METAMODELS FOR COMPUTER-BASED ENGINEERING DESIGN: SURVEY AND RECOMMENDATIONS

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ABSTRACT

The use of statistical techniques to build approximations of expensive computer analysis codes pervades much of today's engineering design. These statistical approximations, or metamodels, are used to replace the actual expensive computer analyses, facilitating multidisciplinary, multiobjective optimization and concept exploration. In this paper we review several of these techniques including design of experiments, response surface methodology, Taguchi methods, neural networks, inductive learning, and kriging. We survey their existing application in engineering design and then address the dangers of applying traditional statistical techniques to approximate *deterministic* computer analysis codes. We conclude with recommendations for the appropriate use of statistical approximation techniques in given situations and how common pitfalls can be avoided.

1 INTRODUCTION

Much of today's engineering analysis consists of running complex computer codes: supplying a vector of design variables (inputs) $\mathbf{x}$ and computing a vector of responses (outputs) $\mathbf{y}$. Despite steady advances in computing power, the expense of running many analysis codes remains non-trivial; single evaluations of aerodynamic or finite-element analyses can take minutes to hours, if not longer. Moreover, this mode of query-and-response often leads to a trial and error approach to design whereby a designer may never uncover the functional relationship between $\mathbf{x}$ and $\mathbf{y}$ and therefore never identify the "best" settings for input values.

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Statistical techniques are widely used in engineering design to address these concerns. The basic approach is to construct *approximations* of the analysis codes that are more efficient to run and yield insight into the functional relationship between $\mathbf{x}$ and $\mathbf{y}$. If the true nature of a computer analysis code is

$$y = f(\mathbf{x}),$$

then a "model of the model" or *metamodel* [62] of the analysis code is

$$\hat{y} = g(x), \text{ and so } y = \hat{y} + \varepsilon$$

where ε represents both the error of approximation and measurement (random) errors. The most common metamodeling approach is to apply the design of experiments (DOE) to identify an efficient set of computer runs ($\mathbf{x}_1$, $\mathbf{x}_2$, ..., $\mathbf{x}_n$) and then use regression analysis to create a polynomial approximation of the computer analysis code. These approximations then can *replace* the existing analysis code while providing:

- a better understanding of the relationship between $\mathbf{x}$ and $\mathbf{y}$,
- easier integration of domain dependent computer codes, and
- fast analysis tools for optimization and exploration of the design space by using approximations in lieu of the computationally expensive analysis codes themselves.

We have found that many applications (including our own) using these methods for computer-based design are statistically questionable because many analysis codes are *deterministic* in which the error of approximation is *not* due to random effects. This calls into question the subsequent statistical analyses of model significance. Consequently, we seek to highlight potential statistical pitfalls in metamodeling and provide general recommendations for the proper use of metamodeling techniques in computer-based engineering design. In Section 2 we present a review of metamodeling techniques including regression, neural networks, inductive learning, and kriging. We conclude Section 2 with an introduction to the general statistical approaches of response surface methodology and Taguchi's robust design. In Section 3 we describe the engineering design context for statistical applications, review existing applications and methods and conclude

with a closer look at deterministic applications of metamodeling. In Section 4 we present some recommendations for avoiding pitfalls in using metamodeling, and in Section 5 we conclude by discussing some more advanced issues that contribute to making metamodeling an active and interesting research area.

2 REVIEW OF METAMODELING TECHNIQUES

Metamodeling involves (a) choosing an experimental design for generating data, (b) choosing a model to represent the data, and then (c) fitting the model to the observed data. There are several options for each of these steps as shown in Figure 1, and we have attempted to highlight a few of the more prevalent ones. For example, building a neural network involves fitting a network of neurons by means of backpropagation to data which is typically hand selected while Response Surface Methodology usually employs central composite designs, second order polynomials and least squares regression analysis.

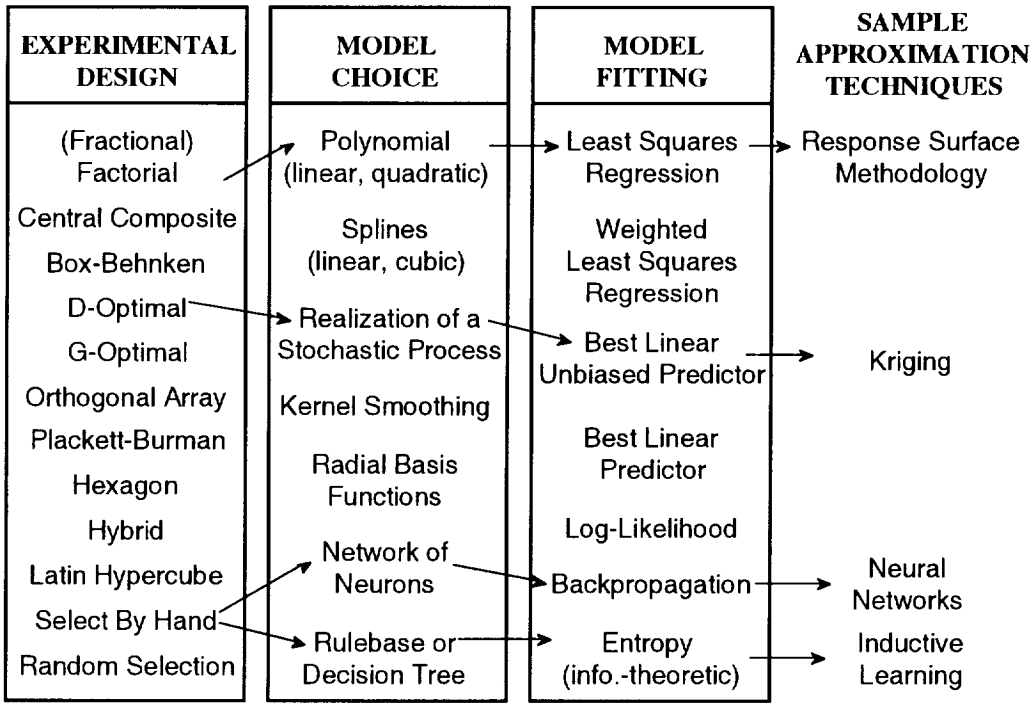


Figure 1. Techniques for Metamodeling

In the remainder of this section we provide a brief overview of several of the options listed in Figure 1. In Section 2.1 the focus is on experimental designs, particularly (fractional) factorial designs, central composite designs and orthogonal arrays. In Section 2.2 we discuss model choice and model fitting, focusing on response surfaces, neural networks, inductive learning and kriging. We conclude with an overview of two of the more common metamodeling techniques, namely, response surface methodology and Taguchi's robust design.

2.1 Experimental Design

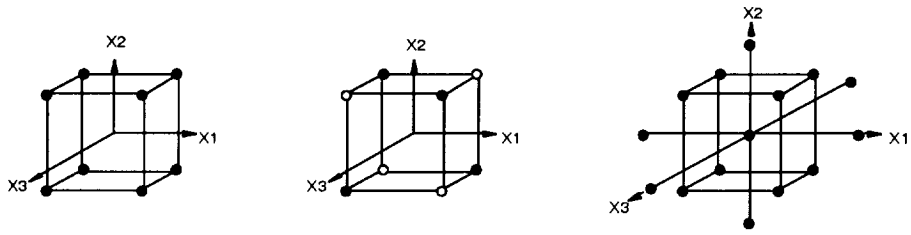
Properly designed experiments are essential for effective computer utilization. In engineering, traditionally a single parameter is varied (perturbed) and the effects are observed. Alternatively, combinations of factor settings are assigned either systematically (e.g., grid search) or randomly to provide an alternative for comparison. Experimental design techniques which were developed for physical experiments are being applied to the design of computer experiments to increase the efficiency of these analyses. In this section an overview of different types of experiment designs is provided along with measures of merit for selecting/comparing different experimental designs.

2.1.1 A Survey of Experimental Designs. An experimental design represents a sequence of experiments to be performed, expressed in terms of *factors* (design variables) set at specified *levels* (predefined values). An experimental design is represented by a matrix $\mathbf{X}$ where the rows denote experiment runs, and the columns denote particular factor settings.

Factorial Designs: The most basic experimental design is a *full factorial design*. The number of design points dictated by a full factorial design is the product of the number of levels for each factor. The most common are 2^k (for evaluating main effects and interactions) and 3^k designs (for evaluating main and quadratic effects and interactions) for k factors at 2 and 3 levels, respectively. A 2^3 full factorial design is shown in Figure 2(a).

