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THE USE OF VARIANCE REDUCTION TECHNIQUES IN THE ESTIMATION OF SIMULATION METAMODELS

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ABSTRACT

Variance reduction techniques can be useful strategies for improving the estimates of simulation metamodel coefficients. Depending upon the goals of the experimenter, the type of metamodel being estimated, and the characteristics of the system being simulated, an appropriate variance reduction technique can be applied. This paper provides a review of recent research that investigates the application of variance reduction techniques in the simulation metamodeling context. One strategy, Schruben and Margolin's (1978) assignment rule, which utilizes a combination of antithetic and common random number streams, is found to be a particularly useful variance reduction technique for the estimation of simulation metamodels.

1 INTRODUCTION

In this paper, we use the term "simulation metamodel" to describe a mathematical equation that relates the input and output variables of a computer simulation model. Since a computer simulation model is, in itself, only a model of the true system, the term *metamodel* is generally used to describe the mathematical model that approximates the relationship between the variables of a simulation model.

For example, in the research of Galbraith and Standridge (1994), the true system of interest is an electronics assembly plant where circuit boards are manufactured. Their computer simulation model mimics the operation of the true system, over time, using input distributions that are estimated from the actual manufacturing facility. The stochastic model components (those requiring random number generators) include assembly times, routing times, time between equipment failures, etc. After validating and verifying the computer simulation model of the manufacturing facility, a metamodel is then used to explain the relationship that exists between the input variables and the simulated output response. The output variable, denoted y, is typically a performance measure of the system (e.g.; mean production time for circuit boards). The controllable input variables (e.g.; type of solder and the method of component placement on circuit boards) are termed factors and denoted $x_i\,(i = 1, \ldots, k)$. An experimenter may be interested in maximizing or minimizing y, determining the sensitivity of y to the input variables, or simply studying the nature of the relationship between y and various x_i.

The type of metamodels most commonly used in simulation studies are polynomial regression models, such as the first-order model

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i\, x_{iu} + \epsilon_u \tag{1}$$

and the second-order model

$$y_u = \beta_0 + \sum_{i=1}^{k} \beta_i\, x_{iu} + \sum_{i=1}^{k} \beta_{ii}\, x_{iu}^2 + \sum_{i<j}\sum \beta_{ij}\, x_{iu} x_{ju} + \epsilon_u \tag{2}$$

where $u = 1, \ldots, n$ is the simulation run number, y_u is the simulated response (often the mean of observations collected during a simulation run), x_{iu} is the setting of the ith input factor on the uth simulation run, the β's are model coefficients to be estimated using regression analysis, and ϵ_u is unexplainable error in the regression model.

Barton (1994) identifies some "alternative" metamodels for simulation studies, including frequency domain approximations, kernel smoothing models, radial basis functions, spatial correlation models, and spline models. The advantage of these alternative models is their ability to fit a wide variety of curvilinear relationships, often in a piecewise manner. The disadvantage of the alternative metamodels is that their use requires sophisticated statistical knowledge. Not many simulation practitioners are familiar with the alternative models and few statistical packages provide routines for the estimation and analysis of such models. In addition, using variance reduction techniques with the alternative models has not yet been investigated. Polynomial regression models, on the other hand, are familiar to many experimenters, most statistical packages support their estimation and analysis, and the application of variance reduction techniques has been investigated in many research studies.

In terms of the type of metamodel, the scope of this paper is limited to traditional polynomial regression metamodels. It is assumed that the experimenter has developed a valid simulation model, identified the output variable of interest y, and selected a set of k controllable input variables x_i. The experimenter's objective is to develop a polynomial regression metamodel that can be used for optimization, prediction, or sensitivity analysis. The question we address in this paper is: What type of variance reduction techniques would be appropriate for the experimenter's simulation metamodeling study?

We present an overview of recent fundamental advances on the application of variance reduction techniques in a simulation metamodeling context. The paper is organized as follows. Section 2 provides references to some examples of simulation metamodeling studies. Section 3 describes commonly used experimental design plans and variance reduction techniques. Section 4 discusses recent research findings on the use of variance reduction techniques in simulation metamodeling studies.

