

SIMULATION METAMODELS

Russell R. Barton
Department of Industrial and Manufacturing Engineering
The Pennsylvania State University
University Park, PA 16802 U.S.A.

ABSTRACT

The simulation community has used *metamodels* to study the behavior of computer simulations for over twenty-five years. The most popular techniques have been based on parametric polynomial response surface approximations. In this advanced tutorial, we discuss developments in this area, including alternative metamodel types and experimental designs.

1 INTRODUCTION

Complex computer simulation models of proposed or existing real systems are often used to make decisions on changes to the system design. Analysts use the simulation model as a surrogate because it is impractical to construct multiple prototype versions of the real system, or because cost or other constraints prohibit experimentation with the real system. These models themselves may be quite complex, and so simpler approximations are often constructed; models of the model, or *metamodels* (Kleijnen, 1987).

The mathematical representation of a simulation model input - output function will be represented as

$$\mathbf{y} = \mathbf{g}(\mathbf{v}) . \quad (1)$$

Here, \mathbf{y} and \mathbf{v} are vector valued, and will usually include random components. The \mathbf{v} vector for a manufacturing simulation might include the following components: the number of machines, machine processing times, machine breakdown time probability distribution parameters, and perhaps all the pseudorandom quantities used in the simulation run. The vector \mathbf{y} might include the average work in process, the average daily throughput, and the average daily operating expenses.

Metamodels are typically developed separately for each component of \mathbf{y} , that is, for each coordinate function of \mathbf{g} . We will restrict our attention to input - output models where: i) y has one component, ii) the random component, if present, is additive, and iii) the list of parameters is

restricted to those that will be in the argument list of the metamodel:

$$y = g(\mathbf{x}) + \varepsilon . \quad (2)$$

The metamodeling task involves finding ways to model g and ways to model ε . We will generally denote the metamodel as f and the predicted output responses as $f(\mathbf{x})$ or \hat{y} .

$$g(\mathbf{x}) \approx f(\mathbf{x}) = \hat{y} \quad (3)$$

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 \mathbf{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 model 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, etc.) and choices for the way to pick the 'best' representation from within a family (e.g. least squares, maximum likelihood, cross validation, etc.). The issues of experiment design and metamodel assessment are related since the selection of an experiment design will be determined in part by its effect on assessment issues.

This review will draw from earlier papers (Barton 1992, 1993, 1994), with a focus on the most promising metamodel and experiment design strategies. For an in-depth discussion of metamodel fitting and validation issues, see Kleijnen and Sargent (1997).

The most popular techniques for constructing f have been based on parametric polynomial response surface approximations. While we review recent developments for polynomial metamodels, we also present alternative metamodeling approaches:

- splines,

- radial basis functions,
- neural networks,
- spatial correlation models, and
- frequency-domain approximations.

The paper is organized to cover each of the metamodeling techniques in sequence, beginning with traditional response surface methodology. For more background and additional metamodeling techniques, see Barton (1993).

2 RESPONSE SURFACE METAMODELING

Response surface methods have been used effectively for over thirty years as metamodels. These methods are the topic of entire texts (Box and Draper 1987, Khuri and Cornell 1987, Myers 1976), but our review must be brief.

Polynomial regression models were developed for the 'exploitation' of response surfaces (1), that is, for optimization. This approach fits first or second order polynomial models to y , the system response. The model is of the form (3) with y a scalar and ε a scalar, although these quantities are often viewed as vectors by considering multiple observations simultaneously.

2.1 Mathematical Form for RS Models

Let $\mathbf{y} = (y_1, \dots, y_n)'$ represent a set of (univariate) outputs of the simulation model run under input conditions $\mathbf{x}_1, \dots, \mathbf{x}_n$, respectively. The ε_i for the multiple observations are assumed to be independent, identically distributed Gaussian quantities with variance σ^2 . The basis functions are usually taken as the products of the power functions, 1, x_j, x_j^2, \dots , giving

$$f(\mathbf{x}) = \sum \beta_k p_k(\mathbf{x}) \quad (4)$$

Here $p_k(\mathbf{x})$ is a product of univariate power functions, such as $(x_1), (x_1)^2, (x_3)^2(x_4)$, etc. Alternatively, the basis may be orthogonal polynomials, $\varphi_k(\mathbf{x})$, providing the same polynomial for f but a different representation:

$$f(\mathbf{x}) = \sum \alpha_k \varphi_k(\mathbf{x}) . \quad (5)$$

The coefficients β_k or α_k are estimated from observed (\mathbf{x}_i, y_i) data points, $i = 1, \dots, n$ via least squares or maximum likelihood estimation, which are identical procedures for Gaussian errors. The resulting estimates can be thought of as random quantities that depend on the random observations. The advantage of (5) over (4) is that the coefficient estimates for the α_k 's will be uncorrelated and will be robust to small changes in the observed data.