The size of a full factorial experiment increases exponentially with the number of factors; this leads to an unmanageable number of experiments. *Fractional factorial designs* are used when experiments are costly and many factors are required. A fractional factorial design is a fraction of a

full factorial design; the most common are $2^{(k-p)}$ designs in which the fraction is $1/2^{(p)}$. A half fraction of the 2^3 full factorial design is shown in Figure 2(b). The reduction of the number of design points in a fractional factorial design is not without a price. The 2^3 full factorial design shown in Figure 2(a) allows estimation of all main effects (x_1, x_2, x_3), all two factor interactions (x_1x_2, x_1x_3 and x_2x_3), as well as the three factor interaction ($x_1x_2x_3$). For the 2^{3-1} fractional factorial indicated by the solid dots in Figure 2(b), the main effects are aliased (or biased) with the two factor interactions. *Aliased effects cannot be estimated independently unless they are known (or assumed) not to exist.*



(a) 2^3 Full Factorial (b) 2^{3-1} Fractional Factorial (c) Composite Design

Figure 2. Basic Three-Factor Designs

Often 2^k and $2^{(k-p)}$ designs are used to identify or *screen* for important factors. When there are many factors, the *sparsity of effects principle* [87] can be invoked whereby the system is assumed to be dominated by main effects and low order interactions. Thus, two level fractional factorial designs are used to "screen" factors to identify those with the greatest effects. The sparsity of effects principle is not always valid, however; Hunter [59] notes that *every* design provides aliased estimates: quadratic and cubic effects, if present, bias the estimates of the mean and main effects when a two level fractional factorial design is used.

One specific family of fractional factorial designs frequently used for screening are two level Plackett-Burman (PB) designs [103]. These are used to study k=n-1 factors in n=4m design points. PB designs in which n is a power of two are called geometric designs and are identical to $2^{(k-p)}$ fractional factorials. If n is strictly a multiple of four, the PB designs are referred to as non-geometric designs and have very messy alias structures. Their use in practical problems is

problematic particularly if the design is saturated (i.e., the number of factors is exactly n-1). If interactions are negligible, however, these designs allow unbiased estimation of all main effects, and require only one more design point than the number of factors; they also give the smallest possible variance [14]. Myers and Montgomery [91] present a more complete discussion of factorial designs and aliasing of effects. Minimum variance and minimum size designs are discussed in Section 2.1.2.

Central Composite and Box-Behnken Designs: To estimate quadratic effects, 3^k or $3^{(k-p)}$ designs can be used but often require an unmanageable number of design points. The most common second order designs, configured to reduce the number of design points, are central composite and Box-Behnken designs.

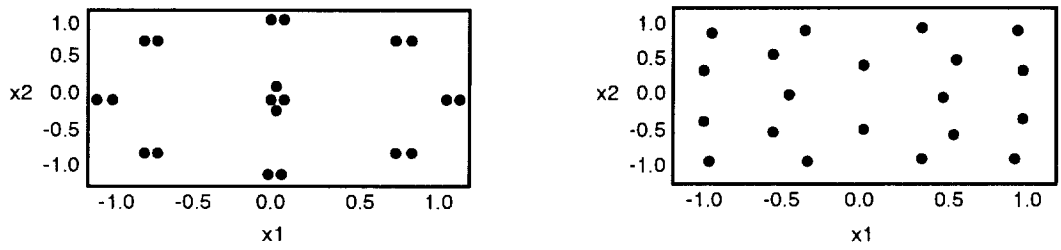
A central composite design (CCD) is a two level ($2^{(k-p)}$ or 2^k) factorial design, augmented by n_0 center points and two "star" points positioned at $\pm\alpha$ for each factor. This design, shown for three factors in Figure 2(c), consists of $2^{(k-p)}+2^k+n_0$ total design points to estimate $2k+k(k-1)/2+1$ coefficients. For three factors, setting $\alpha=1$ locates the star points on the centers of the faces of the cube, giving a face-centered central composite (CCF) design; note that for values of α other than 1, each factor is evaluated at five levels.

Often it is desirable to use the smallest number of factor levels in an experimental design. One common class of such designs is the Box-Behnken designs [15]. These are formed by combining 2^k factorials with incomplete block designs. They do not contain points at the vertices of the hypercube defined by the upper and lower limits for each factor. This is desirable if these extreme points are expensive or impossible to test. More information about CCD and Box-Behnken designs can be found in [87].

Orthogonal Arrays: The experiment designs used by Taguchi, *orthogonal arrays*, are usually simply fractional factorial designs in two or three levels ($2^{(k-p)}$ and $3^{(k-p)}$ designs). These arrays are constructed to reduce the number of design points necessary; two-level L_4, L_{12}, and L_{16} arrays, for example, allow 3, 11, and 15 factors/effects to be evaluated with 4, 12, and 16 design points, respectively. Often these designs are identical to Plackett-Burman designs [78]. The definition of

orthogonality for these arrays and other experiment designs is given in Section 2.1.2. An overview of Taguchi's approach to parameter design is given in Section 2.3.

"Space Filling" Designs: Many researchers advocate the use of "space filling" designs when sampling deterministic computer experiments. As discussed by Booker [13], in the "classical" design and analysis of physical experiments (i.e., using central composite and factorial designs), random variation is accounted for by spreading the sample points out in the design space and by taking multiple data points (replicates), see Figure 3. Sacks, et al. [117] state that the "classical" notions of experimental blocking, replication, and randomization are irrelevant when it comes to deterministic computer experiments; thus, sample points in DACE should be chosen to fill the design space. They suggest minimizing the integrated mean squared error (IMSE) over the design region by using IMSE-optimal designs; the "space filling" design illustrated in Figure 3(b) is an IMSE optimal design.



(a) "Classical" Design (b) "Space Filling" Design

Figure 3. "Classical" and "Space Filling" Designs [adapted from 13]

Koch [63] investigates the use of a modified central composite design which combines half fractions of a CCI and a CCF to more evenly distribute the points throughout the design space. Koehler and Owen [66] describe several Bayesian and Frequentist "space filling" designs, including maximum entropy designs, mean squared-error designs, minimax and maximin designs, Latin hypercubes, randomized orthogonal arrays, and scrambled nets. Minimax and maximin designs were originally proposed by Johnson, et al. [60] specifically for use with computer experiments. Sherwy and Wynn [121] and Currin, et al. [35] use the maximum entropy principle to develop designs for computer experiments. Tang [128] describes orthogonal array-based Latin

hypercubes which he asserts are more suitable for computer experiments than general Latin hypercubes. Park [100] discusses optimal Latin hypercube designs for computer experiments which either minimize IMSE or maximize entropy, spreading the points out over the design region. Morris and Mitchell [89] propose maximin distance designs found within the class of Latin hypercube arrangements since they "offer a compromise between the entropy/maximin criterion, and good projective properties in each dimension." Owen [99] advocates the use of orthogonal arrays as suitable designs for computer experiments, numerical integration, and visualization; a collection of orthogonal array generators is available over the Internet [98]. A review of Bayesian experimental designs for linear and nonlinear regression models is given in [24].

2.1.2 Measures of Merit for Evaluating Experimental Designs. Selecting the appropriate design is essential for effective experimentation: the desire to gain as much information as possible about the response-factor relationships is balanced against the cost of experimentation. Several measures of merit are available and useful for evaluating and comparing experimental designs.

Orthogonality, Rotatability, Minimum Variance, and Minimum Bias: To facilitate efficient estimates of parameters, four desirable characteristics of an experimental design are orthogonality, rotatability, minimum variance, and minimum bias. A design is *orthogonal* if, for every pair of factors x_i and x_j, the sum of the cross-products of the N design points

$$\sum_{u=1}^{N} x_{iu}x_{ju}$$

is zero. For a first order model, the estimates of all coefficients will have minimum variance if the design can be configured so that

$$\sum_{u=1}^{N} x_{iu}^2 = N \ ;$$

the variance of predictions $\hat{y}$ will also have constant variance at a fixed distance from the center of the design, and the design will also be rotatable.

In second order modeling, Hunter [58] suggests that orthogonality is less important: "If the objective of the experimenter is to forecast a response at either present or future settings of $\mathbf{x}$, then an unbiased minimum variance estimate of the forecast $\hat{\mathbf{y}}$ is required. In the late 1950's Box and his co-workers demonstrated that rotatability...and the minimization of bias from higher order terms...were the essential criteria for good forecasting." A design is *rotatable* if $N \bullet Var[\hat{\mathbf{y}}(x)]/\sigma^2$ has the same value at any two locations that are the same distance from the design center. The requirements for *minimum variance* and *minimum bias* designs for second order models are beyond the scope of this work; we refer the reader to [91] for more information.

