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THE EFFECT OF REPEATEDLY SAMPLING AN EMBEDDED METAMODEL ON THE SIMULATION RESPONSE

THESIS

John Kent Patterson, Captain, USAF

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J. Kent Patterson, B.S., M.A.S.

Captain, USAF

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COMMITTEE:

	NAME/DEPARTMENT	SIGNATURE
Advisor	Lt. Col. Paul F. Auclair, Ph.D. Assistant Professor of Operations Research Department of Operational Sciences, AFIT/ENS	Paul F. Auclair
Reader	Dr. Edward F. Mykytka Associate Professor of Operations Research Department of Operational Sciences, AFIT/ENS	Edward F. Mykytka

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Abstract

A metamodel is said to be embedded within a simulation if it is used to replace a submodule of that simulation. Replacing a deterministic module with an embedded deterministic metamodel poses no apparent mathematical problems. However, using a deterministic metamodel to replace a stochastic simulation component could require additional corrective actions.

Intuitively, replacing a stochastic simulation component with a deterministic polynomial metamodel should reduce the variance of the 'parent' simulation. If a simulation component that exhibits variation in its output for a given set of inputs is replaced by a deterministic equation with no comparable variation in its output, the variance of the 'parent' simulation could be reduced inappropriately.

This research investigated the effects of metamodel substitution in two phases. The first case dealt with a set of tandem queues. It was shown that as each queue was sequentially replaced with a metamodel, the total system variance was inappropriately diminished. A theoretical model of the error components was postulated and used to compensate for this missing variation, restoring the parent simulation's variance to approximately its original level. In the second phase, the problem was extended to the case of repeatedly sampling an embedded metamodel. Again, as the theoretical model of the error components predicted, the metamodel substitution inappropriately diminished the variance of the parent simulation in scenarios where there was at least a moderate degree of variance in the submodule that was replaced. The diminished variance was again compensated for by appealing to the theoretical model of error components introduced in the first phase.

In addition, guidelines for metamodel use were presented. In some situations, sampling from a probability distribution is more appropriate than the use of metamodel.

THE EFFECT OF REPEATEDLY SAMPLING AN EMBEDDED METAMODEL ON THE SIMULATION RESPONSE

I. Introduction

Background

Computer simulation, in its broadest sense, is the process of designing a mathematical-logical model of a real system and experimenting with this model on a computer (Pritsker, 1986:6). In this sense, the computer is basically an extension of the analytical approach to reality (Patterson, 1972:60). As analysts have tried to model larger and more complex problems, computer simulation models have grown in size and complexity. The growing size and complexity of simulation models has led researchers to improve methods for organizing, developing, and accelerating the run times of simulation models.

One method of organizing the growing complexity of computer simulation models is the use of hierarchical modeling. In general, hierarchical modeling provides a means for managing system complexity by partitioning the system into logical, usable chunks which can then be independently manipulated (created, changed, extended) (Luna, 1993:132).

> There are several reasons that [a] hierarchical modeling capability is desirable. These include modeling ease (e.g., reducing the time and effort required to develop models), allowing for model reuse (a topic of long standing interest . .), reducing the number of specific models required, allowing for the use of a data base of models . . . , and aiding in model validation. . . (Sargent, 1993:569).

A rather straightforward approach to hierarchical modeling is to decompose a model into 'connected submodels.' (Sargent, 1993:569). A second approach, is to replace one or more of the submodels with a corresponding empirical approximation or metamodel (Sargent, 1993:569). These metamodels are the main focus of this thesis.

Whereas a computer simulation is a model of reality, a metamodel is a model of a computer simulation, and is thus a model of a model; hence, the name *metamodel.* Metamodels are often linear regression models. While this thesis deals exclusively with least squares regression metamodels; piecewise linear models, splines, inverse polynomials, and Fourier transformations may also serve as metamodels (Kleijnen, 1987:149). Other metamodel forms include kernel smoothing, radial basis functions, spatial correlation models, wavelets, and neural networks (Barton, 1993:12) Regardless of its type, a metamodel relates the output of a simulation to its input factors. A metamodel, then, is an empirical model based on an underlying causal (or mechanistic) simulation model.

Metamodels are used for validation, estimation of factor interactions, control, optimization, and so on (Kleijnen, 1987:149). The primary use of the metamodel is to gain insight into the simulation from which the metamodel was built or created.

> The use of a metamodel enables one to interpret the simulated system more easily and more fully, especially with regard to performing sensitivity analysis, evaluating the effect of specific values of the input variables on the response measurements, and answering the 'what-if' question without the need for additional runs. After all, once the metamodel has been developed and validated, further investigation of the real system using this metamodel is simpler and less costly than conducting additional simulation experiments. In addition, the coefficients calculated for the regression metamodel may give the researcher a better understanding of the relationships between the input variables and the response measurement of interest (Friedman, 1985:144).

Since a fully developed and validated metamodel eliminates the need for further simulation runs, the ensuing analyses of the real-world system would generally focus on the metamodel almost exclusively (Ghosh, 1988:70).

Another possible use of metamodels arises, as Kleijnen stated, when, there is a 'parent' simulation that uses the output of a 'lower-level component' simulation. An example might occur in a theater-level military simulation. A larger theater-level simulation might call on a lower-level component simulation to assist in resolving a 'one-on-one' conflict between two aircraft. The lower-level component simulation would determine the probability of a 'kill', which the parent simulation would then use to determine if a 'kill' occurred. It might be possible to replace this lower-level component simulation with a metamodel. When a parent simulation uses the output of a metamodel contained within it, the metamodel is said to be embedded within the parent simulation. When the parent simulation repeatedly uses the output of the embedded metamodel, it is said to repeatedly sample from this embedded metamodel. There are several aspects regarding this process of replacing a lower-level component simulation with a metamodel that should be considered.

One of these considerations is the difference between a stochastic simulation model and a metamodel. A computer simulation is random or stochastic when a random number generator is used to simulate the random nature of the system or process under investigation. In contrast, a least-squares regression function is deterministic; for a given set of inputs, a least squares regression metamodel always yields the same result. Like a least squares regression function, a deterministic simulation always produces the same response for a given set of inputs. Deterministic simulations may be viewed as a special case of random simulations; given a specified set of input parameters, the output assumes a specific value with probability equal to one (Kleijnen, 1987:148).

Thus, if we simply replace a lower-level component in a simulation with a least-squares metamodel, we would expect the output variance of the parent simulation to diminish. If there is a reduction in output variability associated with substituting a metamodel for a lower-level component simulation, can this lack of variability then be replaced? The currently available literature concerning metamodels has yet to address this question.

Problem Statement

There has been little research on the effect of embedded metamodels on the variability of simulation responses. Furthermore, there are no published guidelines that indicate when it is appropriate to substitute a metamodel for a 'lower-level component' simulation.

Objective

The purpose of this work is to 1.) provide insight into how embedded metamodels affect the output of a parent simulation, particularly with regard to repeatedly sampling an embedded metamodel, and 2.) suggest guidelines for their use.

Overview

Chapter II provides some background on metamodels, a survey of relevant research issues regarding embedded metamodels, as well as some examples of metamodel applications. As alluded to earlier, this body of literature offers little guidance regarding embedded metamodels. In Chapter III the issue of substituting a deterministic metamodel for a stochastic simulation component is explored via a simulation model of tandem queues. This process is then generalized in Chapter IV where the issue of repeatedly sampling an embedded metamodel is developed. Having discussed methods for metamodel usage in Chapters III and IV, Chapter V discusses potential pitfalls of inappropriate metamodel uses. Finally, Chapter VI closes this thesis with some conclusions and recommendations.