2.2 Design of Experiments for RS Models

The recent developments for polynomial response surface models have been in the area of experimental design. To introduce these advances, we first describe the design problem. The coefficient vector $\boldsymbol{\beta}$ in (4) is determined by

$$\boldsymbol{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} , \quad (6)$$

where $\mathbf{X} = (\mathbf{1}, \mathbf{x}_1, \dots, \mathbf{x}_n)$ for a first degree (linear) polynomial, and includes products of these columns for higher order polynomials. From (2), we see that, since \mathbf{y} is a random vector, $\boldsymbol{\beta}$ will be random.

Some recent research relates to two properties of $\boldsymbol{\beta}$. First, one would like to minimize the variance of $\boldsymbol{\beta}$. This will make the approximating function f less sensitive to the random perturbations introduced by ε . Second, one may want to estimate some of the coefficients in the $\boldsymbol{\beta}$ vector without making the number of simulation runs needed to estimate all of the coefficients in $\boldsymbol{\beta}$. By leaving terms out of the metamodel (4), the fitting process may produce biased estimates for the remaining coefficients. Both of these properties are affected by the choice of the experimental design strategy. Each is discussed briefly below.

With independent ε_i values the variance-covariance matrix for the coefficient vector $\boldsymbol{\beta}$ is

$$\sum_{\boldsymbol{\beta}} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1} . \quad (7)$$

When the ε_i values are dependent, with covariance matrix \sum_{ε} , the variance-covariance matrix for $\boldsymbol{\beta}$ is

$$\sum_{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\sum_{\varepsilon}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} . \quad (8)$$

Schruben and Margolin (1978) exploited (8) to produce a reduced variance-covariance matrix for $\boldsymbol{\beta}$ by inducing correlation in the ε_i values. The Schruben-Margolin strategy induces positive correlation between runs within a block, and negative correlations between blocks. The usual statistical analysis must be modified for this strategy, as described by Nozari, Arnold, and Pegden (1987) and Tew and Wilson (1992). Tew and Crenshaw (1990) and Tew (1994) discuss the implications when *all* of the random number streams are used as common or antithetic streams across the experiment (no pure error term remains), and Tew and Wilson (1994) discuss combined variance reduction strategies.

The second experiment design issue receiving attention in simulation designs is bias. If there is concern that higher order terms may be present in (2) that are not modeled in (4), then simulation runs over the design space must be chosen differently. Donohue, Houck and Myers (1993) develop two-level factorial designs that protect

against bias in the presence of polynomials of order two. Optimal designs are found for three pseudorandom number generation strategies: independent streams, common random numbers, and Schruben/Margolin CRN/ARN in orthogonal blocks.

Donohue, Houck and Myers (1995) discuss both variance and bias in fitting quadratic models for response surface studies, extending the Schruben and Margolin and Tew and Wilson work. They present four types of low variance and low bias designs for response surface estimation: 3^k factorials, central composite designs, Box-Behnken designs, and small composite designs.

Response surface metamodels for discrete event simulation models must often contend with nonhomogeneous variance. Cheng and Kleijnen (1994) develop optimal design of experiments for fitting metamodels when the response is some output function of a nearly saturated queue. Kleijnen and Van Groenendaal (1994) develop sequential experimental designs for weighted least squares regression metamodels.

3 SPLINE METAMODELS

Any polynomial approximation represented by (4) can be constructed from linear combinations of the functions $\prod x_{jk}$, where the product is over k , and the index j_k may take the same value more than once. This choice for a basis has drawbacks, as mentioned earlier.

