters. Thus, all optimal procedures based on $\mathbf{Z}^*$ are also optimal for procedures based on $\mathbf{Z}$, the untransformed responses.

By Theorem 5, and as before, the model involving $\mathbf{Z}^*$ consist of 3 separate ordinary linear models, one involving $(\mathbf{Z}_1^*, \beta_0, \lambda_1^2)$, one involving $(\mathbf{Z}_2^*, \lambda_2^2)$, and one involving $(\mathbf{Z}_3^*, \beta_1, \lambda_3^2)$, for which optimal procedures are easy to find. Arnold [1981] refers to this situation as a "product of problems" and notes that a procedure for drawing inferences about $\beta_0 (\beta_1)$ based on $\mathbf{Z}_1^* (\mathbf{Z}_3^*)$ that is optimal among procedures based on $\mathbf{Z}_1^* (\mathbf{Z}_3^*)$ is optimal among procedures based on $\mathbf{Z}^*$. (See p. 135 of Nozari, Arnold, and Pegden [1987]). Thus, the situation created by Theorems 5, 6, 7, and 8 is similar to the situation created by Theorems 1, 2, 3, and 4 of Nozari, Arnold, and Pegden [1987] with the exception of the differences in the respective variance components. The remainder of this section is devoted to identifying and interpreting the changes in Results 1, 2, 3, and 4 of Nozari, Arnold, and Pegden [1987] brought on by these variance component differences. (Results 1, 2, 3, and 4 are summarized in Section 1.2).

Result 1 remains unchanged under (35) in that the ordinary least squares estimator of β,

$$\hat{\hat{\beta}} = \begin{bmatrix} \hat{\hat{\beta}}_0 \\ \hat{\hat{\beta}}_1 \end{bmatrix} = (\mathbf{G}^{*\prime}\mathbf{G}^*)^{-1} \mathbf{G}^{*\prime}\mathbf{Z}^* = (\mathbf{G}'\mathbf{G})^{-1} \mathbf{G}'\mathbf{Z}, \tag{42}$$

is the optimal (minimum variance, unbiased) estimator. However, Theorems 6 and 8 indicate that, respectively,

$$\hat{\hat{\beta}}_0 = (2q)^{-1/3} r^{-1} \mathbf{1}_r' \mathbf{Z}_1^* \sim N_1(\beta_0, \lambda_1^2 (2qr)^{-1}), \tag{43}$$

and

$$\hat{\hat{\beta}}_1 = (\mathbf{T}^{*\prime}\mathbf{T}^*)^{-1} \mathbf{T}^{*\prime}\mathbf{Z}_3^* \sim N_{p-1}(\beta_1, \lambda_3^2 (\mathbf{T}^{*\prime}\mathbf{T}^*)^{-1}). \tag{44}$$

Thus, the variances of $\hat{\hat{\beta}}_0$ and the components of $\hat{\hat{\beta}}_1$ have been reduced by $\sigma^2(1 - \rho_+)$. Since $\lambda_3^2 = 0$, the multivariate distribution of $\hat{\hat{\beta}}_1$ given in (44) is degenerate. To clarify, $\lambda_3^2 = 0$ in (44) indicates that if $\mathbf{G}\beta$ is the mean of $\mathbf{Z}$, then β_1 is known perfectly. (In practice of course, the hypothesized linear model $\mathbf{G}\beta$ for simulation experiments is at best a close approximation to the mean of $\mathbf{Z}$ so that $\text{var}(\hat{\hat{\beta}}_1) > 0$).

Result 2 remains unchanged under (35) with the exception that the half-width of the $100(1-\alpha)\%$ confidence interval for β_0 is reduced by the amount of:

$$[(\sigma^2 q(\rho_+ - \rho_-) + \sigma^2 (1 - \rho_+))^{1/2} - (\sigma^2 q(\rho_+ - \rho_-))^{1/2}] t \frac{(r-1)}{(mr)^{1/2}}. \tag{45}$$

Although Results 1 and 2 have changed very little under model (34), Results 3 and 4 have changed fundamentally. Moreover, under the assumption of (36), the statistical test given by Result 3 can be eliminated. This is because the $\text{Cov}(\hat{\hat{\beta}}_1) = 0$. Since β_1 is known with certainty, no statistical testing procedure is required to determine whether $\mathbf{H}\beta_1 = 0$ or $\mathbf{H}\beta_1 \neq 0$. Thus, the testing procedure given by equation (18) and the $100(1-\alpha)\%$ simultaneous confidence interval given by equation (6) of Nozari, Arnold, and Pegden [1987] are inappropriate under model (34).

