Review of Metamodeling Techniques in Support of Engineering Design Optimization

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Computation-intensive design problems are becoming increasingly common in manufacturing industries. The computation burden is often caused by expensive analysis and simulation processes in order to reach a comparable level of accuracy as physical testing data. To address such a challenge, approximation or metamodeling techniques are often used. Metamodeling techniques have been developed from many different disciplines including statistics, mathematics, computer science, and various engineering disciplines. These metamodels are initially developed as "surrogates" of the expensive simulation process in order to improve the overall computation efficiency. They are then found to be a valuable tool to support a wide scope of activities in modern engineering design, especially design optimization. This work reviews the state-of-the-art metamodel-based techniques from a practitioner's perspective according to the role of metamodeling in supporting design optimization, including model approximation, design space exploration, problem formulation, and solving various types of optimization problems. Challenges and future development of metamodeling in support of engineering design is also analyzed and discussed. [DOI: 10.1115/1.2429697]

Keywords: metamodeling, engineering design, optimization

Introduction

To address global competition, manufacturing companies strive to produce better and cheaper products more quickly. For complex systems such as an aircraft, the design is intrinsically a daunting optimization task often involving multiple disciplines, multiple objectives, and computation-intensive processes for product simulation. Just taking the computation challenge as an example, it is reported that it takes Ford Motor Company about 36–160 h to run one crash simulation [1]. For a two-variable optimization problem, assuming on average 50 iterations are needed by optimization and assuming each iteration needs one crash simulation, the total computation time would be 75 days to 11 months, which is unacceptable in practice. Despite continual advances in computing power, the complexity of analysis codes, such as finite element analysis (FEA) and computational fluid dynamics (CFD), seems to keep pace with computing advances [2]. In the past 2 decades, approximation methods and approximation-based optimization have attracted intensive attention. This type of approach approximates computation-intensive functions with simple analytical models. The simple model is often called metamodel; and the process of constructing a metamodel is called metamodeling. With a metamodel, optimization methods can then be applied to search for the optimum, which is therefore referred as metamodel-based design optimization (MBDO).

Continuing on an earlier review [3], Haftka and co-authors [4] discussed in depth the relation between experiments and optimization, i.e., the use of optimization to design experiments, and the use of experiments to support optimization. It also dedicated a section talking about MBDO using slightly different terminologies. The benefits of MBDO were elaborated as follows: (1) it is easier to connect proprietary and often expensive simulation codes; (2) parallel computation becomes simple as it involves running the same simulation at many design points; (3) building metamodels can better filter numerical noise than gradient-based methods; (4) the metamodel renders a view of the entire design space; and (5) it is easier to detect errors in simulation as the entire design domain is analyzed. Simpson et al. [5] gave a very focused review on metamodels and MBDO by going through many popular sampling methods (or experimental design methods), approximation models (metamodels), metamodeling strategies, and applications. Guidelines and recommendations were also given at the end of the paper. A panel discussion about the topic was held in 2002 in the 9th AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization in Atlanta. The summary of the panel discussion was archived in Ref. [6]. Four future research directions were elaborated as: (1) sampling methods for computer experiments; (2) visualization of experimental results; (3) capturing uncertainty with approximation methods; and (4) high-dimensional problems.

In the past few years, new developments in metamodeling techniques have been continuously coming forth in the literature. From the lead author's past five years of experience as a session organizer/chair for the ASME Design Engineering Technical Conference (DETC) on the topic, it also seems that as more and more of these methods being developed, the gap between the research community and design engineers keeps widening. It is probably first because metamodeling is mathematically involving, and second it evolves rapidly with rich information from many disciplines. Therefore, a review of the field from a practitioner's view is seen needed. This review is expected to offer an overall picture of the current research and development in metamodel-based design optimization. Moreover, it is organized in a way to provide a reference of metamodeling techniques for practitioners. It is also hoped that by examining the needs of design engineers, the research community can better align their research directions towards such needs. Though great efforts have been exercised to collect as much relevant and important literature as possible, it is not the intent of the review to be exhaustive on this intensively studied topic.