Unsaturated/Saturated and Supersaturated Designs: In many cases, the primary concern in the design of an experiment is its size. Most designs are *unsaturated* in that they contain at least two more design points than the number of factors. A *saturated* design is one in which the number of design points is equal to one more than the number of factor effects to be estimated. Saturated fractional factorial designs allow unbiased estimation of all main effects with the smallest possible variance and size [14]. The most common examples of saturated designs are the Plackett-Burman two level design and Taguchi's orthogonal arrays. For estimating second order effects, *small composite designs* have been developed to reduce the number of required design points. A small composite design is saturated if the number of design points is $2k+k(k-1)/2+1$ (the number of coefficients to be estimated for a full quadratic model). Myers and Montgomery [91] note that recent work has suggested that these designs may not always be good; additional comments on small composite designs can be found in [16, 77]. Finally, in *supersaturated* designs the number of design points is less than or equal to the number of factors [37, 38].

It is most desirable to use unsaturated designs for predictive models, unless running the necessary experiments is prohibitively expensive. When comparing experiments based on the number of design points and the information obtained, the D-optimal and D-efficiency statistics are often used.

D-optimal and D-efficiency: A design is said to be D-optimal if $|\mathbf{X}'\mathbf{X}|/n^p$ is maximized where $\mathbf{X}$ is the expanded design matrix which has n rows (one for each design setting) and p columns (one

column for each coefficient to be estimated plus one column for the overall mean). The D-efficiency statistic for comparing designs, Eq. (1), compares a design against a D-optimal design, normalized by the size of the matrix in order to compare designs of different sizes.

$$\text{D-efficiency} = (|X'X|_{\text{design}}/|X'X|_{\text{D-optimum}})^{1/p} \tag{1}$$

Other statistics for comparing designs such as G-efficiency, Q-efficiency, and A-optimality have also been formulated, see, e.g., [91]. We now turn to the issues of model choice and model fitting.

2.2 Model Choice and Model Fitting

After selecting an appropriate experimental design and performing the necessary computer runs, the next step is to choose an approximating model and fitting method. Many alternative models and methods exist, but here we review the four which are most prevalent in the literature: response surfaces, neural networks, inductive learning, and kriging.

2.2.1 Response Surfaces. Given a response, y, and a vector of independent factors $\mathbf{x}$ influencing y, the relationship between y and $\mathbf{x}$ is:

$$y = f(\mathbf{x}) + \varepsilon \ , \tag{2}$$

where ε represents random error which is assumed to be normally distributed with mean zero and standard deviation σ. Since the true response surface function $f(\mathbf{x})$ is usually unknown, a response surface $g(\mathbf{x})$ is created to approximate $f(\mathbf{x})$. Predicted values are then obtained using $\hat{\mathbf{y}} = g(\mathbf{x})$.

The most widely used response surface approximating functions are low-order polynomials. For low curvature, a first order polynomial can be used as in Eq. (3); for significant curvature, a second order polynomial which includes all two-factor interactions is available, see Eq. (4).

$$\hat{y} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i \tag{3}$$

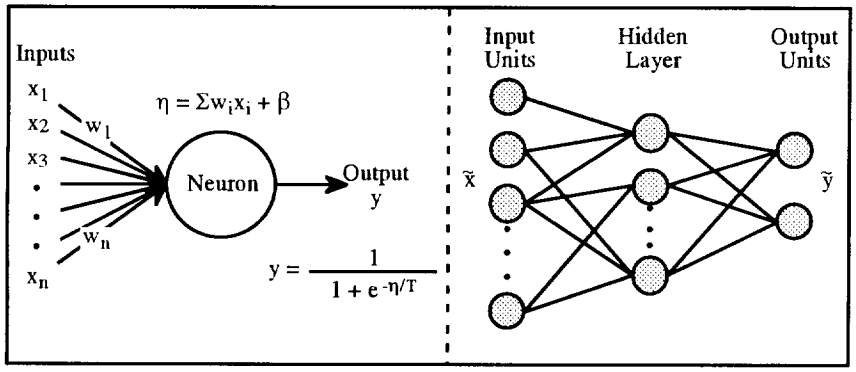
$$\hat{y} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i} \sum_{\substack{j \\ i<j}} \beta_{ij} x_i x_j \tag{4}$$

The parameters of the polynomials in Eq. (3) and Eq. (4) are usually determined by least squares regression analysis by fitting the response surface approximations to existing data. These approximations are normally used for prediction within *response surface methodology (RSM).* A more complete discussion of response surfaces and least squares fitting is presented in [91]. An overview of RSM is given in Section 2.3.

2.2.2 Neural Networks. A neural network is composed of neurons (single-unit perceptrons) which are multiple linear regression models with a nonlinear (typically sigmoidal) transformation on y. If the inputs to each neuron are denoted $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$, and the regression coefficients are denoted by the weights, w_i, then the output, y, might be given by

$$y = \frac{1}{1 + e^{-\eta/T}} \tag{5}$$

where $\eta = \Sigma w_i x_i + \beta$ (where β is the "bias value" of a neuron), and T is the slope parameter of the sigmoid defined by the user. A *neural network* is then created by assembling the neurons into an architecture; the most common of which is the multi-layer feedforward architecture, see Figure 4.



(a) Single-Unit Perceptron (b) Feedforward Two-layer Architecture

Figure 4. Typical Neuron and Architecture

There are two main issues in building a neural network: (1) specifying the architecture and (2) training the neural network to perform well with reference to a training set. "To a statistician, this is equivalent to (i) specifying a regression model, and (ii) estimating the parameters of the model

given a set of data" [30]. If the architecture is made large enough, a neural network can be a nearly universal approximator [115]. Hajela and Berke [54] review the use of neural networks in structural analysis and design.

"Training" a neural network is the determination of the proper values for all weights, w_i, in the architecture and is usually done by backpropagation [115]; this requires a set of n training data points $\{(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2), \ldots, (\mathbf{x}_p,y_p)\}$. For a network with output y, the performance is

$$E = \sum_p (y_p - \hat{y}_p)^2 \tag{6}$$

where $\hat{\mathbf{y}}_p$ is the output that results from the network given input $\mathbf{x}_p$, and E is the total error of the system. The weights are then adjusted in proportion to

$$\frac{\partial E}{\partial y}\frac{\partial y}{\partial w_{ij}}. \tag{7}$$

Neural networks are best suited for approximating deterministic functions in regression-type applications. "In most applications of neural networks that generate regression-like output, there is no explicit mention of randomness. Instead, the aim is function approximation" [30]. Typical applications of neural nets are speech recognition and handwritten character recognition where the data is complex and of high dimensionality. Networks with tens of thousands of parameters have been used but the requisite gathering of training data and calculation of model parameters can be extremely computationally expensive. Cheng and Titterington [30] comment that "...the procedure is to toss the data directly into the NN software, use tens of thousands of parameters in the fit, let the workstation run 2-3 weeks grinding away doing the gradient descent, and *voilá,* out comes the result." Rogers and LaMarsh [111] describe parallel computing efforts aimed at reducing the time required to "train" neural networks.

2.2.3 Inductive Learning. Inductive learning is one of five main paradigms of machine learning that also include neural networks, case-based learning, genetic algorithms, and analytic learning [68]. Of these five, inductive learning is the most akin to regression and metamodeling and is therefore the focus here. An inductive learning system induces rules from examples; the

fundamental modeling constructs are condition-action rules which partition the data into discrete categories and can be combined into decision trees for ease of interpretation, see Figure 5.