Moreover, the statistical testing procedure given by Result 4 for testing H_0: $\mathbf{K}\beta = 0$ versus H_1: $\mathbf{K}\beta \neq 0$ reduces to a simpler test of H_0: $\beta_0 = 0$ versus H_1: $\beta_0 \neq 0$. As before, this is due to the absence of variability for the components of β_1 under (34). Specifically, following the development of Result 4 given on page 136 of Nozari, Arnold, and Pegden [1987], it can be shown that under model (34):

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \overline{\mathbf{z}} \sim N_p(\beta, \tfrac{1}{r} \Delta), \tag{46}$$

where

$$\Delta = \sigma^2 \begin{bmatrix} \frac{(\rho_+ - \rho_-)}{2} & 0' \\ 0 & 0 \end{bmatrix}, \quad (47)$$

and $\overline{z} = \frac{1}{r}\sum_{i=1}^{r} z_i$. Taking $S = \frac{1}{r}\sum_{i=1}^{r}(z_i - \overline{z})(z_i - \overline{z})'$ and letting $\hat{\Delta} = (X'X)^{-1}X'SX(X'X)^{-1}$ yields by (36) and Theorem 17.6 of Arnold [1981]:

$$\hat{\Delta} \sim W_p(r-1, \frac{1}{r-1}\Delta). \quad (48)$$

A proof of (47) is given in Appendix V of Crenshaw [1989]. By (47) and Theorem 17.6 of Arnold [1981], the Wishart distribution in (48) reduces to:

$$\hat{\Delta}_{11} \sim \frac{\sigma^2(\rho_+ - \rho_-)}{2(r-1)}\chi^2_{r-1}, \quad (49)$$

which implies that

$$\frac{(mr)^{1/2}(\hat{\beta}_0 - \beta_0)}{\hat{\lambda}_1} \sim t(r-1), \quad (50)$$

where $\hat{\Delta}_{11}$ is the element of Δ in the first-row and first-column position. A proof of (50) is given in Appendix VI of Crenshaw [1989].

The distribution of the responses generated by model (39) has significantly changed the applicability of the Nozari, Arnold, and Pegden statistical analysis procedure. In particular, the $\sigma^2(1 - \rho_+)$ variance reduction has eliminated the need for Results 3 and 4 all together. For example, equation (50) can be used to conduct hypothesis tests and construct confidence intervals on β_0. Thus, as expected, Result 4 reduces to the procedure of Result 1 and, as with Result 3, hypothesis tests and confidence intervals on β_1 are unavailable. Consequently, under model (35), the objectives of the Nozari, Arnold, and Pegden statistical analysis procedure are attainable for β_0, but unattainable for β_1.

3. EXAMPLE

In the previous section the argument was made for randomly selecting at least one random number stream across all design points in the experiment to ensure a pure error component in the response. This procedure is recommended in all cases. Nevertheless, many simulation analysts, in the spirit of trying to maximize the magnitude of the induced correlations, use *all* available random number streams to induce correlations across design points. In order to explain what can happen in this situation we present, in this section, some simplified examples.

3.1 An Illustrative Example on the Effectiveness of the Combined Use of Common Random Numbers and Antithetic Variates

In this section, a simulation experiment is conducted to illustrate how the implementation of the Schruben-Margolin correlation induction strategy can affect the presence of random error in the response. Consider a simulation experiment consisting of two factors, each with two levels of interest. For the ith replicate of the jth design point, the known function of the factor settings, x_1 and x_2, yield the univariate response y_{ij}, which has mean μ and variance σ^2. The vector, $y_i = (y_{i1}, y_{i2}, ..., y_{im})'$, denotes the m responses of the ith replicate. For a given design point, the linear relation of the univariate response to the level of two factors is given by:

$$y_{ijn} = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2j} + \varepsilon_{(ij)n}, \quad (51)$$

where

y_{ijn} = the response for the nth run of the simulation using the ith and jth level of the factor settings;

β_0 = the overall mean response;

x_{1i} = the fixed effect of the ith level of the factor setting;

x_{2j} = the fixed effect of the jth level of the factor setting;

$\varepsilon_{(ij)n}$ = the residual error for the nth computation of the simulation at factor levels x_{1i}, and x_{2j} where $\{\varepsilon_{(ij)n}$: for all i, j, k, n$\}$ IID $\sim N(0, \sigma^2)$.