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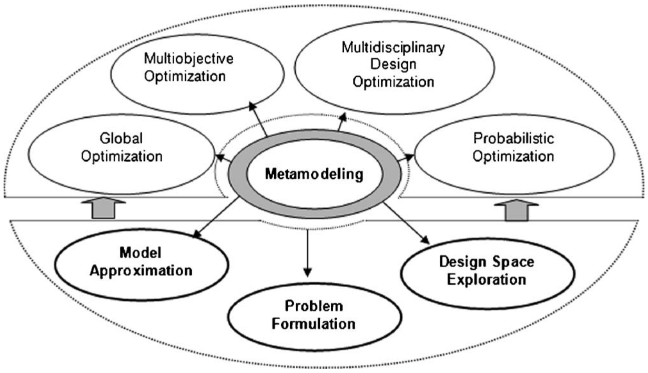

Fig. 1 Metamodeling and its role in support of engineering design optimization

Table 1 Commonly used metamodeling techniques

Experimental Design/Sampling Methods	Metamodel Choice	Model Fitting
- Classic methods • (Fractional) factorial • Central composite • Box-Behnken • Alphabetical optimal • Plackett-Burman - Space-filling methods • Simple Grids • Latin Hypercube • Orthogonal Arrays • Hammersley sequence • Uniform designs • Minimax and Maximin - Hybrid methods - Random or human selection - Importance sampling - Directional simulation - Discriminative sampling - Sequential or adaptive methods	- Polynomial (linear, quadratic, or higher) - Splines (linear, cubic, NURBS) - Multivariate Adaptive Regression Splines (MARS) - Gaussian Process - Kriging - Radial Basis Functions (RBF) - Least interpolating polynomials - Artificial Neural Network (ANN) - Knowledge Base or Decision Tree - Support Vector Machine (SVM) - Hybrid models	- (Weighted) Least squares regression - Best Linear Unbiased Predictor (BLUP) - Best Linear Predictor - Log-likelihood - Multipoint approximation (MPA) - Sequential or adaptive metamodeling - Back propagation (for ANN) - Entropy (inf.-theoretic, for inductive learning on decision tree)

Roles of Metamodeling in Support of Design Optimization

Intensive research has been done in employing metamodeling techniques in design and optimization. These include research on sampling, metamodels, model fitting techniques, model validation, design space exploration, optimization methods in support of different types of optimization problems, and so on. Through the years it has become clear that metamodeling provides a decision-support role for design engineers. What are the supporting functions that metamodeling can provide? From our experience and informal interviews with design engineers, with reference to the literatures [7], the following lists some of the areas that metamodeling can play a role.

1. Model approximation: Approximation of computation-intensive processes across the entire design space, or global approximation, is used to reduce computation costs;
2. Design space exploration: The design space is explored to enhance the engineers' understanding of the design problem by working on a cheap-to-run metamodel;
3. Problem formulation: Based on an enhanced understanding of a design optimization problem, the number and search range of design variables may be reduced; certain ineffective constraints may be removed; a single objective optimization problem may be changed to a multiobjective optimization problem or vice versa. Metamodels can assist the formulation of an optimization problem that is easier to solve or more accurate than otherwise; and
4. Optimization support: Industry has various optimization needs, e.g., global optimization, multi-objective optimization, multidisciplinary design optimization, probabilistic optimization, and so on. Each type of optimization has its own challenges. Metamodeling can be applied and integrated to solve various types of optimization problems that involve computation-intensive functions.

As illustrated in Fig. 1, metamodeling supports various design activities that are enclosed in small ellipses. The bottom half includes model approximation, problem formulation, and design space exploration, which form a common supportive base for all types of optimization problems. The upper half lists four major types of optimization problems of interests to design engineers. For each of the above-mentioned areas, related recent development is reviewed in this work. General consensus that has been reached thus far in the research community is also given.

Model Approximation

Approximation, or metamodeling, is the key to metamodel-based design optimization. Conventionally the goal of approximation is to achieve a global metamodel as accurate as possible at a reasonable cost. In this section, we focus on global metamodeling and discuss MBDO in later sections.

Table 1 categorizes the metamodeling techniques according to sampling, model types, and model fitting [5]. This review discusses each of these categories in more detail.