The high order polynomial achieves a good fit by adjusting coefficients to achieve cancellation of large oscillations over most of the range. This reliance on cancellation makes high order polynomial fits non-robust. If a quadratic approximation to the function is adequate, then global polynomial basis functions can be used to build the approximating metamodel. If a more accurate representation is needed, the simulation modeler should consider other basis functions from which to build the metamodel.

Spline models have been used widely for approximation of deterministic simulation responses. Myers et al. (1996) describe the use of splines for linking submodels for system-level design, using the aerospace design software ASTROS (Neill et al. 1990).

3.1 Mathematical Form for Spline Models

The difficulties with polynomial basis functions are avoided if: i) they are applied to a small region and, ii) only low order polynomials are used. This is the motivation for metamodels based on piecewise polynomial basis functions. When continuity restrictions are applied to adjacent pieces, the piecewise polynomials are called splines. The (univariate) metamodel can be written as

$$f(x) = \sum c_j B_j(x) \quad (9)$$

where the B_j are the quadratic or cubic piecewise polynomial basis functions. The basis functions can be described most simply for the univariate case. The domain is divided into intervals $[t_1, t_2), [t_2, t_3) \dots [t_{n-1}, t_n)$ whose endpoints are called knots. Two sets of spline basis functions are commonly used, the truncated power function basis and the B-spline basis (deBoor 1978).

Since most simulation model output functions will not be deterministic, interpolating splines will not be satisfactory. The motivation for *smoothing splines* is based on an explicit tradeoff between the fit/accuracy of the approximation at known points and smoothness of the resulting metamodel. The fit term is represented as a sum of squared differences of the metamodel and simulation model responses at each of the experimental runs. The smoothness is represented by an integral of the square of some derivative over the region of validity of the metamodel. The relative weight of these objectives is captured by the smoothing parameter, λ : $\lambda = 0$ provides interpolation with no constraint on smoothness. The function that minimizes this quantity will be a spline of order k , which is in C^{k-2} (continuous derivatives up to the $(k-2)^{\text{th}}$ derivative) and is a piecewise polynomial with terms up to x^{k-1} . The knots will occur at points in x corresponding to the observed data, x_j .

An important issue is the selection of the value for the smoothing parameter λ . The value may be chosen by visual examination of the fit, or by minimizing cross validation (like residual sum of squares), or generalized cross validation (GCV) (an adjusted residual sum of squares). Eubank (1988) and Craven and Wahba (1979) discuss these approaches.

Three classes of spline metamodels can be described as solutions to special cases of this smoothness vs. fit tradeoff: spline smoothing, spline interpolation (described earlier), and least squares or regression splines. The key differences are summarized below.

Smoothing Splines: k is chosen by the user, knots are not pre-specified, but they will occur at the x_j values in the optimal solution (i.e., $t_j = x_j$), λ can be chosen based on the user's preference or by generalized cross validation.

Spline Interpolation: k is chosen by the user, knots are not pre-specified, but they will occur at the x_j values in the optimal solution, $\lambda = 0$.

Regression Splines: k is chosen by the user, preferably near local maxima/minima and inflection points, knots are chosen by the user, $\lambda = 0$.

3.2 Multivariate Splines

The extension of the univariate spline metamodels to multivariate situations has been an active area of recent research. Tensor products of univariate splines can be used for multivariate metamodels (deBoor 1978). Tensor product approximation requires a full factorial experiment

design to estimate the parameters of the metamodel. Univariate splines are fit for each factor, for each level of every other factor. There is no requirement for either equal numbers of levels across all design factors, or equal spacing within one factor. Because tensor product splines require many experimental runs on a complete rectangular grid, and because there are numerical difficulties in calculating the spline coefficients for metamodels with many input parameters, several alternative multivariate spline models have been proposed. Interaction splines were presented by Wahba (1986). These models are linear combinations of products of at most two univariate splines.

Multivariate Adaptive Regression Spline (MARS) models (Friedman 1990) use a stepwise procedure to recursively partition the simulation input parameter space. The univariate product degree and the knot sequences are determined in a stepwise fashion based on the GCV score. The Π model (Breiman 1991) also uses a stepwise procedure for selecting a linear combination of products of univariate spline functions to be included in the metamodel. For all of these regression spline methods, the authors assume that the set of data values $\{(\mathbf{x}_i, y_i)\}$ to be fit are given. There is no discussion about the design of the simulation experiment to provide the best fit of f to g over some region of interest.