In order to demonstrate the impact of using all streams to induce correlations for this example, the error term in model (51) was decomposed into two components: $\varepsilon_{1(ij)n}$ and $\varepsilon_{2(ij)n}$. That is, $\varepsilon_{(ij)n} = \varepsilon_{1(ij)n} + \varepsilon_{2(ij)n}$, where $\varepsilon_{1(ij)n}$ IID $\sim N(0, \sigma_1^2)$ and $\varepsilon_{2(ij)n}$ IID $\sim N(0, \sigma_2^2)$, such that $\sigma^2 = (\sigma_1^2 + \sigma_2^2)$. (Note that, unlike most simulation models, the model in (51) is completely known and is not an hypothesized approximation to the true relationship between the response of interest and the settings of the factors.)

For this example, the simulation experiments were performed using the tabulation method of the Normal distribution function with 10 independent replications made at each of the four design points. The purpose of this example is to study the effect that the different factor levels have on the mean response. To study this system, a 2^2 factorial design was employed for factor levels x_1 and x_2 given in Table 1. This 2^2 factorial design is orthogonally blockable into two blocks of four design points each. The x_1x_2 interaction was used to divide the experiment into two incomplete blocks of two design points each. Table 2 shows how the treatments were assigned to the blocks so as to confound x_1x_2 with the block effect induced by the assignment of common random number streams and antithetic random number streams as prescribed by the Schruben-Margolin strategy.

Table 1. Factor Levels for Example 1

Factors	Selected Levels
x_1	-1 ≡ 1.0
	+ 1 ≡ 2.0
x_2	-1 ≡ 2.0
	+ 1 ≡ 3.0

Including the block effect, the complete mathematical model for this experiment is given by:

$$y_{lij} = \beta_0 + B_l + \beta_1 x_{1i} + \beta_2 x_{2j} + \varepsilon_{1(ijn)} + \varepsilon_{2(ij)n} \quad (52)$$

where B_l = the random effect of the lth block, confounded with the

x_1x_2 interaction such that $\{B_l: l = 1, 2,\}$ IID ~ $N(\mu_{ij}, \sigma_B^2)$ $\mu_{ij} = 0$, if the x_1x_2 interaction does not exist. The block effect B_l is random due to the random selection of the set of random number streams, $\mathbf{R}_1$ and $\mathbf{R}_2$, that are used by all design points in Block 1 to drive the two error components, $\varepsilon_{1(ij)n}$ and $\varepsilon_{2(ij)n}$, respectively. For all design points in Block 2, the antithetic streams, $\overline{\mathbf{R}}_1$ and $\overline{\mathbf{R}}_2$ are used to drive $\varepsilon_{1(ij)n}$ and $\varepsilon_{2(ij)n}$, respectively. (See the assignment rule given in Section 1.)

To provide the desired sign pattern for the induced correlations as prescribed by the Schruben-Margolin correlation induction strategy, this example was structured so as to maintain the following properties across all four design points:

1. The response y has the same *monotonic* dependence on the ith random number sampled within a run when all other random numbers are fixed (i = 1, 2, ...).
2. Random numbers are assigned to the error term in a *synchronized* manner so that the stochastic characteristics generated are the same for every alternative within the same block (j = 1, 2).

For a detailed discussion of the Schruben-Margolin correlation induction strategy, see Section 1.1.

For this example, the first set of runs utilized all streams to induce correlations across design points. The resulting set of simulation responses are displayed in Table 3. The corresponding sample correlation matrix is given by:

$$\hat{\text{Corr}}(y) = \begin{bmatrix} 1.0000 & 1.0000 & -.9998 & -.9998 \\ 1.0000 & 1.0000 & -.9998 & -.9998 \\ -.9998 & -.9998 & 1.0000 & 1.0000 \\ -.9998 & -.9998 & 1.0000 & 1.0000 \end{bmatrix}, \tag{53}$$

and the resulting sample covariance matrix of $(\hat{\beta} = \hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2)'$ is given by:

$$\hat{\text{Cov}}(\hat{\beta}) = \begin{bmatrix} 0.0006 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 \end{bmatrix}. \tag{54}$$