Sampling. "Classic" experimental designs originated from the theory of Design of Experiments when physical experiments are conducted. These methods focus on planning experiments so that the random error in physical experiments has minimum influence in the approval or disapproval of a hypothesis. Widely used "classic" experimental designs include factorial or fractional factorial [8], central composite design (CCD) [8,9], Box-Behnken [8], alphabetical optimal [10,11], and Plackett-Burman designs [8]. These classic methods tend to spread the sample points around boundaries of the design space and leave a few at the center of the design space. As computer experiments involve mostly systematic error rather than random error as in physical experiments, Sacks et al. [12] stated that in the presence of systematic rather than random error, a good experimental design tends to fill the design space rather than to concentrate on the boundary. They also stated that "classic" designs, e.g., CCD and *D*-optimality designs, can be inefficient or even inappropriate for deterministic computer codes. Simpson et al. [13] confirmed that a consensus among researchers was that experimental designs for deterministic computer analyses should be space filling.

Koehler and Owen [14] described several Bayesian and frequentist "space filling" designs, including maximum entropy design [15], mean squared-error designs, minimax and maximin designs [16], Latin hypercube designs, orthogonal arrays, and scrambled nets. Four types space filling sampling methods are relatively more often used in the literature. These are orthogonal arrays [17–19], various Latin hypercube designs [20–24], Hammersley sequences [25,26], and uniform designs [27]. Hammersley sequences and uniform designs belong to a more general group called low discrepancy sequences [28]. The code for generating orthogonal arrays is available online at http://lib.stat.cmu.edu/design/owen.html and http://ie.uta.edu/index.cfm/ by Chen [28]. Hammersley sampling is found to provide better uniformity than Latin hypercube designs. Several uniform designs are available on-line at URL: http://www.math.hkbu.edu.hk/UnifromDesign. A comparison of these sampling methods is in Ref. [29]. It is found that the Latin hypercube design is only uniform in one-dimensional (1D) projection while the other methods tend to be more uniform in the entire space. Also found is that the "appropriate" sample size depends on the complexity of the function to be approximated. In general, more sample points offer more information of the function, however, at a higher expense.

For low-order functions, after reaching a certain sample size, increasing the number of sample points does not contribute much to the approximation accuracy. Moreover, when certain optimality criteria are used to generate samples, these optimality criteria such as maximum entropy are concerned with the sample distribution and are independent to the function. While the approximation accuracy depends on whether sample points capture all the features of the function itself. Therefore those optimality criteria are not perfectly consistent with the goal of improving approximation, due to which the additional computational cost of searching for the optimal sample is often not well justified.

The Monte Carlo simulation (MCS) method, which is a random sampling method, is still a popular sampling method in industry, regardless of its inefficiency. It is probably because the adequate and yet efficient sample size at the outset of metamodeling is unknown for any black-box function. Improved from the Monte Carlo simulation method, the importance sampling (IS) bears the potential of improving its efficiency while maintain the same level of accuracy as MCS [30]. Zou and colleagues developed a method based on an indicator response surface, in which IS was performed in a reduced region around the limit state [31–33]. Another variation of MCS is directional simulation [34–36]. A new discriminative sampling method has been developed when the sampling goal was for optimization instead of global metamodeling [37–39]. With its original inspiration from Ref. [40], this sampling method is space filling and reflects the goal of sampling; it is a more aggressive MCS method. Comparatively, these MCS-rooted methods are less structured but offer more flexibility. If any knowledge of the space is available, these methods may be tailored to achieve higher efficiency. They may also play a more active role for iterative sampling-metamodeling processes.

Mainly due to the difficulty of knowing the "appropriate" sampling size *a priori*, sequential and adaptive sampling has gained popularity in recent years. Lin [41] proposed a sequential exploratory experiment design (SEED) method to sequentially generate new sample points. Jin et al. [42] applied simulated annealing to quickly generate optimal sampling points and the method has been incorporated into the software iSight [43]. Sasena et al. [44] used the Bayesian method to adaptively identify sample points that gave more information. Wang [45] proposed an inheritable Latin hypercube design for adaptive metamodeling. Samples are repetitively generated fitting a Kriging model in a reduced space [46]. Jin et al. [47] compared a few different sequential sampling schemes and found that sequential sampling allows engineers to control the sampling process and it is generally more efficient than one-stage sampling. One can custom design flexible sequential sampling schemes for specific design problems.