2 APPLICATIONS OF METAMODELS

There are many articles in the simulation literature that use simulation metamodels to study real-world systems. A few such studies are mentioned here. Gordon, Ausink, and Berdine (1994) develop a simulation model of a spacecraft in orbit. The simulation model has 6 stochastic components (e.g.; changes in solar radiation and changes in transmission voltage) and 5 controllable input variables (e.g.; tracking error and thrust input) that effect the output variable of interest (cost of controlling the spacecraft's orbit). A second-order metamodel is developed in order to efficiently learn about the relationships that exist between cost and the controllable input variables.

Kuei and Madu (1994) and Madu and Kuei (1992) develop simulation models of 2 machine maintenance queueing systems in order to determine the number of machines and repair persons needed for various service levels (the output variable of interest). The simulation models have a number of stochastic components (e.g.; machine repair times and time between failures) and a number of controllable input variables (e.g.; number of repair persons and number of standby machines). Second-order metamodels of the simulations are developed in order to advise management on issues related to the service levels of the maintenance systems.

Friedman and Pressman (1988) develop simulation models of 3 systems with known theoretical solutions in order to ascertain whether simulation metamodels can be trusted. The first system is an M/M/s queueing system. A metamodel relating time-in-system to 3 input variables (arrival rate, service rate, and number of servers) is developed. The second system is time-shared computer system with a single central processing unit. A metamodel relating job response time to 3 input variables (arrival rate, service rate, and proportion of time used for overhead) is developed. The third simulation is an order-level inventory control system. A metamodel relating annual inventory costs to 3 input variables (item demand, review period, and target inventory level) is developed. For each of the simulated systems, a first-order metamodel using natural logarithms of the variables

$$\ln y_u = \ln \beta_0 + \beta_1 \ln x_{1u} + \beta_2 \ln x_{2u} + \beta_3 \ln x_{3u} + \ln \epsilon_u \tag{3}$$

or, equivalently, the multiplicative model

$$y_u = \beta_0 \ (x_{1u})^{\beta_1} \ (x_{2u})^{\beta_2} \ (x_{3u})^{\beta_3} \ \epsilon_u \tag{4}$$

provides results similar to the analytic solution.

There are many other studies that develop simulation metamodels of real-world systems. Excellent sources of such applications can be found in the *Proceedings of the Winter Simulation Conference* and in the *Simulation* journal.

3 BACKGROUND INFORMATION

In this section we discuss experimental design plans and variance reduction techniques that are particularly useful in simulation metamodeling studies.

3.1 Experimental Design Plans

In order to estimate the β coefficients of the polynomial regression model in (1) or (2), experimental data must be collected. Specifically, information on the response variable y at a variety of input conditions x_{iu} is needed. *Experimental design* is a scientific approach to deciding how to collect such information.

Classical experimental design procedures involve finding efficient approaches to collecting and analyzing data for the development of a mathematical model of a system.

In a simulation context, an experimental design must specify the values of the k controllable input factors (x_i ; $i = 1, \ldots, k$) on each simulation run such that the β coefficients can be efficiently estimated. For the first-order model in (1), the most commonly used experimental designs are the 2-level (full or fractional) factorial plans. These designs minimize the variances of the estimated β coefficients. Other first-order designs have been developed for specific experimental goals (e.g.; screening designs) but the properties of the factorial plans make them the most widely used first-order designs.

For the second-order model in (2), a number of experimental designs have been developed for the efficient estimation of the β coefficients. The 3-level factorial designs are often used because of their intuitive appeal, but these designs have the drawback of requiring a large number of experiments. For example, if a simulation model has k=7 input factors, then a full 3-level factorial plan requires $3^7 = 2187$ simulation runs for 1 replication of the experimental design. A 1/3 fractional replication would require 729 runs. For complex simulation models, the computer time needed to collect the data for 3-level factorial designs may be prohibitively large.

There are many other commonly used second-order designs that have desirable properties in certain situations (e.g.; Box-Behnken, central composite, equiradial, Notz, and small composite designs). Thus, unlike the case of fitting a first-order metamodel, an experimenter has a wide variety of choices for an efficient second-order experimental design. However, despite the design choices available, the central composite design is the most popular of the second-order designs.