II. Background

Overview

Metamodels have been used by the simulation community for almost twenty years (Barton, 1993:12). Despite impressive advances in computing and simulation capabilities, metamodels continue to be effective representations of input-output relationships due to their ease of use and straight-forward application.

> The value of metamodels lies in their simplicity. A simple model is easy to understand, and so it is possible to gain insight from a metamodel of a complex situation whose structure defies obvious insight into its behavior. A simple model is also a fast running model, and so simulation metamodels can be used for interactive "what it?" studies in place of the time consuming original code (Barton. 1993:12).

Metamodels may be represented as piecewise linear models, splines, inverse polynomials, Fourier transformations, kernel smoothing, radial basis functions, spatial correlation models, wavelets, or neural networks. However, they often are polynomial regression metamodels of the form (Kleijnen, 1987:149)

$$y = g(\mathbf{x}) + \varepsilon \tag{2.1}$$

where y is the actual value, g(**x**) is the true metamodel, and ε is the error. In practice, the true metamodel is rarely known and must be estimated by

$$g(\mathbf{x}) \approx f(\mathbf{x}) = \hat{y} \tag{2.2}$$

where f(**x**) is the polynomial approximation of g(**x**) and $\hat{y}$ is the metamodel estimate of the actual value of y. For reasons of practicality and interpretability, polynomial metamodels frequently are limited to first and second order linear models (Kleijnen, 1987:200).

Research Issues

Most of the research pertaining to metamodels has focused on the technical details of actually developing and exploiting their many possible forms. Other research related to developing metamodels includes analysis of error components (Tew, 1994:7) and alternatives to polynomial regressions (Barton, 1992:289; Barton, 1993:12).

Developing and interpreting metamodels raises a host of issues.

> The major issues in metamodeling include: i) the choice of a functional form for f, ii) the design of experiments, i.e., the selection of a set of **x** points at which to observe y (run the full model) to adjust the fit of f to g, the assignment of random number streams, the length of runs, etc., and iii) the assessment of the adequacy of the fitted metamodel (confidence intervals, hypothesis tests, lack of fit and other diagnostics). The functional form will generally be described as a linear combination of basis functions from a parametric family. So there are choices for families (e.g., polynomials, sine functions, piecewise polynomials, wavelets, etc.) and choices for the way to pick the 'best' representation from within the family (e.g. least squares, maximum likelihood, cross validation, etc.). The issues of experimental design and metamodel assessment are related since the selection of an experimental design will be determined in part by its effects on assessment issues (Barton, 1992:290).

The experimental design used to create the metamodel has also been an area of research. Response Surface Methodology (RSM) techniques have been the traditional method for gradient information and sensitivity analysis (Wilson, 1987:378).

> Response surface methodology comprises a group of statistical techniques for empirical model building and model exploitation. By careful design and analysis of experiments, it seeks to relate a *response*, or *output* variable to the levels of a number of *predictors*, or *input* variables, that affect it (Box, 1987:1).

The reader is referred to Box and Draper (1987) for a more complete discussion of RSM. However, as research into RSM for gradient information and sensitivity analysis has diminished, alternatives have been investigated. These alternatives include frequency-domain methods, perturbation analysis, and likelihood-ratio methods (Wilson, 1987:378). These alternatives represent areas of research into other methods of model development, other than the traditional methods of RSM. In comparison to these alternatives for gradient information and sensitivity analysis, the mathematical and statistical foundations of RSM are more transparent and more developed (Wilson, 1987:378).

Clearly, while researchers and practitioners have focused on metamodel development, design, applications, and forms, the current literature also indicates that metamodels continue to be the object of ongoing research. Sargent's summary of 11 different metamodel research issues included:

1. What type of Goodness of Fit criterion should be used for the metamodel?
2. What are the trade-offs between simplicity and complexity (using, e.g., variance reduction techniques) in designs?
3. What is the required level of accuracy for the metamodel?
4. How to determine the validity of the metamodel with respect to the real system? (Sargent, 1991:892).

While there have been references to the possibility of embedding metamodels within a simulation, little progress has been made in this area (Sargent, 1991).

Metamodel Uses

The use of metamodels to provide insight into more complex systems has been the most common application of metamodels (Ghosh, 1988:70). Specific examples of using metamodels to provide insight into complicated systems include Ghosh's evaluation of a computer's multiprocessor performance and Kleijnen's sensitivity analysis of the greenhouse effect (Kleijnen, 1990; Ghosh, 1988). Ghosh's research was significant in that it was the first to fully explore the methodology issues regarding metamodel research of multiprocessor performance (Ghosh, 1988:70). Kleijnen's sensitivity analysis revealed the importance of key model inputs affecting the greenhouse effect, like the ocean, which unexpectedly was quadratic in nature, and provided insight into a 'bug' in the dike-raising module of the simulation (Kleijnen, 1990:17). These results are typical of metamodel applications in that significant effects are determined and errors in model formulation are revealed. For additional examples, the reader is referred to the extensive list of documented metamodel applications, forms, and uses contained in (Kleijnen, 1987).

Embedded Metamodels

Sargent elaborated on the concept of embedded metamodels in the context of hierarchical modeling. He suggested the use of metamodels to replace one or more 'lower-level components' in a parent simulation. He added, "This approach needs considerable development prior to becoming feasible" (Sargent, 1993:570). Sargent did not list the specifics of the required development, but they would presumably include such issues as the inappropriate reduction in the variability of the simulation output and the methods needed to restore it.

Central to the issue of inappropriately reducing the variance of a simulation model is the potential practice of replacing a *stochastic* simulation component with a *deterministic* polynomial expression. This area of research appears to be unexplored. There has been some work in replacing 'lower-level components' in deterministic simulations with metamodels. In fact, Kleijnen used a metamodel to serve as a 'lower-level component' of a larger deterministic simulation (Kleijnen, 1990:12). Kleijnen's application of replacing a deterministic simulation component with a deterministic metamodel was completely appropriate and consistent.. The problems with metamodel substitutions originate when a *deterministic* metamodel replaces a *stochastic* simulation component. These problems revolve around identifying and possibly replacing the variability present in the simulation without the embedded metamodel, but diminished in the simulation that contains an embedded metamodel. The currently available literature does not address this aspect of metamodel use.

III. Metamodel Effects on Variation

Introduction

Replacing a stochastic simulation component with a deterministic embedded metamodel will probably decrease the overall variation of the 'parent' simulation. This conjecture was tested using a simulation of tandem queues. By comparing the output variance of the parent simulation with that of a simulation containing one or more metamodels, the effect of metamodel substitution on simulation output was examined.

Components of Variation

A number of components or random events generated within a simulation affect the mean and the variance its response. In a stochastic simulation, several of these components will have their own sources of variability. The variance of a simulation response, then, can be conceptualized as a function of the variances of each of its components. Although a simulation might actually contain a large number of components, the conceptual model of its variance could be limited to those components that have an identifiable and quantifiable effect on either the mean or the variance of the simulation output. These individual components, or elements, could reasonably be restricted to the major subroutines or processes contained in the simulation. For *n* such elements, we could express the mean μ_s, and variance σ_s^2, of the simulation as

$$\mu_s = \mu_1 + \ldots + \mu_n \tag{3.1}$$

and

$$\sigma_s^2 = \sigma_1^2 + \ldots + \sigma_n^2 \tag{3.2}$$

respectively, where μ_i and σ_i^2 represent the mean and variance of the *i*th component of the simulation. If one of these components were deterministic in nature, its mean, given a fixed set of inputs, would be constant, and therefore its variance about that mean would equal zero. Equations 3.1 and 3.2 contain some implicit assumptions. The first assumption is that the components which have these variances are independent, and secondly, that their variances are indeed additive. Depending on the actual simulation, these assumptions may or may not be true.