Metamodeling. Metamodeling evolves from classical design of experiments (DOE) theory, in which polynomial functions are used as response surfaces, or metamodels. Besides the commonly used polynomial functions, Sacks et al. [12,48] proposed the use of a stochastic model, called Kriging [49], to treat the deterministic computer response as a realization of a random function with respect to the actual system response. Neural networks have also been applied in generating the response surfaces for system approximation [50]. Other types of models include radial basis functions (RBF) [51,52], multivariate adaptive regression splines (MARS) [53], least interpolating polynomials [54], and inductive learning [55]. A combination of polynomial functions and artificial neural networks has also been archived in Ref. [56]. There is no conclusion about which model is definitely superior to the others. However, insights have been gained through a number of studies [2,5,13,28,57,58]. In recent years, Kriging models and related Gaussian processes are intensively studied [59–64]. A well written Kriging modeling code (in Matlab) is downloadable from the internet URL: http://www2.imm.dtu.dk/~hbn/dace/ [65].

In general the Kriging models are more accurate for nonlinear problems but difficult to obtain and use because a global optimization process is applied to identify the maximum likelihood estimators. Kriging is also flexible in either interpolating the sample points or filtering noisy data. On the contrary, a polynomial model is easy to construct, clear on parameter sensitivity, and cheap to work with but is less accurate than the Kriging model [13]. However, polynomial functions do not interpolate the sample points and are limited by the chosen function type. The RBF model, especially the multiquadric RBF, can interpolate sample points and at the same time is easy to construct. It thus seems to reach a tradeoff between Kriging and polynomials. Recently, a new model called support vector regression (SVR) was used and tested [66]. SVR achieved high accuracy over all other metamodeling techniques including Kriging, polynomial, MARS, and RBF over a large number of test problems. It is not clear, however, what are the fundamental reasons that SVR outperforms others. The least interpolating polynomials use polynomial basis functions and also interpolate responses. They choose a polynomial basis function of "minimal degree" as described by Ref. [54] and hence are called "least interpolating polynomials." This type of metamodel deserves more study. In addition, Pérez et al. [67] transformed the matrix of second-order terms of a quadratic polynomial model into the canonical form to reduce the number of terms. Messac and his team developed an extended RBF model [68] by adding extra terms to a regular RBF model to increase its flexibility, based on which an optimal model could be searched for. Turner and Crawford proposed a NURBS-based metamodel, which was applied only to low-dimensional problems [69].

If gradient information can be reliably and inexpensively obtained, gradient information can be utilized in metamodeling [70,71]. A multipoint approximation (MPA) strategy has also received some attention [72–75]. MPA uses blending functions to combine multiple local approximations, and usually gradient information is used in metamodeling. Metamodels can also be constructed when design variables are modeled as fuzzy numbers [76,77].

Each metamodel type has its associated fitting method. For example, polynomial functions are usually fitted with the (weighted) least square method; the kriging method is fitted with the search for the best linear unbiased predictor (BLUP). Simpson et al. [5] gave a detailed review on the equations and fitting methods for common metamodel types.

In general computer experiments have very small random error which might be caused by the pseudorandom number generation or rounding [78]. Giunta et al. [79] found that numerical noises in computing the aerodynamic drag of high speed civil transport (HSCT) caused many spurious local minima of the objective function. The problem was due to the discontinuous variations in calculating the drag by using the panel flow solver method. Madsen et al. [80] stated that noises could come from the complex numerical modeling techniques of CFD such as turbulence models, incomplete convergence, and discretization. In case of physical or noisy computer experiments, it is found that Kriging and RBF are more sensitive to numerical noise than polynomial models [13,81]. However, Kriging, RBF, and artificial neural network (ANN) could be modified to handle noises, assuming the signal to noise ratio is acceptable [82].