By applying formulas (17), (23), (24), and (25) to the generated simulation responses, the following results were obtained: $\hat{\sigma}^2$ = 3.6080, $\hat{\tau}_1^2$ = 0.0026, $\hat{\tau}_2^2$ = 12.9842, and $\hat{\tau}_3^2$ = 0.0009. Observe that $\hat{\tau}_1^2$, and $\hat{\tau}_3^2$ are not practically, significantly different from 0. Thus, as expected, when all streams are utilized under the Schruben-Margolin strategy in conjunction with a linear model, no pure error is observed in the responses.

To demonstrate when a measure of pure error is present in the simulation model, a second set of simulation runs were performed under conditions similar to experiment 1, except that stream two, which drives $\varepsilon_{2(ij)n}$ of the error term, was randomly selected across all design points. The resulting set of generated responses are displayed in Table 4. The corresponding sample correlation matrix is given by:

$$\hat{\text{Corr}}(y) = \begin{bmatrix} 1.0000 & .7451 & -.5998 & .0982 \\ .7451 & 1.0000 & -.5930 & .2504 \\ -.5998 & -.5930 & 1.0000 & -.4402 \\ .0982 & .2504 & -.4402 & 1.0000 \end{bmatrix}, \tag{55}$$

and the resulting sample covariance matrix of $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2)'$ is given by:

$$\hat{\text{Cov}}(\hat{\beta}) = \begin{bmatrix} .8577 & .3593 & -.2682 \\ .3592 & .5797 & -.2193 \\ -.2682 & -.2192 & .4467 \end{bmatrix}. \tag{56}$$

The following results, again, were obtained from formulas (17), (23), (24), and (25): $\hat{\sigma}^2$ = 3.3210, $\hat{\tau}_1^2$ = 3.0718, $\hat{\tau}_2^2$ = 5.3699, and $\hat{\tau}_3^2$ = 1.7552. Of note is that with pure error in the simulation model, $\hat{\tau}_1^2$, and $\hat{\tau}_3^2$ are practically, significantly different from 0.

To complete this first example, another set of simulation runs were made. These runs were conducted to demonstrate the effect that an incorrectly hypothesized model can have on the statistical results, or more directly, how the results obtained from an incorrectly specified model can mask the absence of random error in the response. This second set of runs were performed exactly as the first set, except that a non-linear model was used to generate the simulation responses. The non-linear model used for this experiment is given by:

$$y_{ijn} = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2j} + (x_{1i}^2 x_{2j}^2)\varepsilon_{(ij)n} \tag{57}$$

where

y_{ijn} = the response for the nth run of the simulation using the ith and jth level of the factor settings;
β_0 = the overall mean response;
x_{1i} = the fixed effect of the ith level of the factor setting;
x_{2j} = the fixed effect of the jth level of the factor setting;
$\varepsilon_{(ij)n}$ = the residual error for the nth computation of the simulation at factor levels x_{1j}, and x_{2j} where $\{\varepsilon_{(ij)n}$: for all i, j, k, n$\}$ IID ~ $N(0, \sigma^2)$.

Equation (57) represents the correct relationship between the response and the levels of the input factors. However, for this experiment, the linear model in (51) was used as the hypothesized metamodel. Thus, there will be a lack-of-fit component present in the results.

Table 5 gives the resulting responses generated, where all streams were utilized under model (57). Again, random number streams, $\mathbf{R}_1$ and $\mathbf{R}_2$, are used to drive the two error components of, $\varepsilon_{1(ij)n}$ and $\varepsilon_{2(ij)n}$, respectively. for all design points in Block 1, and the antithetic streams, $\overline{\mathbf{R}}_1$ and $\overline{\mathbf{R}}_2$, are used to drive the error components in Block 2. The corresponding sample covariance matrix of $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2)'$ is given by:

$$\hat{\text{Cov}}(\hat{\beta}) = \begin{bmatrix} 47.8000 & 81.3000 & 127.2000 \\ 81.3000 & 137.7000 & 216.2000 \\ 127.5000 & 216.5000 & 340.0000 \end{bmatrix}. \tag{58}$$