4 RADIAL BASIS FUNCTION METAMODELS

Radial basis functions (RBF) provide an alternative approach to multivariate metamodeling. In an empirical comparison, Franke (1982) found radial basis functions to be superior to thin plate splines, cubic splines and B-splines, and several others. Tu and Barton (1997) found them to provide effective metamodels for electronic circuit simulation models.

4.1 Mathematical Form for RBF Models

The original development by Hardy (1971) introduced, among others, simple 'multiquadric' basis functions

$$f(\mathbf{x}) = \sum a_i \|\mathbf{x} - \mathbf{x}_i\|, \quad (10)$$

where the sum is over the observed set of system responses, $\{(\mathbf{x}_i, y_i)\}$ and $\|\cdot\|$ represents the Euclidean norm. The coefficients a_i are found simply by replacing the left hand side of (10) with $g(\mathbf{x}_i)$, $i = 1, \dots, n$, and solving the resulting linear system.

4.2 Design of Experiments for RBF Models

Unfortunately, the condition number of the linear system deteriorates rapidly with increasing dimension and increasing numbers of data values to be fitted. Also, since this is an interpolation method, its direct application to

simulation metamodeling is limited. Dyn, Levin, and Rippa (1986) and Dyn (1987) solve both of these problems by finding effective preconditioners for the linear system, and by executing only the first few iterative steps in solving the system of equations to provide a smooth fit to noisy data.

The issue of solvability has been addressed recently by Ball et al. (1992) and Sun (1993). Ball et al. provide upper and lower bounds on the l_2 norm of the matrix of equation coefficients (Hardy matrix), and Sun gives necessary and sufficient conditions on the location of the design points for the Hardy matrix to be nonsingular.

Radial basis functions also arise for a class of spline functions. The so called thin plate splines have radial basis functions of $\|\mathbf{x} - \mathbf{x}_i\|^2 \log \|\mathbf{x} - \mathbf{x}_i\|$. Like smoothing splines, the radial basis functions, as well as their coefficients in the metamodel, depend on the location of the observed values \mathbf{x}_i .

5 NEURAL NETWORK METAMODELS

Neural networks can be thought of as flexible parallel computing devices for producing responses that are complex functions of multivariate input information. They can approximate arbitrary smooth functions and can be fitted using noisy response values. Neural networks are networks of numerical processors, whose inputs and outputs are linked according to specific topologies. For an introduction to neural networks, see Lippman (1987), Wasserman (1989) or Måsson and Wang (1990). There is a brief overview by Wilson and Sharda (1992). Networks used for function approximation are typically multi-layer feedforward networks. Feedforward layered networks have the flexibility to approximate smooth functions arbitrarily well, provided sufficient nodes and layers. This follows from the work of Kolmogorov (1961) whose results imply that any continuous function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ can be exactly reproduced over a compact subset by a three-layer feedforward network. While there are some approximation schemes using three layers, most approximations use a two layer network structure, with a single output node for models having a univariate dependent variable.

The overall metamodel is then a linear combination of linear or nonlinear functions of the argument vector \mathbf{x} .

Strictly speaking, neural networks are assumed to use functions that are threshold functions. It is useful to allow more general functions, however and to think of neural networks as a technique for computing metamodel coefficients and predicted values rather than as representing a particular class of modeling techniques. All of the metamodels discussed in this paper can be implemented using a neural network structure.

6 SPATIAL CORRELATION METAMODELS

Sacks, Welch, Mitchell, and Wynn (1989) and numerous references therein develop a *spatial correlation* parametric regression modeling approach that shares some common features with spline smoothing and kernel metamodeling. The expected smoothness of the function is captured in a spatial correlation function. Spatial correlation models, also called kriging models, have recently become popular for deterministic simulation metamodels (Simpson et al. 1998, Trosset and Torczon 1997, Karimi, Booker and Mong 1996).