Model Validation. Metamodels, especially global metamodels, are to be validated before being used as a "surrogate" of the computation-intensive processes. Model validation has been a challenging task, and it shares common challenges with the verification and validation of other computational models [83,84]. Meckesheimer et al. [26,85] studied the cross-validation method. One starts with a dataset, $S\{X,Y\}$, consisting of N input–output data pairs $(\mathbf{x};y)$, where y is the disciplinary model response at the design sample point, $\mathbf{x}$, and N is the total number of disciplinary model runs. In p-fold cross validation, the initial data set is split into p different subsets, that is, $S\{X,Y\}=S1\{X1,Y1\},S2\{X2,Y2\},\ldots,Sp\{Xp,Yp\}$. Then, the metamodel is fit p times, each time leaving out one of the subsets from training, and using the omitted subset to compute the error measure of interest. A variation of p-fold cross validation is the leave-k-out approach, in which all possible $\binom{N}{k}$ subsets of size k are left out, and the metamodel is fit to each remaining set. Each time, the error measure of interest is computed at the omitted points. This approach is a computationally more expensive version of p-fold cross validation. Mitchell and Morris [86] described how the cross-validation error measure could be computed inexpensively for the special case of $k=1$; this is called leave-one-out cross validation. Based on the observations from the experimental study conducted to assess the leave-k-out cross-validation strategy [26], a value of $k=1$ was recommended for providing a prediction error estimate for RBF and low order polynomial metamodels, but not for kriging metamodels. Choosing k as a function of the sample size used to construct the metamodel N (that is, $k=0.1N$ or $k=\sqrt{N}$) was instead recommended for estimating the prediction error for kriging metamodels. Lin [41] found through intensive testing that the leave-one-out cross validation is an insufficient measurement for metamodel accuracy. The leave-one-out cross validation is actually a measurement for degrees of insensitivity of a metamodel to lost information at its data points, while an insensitive metamodel is not necessarily accurate. A "validated" model by leave-one-out could be far from the actual as the data points may not be able to capture the actual. Designers are in danger of accepting an inaccurate metamodel that is insensitive to lost information at data points, and inaccurate and insensitive metamodels might be the results of poor experimental designs (clustering points or correlated data points). On the other hand, with leave-one-out cross validation we are in danger of rejecting an accurate metamodel that is also sensitive to lost information at data points.

Given that cross validation is insufficient for assessing models, employing additional points is essential in metamodel validation. When additional points are used for validation, there are a number of different measures of model accuracy. The first two are the root mean square error (RMSE) and the maximum absolute error (MAX), defined below

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{m} (y_i - \hat{y}_i)^2}{m}} \tag{1}$$

$$\mathrm{MAX} = \max|y_i - \hat{y}_i|, \quad i = 1, \ldots, m \tag{2}$$

where m is the number of validation points; and $\hat{y}_i$ is the predicted value for the observed value y_i. The lower the value of RMSE and/or MAX, the more accurate the metamodel. RMSE is used to gauge the overall accuracy of the model, while MAX is used to gauge the local accuracy of the model. An additional measure is also used is the R square value, i.e.

$$R^2 = 1 - \frac{\sum_{i=1}^{m} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{m} (y_i - \bar{y})^2} \tag{3}$$

where $\bar{y}$ is the mean of the observed values at the validation points. It is to be noted that Eq. (3) is computed for the additional validation points, which differs from the traditional use of R square [61]. Variations of the three measures exist in the literature [13].

Design Space Exploration

Given a reasonably accurate metamodel, the design space can be explored to obtain deeper insight into the design problem and better formulate the optimization problem. Most of today's design tools such as computer aided design (CAD) aim at improving the productivity of a design engineer. The relationship between design variables and product performance is usually embedded in complex equations or models in FEA or CFD codes. Engineers, by experience, often only have a vague idea about such relationship. A common method an engineer uses to understand a design problem is through sensitivity analysis and "what if" questions. Sensitivity analysis, however, is based on a fixed condition with the variation of one variable. If the condition is changed, the sensitivity information changes as well. An engineer still cannot have an idea of the overall structure of the problem. The metamodeling approach can assist the engineer to gain insight to the design problem, currently, through two channels. The first is through the metamodel itself. Given the metamodel, one can analyze the properties of the metamodel to gain a better understanding of the problem. A good example is for the quadratic polynomial metamodel, if all the design variables are normalized to $[-1,1]$, then the magnitude of the coefficients in the metamodel indicates the sensitivity or importance of the corresponding term [87]. This is in fact used for screening of design variables. The second way of enhancing the understanding is through visualization.