The central composite designs require that each input variable x_i be set at 5 different levels, but require far fewer runs than the 3-level factorial designs. A central composite design consists of 3 parts: a 2-level factorial design, an axial design, and one (or more) experimental run at the center of the design. The number of runs required is $2^k + 2k + 1$, or 143 when k=7. Depending upon the levels of the variables chosen for the axial portion, the central composite design can be developed to have a variety of desirable properties. Since one part of the design is a first-order 2-level factorial, experimenters often fit a first-order model before augmenting the design with an axial portion in order to fit a second-order model. This capability of being performed sequentially is one of the main reasons for the popularity of the central composite design.

Table 1 illustrates a central composite design for a metamodel with $k = 3$ input variables. The top portion of the design (runs 1–8) is a 2-level factorial plan with the x_i levels specified as +1 and −1 for each variable. (The experimenter must "code" the levels of each controllable input variable such that +1 corresponds to the highest value and −1 corresponds to the lowest value within the region of experimentation.) The bottom of the design (runs 10–15) is the axial portion with the 3 levels specified as $+\alpha$, 0, and $-\alpha$. The design also includes 1 experiment (run #9) at the center of the region, $x_1 = x_2 = x_3 = 0$.

Table 1: $k = 3$ Central Composite Design

Run #	Input Variables		
u	x_1	x_2	x_3
1	+1	+1	+1
2	+1	+1	−1
3	+1	−1	+1
4	+1	−1	−1
5	−1	+1	+1
6	−1	+1	−1
7	−1	−1	+1
8	−1	−1	−1
9	0	0	0
10	$+\alpha$	0	0
11	$-\alpha$	0	0
12	0	$+\alpha$	0
13	0	$-\alpha$	0
14	0	0	$+\alpha$
15	0	0	$-\alpha$

Classical experimental design procedures require that the experimenter choose the high and low levels of each factor. These levels would generally be selected such that the output variable y is adequately described by the second-order metamodel in (2). Other issues facing the experimenter are the number of experiments to perform at the center and the number of times to replicate each design point.

In a simulation context, the experimenter has a number of additional experimental design considerations. Here we assume that the length of the simulation runs, the length of any warm-up period, the initial conditions, and other such tactical issues have already been addressed. (See Nelson 1992 for recommendations concerning these tactical issues.) There is also the strategic issue of how to assign random number streams to the stochastic model components. The use of independent streams for each stochastic model component on each simulation run would result in independent output responses (similar to most real-world studies). However, due to the high variability often associated with simulation output, the use of a technique to reduce variability through the manipulation of random number streams can be desirable.

The next section discusses the variance reduction techniques that are applicable to simulation metamodeling studies.

3.2 Variance Reduction Techniques

Variance reduction techniques were originally developed for the estimation of integrals in mathematics and physics (Kleijnen 1977). In order to use these techniques in simulation, changes were needed due to the autocorrelation of simulated observations and the complex relationships between stochastic model components and simulated response output. Fishman (1974) appears to be the first researcher to investigate the use of variance reduction techniques in the design of simulation experiments. Unfortunately, the results of that study were pessimistic. Since that time, new research studies have brought optimism into the area. In this paper, we briefly describe 4 variance reduction techniques (common random numbers, antithetic random numbers, the assignment rule, and control variates) that are potentially useful in simulation metamodeling studies.

Consider the simulation of an M/M/1 queueing system. Let the output variable y be the steady state time-in-system, and let the single input variable x be the server utilization. Suppose the experimental design involves 2 replications of the following 2 design points: x=0.5 and x=0.7. Another aspect of the experimental design is the assignment of random number streams to the 2 stochastic model components: arrivals and services. Let the vector $\boldsymbol{R}_i$ ($i = 1, \ldots$) denote the ith stream of uniform (0, 1) random numbers used to generate stochastic inputs. If no variance reduction technique is used, the experimental design might be performed using the stream assignments shown in Table 2. This assignment of a unique random number stream to each stochastic component on each simulation run is termed *independent random numbers,* resulting in independent output responses, y_u ; $u = 1, \ldots, 4$.