6.1 Mathematical Form for Spatial Models

The model assumption is

$$y(\mathbf{x}) = g(\mathbf{x}) + Z(\mathbf{x}). \quad (11)$$

Z is assumed to be a Gaussian stochastic process with spatial correlation function

$$\text{Cov}(Z(\mathbf{u}), Z(\mathbf{v})) = R(\mathbf{u}, \mathbf{v}) = \exp(-\sum \theta_j (u_j - v_j)^p). \quad (12)$$

The value of p is sometimes fixed at 2, and $g(\mathbf{x})$ is usually approximated by a constant, or a linear function of \mathbf{x} . The values θ_j are estimated by maximum likelihood, and are used to calculate approximate expected values of (12) to provide the metamodel $f(\mathbf{x})$. This metamodel family has been used to model deterministic simulation models, but Sacks, et al. suggest the addition of a stochastic term for nondeterministic simulation metamodeling. Mitchell and Morris (1992) discuss this extension, as well as other correlation functions.

6.2 Design of Experiments for Spatial Correlation Metamodels

Currin et al. (1991) discuss the design of simulation experiments for estimating the p and θ_j parameters in (12). Factorial designs are not appropriate for fitting these parameters. In the case of a factorial design on r factors, if there are fewer than r factors active in the model, the design will be projected effectively on the remaining factors, giving duplicate points. For the spatial correlation model, this leads to difficulties: the covariance matrix R will not be full rank, and the likelihood function will be impossible to maximize. Latin hypercube designs avoid this problem, but often provide a poor coverage of the space. Sacks, et al. (1989) consider initial Latin hypercube experiment designs followed by the sequential addition of points to minimize mean squared error integrated over the region of interest.

The spatial correlation model provides a very good fit with relatively small designs. Orthogonal arrays of

strength r (Owen 1992) are an attractive class of sparse designs because they provide balanced (full factorial) designs for any projection onto r factors.

Alternative approaches to improve on the coverage of Latin hypercube designs are proposed by Handcock (1992), Salagame and Barton (1993) and Corsten and Stein (1994). All are hierarchical designs, in which the design space is first subdivided into regions to maintain balance, and sub-designs are constructed for a subset of the regions.

Morris et al. (1993) expand the spatial correlation model to consider the case where function and derivative information is available. Considered example with Latin hypercube, D -optimal, and two hybrid design procedures designed to have the properties of both Latin hypercube and D -optimality. One of the hybrid methods provided the smallest prediction error.

7 FREQUENCY DOMAIN METAMODELS

Viewing variations of g over its domain in terms of spatial correlation leads naturally to the idea of Fourier basis functions for representing an approximation to g in (2). While such an approach is possible, it is prone to difficulties (as is the global polynomial model) because the Fourier decomposition is based on basis functions with global support. Close approximations of g by a metamodel using a Fourier basis depends heavily on cancellation to achieve the desired form, which may result in a lack of robustness.

This is less of an issue when modeling dynamic phenomena. Schruben and Cogliano (1987) use Fourier decomposition to determine steady state input output structure by deliberately varying input parameters sinusoidally. There have been a series of papers since then discussing the design of experiments for this class of metamodels (see for example Morrice 1991, Buss 1990, Jacobson et al. 1992, and Morrice and Schruben 1993).

For static metamodels, wavelet basis functions provide a decomposition in both location and frequency, providing local rather than global basis functions. The wavelet basis elements have finite support, and are adjusted by dilation factors to achieve a good fit (Daubechies 1988). This methodology is still in the early stages of development. At present, applications of wavelet models have been limited to functions of one or two variables; in particular, to the construction of a smoothed visual image from noisy image intensity data.

8 CONCLUSION

Developments for both response surface models and nontraditional models provide increased efficiency and applicability for these methods. In particular, recent work in the areas of spatial correlation and radial basis functions has clarified the importance of experimental design for

non-traditional models. While the fitting capability of these alternative methods is exciting, at the present time it is based on a small set of examples (see Ilgenstein and Sargent 1994, and Laslett 1994). A more extensive computational comparison of the methods is needed, but this will have to wait for more generally available computer codes for the newer metamodeling methods.

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AUTHOR BIOGRAPHY

RUSSELL R. BARTON is a Professor in the Department of Industrial and Manufacturing Engineering at The Pennsylvania State University. He received a B.S. in electrical engineering from Princeton University in 1973 and a Ph.D. in operations research from Cornell University in 1978. His current research interests include graphical methods for experiment design, optimization and metamodeling methods for simulation models, and statistical issues in modeling manufacturing yield.