As expected, the sample correlation matrix for this example was exactly the same as in experiment 1, and is given by equation (53). Using the responses generated from model (57), the following results were obtained from formulas (17), (23), (24), and (25), respectively: $\hat{\sigma}^2$ = 1475.010, $\hat{\tau}_1^2$ = 172.010, $\hat{\tau}_3^2$ = 3418.072, and $\hat{\tau}_3^2$ = 859.976. Notice the huge variations in the responses generated

Table 2. Assignment of Treatment Combinations to Blocks for Example 1			
Block J (Random Number Assignment)	Response Index k	Treatment Combination x_1	x_2
1 (Common Streams **R**)	1	-1	-1
	2	+1	+1
2 (Antithetic Streams $\overline{\mathbf{R}}$)	3	-1	+1
	4	+1	-1

Table 3. Simulation Responses Generated for Experiment 1 Using All Streams							
Response index k	1	2	1	2	Averages within:		
Replication Number i	Block j 1		Block j 2		Blocks $\bar{y}_{i1.}$	$\bar{y}_{i2.}$	Replications $\bar{y}_{i..}$
1	5.28	9.28	12.86	12.86	7.28	12.86	10.07
2	6.16	10.16	11.81	11.81	8.16	11.81	9.98
3	8.33	12.33	9.66	9.66	10.33	9.66	9.99
4	8.50	12.50	9.49	9.49	10.50	9.49	9.99
5	9.10	13.10	8.89	8.89	11.10	8.89	9.99
6	8.51	12.51	9.48	9.48	10.51	9.48	9.99
7	8.15	12.15	9.84	9.84	10.15	9.84	9.99
8	9.66	13.66	8.33	8.33	11.66	8.33	9.99
9	11.24	15.24	6.75	6.75	13.24	6.75	9.99
10	11.13	15.13	6.86	6.86	13.13	6.86	9.99
Averages across Replications	$\bar{y}_{.1k}$		$\bar{y}_{.2k}$		$\bar{y}_{.1.}$	$\bar{y}_{.2.}$	$\bar{y}_{...}$
	8.60	12.60	9.39	9.39	10.60	9.39	9.99

Table 4. Simulation Responses Generated for Experiment 2 Using One Stream							
Response index k	1	2	1	2	Averages within:		
Replication Number i	Block j 1		Block j 2		Blocks $\bar{y}_{i1.}$	$\bar{y}_{i2.}$	Replications $\bar{y}_{i..}$
1	7.02	9.24	9.98	8.60	8.13	9.29	8.71
2	5.64	10.73	10.41	10.72	8.18	10.56	9.37
3	10.30	12.38	9.99	11.15	11.34	10.57	10.95
4	7.74	11.50	12.07	6.52	9.62	9.29	9.45
5	7.68	10.94	8.89	10.55	9.31	9.72	9.51
6	3.79	8.86	12.80	9.53	6.32	11.16	8.74
7	8.32	13.66	10.27	9.63	10.99	9.95	10.47
8	5.64	11.46	9.66	9.13	8.55	9.39	8.97
9	8.14	14.88	9.16	11.77	11.51	10.46	10.98
10	10.73	15.28	8.49	9.01	13.00	8.75	10.87
Averages across Replications	$\bar{y}_{.1k}$		$\bar{y}_{.2k}$		$\bar{y}_{.1.}$	$\bar{y}_{.2.}$	$\bar{y}_{...}$
	7.50	11.89	10.17	9.66	9.69	9.91	9.80

Table 5. Simulation Responses Generated for Experiment 3 Using All Streams

Response index k	1	2	1	2	Averages within:		
Replication Number i	Block j				Blocks		Replications
	1		2		$\bar{y}_{i1.}$	$\bar{y}_{i2.}$	$\bar{y}_{i..}$
1	-2.88	-85.92	35.74	55.76	-44.40	45.75	0.67
2	0.64	-54.24	26.29	38.96	-26.80	32.62	2.91
3	9.32	23.88	6.96	4.56	16.60	5.75	11.17
4	10.00	30.00	5.41	1.84	20.00	3.62	11.81
5	12.40	51.60	0.01	-7.76	32.00	-3.87	14.06
6	10.04	30.36	5.32	1.68	20.20	3.58	11.85
7	8.60	17.40	8.56	7.44	13.00	8.00	10.50
8	14.64	71.76	-5.03	-16.72	43.20	-10.87	16.16
9	20.96	128.64	-19.25	-42.00	74.80	-30.62	22.09
10	20.52	124.68	-18.26	-40.24	72.60	-29.25	21.67
Averages across Replications	$\bar{y}_{.1k}$		$\bar{y}_{.2k}$		$\bar{y}_{.1.}$	$\bar{y}_{.2.}$	$\bar{y}_{...}$
	10.42	33.81	4.57	0.35	22.12	2.46	12.28