Equations 3.1 and 3.2, also, provide a mechanism for assessing the effect of replacing a major simulation component with a metamodel. If a component that is stochastic in nature is replaced by a deterministic function, the variance of the simulation response could be artificially diminished.

Central to examining the appropriateness of replacing a stochastic component of a simulation with a deterministic component is the concept of relative variance. Relative variance is defined as:

$$\text{Relative Variance} = \frac{\sigma_c^2}{\sigma_s^2} \tag{3.3}$$

where σ_c^2 represents the variance of an individual component or the sum of the variances of a set of components and σ_s^2 represents the variance of the parent simulation. The relative variance can be small either because the components simply have low variations intrinsically, or because there are so many sources of variation within the simulation that the components' relative contributions to the output variance is small. Using Equation 3.3, Figure 3-1 illustrates the effect on σ_s^2 (the variance of the parent simulation) of substituting either 1, 2, 5, or 10 metamodels into simulations consisting of up to 100 components with equal variance, σ_i^2. In regions, such as the upper right portion of Figure 3-1, where the replaced components contribute negligibly to the simulation output variance, the metamodel substitution would be expected to have little impact. In the lower left portion of Figure 3-1, where the replaced components accounted for much of the output variance, the metamodel substitution would likely result in a major reduction in variance.

The presentation in Figure 3-1 can be generalized by partitioning the components of variance into two terms: σ_m^2, the components of variance corresponding to those elements replaced by one or more metamodels, and σ_r^2, the components of variance for the remaining elements not replaced by metamodels. The total variance in the simulation is simply given by $\sigma_m^2+\sigma_r^2$. The ratio $\sigma_m^2/(\sigma_m^2+\sigma_r^2)$ represents the proportion of the output variance lost due to one or more metamodel substitutions, while $\sigma_r^2/(\sigma_m^2+\sigma_r^2)$ indicates the proportion of the output variance remaining. It is evident that these two ratios will always sum to one. The line in Figure 3-2 depicts the theoretical relationship between these two ratios.

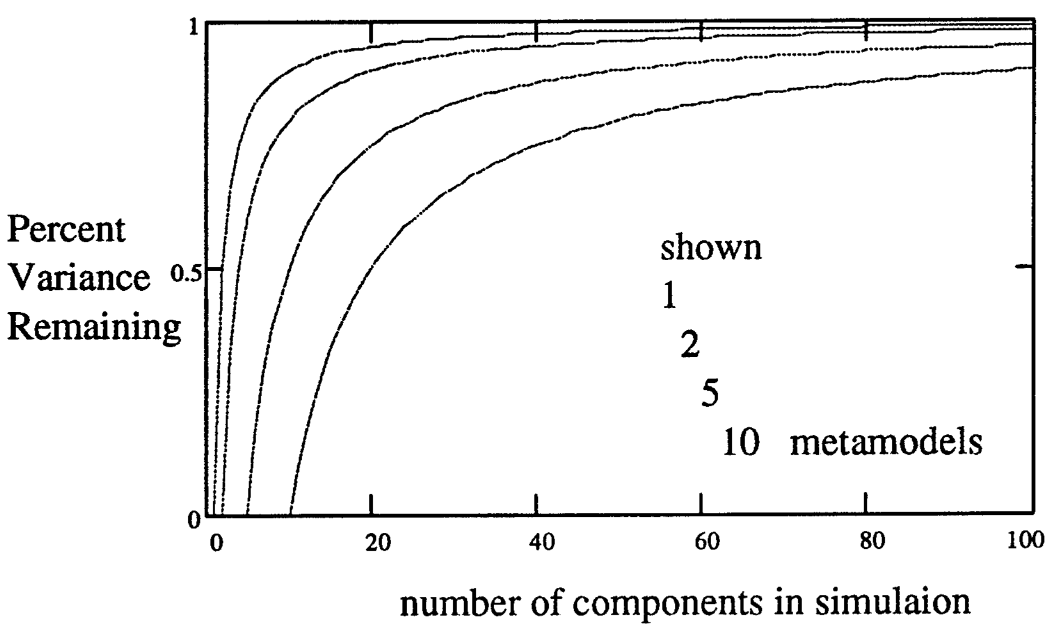


Figure 3-1 Relative Percent of Variation Remaining

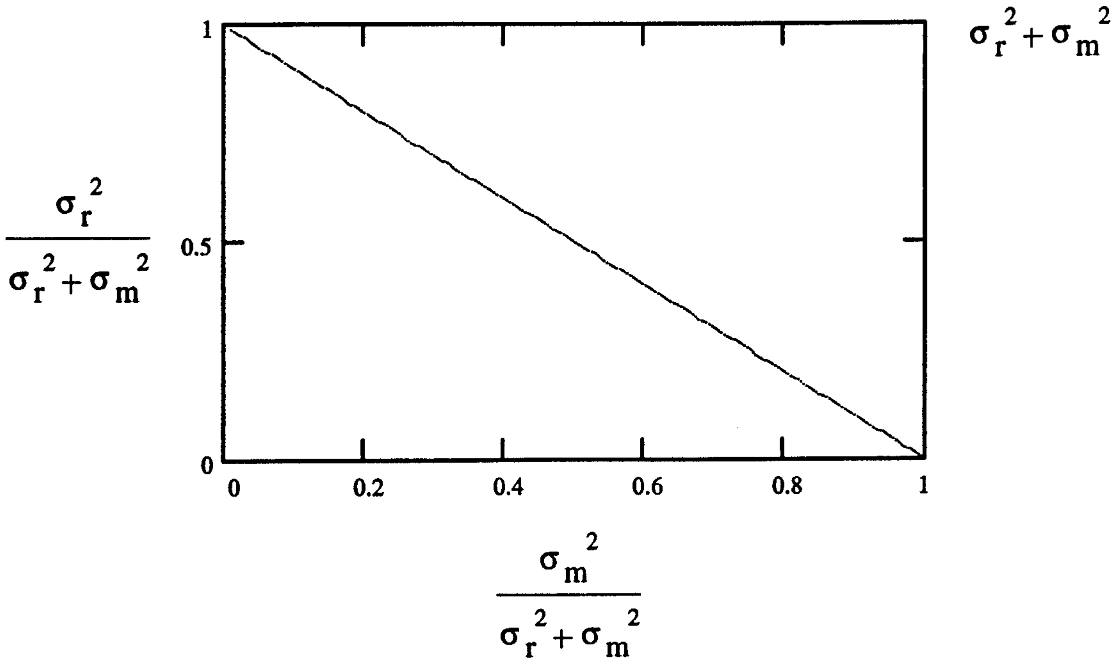


Figure 3-2 Percent of Simulation Replaced by Metamodels

Figures 3-1 and 3-2 indicate that substituting a deterministic function for a stochastic simulation component would inappropriately reduce the output variance of the parent simulation. Although not depicted in either figure, the mean of the simulation output would probably not be significantly affected by metamodel substitutions, assuming that the metamodel adequately estimates the mean. Since a properly validated metamodel provides an approximately unbiased estimate of the mean, the overall system mean should be largely unaffected. To test these conjectures an experiment was performed.

Experiment Background

Because of its convenient mathematical properties, a simulation of tandem queues consisting of 5 M/M/1 queues was performed. The performance measure of interest in the simulation was queue length. Since each M/M/1 queue in the system is independent, the total number of entities waiting in the system is simply the sum of the individual queue lengths (Ross, 1993:374). If L_s represents the total queue length for the tandem queuing system and L_i, i = 1, 2, . . . , 5, represents the queue length for each of the individual M/M/1 queues, then

$$L_s = L_1 + L_2 + L_3 + L_4 + L_5 \qquad (3.4)$$

Similarly, the variance of the system queue length is the sum of the variances for each of the queue lengths. Thus, in this situation, the simulation output is indeed additive.