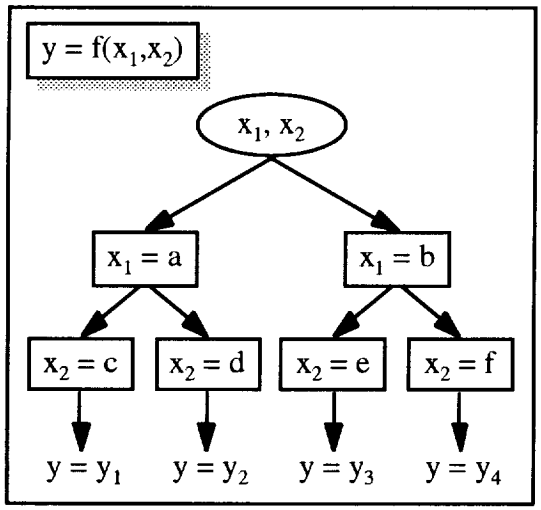


Figure 5. A Decision Tree

Training data are required in the form $\{(\mathbf{x}_1,y_1),(\mathbf{x}_2,y_2), \ldots, (\mathbf{x}_n,y_n)\}$ where $\mathbf{x}_i$ is a vector of attribute values (e.g., processing parameters and environmental conditions), and each y_i is a corresponding observed output value. Although attributes and outputs can be real-valued, the method is better suited to discrete-valued data; real values must often be transformed into discrete representations [41]. Once the data has been collected, training algorithms build a decision tree by selecting the "best" divisive attribute and then recursively calling the resulting data subsets. Although trees can be built by selecting attributes randomly, it is more efficient to select attributes that minimize the amount of information needed for category membership. The mathematics of such an information-theoretic approach are given in [41].

Many of the applications of inductive learning have been in process control and diagnostic systems, and inductive learning approaches can be used to automate the knowledge-acquisition process of building expert systems. Furthermore, although decision trees appear best suited for applications with discrete input and output values, there are also applications with continuous variables that have met with greater success than standard statistical analysis. Leech [71] reports a process-control application where "Standard statistical analysis methods were employed with

limited success. Some of the data were non-numerical, the dependencies between variables were not well understood, and it was necessary to simultaneously control several characteristics of the final product while working within system constraints. The results of the statistical analysis, a set of correlations for each output of interest, were difficult for people responsible for the day-to-day operation to interpret and use." Additional examples can be found in [41, 68].

2.2.4 Kriging. Since many computer analysis codes are deterministic and therefore not subject to measurement error, the usual measures of uncertainty derived from least-squares residuals have no obvious meaning (cf., [117]). Consequently, some statisticians (see, e.g., [13, 66, 117, 138]) have suggested modeling responses as a combination of a polynomial model plus departures of the form:

$$y(\mathbf{x}) = f(\mathbf{x}) + Z(\mathbf{x}) \tag{8}$$

where $y(\mathbf{x})$ is the unknown function of interest, $f(\mathbf{x})$ is a known polynomial function of $\mathbf{x}$, and $Z(\mathbf{x})$ is the realization of a normally distributed Gaussian random process with mean zero, variance σ^2, and non-zero covariance. The $f(\mathbf{x})$ term in Eq. (8) is similar to the polynomial model in a response surface and provides a "global" model of the design space; in many cases $f(\mathbf{x})$ is simply taken to be a constant term, see, e.g., [117, 139].

While $f(\mathbf{x})$ "globally" approximates the design space, $Z(\mathbf{x})$ creates "localized" deviations so that the kriging model interpolates the n_s sampled data points. The covariance matrix of $Z(\mathbf{x})$ is given by:

$$\mathrm{Cov}[Z(\mathbf{x}^i),Z(\mathbf{x}^j)] = \sigma^2\, \mathbf{R}([R(\mathbf{x}^i,\mathbf{x}^j)]. \tag{9}$$

where $\mathbf{R}$ is the correlation matrix, and $R(\mathbf{x}^i,\mathbf{x}^j)$ is the correlation function between any two of the n_s sampled data points $\mathbf{x}^i$ and $\mathbf{x}^j$. $\mathbf{R}$ is a (n_s x n_s) symmetric matrix with ones along the diagonal. The correlation function $R(\mathbf{x}^i,\mathbf{x}^j)$ is specified by the user; Sacks, et al. [117] and Koehler and Owen [66] discuss several correlation functions which may be used. In our work, we have employed a Gaussian correlation function of the form:

$$R(\mathbf{x}^i,\mathbf{x}^j) = \exp[-\sum_{k=1}^{n_s}\theta_k\left|x_k^i - x_k^j\right|^2] \tag{10}$$

where θ_k are the unknown correlation parameters used to fit the model, and the x_k^i and x_k^j are the k^{th} components of sample points $\mathbf{x}^i$ and $\mathbf{x}^j$. In some cases using a single correlation parameter gives sufficiently good results, see, e.g., [94, 117].

Predicted estimates, $\hat{y}(\mathbf{x})$, of the response $y(\mathbf{x})$ at untried values of $\mathbf{x}$ are given by:

$$\hat{y} = \hat{\beta} + \mathbf{r}^T(\mathbf{x})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{f}\hat{\beta}) \tag{11}$$

where $\mathbf{y}$ is the column vector of length n_s which contains the values of the response at each sample point, and $\mathbf{f}$ is a column vector of length n_s which is filled with ones when $f(\mathbf{x})$ is taken as a constant. In Eq. (11), $\mathbf{r}^T(\mathbf{x})$ is the correlation vector of length n_s between an untried $\mathbf{x}$ and the sampled data points $\{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^{ns}\}$ and is given by:

$$\mathbf{r}^T(\mathbf{x}) = [R(\mathbf{x},\mathbf{x}^1), R(\mathbf{x},\mathbf{x}^2), \ldots, R(\mathbf{x},\mathbf{x}^{ns})]^T \tag{12}$$

In Eq. (11), $\hat{\beta}$ is estimated using Eq. (13).

$$\hat{\beta} = (\mathbf{f}^T\mathbf{R}^{-1}\mathbf{f})^{-1}\mathbf{f}^T\mathbf{R}^{-1}\mathbf{y}. \tag{13}$$

The estimate of the variance, $\hat{\sigma}^2$, from the underlying global model (not the variance in the observed data) is given by

$$\hat{\sigma}^2 = \frac{(\mathbf{y} - \mathbf{f}\hat{\beta})^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{f}\hat{\beta})}{n_s} \tag{14}$$

where $f(\mathbf{x})$ is assumed to be the constant $\hat{\beta}$. The maximum likelihood estimates (i.e., "best guesses") for the θ_k in Eq. (10) used to fit the model are found by maximizing [13]:

$$-\frac{[n_s \ln(\hat{\sigma}^2) + \ln|\mathbf{R}|]}{2} \tag{15}$$

for $\theta_k > 0$ where both $\hat{\sigma}^2$ and $|\mathbf{R}|$ are both functions of θ_k. While any values for the θ_k create an interpolative approximation model, the "best" kriging model is found by solving the k-dimensional unconstrained nonlinear optimization problem given by Eq. (15).

Depending on the choice of correlation function in Eq. (10), kriging can either "honor the data," providing an exact interpolation of the data, or "smooth the data," providing an inexact interpolation [34]. Finally, it should be noted that kriging is different from fitting splines (i.e., non-parametric regression models). In several comparative studies kriging performs as well as, if not better than, splines [69].

2.2.4 Additional Metamodeling Approaches. For the reader's convenience, we include references for some alternative metamodeling techniques which have not been discussed in the previous subsections. Rasmussen [106] offers an accumulated approximation technique for structural optimization which refines the approximation of objective and constraint functions by accumulating the function values of previously visited points. Similarly, Balling and Clark [4] describe weighted and gradient-based approximations for use with optimization which utilize weighted sums of exact function values at sample points. Friedman [45] describes multivariate adaptive regression splines (MARS): a flexible regression modeling method based on recursive partitioning and spline fitting for high dimensional data. Dyn, et al. [39] use radial basis functions to build global approximation surfaces to interpolate smooth data. Wang, et al. [137] present multivariate Hermite approximations for multidisciplinary design optimization which uses data generated during the course of iterative optimization; it is compared against linear, reciprocal, and other standard approximations but shows inefficiencies because it requires more data points. Finally, Friedman and Steutzle [46] introduce projection pursuit regression which works well in high-dimensional (< 50) data and with large data sets (can handle 200,000+ data points); project pursuit regression takes the data and generates different projections of it along linear combinations of the variables; an optimizer finds the best projections and builds a predictor by summing them together with arbitrary levels of precision.

This concludes our discussion on experimental design, model selection and model fitting. We now turn to more general methods for experimental design and modeling building.

2.3 Experimentation and Metamodeling Strategies

Two widely used methods incorporating experimental design, model building, and prediction are response surface methodology and Taguchi's robust design or parameter design. A brief overview of these two approaches is provided.

2.3.1 Response Surface Methodology (RSM). Different authors describe RSM differently. Myers, et al. [90] define RSM as "a collection of tools in design or data analysis that enhance the exploration of a region of design variables in one or more responses." Box and Draper [16] state that, "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." Finally, Myers and Montgomery [91] state that RSM "is a collection of statistical and mathematical techniques useful for developing, improving, and optimizing process. It also has important applications in the design, development, and formulation of new products, as well as in the improvement of existing product designs."