Table 6. Simulation Responses Generated for Experiment 4 Using One Stream

Response index k	1	2	1	2	Averages within:		
Replication Number i	Block j				Blocks		Replications
	1		2		$\bar{y}_{i1.}$	$\bar{y}_{i2.}$	$\bar{y}_{i..}$
1	4.08	-87.36	9.82	-12.40	-41.64	-1.29	-21.46
2	-1.44	-33.72	13.69	21.52	-17.58	17.60	0.01
3	17.20	25.68	9.91	28.40	21.44	19.15	20.29
4	6.96	-6.00	28.63	-45.68	0.48	-8.52	-4.02
5	6.72	-26.16	0.01	18.80	-9.72	9.40	-0.16
6	-8.84	-101.04	35.20	2.48	-54.94	18.84	-18.05
7	9.28	71.76	12.43	4.08	40.52	8.25	24.38
8	-1.44	-7.44	6.94	-3.92	-4.44	1.51	-1.46
9	8.56	115.68	2.44	38.32	62.12	20.38	41.25
10	18.92	130.08	-3.59	-5.84	74.50	-4.71	34.89
Averages across Replications	$\bar{y}_{.1k}$		$\bar{y}_{.2k}$		$\bar{y}_{.1.}$	$\bar{y}_{.2.}$	$\bar{y}_{...}$
	6.00	8.14	11.54	4.57	7.07	8.06	7.56

from model (57) as compared to the responses obtained in the first set of runs. The responses generated from the non-linear model in (57) give the true relationship between the response of interest and the input factors. However, the statistical analysis for this experiment was conducted under the assumption that the true relationship between the response of interest and the input factors is given by the linear model in (51). Thus, since the only change from (51) to (57) is the inclusion of the non-linear term, $(x_{1i}^2, x_{2j}^2)\epsilon_{(ij)n}$, this variation must be due to the lack-of-fit in the model, and not the procedure used to perform the simulation experiment.

Model (57) was also used to generate the responses for a fourth set of runs, where the second stream, $\mathbf{R}_2$, was randomly selected across design points. Model (57) again represents the true relationship between the response of interest and the levels of the input factors, and as before, the hypothesized metamodel will be given by model (51). The responses are given in Table 6, and the corresponding sample covariance matrix of $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2)'$ is given by:

$$\hat{\text{Cov}}(\hat{\beta}) = \begin{bmatrix} 462.0000 & 462.5000 & 279.0000 \\ 472.2000 & 506.7000 & 264.7000 \\ 278.7000 & 264.7000 & 268.2000 \end{bmatrix}. \quad (59)$$

The correlation matrix for this experiment was identical to the one for experiment 2, and is given in equation (55). The following $\hat{\sigma}^2$ results were obtained from formulas (17), (23), (24), and (25): = 1732.5160, $\hat{\tau}_1^2$ = 1662.8000, $\hat{\tau}_2^2$ = 1784.4520, and $\hat{\tau}_3^2$ = 1394.9030. These results indicate a moderate increase in σ^2, but, as expected, a significant increase results in $\hat{\tau}_1^2$ and $\hat{\tau}_3^2$. These relatively simple simulation experiments have eloquently illustrated the appropriateness for a measure of pure error in a simulation experiment. They also show how a lack-of-fit of the hypothesized model tends to distort the results of the statistical analysis.

4. CONCLUSIONS

Clearly, the results of Section 2 together with the examples discussed in Section 3 suggest that, in order to legitimize a proper statistical analysis of the output responses from a simulation experiment conducted under the Schruben-Margolin correlation-induction strategy, at least one random number stream must be randomly selected across all design points in the experiment. In practice, this rule should be followed for *any* simulation experiment where correlations are induced across design points by the methods of common random numbers or antithetic variates. The obvious question left unanswered is: For a given simulation model, which random number stream(s) should be randomly selected across the design points? This issue will be taken up in future work.

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