Using this simulation, the effect of replacing simulation components with metamodels was examined. As one or more of the queues were replaced by a metamodel, the effect on the mean and variance of the system could be compared to the mean and variance of the corresponding system which contained no metamodel components.

Queue Experiment

Five M/M/1 queues with identical arrival rates (λ=16/hr) and service rates (μ=18/hr) were simulated for 28 days of operation. The simulation statistics were cleared after approximately 8 days to remove any bias due to start-up conditions. Ten replications were conducted for each queue. The mean and variance of these ten replications for each queue are shown in Table 3-1.

Table 3-1 **Queue Simulation Results**

Queue	Queue Length	
Number	Mean	Variance
1	6.565	0.238795
2	7.017	0.261146
3	6.772	0.247496
4	6.940	0.213511
5	6.977	0.278790

The mean number of customers in a tandem queuing system consisting of five M/M/1 queues could be estimated by the sum of the mean queue lengths listed in Table 3-1. Alternatively, the mean number of customers in the system could be estimated by the sum of simulation and metamodel estimates. The metamodel selected to represent the mean length of an M/M/1 queue was previously developed by Friedman (1985).

> The system modeled an M/M/s queue, with a single service facility and a single waiting line; demands were assumed to arrive according to Poisson process with a constant average arrival rate (ARR) and service times were assumed to follow an exponential distribution with a constant average service time (1/SVC). The performance measure of interest, average number of demands waiting for service (LQ) was generated at the end of each 15-week run (Friedman, 1985:145).

The form of their metamodel is:

$$\ln(LQ)=2.9517+15.0099\cdot\ln(ARR)-14.7682\cdot\ln(SVC)-14.8217\cdot\ln(NSVR) \qquad (3.5)$$

For an arrival rate of $\lambda=16$/hour, service rate of $\mu=18$ / hour, and a single server, the metamodel yields an expected queue length of 6.569, as opposed to the expected steady state value of 7.111 (Ross, 1993:360).

To examine the effect of replacing a stochastic simulation component with a deterministic metamodel, the simulated queuing results were sequentially replaced by the Friedman metamodel result. Thus, the first metamodel replaced the first queuing simulation, the second metamodel replaced the second simulation, and ultimately the fifth metamodel replaced the last remaining simulation.

The results of the metamodel substitution experiment are summarized in Table 3-2.

Table 3-2 Metamodel Substitution Results

	System Variation			*Total Length of Queues*		
	Actual	Original	% Original	Actual	Original	% Original
All 5 components simulated **	1.24	1.24	100.00	34.27	34.27	100.00
Replace first component w/ MM	1.00	1.24	80.73	34.28	34.27	100.01
Replace first and second components w/ MMs	0.74	1.24	59.68	33.83	34.27	98.70
Replace first through third components w/ MMs	0.49	1.24	39.68	33.62	34.27	98.11
Replace first through fourth components w/ MMs	0.28	1.24	22.50	33.25	34.27	97.03
Replace all five components w/ MMs	0.00	1.24	0.00	32.85	34.27	95.84
** Original System						

As each of the i components was sequentially replaced by a metamodel, the variability of the entire system decreased. In the extreme, when each of the 5 components were replaced by a metamodel, the variability of the estimated queue length was zero. Because the metamodel was properly specified and approximately unbiased, there was no significant difference, at an $\alpha = .10$ level, between the total queue length of the original system and the total queue lengths predicted by any of the simulations that contained one or more metamodels.

Error Replacement

Each of the metamodel substitutions in the experiment actually produced a new or modified model consisting of a different mix of simulation and metamodel components. The reduction in simulation output variance due to metamodel substitution resulted from ignoring the variance of the embedded metamodels. The variance of a metamodel response is generally not the same as the variance of the simulation component it replaced. A procedure to compensate for the inappropriately diminished variance of the simulation output could attempt to restore the variance that was present in the original simulation. On the other hand, an alternative procedure might focus on estimating the variance of the new or modified model. The question of which approach is preferable is a philosophical modeling issue that has yet to be resolved.

The Mean Square Error (MSE) of a properly specified least-squares metamodel is an unbiased estimator of the variance of the simulation response at a given design point. In contrast, the variance of a least squares metamodel response is a function of the variances of the regression coefficients and the covariances between pairs of regression coefficients (Neter, 1990:244). This variance is given by

$$s^2(\hat{Y}_h) = MSE(\mathbf{X}_h'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_h) \qquad (3.6)$$

where the **X** matrix is the original design matrix, and the $\mathbf{X}_h$ vector is the vector of the specific point about which the variance is to be determined.

Equation 3.6 is the variance of the expected *mean* response of the simulation at a specific design point, as opposed to the variance of a predicted response of an *individual outcome* at a specific design point. The variance of a predicted response of an *individual outcome* at a specific design point must also consider the variance about the conditional mean. Thus, the variance of a predicted response of an *individual outcome* at a specific design point is (Neter, 1990:246).

$$s^2(\hat{Y}_{h(new)}) = MSE(1+\mathbf{X}_h'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_h) \qquad (3.7)$$

Equation 3.7 represents the component of variance that the metamodel contributes to the simulation output for an individual response. For *r* individual responses, the variance of the sample mean is simply the estimated population variance divided by *r*. Under the assumption that the metamodel provides a valid measure of the variance of individual outcomes, the variance of the mean response of *r* replications could be estimated by

$$\text{Component Variation} = \frac{MSE(1+\mathbf{X}_h'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_h)}{r} \qquad (3.8)$$

Equation 3.8 could be used to adjust the precision of the original metamodel to more closely correspond to that of the replaced simulation component. In this study, Equation 3.8 was used to compensate for the inappropriate variance reduction induced by ignoring the variance of embedded metamodels.

Figure 3-3 depicts the results of the metamodel substitution experiment and the use of Equation 3.8 to compensate for the inappropriate reduction in the variance of the simulation output. The Xs denote the loss of system variability as first one, then more of each of the queues were replaced by a metamodel. When all five of the queues were replaced with metamodels, the system variation was zero. The diamonds denote the variance of the overall system present when the variance of the metamodel response was estimated by Equation 3.8 with $r = 10$ replications. In this instance, application of Equation 3.8 appeared to adequately account for the inappropriate reduction in the variance of the simulation output.