The "collection of statistical and mathematical techniques" of which these authors speak refers to the design of experiments (Section 2.1), least squares regression analysis and response surface model building (Section 2.2.1), and "model exploitation," exploring a factor space seeking optimum factor settings. The general RSM approach includes all or some of the following steps:

i) *screening:* when the number of factors is large or when experimentation is expensive, screening experiments are used to reduce the set of factors to those that are most influential to the response(s) being investigated;

ii) *first order experimentation:* when the starting point is far from the optimum point or when knowledge about the space being investigated is sought, first order models and an approach

such as steepest ascent are used to "rapidly and economically move to the vicinity of the optimum" [88];

iii) *second order experimentation:* after the best solution using first order methods is obtained, a second order model is fit in the region of the first order solution to evaluate curvature effects and to attempt to improve the solution.

A more detailed description of RSM techniques and tools can be found in [91], and a comprehensive review of RSM developments and applications from 1966-1988 is given in [90]. In Section 3 we review recent applications in aerospace and mechanical engineering design, but first we discuss Taguchi's robust design approach.

2.3.2 Taguchi's Robust Design. Genichi Taguchi developed an approach for industrial product design built on statistically designed experiments. Taguchi's robust design for quality engineering includes three steps: *system design, parameter design, and tolerance design* [18]. The key step is parameter design within which statistical experimentation is incorporated.

Rather than simply improving or optimizing a response value, the focus in parameter design is to identify factor settings that minimize variation in performance and adjust the mean performance to a desired target in order to minimize the associated loss. Factors included in experimentation include *control factors* and *noise factors*; control factors are set and held at specific values, while noise factors cannot be controlled, e.g., shop floor temperature. The evaluation of mean performance and performance variation is accomplished by "crossing" two orthogonal arrays (Section 2.1.1). Control factors are varied according to an inner array, or "control", array, and for each run of the control array, noise factors are varied according to an outer, or "noise", array. For each control factor experiment, a response value is obtained for each noise factor design point. The mean and variance of the response (measured across the noise design points) are calculated. The performance characteristic used by Taguchi is a *signal-to-noise (S/N)* ratio defined in terms of the mean and variance of the response. Several alternate *S/N* ratios are available based on whether lower, higher, or nominal response values are desired, see, e.g., [112].

The Taguchi approach does not explicitly include model building and optimization. Analysis of experimental results is used to identify factor effects, to plan additional experiments, and to set factor values for improved performance. A comprehensive discussion of the Taguchi approach is given in [102, 112]. Taguchi methods have been used extensively in engineering design and are often incorporated within traditional RSM for efficient, effective, and *robust* design [91]. These applications and their implications for engineering design are discussed next.

3 METAMODELING IN ENGINEERING DESIGN

How are the metamodeling techniques of the previous section employed in engineering design? All of these techniques can be used to create approximations of existing computer analyses, and produce fast analysis modules for more efficient computation. These metamodeling techniques also yield insight into the functional relationship between input and output parameters.

Where would such models be useful? A designer's goal is usually to arrive at improved or robust solutions which are the values of design variables that best meet the design objectives as shown in Figure 6. A search for these solutions usually relies on an optimization technique which generates and evaluates many potential solutions in the path toward design improvement; thus, fast analysis modules are an imperative.

When are metamodels useful or appropriate? In the later stages of design when detailed information about specific solutions is available, highly accurate analysis is essential. In the early stages of design, however, the focus is on generating, evaluating, and comparing potential conceptual configurations. The early stages of design are characterized by a large amount of information, often uncertain, which must be managed. To ensure the identification of a "good" system configuration, a comprehensive search is necessary. In this case, the tradeoff between accuracy and efficiency may be appropriate. The creation of metamodels allows fast analysis, facilitating both *comprehensive and efficient* design space search at the expense of a (hopefully slight) loss of accuracy.

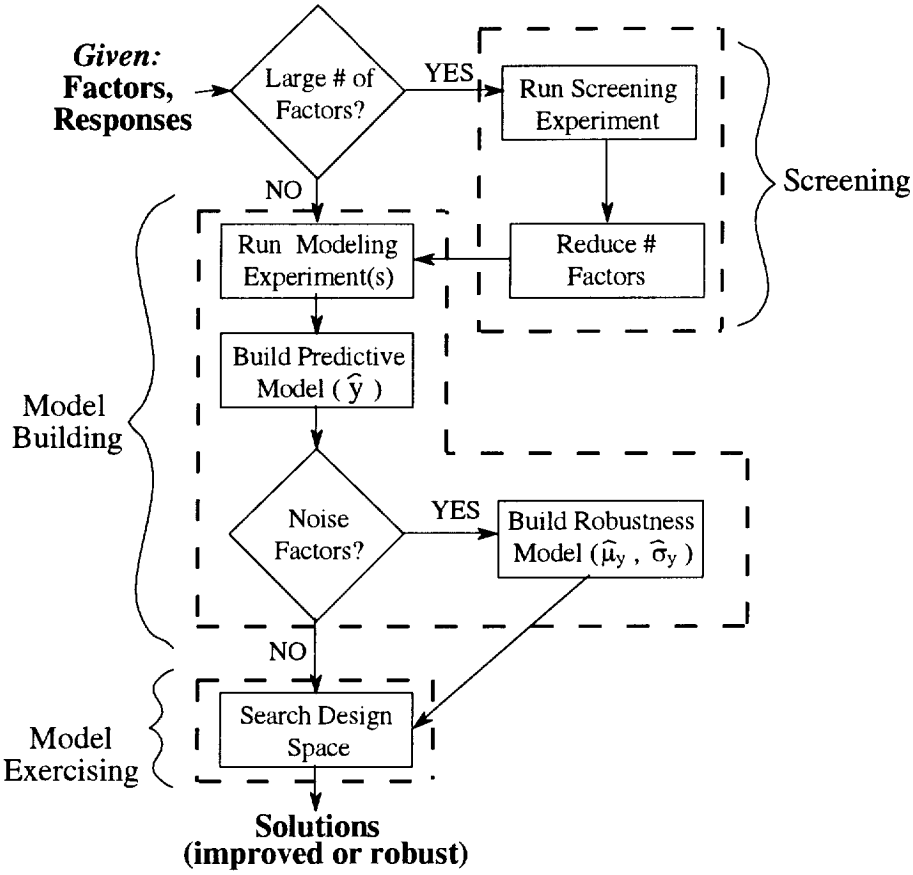


Figure 6. Principal Use of Statistics in Computer-Based Design

Having established our engineering design "context" for using metamodels, we present a review of several statistical applications in engineering design in Section 3.1. In Section 3.2 we discuss a general statistical methods which have been developed for engineering applications, and we conclude by discussing some of the pitfalls associated with the application of statistical techniques to deterministic computer experiments in Section 3.3. This then paves the way for Section 4, guidelines for the appropriate use of statistics in computer-based design.

3.1 Applications in Engineering Design

3.1.1 DOE, RSM, and Taguchi's Robust Design. In Table 1 we present a survey of several engineering applications of design of experiments, response surface methodology, and Taguchi's

robust design approach. Most of these examples come from aerospace and mechanical engineering design applications presented at conferences in recent years. A review of approximation concepts used in structural design can be found in [7].

Some observations regarding our findings are as follows.

- Central composite designs and D-optimal designs seem to be preferred among aerospace engineers while orthogonal arrays (OAs) are preferred by mechanical engineers; grid and random point searches are seldom used since they are less efficient.
- Optimization seems to be the principal driver for aerospace applications of DOE and RSM; these types of applications typically involve the use of computer intensive analysis and optimization routines, and DOE and RSM is a logical choice for increased efficiency.
- Mechanical engineers usually use OAs and Taguchi's approach for robust design and the signal-to-noise ratio for parameter and tolerance design.
- Very few designers actually model Taguchi's loss function directly (see, e.g., [9]); many prefer to model the response instead.
- Most applications use second order response surface models; there are only a few cases where higher order (see, e.g., [136]) and mixed polynomial models (see, e.g., [113]) are used for engineering design.
- When orthogonal arrays are used, special care must be taken to avoid aliasing main effects with interactions, unless the interactions are known (or assumed) to be insignificant.
- Most applications utilize least squares regression analysis when fitting a model; only a few use stepwise regression, and this is usually because the model is not second order.