Table 2: Independent Random Numbers

Run #	Replication	x	Arrival Stream	Service Stream
1	1	0.5	$\boldsymbol{R}_1$	$\boldsymbol{R}_5$
2	1	0.7	$\boldsymbol{R}_2$	$\boldsymbol{R}_6$
3	2	0.5	$\boldsymbol{R}_3$	$\boldsymbol{R}_7$
4	2	0.7	$\boldsymbol{R}_4$	$\boldsymbol{R}_8$

The variance reduction technique of *common random numbers* uses the same stream more than once in order to induce positive correlations and reduce the variances of certain output statistics. The technique can be used within a simulation run (generating data for 2 or more stochastic model components with the same random number stream) and/or between simulation runs (generating data for different sets of input conditions using the same random number stream). For the M/M/1 queueing system considered here, Tables 3 and 4 respectively illustrate experimental designs that use common random numbers *within* and *between* simulation runs.

Table 3: Common Random Numbers Within Runs

Run #	Replication	x	Arrival Stream	Service Stream
1	1	0.5	$\boldsymbol{R}_1$	$\boldsymbol{R}_1$
2	1	0.7	$\boldsymbol{R}_2$	$\boldsymbol{R}_2$
3	2	0.5	$\boldsymbol{R}_3$	$\boldsymbol{R}_3$
4	2	0.7	$\boldsymbol{R}_4$	$\boldsymbol{R}_4$

Table 4: Common Random Numbers Between Runs

Run #	Replication	x	Arrival Stream	Service Stream
1	1	0.5	$\boldsymbol{R}_1$	$\boldsymbol{R}_3$
2	1	0.7	$\boldsymbol{R}_1$	$\boldsymbol{R}_3$
3	2	0.5	$\boldsymbol{R}_2$	$\boldsymbol{R}_4$
4	2	0.7	$\boldsymbol{R}_2$	$\boldsymbol{R}_4$

The variance reduction technique of *antithetic random numbers* uses antithetic pairs of random numbers in order to induce negative correlations that lead to reduced variability of certain output statistics. Antithetic streams, defined as $\overline{\boldsymbol{R}}_i = \boldsymbol{1} - \boldsymbol{R}_i$, are also uniformly distributed on the (0, 1) interval. Unlike common random numbers, replications of design points can be made with antithetic streams (see Table 5).

Table 5: Antithetic Random Numbers

Run #	Replication	x	Arrival Stream	Service Stream
1	1	0.5	$\boldsymbol{R}_1$	$\boldsymbol{R}_3$
2	1	0.7	$\boldsymbol{R}_2$	$\boldsymbol{R}_4$
3	2	0.5	$\overline{\boldsymbol{R}}_1$	$\overline{\boldsymbol{R}}_3$
4	2	0.7	$\overline{\boldsymbol{R}}_2$	$\overline{\boldsymbol{R}}_4$

There are many possibilities for combining the strategies of independent, common, and antithetic random number streams. The third variance reduction technique discussed in this paper, Schruben and Margolin's (1978) assignment rule, is just one way of combining these strategies. The assignment rule uses common and antithetic random number streams in pairs of "orthogonal" blocks in order to induce both positive and negative correlations that result in reduced variability of certain metamodel coefficients. (See Box and Draper 1987 for the design requirements of orthogonal blocking.) If we incorrectly assume that the 2 design points, x=0.5 and x=0.7, of the M/M/1 queueing example represent orthogonal blocks, then Table 6 illustrates the assignment rule strategy.

Table 6: The Assignment Rule*

Run #	Replication	x	Arrival Stream	Service Stream
1	1	0.5	$\boldsymbol{R}_1$	$\boldsymbol{R}_3$
2	1	0.7	$\overline{\boldsymbol{R}}_1$	$\overline{\boldsymbol{R}}_3$
3	2	0.5	$\boldsymbol{R}_2$	$\boldsymbol{R}_4$
4	2	0.7	$\overline{\boldsymbol{R}}_2$	$\overline{\boldsymbol{R}}_4$

* A design with k=1 factor does not form orthogonal blocks so this design only illustrates the assignment rule, *in concept*.

Another variance reduction technique that is used in simulation metamodeling is *control variates*. Unlike the 3 techniques described previously, the use of control variates does not affect the random number stream assignments. The control variates technique only changes the statistical estimators of the metamodel coefficients. The basic idea of control variates is to identify one or more random variables whose expectations are known and correlated with the simulated output variable of interest. The new estimator is computed as the old estimator plus a linear combination of the control variables. See Bauer and Wilson (1992) and Lavenberg, Moeller, and Welch (1982) for more information on control variates.