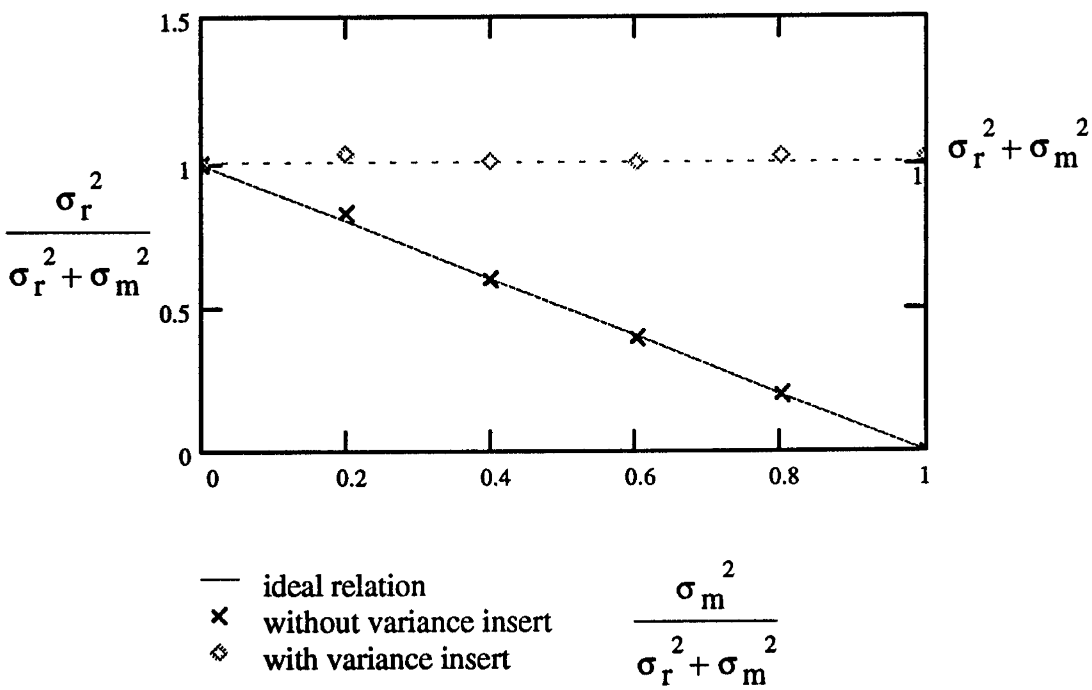


Figure 3-3 Percent Variation Remaining with and without Variance Reinsertion

Thus, for a simple set of tandem queues, the variance of the simulation response was diminished by replacing stochastic simulation components with deterministic metamodels. Furthermore, a postulated method of accounting for the inappropriate variance reduction restored the output variance to approximately the same level as the original simulation. Since, for a given design point, the metamodels closely approximate the simulation mean, the use of metamodels did not significantly affect the mean of the tandem queuing system, as shown in Table 3-2.

This experiment showed that for a simple singly sampled embedded metamodel it was possible to compensate for the variance diminished by the use of metamodels. This example dealt with the use of a polynomial metamodel and relied on the linear model assumption of normally distributed residuals. The next chapter generalizes this approach to the case of repeatedly sampling an embedded metamodel.

IV. Repeatedly Sampling an Embedded Metamodel

Introduction

It has been established that, in some cases, an embedded metamodel reduces the variability of the overall simulation model, and that there is at least one method of compensating for that diminished variability. This chapter extends the model established in Chapter III to the case of repeatedly sampling an embedded metamodel. The results of an experiment show that the variability of the parent simulation is again, inappropriately reduced, and that the methods developed in Chapter III can be adapted to restore the variance of the parent simulation to approximately the same level of variation originally present.

Background of Model

The model needed for this type of experiment was fairly specific: a stochastic simulation with several submodules, each of which must have a quantifiable mean and variance. The output of each of these submodules must feed into an overall parent simulation which, again, must have both a quantifiable mean and variance

The simulation created to meet these requirements dealt with the scenario of a car dealer who buys four cars, the same type of car (e.g. a corvette), every day, from four different cities located near each other. The buyer visits these cities and buys each car at a price which depends on six characteristics: miles, age, number of wrecks, appearance, rust, and color. The buyer's estimate of the price of the car based on these six factors is assumed to be the 'true,' or simulated, price of the car. It is assumed that no other factors affect the price of the car. The simulation variable of interest is the total cost of buying the four cars each day.

The dealer considered purchasing cars over the phone and wished to build a metamodel to estimate car prices based on the most important input factors. It was assumed that data would be collected over some time period (200 days) and that this data would be used to create a metamodel for use in the future. The data for these 200 days was created by generating the information for each of the six input variables. Equation 4.1 was used to generate the 'true' prices of the cars.

$$y = 34000 - 800 \cdot Age + 72 \cdot Appearance - 20 \cdot Color - 0.03839 \cdot Miles - 367 \cdot Rust - 100 \cdot Wrecks \tag{4.1}$$

A random component, distributed $N(0,\sigma^2)$, was added Equation 4.1 to create a specific level of variance in the data base. The variance, σ^2, in the random component was set to three different levels to examine the effect of repeatedly sampling a metamodel in situations ranging from low to high variation. Further details of how the data base was generated are included in Appendix A.

Experiment

There were three scenarios for this experiment, each with a different level of variance in the simulation response. The 'low,' 'medium,' and 'high' scenarios had standard deviations of 100, 1500, and 4000 dollars respectively, in the random component added to Equation 4.1. In each of these scenarios, a metamodel was created from 200 days of data. Only terms with a p-value of 0.10 or less were included in these models, which are presented in Appendix B.

In each of the three scenarios, 50 'days' of operation beyond the data collection period were simulated for each city. All the cities were assumed to be the same in every way, and each represented a submodule of the larger simulation. The output for a single day's operation was the total cost of purchasing a car in each of the four cities. The output for the entire simulation of 50 days was the mean daily car buying cost incurred by the dealer. Figure 4-1 shows the model of the simulation.

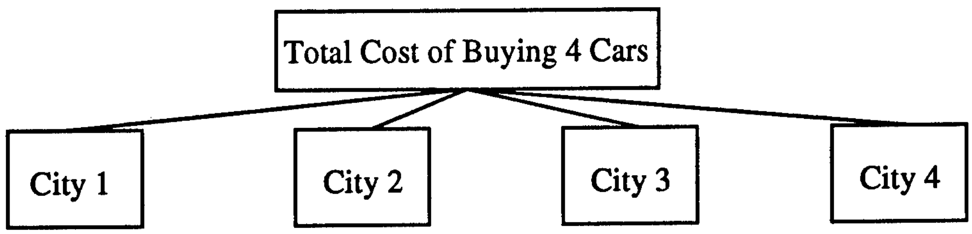


Figure 4-1: **Diagram of Simulation**

Each city submodule was sampled once for each day of the simulation. When an embedded metamodel replaced one of the simulation components, it was also sampled once for every day of the simulation. Thus, this experiment illustrated the concept of repeatedly sampling an embedded metamodel.

First, the mean and variance of the daily car buying experiment for the completely simulated original system were calculated. The mean and variance for the original system were then compared to those of the models containing one or more metamodels. In agreement with the results from Chapter III, the mean was nearly constant in all 3 scenarios (low, medium, high), but the variance of the simulation output was inappropriately diminished in both the medium and high scenarios. In the low scenario, with little variation present initially, there was no significant loss in the output variance. Table 4-1 and Figure 4-2 show this reduction in the output variance as first one, then another, of the metamodels replaced the simulation components. The values depicted in Table 4-1 and Figure 4-2 indicate the percentage of the original output variance present for each scenario.