Table 1. Survey of Engineering Applications of DOE, RSM, and Taguchi's Robust Design

Paper	Experimental Design					Response Surface Method				Taguchi Method		
						Fit Using:						
	Fractional Factorial	CCD	D-optimal	OAs	Grid/Random	Least Square	Stepwise	Order of Equation	Optimize/Improve	Robust Design	Consider Interactions	S/N, Loss, or Resp.
Balabanov, et al. [3]		x				x		2nd	x	x		
Bauer and Krebs [8]	x			x		x		2nd	x	x		S/N
Beard and Sutherland [9]					x					x	x	L
Chen, et al. [25]		x				x		2nd		x		R
Chi and Bloebaum [31]				x					x			R
Engelund, et al. [40]		x				x		2nd	x			
Gadallah and ElMaraghy [47]				x		x		2nd	x	x	x	S/N
Giunta, et al. [51]			x			x		2nd	x			
Giunta, et al. [53]		x	x		x	x		2nd	x			
Healy, et al. [55]				x			x	2nd	x		x	
Hong, et al. [56]				x		x		2nd		x	x	S/N
Koch, et al. [64]		x				x		2nd	x			
Korngold and Gabriele [67]	x							2nd	x			
Li, et al. [74]					x			2nd		x	x	S/N
Mavris, et al. [81]		x				x		2nd		x		R
Mavris, et al. [83]		x				x		2nd		x		R
Roux, et al. [113]			x				x	Mix	x			
Rowell, et al. [114]	x	x			x			2nd	x	x	x	
Stanley, et al. [126]				x					x		x	R
Sundaresan, et al. [127]				x					x		x	R
Unal, et al. [130]			x			x		2nd	x			
Unal, et al. [131]				x					x		x	R
Unal, et al. [132]		x	x	x		x		2nd	x			R
Unal, et al. [133]		x				x		2nd	x			
Venter, et al. [136]					x		x	4th	x			
Yu and Ishii [146]	x					x		2nd		x	x	R

3.1.1 Kriging Applications. Kriging, also referred to as DACE (Design and Analysis of Computer Experiments after the inaugural paper [117]) modeling, has found limited use in engineering design applications perhaps because of the lack of readily available software to fit kriging models, the added complexity of fitting a kriging model, or the additional effort required to use a kriging model. Simpson, et al. [124] detail a preliminary comparison of second order response surface models and kriging models for the multidisciplinary design of an aerospike nozzle which has three geometry (design) variables; neither the kriging models nor the response surface models consistently outperform the other in this engineering example. Giunta [50] presents an investigation into the use of kriging for the multidisciplinary design optimization of a High Speed Civil Transport aircraft. He explores a five and a ten variable design problem, observing that the kriging and response surface modeling approaches yield similar results due to the quadratic trend of the responses. Osio and Amon [94] have developed an extension of DACE modeling for

numerical optimization which uses a multistage strategy for refining the accuracy of the model; they have applied their approach to the thermal design of an embedded electronic package which has 5 design variables. Booker, et al. [12] solve a 31 variable helicopter rotor structural design problem using an similar approximation methodology based on kriging. Booker [11] extend the helicopter rotor design problem to include 56 structural variables to examine the aeroelastic and dynamic response of the rotor. Welch, et al. [138] describe a kriging-based approximation methodology which they use to identify important variables, detect curvature and interactions, and produce a useful approximation model for two 20 variable problems using only 30-50 runs of the computer code; they claim their method can cope with up to 30-40 variables provided factor sparsity can be exploited. Trosset and Torczon [129] have developed a numerical optimization strategy which incorporates DACE modeling and pattern search methods for global optimization. Cox and John [32] have developed the Sequential Design for Optimization method which uses lower confidence bounds on predicted values of the response for the sequential selection of evaluation points during optimization. Both approaches have shown improvements over traditional optimization approaches when applied to a variety of standard mathematical test problems.

3.2 Existing Methods and Tools in Engineering Design

In this section we present some methods and tools developed specifically for engineering which incorporate statistical techniques from Section 2. Since the Taguchi approach and RSM have been widely applied in engineering design, a literature review comparing these approaches is given first. This is followed by an overview of some methods and "tools" that have been developed for general design applications. These include the Robust Concept Exploration Method, the Variable-Complexity Response Surface Modeling Method, and Concurrent SubSpace Optimization to name a few.

3.2.1 Taguchi Approach vs. RSM. The Taguchi approach and RSM have been applied extensively in engineering design. It is commonly accepted that the principles associated with the Taguchi approach are both useful and very appropriate for industrial product design. Ramberg, et

al. [105] suggest that "the loss function and the associated robust design philosophy provide fresh insight into the process of optimizing or improving the simulation's performance." Two aspects of the Taguchi approach are often criticized: the choice of experimental design (orthogonal arrays, inner and outer) and the loss function (signal-to-noise ratio). It has been argued and demonstrated that the use of a single experiment combining control and noise factors is more efficient [122, 131, 139]. The drawbacks of combining response mean and variance into a single loss function (signal-to-noise ratio) are well-documented. Many authors advocate measuring the response directly and separately tracking mean and variance (cf., [27, 105, 139]). However, Shoemaker, et al. [122] warn that a "potential drawback of the response-model approach is that it depends more critically than the loss-model approach on how well the model fits."

Given the wide acceptance of Taguchi robust design principles and the criticisms, many advocate a combined Taguchi-RSM approach or simply using traditional RSM techniques within the Taguchi framework [78, 90, 91, 105]. We believe that orthogonal inner and outer arrays, and single composite experiments each have advantages and disadvantages and appropriate uses, and that separate observation of mean and variance leads to useful insight. Regardless, the core principles of both Taguchi and RSM provide a foundation for many of the specific design methods discussed in Section 3.2.2.

3.2.2 An Overview of Existing Methods. The *Robust Concept Exploration Method (RCEM)* facilitates quick evaluation of different design alternatives and generation of top-level design specifications in the early stages of design [25, 26]. Foundational to the RCEM is the integration of robust design principles, DOE, RSM, and the compromise Decision Support Problem (a multiobjective decision model). The RCEM has been applied to the multiobjective design of a High Speed Civil Transport [25, 65], a family of General Aviation Aircraft [123], a turbine lift engine [64], a solar-powered irrigation system [28], and a flywheel [70]; to manufacturing simulation [101]; and to maintainability design of aircraft engines [93]. A preliminary investigation into the use of DOE and neural networks to augment the capabilities of response surface modeling within the RCEM is given in [29].

The *Variable-Complexity Response Surface Modeling (VCRSM)* Method uses analyses of varying fidelity to reduce the design space to the region of interest and build response surface models of increasing accuracy (see, e.g., [51, 52]). The VCRSM method employs DOE and RS modeling techniques and has been successfully applied to the multidisciplinary wing design of a high speed civil transport (see, e.g., [2, 3, 51, 53, 61]), to the analysis and design of composite curved channel frames [80], to the structural design of bar trusses [113], to predict the fatigue life of structures [135], to reduce numerical noise inherent in structural analyses [53, 136] and shape design problems using fluid flow analysis [92], and to facilitate the integration of local and global analyses for structural optimization [48, 104, 134]. Coarse-grained parallelization of analysis codes for efficient response surface generation has also been investigated [17, 61].

Concurrent SubSpace Optimization (CSSO) uses data generated during concurrent subspace optimizations to develop response surface approximations of the design space. Optimization of these response surfaces forms the basis for the subspace coordination procedure. The data generated by the subspace optimizers is not uniformly centered about the current design as in CCD or other sampling strategies, but instead follows the descent path of the subspace optimizers. In [109, 108, 110], interpolating polynomial response surfaces are constructed which have either a first or second order basis for use in the CSSO coordination procedure. In [140, 141], a modified decomposition strategy is used to develop quadratic response surfaces for use in the CSSO coordination procedure. Finally, in [118-120] artificial neural network response surfaces are developed for use in the CSSO coordination procedure.

Robust Design Simulation (RDS) is a stochastic approach which employs the principles of Integrated Product and Process Development (IPPD) for the purpose of determining the optimum values of design factors and proposed technologies (in the presence of uncertainty) which yield affordable designs with low variability. Toward this end, RDS combines design of experiments and response surface metamodels with Monte Carlo simulation and Fast Probability Techniques (see, e.g., [6]) to achieve customer satisfaction through robust systems design [83]. RDS has been applied to the design of a High Speed Civil Transport aircraft [81, 83] and very large

transports [82]. RDS has also been used to study the economic uncertainty of the HSCT [36, 84] and the feasibility/viability of aircraft [85].