4 RECENT RESEARCH

In this section, we summarize the findings of current metamodeling research that investigates the variance reduction techniques described above. Each of these 19 studies makes a significant contribution to the simulation metamodeling literature.

Schruben and Margolin (1978) develop and present the assignment rule, thereby sparking research interest in this area. The authors appropriately comment that the assignment rule's "true value for simulation has yet to be fully realized."

Hussey, Myers, and Houck (1987a, 1987b) investigate the assignment rule in comparison to independent streams and common streams using 4 variance-related design criteria (generalized variance, integrated variance, prediction variance, and variance of slopes). For both first- and second order metamodels, the assignment rule is found to be the preferred variance reduction technique in most, but not all, experimental settings.

Nozari, Arnold, and Pegden (1987) develop statistical inference procedures for analyzing metamodeling data obtained with the assignment rule strategy. Appropriate confidence intervals and hypothesis tests on the β coefficients of linear models are derived.

Tew and Crenshaw (1990) examine the effect that the absence of a pure error component has on the statistical analysis procedures associated with the estimation of metamodel coefficients. They show that in order to legitimize a proper statistical analysis, at least one random number stream must be randomly selected across all design points. The authors also point out that inducing too much correlation within a simulation design results in a poor estimate of the experimental error variance.

Using first-order designs, Tew (1991) investigates the use of independent versus correlated replications of the assignment rule strategy. Correlated replications are achieved by using various combinations of common and antithetic stream sets. Tew illustrates that the variances of the metamodel coefficients can be reduced by using correlated replications but, unfortunately, the bias of the coefficients was not considered in this study.

Tew and Wilson (1992) develop statistical procedures for checking the assumptions associated with the assignment rule, which include multivariate normality and the assumed correlation structure. Additionally, statistical tests for lack-of-fit to the assumed metamodel are presented. Joshi and Tew (1995) extend these statistical procedures to the common random number streams strategy.

Kleijnen (1992) compares ordinary and estimated generalized least squares for computing the metamodel's β coefficients when common random number streams are used. Interval estimates computed using the ordinary least squares estimators have good coverage probabilities. Also, it is found that common random number streams reduce the confidence interval widths of all β coefficients except the intercept, β_0.

Donohue, Houck, and Myers (1992, 1995) compare the assignment rule with common and independent streams using 2 mean squared error criteria (MSE of predicted responses and MSE of slope coefficients). For second-order metamodels, the assignment rule performs well in terms of both design criteria; common streams perform well only in terms of the MSE of slopes criterion.

Using central composite designs, Tew (1992) investigates the use common random numbers across design points and antithetic random numbers across replications in comparison to independent random number streams. The variances of the second-order metamodel coefficients are reduced by using Tew's common/antithetic combination strategy. Bias of the metamodel coefficients was not considered here.

Schruben et al. (1992) consider the use of antithetic random number streams in the context of Taguchi's parameter design framework. A simple example illustrates that this variance reduction technique may be beneficial for robust designs in a simulation setting. However, further research using variance reduction techniques combined with Taguchi analysis strategies is called for.

Donohue, Myers, and Houck (1993a, 1993b) investigate the use of independent streams, common streams, and the assignment rule for fitting a first-order metamodel and for sequentially fitting a first- and second-order metamodel using a central composite design. In terms of 2 different mean squared error criteria, the assignment rule was found, in general, to perform the best of the 3 variance reduction techniques.

Extending the earlier work of Crenshaw and Tew, Zeimer and Tew (1994) address the problem of selecting an appropriate method for generating experimental error when correlated replications of design points are used. The authors find that the selection of such a generator is closely linked to its ability to maintain a prescribed correlation structure. Benefits can be achieved from the use of correlated replications if the desired correlation structures are achieved.

Control variates, in combination with common and antithetic random number streams, are investigated by Tew and Wilson (1994). For first-order metamodels, the combined technique is shown to be superior over any of the techniques used individually. Kwon and Tew (1994) extend this research by comparing 3 different methods of combining control variates with common and antithetic streams. The use of both control variates and antithetic streams is shown to perform the best in terms of prediction variance.

Lastly, the most recently published research involves the application of yet another variance reduction technique in a simulation metamodeling study. Hesterberg (1995) uses the *importance sampling* technique in a case study of oil inventory reliability at a large electric power plant and finds the technique to be very efficient. Further research on this variance reduction technique appears warranted.

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