Table 4-1 Queue Simulation Results for Embedded Metamodels			
	Scenario		
	Low	Medium	High
Original System	100	100	100
1 Metamodel Used	100	98	95.6
2 Metamodels Used	99.8	88.4	86.7
3 Metamodels Used	100	86.7	75.5
4 Metamodels Used	100	83.8	60.9

(Values shown are percent of original output variance)

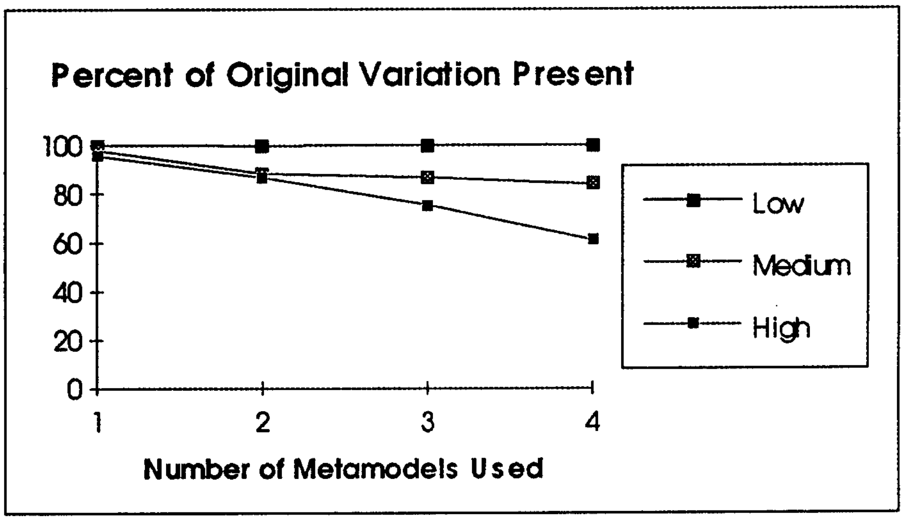


Figure 4-2 Percent of Original Variation Present

Error Replacement

Having demonstrated the potential for an inappropriate loss of output variance when a stochastic simulation model repeatedly samples a deterministic metamodel, the problem of compensating for the diminished output variance remains. To account for the inappropriate variance reduction, the techniques described in Chapter III were reapplied to the current problem with two significant differences. Since the queues examined in Chapter III were identical, Equation (3.8)

$$\text{Component Variation} = \frac{MSE \cdot (1 + \mathbf{X}_h^T \cdot (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}_h)}{r} \quad (3.8)$$

required, only one $\mathbf{X}_h$ vector or design point. In the current problem, however, every car purchase represented a unique design point and corresponding $\mathbf{X}_h$ vector. In addition, there were 10 replications used in Chapter III, so *r* was equal to 10. In this problem, there were no replications, and r was equal to one.

An even more fundamental difference between the two problems lies in the method of compensating for the inappropriate reduction of the output variance. In Chapter III, the variance of the mean queue length was calculated once for each queue. The variance of the mean queue length for the entire system was simply the sum of those variances. In the current repeated sampling problem, a different approach was required. The diminished variance had to be compensated for every time the metamodel was sampled. Assuming an adequate linear polynomial metamodel, the distribution of any predicted individual response would be approximately normally distributed with a mean of zero and a variance, σ_{cv}^2, given by Equation 3.8. Thus, one possible method of compensating for the inappropriate variance reduction in the repeated sampling case would be to generate a $N(0,\sigma_{cv}^2)$ random variate and add it to the metamodel response every time the metamodel is sampled. This modified metamodel response is given by

$$\hat{y}' = f(x) + N(0,\sigma_{cv}^2) \quad (4.2)$$

where f(**x**) is the metamodel and $N(0,\sigma_{cv}^2)$ represents a random sample from the specified Normal distribution.

When the modified metamodels were applied to each of the three scenarios (low, medium, high), the general results of Chapter III were again duplicated. In both of the medium and high variance scenarios the modified metamodel successfully compensated for the inappropriate reduction in the output variance. There was no variance reduction problem in the low-variance scenario, and the modified metamodel had virtually no effect on the statistical quality of its output. The results of this experiment are summarized in Figure 4-3 through 4-5.

Figure 4-3, shows that when the original component has low variability, or is nearly deterministic, replacing that component with a truly deterministic metamodel has little impact on the output variance of the parent simulation. In this case, use of the modified metamodel neither improved nor degraded the of output variance. In Figure 4-4, the expected effect of replacing stochastic subcomponents with deterministic components begins to emerge. The level of variance of the parent simulation was approximately restored to its original level through the use of the modified metamodel. Finally, in Figure 4-5, the effect on the variance of the simulation output when stochastic subcomponents are replaced with deterministic metamodels is most readily apparent. Again, the variance of the simulation output was approximately restored to its original level by the variance compensation actions.

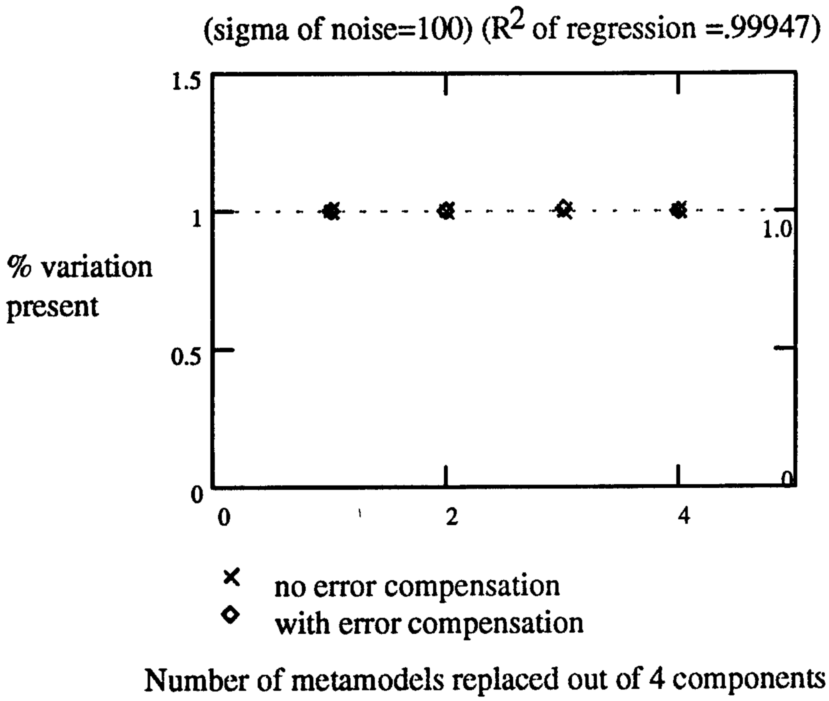
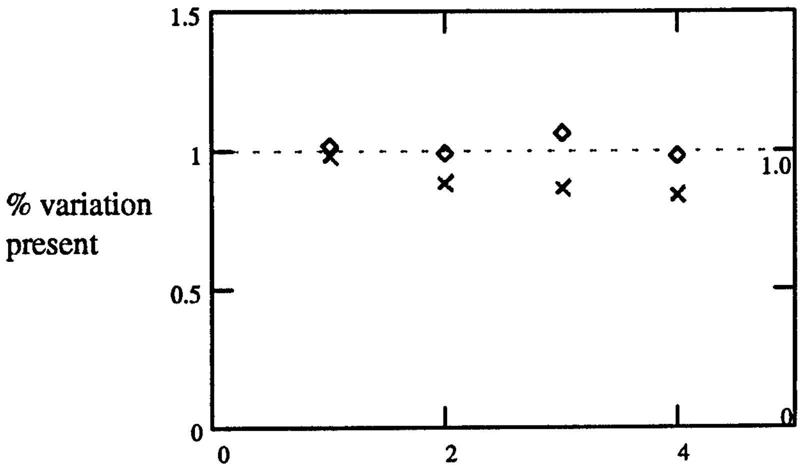


Figure 4-3 Low Variance Scenario

(sigma of noise=1500) (R^2 of regression =.7555)