NORMAN/DEBORA is a TCAD (Technology Computer Aided Design) system incorporating advanced sequential DOE and RSM techniques to aid in engineering optimization and robust design [22]. NORMAN/DEBORA includes a novel design of experiments concept—Target Oriented Design—a unique parameter transformation technique—RATIOFIND—and a non-linear, constrained optimizer—DEBORA [23]. It has been successfully employed for semiconductor integrated circuit design and optimization [20, 21, 23, 57]. An updated and more powerful version of NORMAN/DEBORA is being offered as LMS Optimus [75].

The *Probabilistic Design System (PDS)* being developed at Pratt and Whitney uses Box-Behnken designs and response surface methodology to perform probabilistic design analysis of gas turbine rotors [43, 42]. Fox [44] describes twelve criteria which are used to validate the response surfaces which are used in combination with cheap-to-run analyses in a Monte Carlo Simulator to estimate the corresponding distributions of the responses and minimum life of system components. Adamson [1] describes issues involved with developing, calibrating, using, and testing the PDS and discusses Pratt and Whitney's plans to validate the PDS by designing, building, and testing actual parts.

DOE/Opt is a prototype computer system for DOE, RSM, and optimization [10]. It has been used in semiconductor process/device design including process/device optimization, simulator tuning, process control recipe generation, and design for manufacturability.

Hierarchical and Interactive Decision Refinement (HIDER) is a methodology for concept exploration in the early stages of design. It integrates simulation, optimization, statistical techniques, and machine learning to support design decision making [107, 142]. The methodology is used to hierarchically refine/reduce "a large initial design space through a series of multiple-objective optimizations, until a fully specified design is obtained" [142]. HIDER uses the Adaptive Interactive Modeling System (AIMS) [76] to decompose the design space using distance-

based, population-based, and hyperplane-based algorithms. HIDER and AIMS have been applied to the design of a cutting process [76], a diesel engine [142, 143], and a wheel loader [107].

Other approaches incorporating statistical techniques in engineering design exist; only a few have been included here. Our focus is not on the methods, but on the appropriateness of the statistical techniques; many of the examples to which these methods have been applied employ deterministic computer experiments in which the application of statistical techniques is questionable. Associated issues are discussed in the next section.

3.3 A Closer Look at Experimental Design for Deterministic Computer Experiments

Since engineering design usually involves exercising deterministic computer analysis codes, the use of statistical techniques for creating metamodels warrants a closer look. Given a response of interest, y, and a vector of independent factors **x** thought to influence y, the relationship between y and **x** (see Eq. (2)) includes the random error term ε. To apply least squares regression, error values at each data point are assumed to have identical and independent normal distributions with means of zero and standard deviations of σ, or ε_i i.i.d. $N(0,\sigma^2)$, see Figure 7(a). The least squares estimator then minimizes the sum of the squared differences between actual data points and predicted values. This is acceptable when no data point actually lies on the predicted model because it is assumed that the model "smoothes out" random error. Of course, it is likely that the regression model itself is merely an approximation of the true behavior of **x** and y so that the final relationship is

$$y = g(\mathbf{x}) + \varepsilon_{bias} + \varepsilon_{random} \tag{16}$$

where ε_{bias} represents the error of approximation. However, for deterministic computer analyses as shown in Figure 7(b), ε_{random} has mean zero *and* variance zero, yielding the relationship

$$y = g(\mathbf{x}) + \varepsilon_{bias}\,. \tag{17}$$

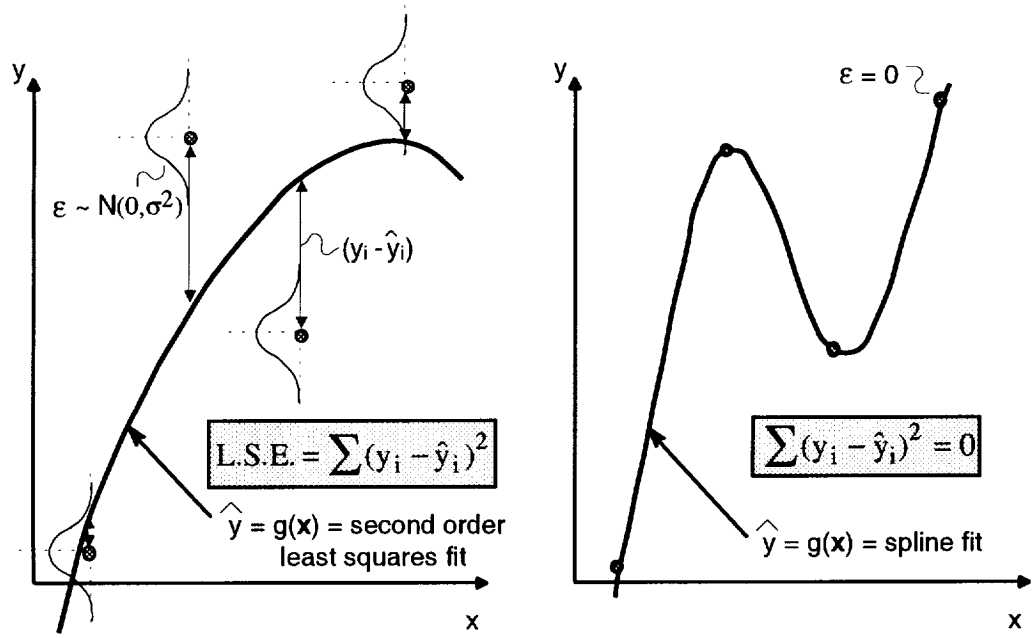


Figure 7. Deterministic and Non-Deterministic Curve Fitting

The deterministic case in Eq. (17) conflicts sharply with the methods of least squares regression. Unless ε_{bias} is i.i.d. $N(0,\sigma^2)$ the assumptions for statistical inference from least squares regression are violated. Further, since there is no random error it is not justifiable to smooth across data points; instead *the model should hit each point exactly and interpolate between them* as in Figure 5(b). Finally, most standard tests for model and parameter significance are based on computations of ε_{random} and therefore cannot be computed. These observations are supported by literature in the statistics community; as Sacks, et al. [117] carefully point out that because deterministic computer experiments lack random error:

- response surface model adequacy is determined solely by systematic bias,
- the usual measures of uncertainty derived from least-squares residuals have no obvious statistical meaning (deterministic measures of uncertainty exist, e.g., max. $|\hat{\mathbf{y}}(\mathbf{x}) - \mathbf{y}(\mathbf{x})|$ over $\mathbf{x}$, but they may be very difficult to compute), and
- the classical notions of experimental blocking, replication and randomization are irrelevant.

Furthermore, some of the methods for the design and analysis of physical experiments (see, e.g., [14, 16, 91] are not ideal for complex, deterministic computer models. "In the presence of systematic error rather than random error, statistical testing is inappropriate" [139]. A discussion of how the model *should* interpolate the observations can be found in [116].

So where can these methods go wrong? Unfortunately it is easy to misclassify the ε_{bias} term from a deterministic model as ε_{random} and then proceed with standard statistical testing. Several authors have reported statistical measures (e.g., F-statistics and root mean square error) to verify model adequacy, see, e.g., [55, 64, 132, 136, 139]. However, these measures have no statistical meaning since they assume the observations include a random error term with a mean of zero and a non-zero standard deviation. Consequently, the use of stepwise regression for polynomial model fitting is also inappropriate since it utilizes F-statistics when adding/removing model parameters.

Some researchers (see, e.g., [51, 53, 92, 135, 136]) have used metamodeling techniques for deterministic computer experiments containing numerical noise. Metamodels are used to smooth the numerical noise which inhibits the performance of gradient based optimizers (cf., [53, 4]). When constructing the metamodels, the numerical noise is used as a surrogate for random error, and the standard least-squares approach is then used to determine model significance. The idea of equating numerical noise to random error warrants further investigation into the sources and nature of this "deterministic" noise.