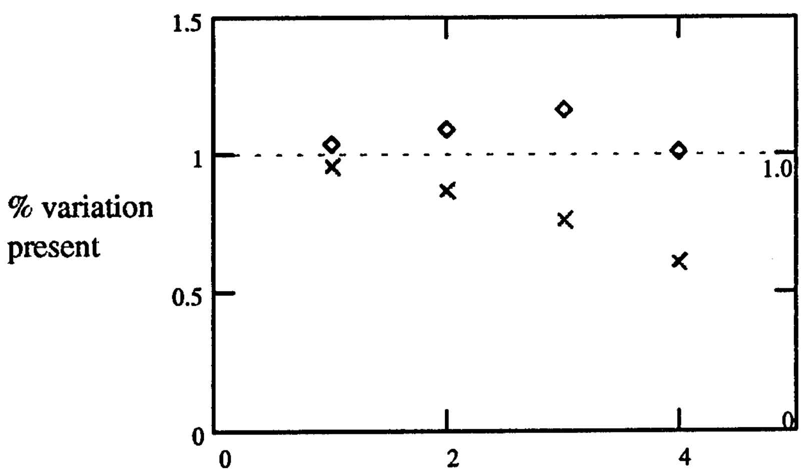


× no error compensation
◇ with error compensation

Number of metamodels replaced out of 4 components

Figure 4-4 Medium Variance Scenario

(sigma of noise=4000) (R^2 of regression =.38875)



× no error compensation
◇ with error compensation

Number of metamodels replaced out of 4 components

Figure 4-5 High Variance Scenario

Conclusion

The inappropriate reduction in the variance of the simulation output when stochastic components were replaced with deterministic metamodels seemed to apply to repeated sampling, as it did for the non-repeated sampling of Chapter III. When there was a significant level of variation initially present in a simulation component, replacing that component with a metamodel inappropriately diminished the variation of the simulation response. However, by compensating for this diminished error, the variance of the simulation could be restored to approximately its original level. The general solution method introduced in Chapter III, to compensate for this diminished variance also appeared to be effective for the repeated sampling case. In the scenario containing low variance initially, the variance compensation method appeared to neither improve nor degrade the level of the variance present.

V. Metamodels and Distributions

Introduction

In Chapters III and IV the focus was on the variance of the simulation output and when it might be inappropriately diminished due to a metamodel substitution. However, a discussion of embedded metamodels would be incomplete without discussing when an embedded metamodel is not appropriate at all. In some situations simply sampling a random number from a known distribution is more appropriate than inserting a metamodel.

Distributions vs Metamodels

A response surface approximates a mechanistic, or theoretical model. If there is a fairly well-defined output measure for a given set of inputs, a response surface or metamodel would be appropriate. Although the randomness in observed or simulated data creates a degree of uncertainty in the exact value of the expected output of any individual observation, it is possible that this random variation could be relatively small, if not nearly zero. An example of such a mechanistic model is Einstein's famous equation

$$E = m \cdot c^2 \tag{5.1}$$

which states that a given amount of mass, *m*, will yield a specific amount of energy, *E*, when the mass is converted to energy.

On the other hand, some outputs conform more to a probability distribution than to a mechanistic model. For example, the time to failure for a light bulb is described fairly well by an exponential distribution. It is not defined by a mechanistic input/output relationship. Thus, it is better modeled by sampling from a probability distribution.

The case mentioned in Chapter I of a theater-level combat model calling a lower-level engagement model to resolve a one-on-one conflict between two aircraft is not so clear. Using a metamodel as a surrogate for an engagement model implies an underlying model that yields credible results (e.g., an integer number of survivors). Without an underlying a mechanistic model, either a theoretical or empirical distribution might be a far more appropriate representation.

Conclusion

When deciding on whether to use an embedded metamodel, it is important to consider whether there is a well defined mechanistic input/output relationship that warrants the use of a metamodel. If there is not a well defined mechanistic input/output relationship, then perhaps it is more appropriate to sample from a probability distribution, or in some cases, simply use the simulation subcomponent the metamodel was being evaluated to replace.

VI. Conclusions and Recommendations

Introduction

As stated previously, the purpose of this research was to 1.) provide insight into how embedded metamodels affect the output of a 'parent' simulation, particularly with regard to repeatedly sampling an embedded metamodel, and 2.) suggest guidelines for their use. Conclusions from preceding chapters are formalized here. In addition, recommendations for additional research are presented.

Conclusions

The theoretical framework for the components of the system variance discussed in Chapter III appeared to correctly predict the effect of a metamodel substitution for singly sampled metamodels, namely an inappropriate reduction in the system variation. When this effect was tested, the empirical results were consistent with the conjecture of an inappropriate reduction in the variance. Using the same theoretical framework for the components of the system variance and exploiting the properties of the linear model, the system variance was returned to approximately its original level, for both the singly and repeatedly sampled embedded metamodel, further validating the theoretical framework for the components of the system variance. Finally, metamodels are not always appropriate substitutes for simulation components. Some simulation components are better represented by distributions of outcomes rather than empirical models.

Recommendations

The conjecture that different types of simulations can be represented by either a metamodel or a sample from a known probability distribution needs to be further explored and defined. The techniques described in Chapters III and IV for compensating for the missing level of variance need to be extended and tested on larger simulations to determine if these results are also consistent and to validate the theoretical framework for the components of the system variance. Lastly, this thesis was limited to linear polynomial metamodels. Other types of metamodels should be examined for the possibility of compensating for inappropriately diminished variance.

Appendix A: Data Base Generation

The database for this research was created in EXCEL. The 200 random numbers for each input variable (age, miles, number of wrecks, appearance, rust, and color) were created using the random number generation. The 200 random numbers were created from the following distributions:

1. Age = Uniform(0,7) years
2. Appearance = Binomial (p=.2) 15 trials
3. Number of Wrecks = Binomial (p=.1) 10 trials
4. Color = Uniform (1,10)
5. Rust = Binomial (p=.1) 8 trials

Miles needed to be 'loosely' tied to age. A random number was drawn from a Normal (15, 5) distribution where the units are thousands of miles. This was then multiplied by *age* to get *miles.*

The six factors were related to the price of the car by

$$y=34000-800\cdot Age+72\cdot Appearance-20\cdot Color-0.0389\cdot Miles-367\cdot Rust-100\cdot Wrecks$$

(4.1)

To provide and control the variance of the model, a column of 'noise' was created and added to Equation 4-1. This noise was set to 3 different levels corresponding to each of the 3 scenarios. Part of the database follows.