How can model accuracy be tested? R-Squared (the model sum of squares divided by the total sum of squares) and R-Squared_adjusted (which takes into account the number of parameters in the model) are the only measures for verifying model adequacy in deterministic computer experiments. This measure is often insufficient; a high R-Squared value can be deceiving. Residual plots may be helpful for verifying model adequacy, identifying trends in data, examining outliers, etc; however, *validating the model using additional (different) data points is essential.* Maximum absolute error, average absolute error, and root mean square error for the additional validation points can be calculated to assess model accuracy, see, e.g., [124, 136]. Otto, et al. [95, 96] and Yesilyurt and Patera [145] have developed a Bayesian-validated surrogate approach

which uses additional validation points to make qualitative assessments of the quality of the approximation model and provide theoretical bounds on the largest discrepancy between the model and the actual computer analysis. They have applied their approach to optimization of multi-element airfoils [96], design of trapezoidal ducts and axisymmetric bodies [97], and optimization of an eddy-promoter heat exchanger [144, 145]. Finally, an alternative method which does not require additional points is leave-one-out cross validation [86]. Each sample point used to fit the model is removed one at a time, the model is rebuilt without a sample point, and the difference between the model without the sample point and actual value at the sample point is computed for all of the sample points.

Given the potential problems in applying least-squares regression to deterministic applications, the trade-off then is between *appropriateness* and *practicality*. If a response surface is created to model data from a deterministic computer analysis code using experimental design and least squares fitting, and if it provides good agreement between predicted and actual values, then there is no reason to discard it. It should be used, albeit with caution. However, it is important to understand the fundamental assumptions of the statistical techniques employed to avoid misleading statements about model significance. In the next section we offer some guidelines for the appropriate use of statistical metamodeling with deterministic computer analyses.

4 GUIDELINES AND RECOMMENDATIONS

How can a designer apply metamodeling tools while avoiding the pitfalls described in Section 3.3? This can either be answered from the bottom up (tools -> applications, Section 4.1) or from the top down (motives -> tools, Section 4.2).

4.1 Evaluation of Metamodeling Techniques

There are two components to this section. The first is an evaluation of the four metamodeling techniques described in Section 2.2. The second component is choosing an experimental design which has more direct applicability to response surface methods. Determining what experimental

designs are most appropriate for the other metamodeling techniques discussed in Section 2.2 are open research areas.

4.1.1 Evaluation of Model Choice and Model Fitting Alternatives. Some guidelines for the evaluation of the metamodeling techniques presented in Section 2.2 are summarized in Table 2.

Table 2. Recommendations for Model Choice and Use

Model Choice	Characteristics/Appropriate Uses
Responses Surfaces	• well-established and easy to use • best suited for applications with random error • appropriate for applications with < 10 factors
Neural Networks	• good for highly nonlinear or very large problems (~10,000 parameters) • best suited for deterministic applications • high computational expense (often > 10,000 training data points); best for repeated application
Rule Induction / Inductive Learning	• best when factors and responses are discrete-valued • form of model is rules or decision tree; better suited to diagnosis than engineering design
Kriging	• extremely flexible but complex • well-suited for deterministic applications • can handle applications with < 50 factors • limited support is currently available for implementation

Response Surfaces: primarily intended for applications with random error; however, they have been used successfully in many engineering design applications. It is the most well-established metamodeling technique and is probably the easiest to use, provided the user is aware of the possible pitfalls described in Section 3.3.

Neural Networks: nonlinear regression approach best suited to deterministic applications which require repeated use. Building a neural network for a one-shot use can be extremely inefficient due to the computational overhead required.

Inductive Learning: modeling technique most appropriate when input and output factors are primarily discrete-valued or can be grouped. The predictive model, in the form of condition-action rules or a decision tree, may lack the mathematical insight desired for engineering design.

Kriging: an interpolation method capable of handling deterministic data which is extremely flexible due to the wide range of correlation functions which may be chosen. However, the method is more complex than response surface modeling and lacks readily available computer support software.

4.1.2 Evaluation of Experimental Designs. There are many voices in the discussion of the relative merits of different experimental designs, and it is therefore unlikely that we have captured them all. The opinions on the appropriate experimental design for computer analyses vary; the only consensus reached thus far is that designs for non-random, deterministic computer experiments should be "space filling." Several "space filling" designs were discussed previously in Section 2.1.1. For a comparison of some specific design types, we refer the reader to the following articles.

- Myers and Montgomery [91] provide a comprehensive review of experimental designs for fitting second order response surfaces. They conclude that hybrid designs are useful, if the unusual levels of the design variables can be tolerated; with computer experiments this is unlikely to be a problem.
- Carpenter [19] examines the effect of design selection on response surface performance. He compares 2^k and 3^k factorial designs, central composite designs, minimum point designs, and minimum point designs augmented by additional randomly selected points; he favors the augmented point designs for problems involving more than 6 variables.
- Giovannitti-Jensen and Myers [49] discuss several first and second order designs, observing that the performance of rotatable CCD and Box-Behnken designs are nearly identical. They note that "hybrid designs appear to be very promising."
- Lucas [79] compares CCD, Box-Behnken, uniform shell, Hoke, Pesotchinsky, and Box-Draper designs, using the D-efficiency and G-efficiency statistics.
- Montgomery and Evans [88] compare six second order designs: (a) 3^2 factorial, (b) rotatable orthogonal CCD, (c) rotatable uniform precision CCD, (d) rotatable minimum bias CCD, (e)

rotatable orthogonal hexagon, and (f) rotatable uniform precision hexagon. Comparison criteria include average response achievement and distance from true optimum.

- Lucas [77] compares symmetric and asymmetric composite and smallest composite designs for different numbers of factors using the D-efficiency and G-efficiency statistics.

4.2 Recommendations for Metamodeling Uses

Most metamodeling applications are built around creating low order polynomials using central composite designs and least squares regression. The popularity of this approach is due, at least in part, to the maturity of RSM, its simplicity, and readily accessible software tools. However, RSM breaks down when there are many (>10) factors or highly nonlinear responses. Furthermore, there are also dangers in applying RSM blindly in deterministic applications as discussed in Section 3.3. Alternative approaches to metamodeling (see Section 4.1.1) address some of these limitations. Our recommendations are:

- If many factors must be modeled in a deterministic application, neural networks may be the best choice despite their tendency to be computationally expensive to create.
- If the underlying function to be modeled is deterministic and highly nonlinear in a moderate number of factors (less than 50, say), then kriging may be the best choice despite the added complexity.
- In deterministic applications with a few fairly well behaved factors, another option for exploration is using the standard RSM approach augmented by a Taguchi outer (noise) array.

RSM/OA approach: The basic problem in applying least-squares regression to deterministic applications is the lack of ε_{random} in Eq. (17). However, if some input parameters in the computer analysis are classified as noise factors, and if these noise factors are varied across an outer array for each setting of the control factors, then essentially a series of *replications* are generated to approximate ε_{random}. This is justified if it is reasonable to assume that, were the experiments performed on an actual physical system, the random error observed would have been due to these noise factor fluctuations. Statistical testing of model and parameter significance can then be

performed, and models of both mean response and variability are created from the same set of experiments. Further discussion and a preliminary investigation into such an approach is given in [72].

5 SUMMARY AND CLOSING REMARKS

In this paper we survey some applications of statistics in engineering design and have discussed the concept of *metamodeling*, refer to Section 1 and Figure 6. However, applying these techniques to deterministic applications in engineering design can cause problems, see Sections 3.1 and 3.3. We present recommendations for applying metamodeling techniques in Section 4, but these recommendations are by no means complete. Comprehensive comparisons of these techniques must be performed; preliminary and ongoing investigations into the use of kriging as an alternative metamodeling technique to response surfaces is described in [124].

The difficulties of large problem size and non-linearity are ever-present. In particular, an issue of interest to us is the *problem of size* [65]. As the number of factors in the problem increases, the cost associated with creating metamodels begins to out-weigh the gains in efficiency. In addition, often screening is insufficient to reduce the problem to a manageable size. This difficulty is compounded by the *multiple response problem*—complex engineering design problems invariably include multiple measure of performance (responses) to be modeled. The screening process breaks down when attempting to select the most important factors for more than one response since each response may require different important factors. The general question arising from these problems, then, is *how can these experimentation and metamodeling techniques be used efficiently for larger problems (problems with greater than 10 factors after screening)?* One approach is problem partitioning or decomposition. Using these techniques, a complex problem may be broken down into smaller problems allowing efficient experimentation and metamodeling, which again leads to *comprehensive and efficient* exploration of a design space [63]. A significant literature base exists of techniques for breaking a problem into smaller problems; a good review of such methods can be found in [73]. Detailed reviews of multidisciplinary design optimization

approaches for formulating and concurrently solving decomposed problems are presented in [125] and [33], and a comparison of some of these approaches is given in [5].

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