		First 50 of a Set of 200: Shows Medium Case of Variation							
Case	N(0,1500)	U(15K,5K)	Miles	Age	# Wrecks	Appearan	Rust	Color	Paid-1
1	197.88	15426	28035	1.82	2	2	1	2	31203
2	1352.60	18298	92099	5.03	0	2	2	4	27125
3	133.57	10335	23077	2.23	0	2	0	3	31554
4	79.04	17377	731	0.04	2	6	0	7	34116
5	419.47	12349	62249	5.04	2	4	0	2	28041
6	-859.72	23149	7225	0.31	1	7	1	9	32461
7	827.33	12167	67565	5.55	2	2	0	9	27555
8	1226.72	15990	57434	3.59	1	2	2	3	29407
9	1614.60	18836	73705	3.91	1	1	2	2	28860
10	4210.05	14583	101677	6.97	4	1	2	1	27642
11	-1216.81	14523	90305	6.22	2	2	2	9	23377
12	-814.00	4765	10665	2.24	2	4	3	1	29947
13	347.74	6298	2011	0.32	1	3	1	1	33749
14	-329.73	13854	26335	1.90	2	1	0	10	30815
15	-1375.50	23885	81937	3.43	3	2	3	0	25474
16	221.05	25575	58171	2.27	1	4	1	3	29934
17	1125.90	14021	30579	2.18	2	2	2	0	31410
18	-348.33	14799	50844	3.44	1	3	1	6	28584
19	-1495.21	2164	2991	1.38	2	4	2	6	30523
20	2610.59	12117	72902	6.02	1	1	1	9	28428
21	1508.66	15684	52912	3.37	0	2	1	1	30529
22	57.79	6983	20778	2.98	1	4	2	3	30271
23	47.57	11214	59297	5.29	1	2	1	1	27199
24	-3157.70	12965	1030	0.08	1	2	1	9	30242
25	1798.47	17508	101077	5.77	0	3	1	4	27069
26	-3092.38	12053	14811	1.23	3	2	3	1	28081
27	-967.19	20917	94634	4.52	3	2	0	2	25581
28	176.49	17327	57769	3.33	1	1	1	6	28769
29	-614.05	20902	47309	2.26	0	2	1	3	29477
30	-158.71	18039	10004	0.55	2	3	1	1	32643
31	803.39	16528	57392	3.47	2	3	0	2	29803
32	-412.44	18638	125938	6.76	2	2	0	6	23177
33	1991.58	27612	112086	4.06	0	4	1	8	28212
34	187.35	13904	60887	4.38	0	3	1	8	28037
35	1086.14	6307	19881	3.15	0	3	1	4	31571
36	-2373.79	14110	69105	4.90	0	4	0	6	25232
37	1151.61	10182	32372	3.18	0	2	1	3	31088
38	-2001.88	16118	18407	1.14	3	1	0	7	30013
39	-286.13	20976	26206	1.25	2	1	1	8	31060
40	4772.45	14126	2526	0.18	1	3	1	1	38261
41	1849.17	17195	41616	2.42	2	4	1	2	32001
42	1503.53	12053	57328	4.76	0	3	0	7	29565
43	-1361.41	8315	38416	4.62	1	1	1	1	27054
44	1684.56	13764	65395	4.75	1	4	1	3	29143
45	-657.61	18087	66401	3.67	3	2	2	5	26866
46	2329.10	21567	65480	3.04	1	1	0	8	31193
47	2425.36	15450	44443	2.88	1	3	0	3	32469
48	-79.61	18844	96408	5.12	0	2	1	10	25713
49	181.34	13376	38985	2.91	1	3	1	6	29988
50	1683.91	22965	116455	5.07	2	4	1	1	26850

Appendix B: Metamodels for Chapter IV

This appendix presents the fitted metamodel and corresponding ANOVA table for each of the three scenarios (low, medium, and high variance). All metamodels were developed using terms with p-values of significance of not greater than .10. Also, all metamodels have p-values for overall significance of the model of not greater than 1 E-17.

Low Variance Scenario: (σ^2_{noise}=100 dollars) (R^2 of Equation = .9993)

$$\hat{y} = 34023.13 - 0.03904 \cdot miles - 794.555 \cdot age - 109.871 \cdot wrecks + 73.591 \cdot appearance - 367.04 \cdot rust - 20.828 \cdot color$$

Regression Statistics					
Multiple R		0.999467035			
R Square		0.998934353			
Adjusted R Square		0.998901224			
Standard Error		98.20757802			
Observations		200			
Analysis of Variance		Sum of	Mean		Significance
	df	Squares	Square	F	of F
Regression	6	1744901549	290816924.8	30152.94089	7.0013E-284
Residual	193	1861432.577	9644.728381		
Total	199	1746762981			
	Coefficients	Std Error	t Statistic	P-value	
Intercept	34023.12747	25.60769733	1328.628929	0	
miles	-0.03903782	0.000368809	-105.848328	6.5876E-177	
age	-794.555046	6.738454719	-117.913539	4.3214E-186	
wrecks	-109.871007	7.451914156	-14.743998	9.70993E-34	
appear	73.591407	4.673888194	15.74522195	8.26041E-37	
rust	-367.036552	9.151668955	-40.1059691	2.71574E-97	
color	-20.8274553	2.339816596	-8.9013196	3.44029E-16	

Medium Variance Scenario: (σ^2_{noise}=1400 dollars) (R^2 of Equation = .7555)

$$\hat{y} = 33984.00 - 0.03807 \cdot miles - 748.549 \cdot age - 474.439 \cdot rust$$

Regression Statistics					
Multiple R		0.869204378			
R Square		0.755516251			
Adjusted R Square		0.751774152			
Standard Error		1619.527333			
Observations		200			
Analysis of Variance		Sum of	Mean		Significance
	df	Squares	Square	F	of F
Regression	3	1588643493	529547831.1	201.8964254	1.09158E-59
Residual	196	514082281.2	2622868.781		
Total	199	2102725775			
	Coefficients	Std Error	t Statistic	P-value	
Intercept	33984.00072	257.3527148	132.0522332	9.3657E-196	
miles	-0.03806599	0.006061683	-6.27977248	2.08872E-09	
age	-748.54866	110.1077442	-6.79832891	1.20514E-10	
rust	-474.439147	146.2709828	-3.243563	0.001384438	

High Variance Scenario: (σ^2_{noise}=4000 dollars) (R^2 of Equation = .3888)

$$\hat{y} = 36065.98 - 0.05975 \cdot miles - 508.371 \cdot age - 840.412 \cdot rust$$

Regression Statistics					
Multiple R		0.623495361			
R Square		0.388746465			
Adjusted R Square		0.369743765			
Standard Error		4115.28689			
Observations		200			
Analysis of Variance		Sum of	Mean		Significance
	df	Squares	Square	F	of F
Regression	6	2078751674	346458612.3	20.45743256	1.75837E-18
Residual	193	3268568135	16935586.19		
Total	199	5347319809			
	Coefficients	Std Error	t Statistic	P-value	
Intercept	36065.98138	1073.064047	33.61027842	5.53761E-84	
miles	-0.05975387	0.015454561	-3.86642286	0.000149508	
age	-508.371356	282.3679692	-1.80038606	0.073314067	
wrecks	-480.637942	312.2647483	-1.53920013	0.125343999	
appear	-250.001362	195.8544463	-1.27646508	0.203278791	
rust	-840.411605	383.4912136	-2.19147551	0.029578142	
color	-123.495297	98.04759221	-1.25954441	0.209309016	

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Vita

Captain John Kent Patterson was born on October 3, 1963 in Clearwater, Florida. He graduated from Oakville Senior High School in St. Louis, Missouri in 1982 and attended the United States Air Force Academy graduating with a Bachelor of Science in Operations Research in May of 1986. Upon graduation he received a regular commission in the USAF and served his first tour of duty at Randolph AFB. He served as the Chief of Production Reports Branch of HQ Recruiting Service. He then volunteered for an assignment to perform missile operations at Malmstrom AFB, Montana. During this tour he held many positions to include those of Senior Evaluator Deputy Commander and Senior Instructor Commander Minuteman II/CDB weapon system. At the completion of this assignment he entered the School of Engineering, Air Force Institute of Technology (AFIT), in August of 1993. Upon competition of his studies at AFIT, he was selected for assignment to HQ ACC Analysis Squadron, Langley AFB, DSN 574-2065.

Permanent Address: 5854 White Pine Dr.
St. Louis, MO, 63129

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13. ABSTRACT *(Maximum 200 words)*

This study investigated the effect on simulation output of repeatedly sampling an embedded metamodel. A metamodel is said to be embedded within a simulation if it is used to replace a submodule of that simulation. Replacing a deterministic module with an embedded deterministic metamodel poses no apparent mathematical problems. However, using a deterministic metamodel to replace a stochastic simulation component could require additional corrective actions. This research was perfromed in two phases. The first phase dealt with a set of tandem queues. It was shown that as each queue was sequentially replaced with a metamodel, the total system variance was inappropriately diminished. A theoretical model of the error components was postulated and used to compensate for this missing variation, restoring the parent simulation's variance to approximately its original level. In the second phase, the problem was extended to the case of repeatedly sampling an embedded metamodel with similar results. In addition, guidelines for metamodel use were presented. In some situations, sampling from a probability distribution is more appropriate than the use of metamodel.

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	16. PRICE CODE

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