Visualization of multi-dimensional data alone has been an interesting topic, and many methods have been developed over the years [88,89]. Winer and Bloebaum developed a visual design steering method based on the concept of graph morphing [90,91]. Eddy and Kemper proposed cloud visualization for the same purpose [92]. Also, SGI and Ford integrated parallel computation and metamodeling for rapid visualization of design alternatives [93]. Visualization methods for multidimensional data sets and identifying Pareto Frontiers for multiobjective optimization problems are also recently developed [94–97]. Ligetti and Simpson [98] and Ligetti et al. [99] proved that both the design efficiency and effectiveness could be improved by using the metamodel approach in graphical design interface. A recent study by the group [100] suggested as the problem size increases, the impact of the metamodel-based approach on design effectiveness decreases. It was also stated that we needed to better understand what graphical capability within a design interface would be effective and why [100]. This study reflects our opinion that the research on visualization needs to go more in depth on understanding the needs of engineers and on designing the best intuitive interface in support of design. Questions needing to be answered include, to list a few: What are the more intuitive and easy-to-understand visualization techniques? What data in design need to be visualized? Why? What are the interactive means that the tool should and can provide to users? How will the visual aid help a designer to enhance the understanding of the problem or better direct the design?

Problem Formulation

Building a design optimization model is the first and yet critical step for design optimization. The quality of the optimization model directly affects the feasibility, cost, and effectiveness of optimization. The optimization problem, however, is usually formulated only from experience in making following decisions: (1) the objective function(s) and, in certain cases, goals; (2) the constraint function(s) and limits; (3) the design variables; and (4) the search range of each design variable. Metamodeling and design space exploration can help the engineer to decide on a reasonable goal for objectives and limits on constraints. Some of the objectives or constraints can be eliminated, combined, or modified. More importantly, metamodeling helps significantly in reducing the number of design variables and their range of search. In return, the reduction of dimensionality and search space is important for metamodeling because the sampling cost is directly influenced by the number of variables and their search range.

On the issue of reducing the number of design variables, the early work of Box and Draper [101] introduced a method to gradually refine the response surface to better capture the real function by "screening" out unimportant variables. Welch et al. [102] documented a systematic approach for screening the variables. The *variable-complexity response surface modeling* method used analyses of varying fidelity to reduce the design space to the region of interest [11,103]. The dimensionality was found difficult to reduce for multidisciplinary and multiobjective design problems, however, due to conflicting objectives [2].

In design engineering optimization, engineers tend to give very conservative lower and upper bounds for design variables at the stage of problem formulation. This is often due to the lack of sufficient knowledge of function behavior and interactions between objective and constraint functions at this early stage. Chen and her co-authors [104] developed heuristics to lead the surface refinement to a smaller design space. Wujek and Renaud [105,106] compared a number of move-limit strategies that all focused on controlling the function approximation in a more "meaningful" design space. Many researchers advocated the use of a sequential metamodeling approach using move limits [107] or trust regions [108,109]. For instance, the concurrent subspace optimization procedure used data generated during concurrent subspace optimization to develop response surface approximations of the design space, which formed the basis of the subspace coordination procedure [110]. Wang and colleagues developed the adaptive response surface method (ARSM), which systematically reduced the size of the design space by discarding portions of it that corresponded to objective function values larger than a given threshold value at each modeling-optimization iteration [45,111]. Heuristic approaches were also developed to gradually concentrate on a smaller design space [46,112,113].

Support of Various Optimization Needs

Due to various needs in design, a design optimization problem could be global optimization, multiobjective optimization in order to satisfy multiple design objectives, multidisciplinary design optimization where coupling between functions is present, or probabilistic optimization when uncertainties of variables are considered (see Fig. 1). In all these various optimization problems, metamodeling has been intensively used.

In general, classical gradient-based optimization methods have several limitations that hinder the direct application of these methods in modern design.

1. First, gradient-based optimization methods require explicitly formulated and/or cheap-to-compute models, while engineering design involves implicit and computation-intensive models such as FEA, CFD, and other simulation models with unreliable and expensive gradient information;
2. Second, gradient-based methods often output a single optimal solution, while engineers prefer multiple design alternatives;
3. Third, the gradient-based optimization process is sequential, nontransparent, and provides nearly no insight to engineers; and
4. Finally, to apply the optimization methods, high-level expertise on optimization is also required for engineers.

The advantages of applying metamodeling in optimization are manifold: (1) the efficiency of optimization is greatly improved with metamodels; (2) because the approximation is based on sample points, which could be obtained independently, parallel computation is supported (assuming an optimization requires 50 expensive function evaluations and each takes 2 h, these 50 evaluations can be computed in parallel and thus the total amount of time is 2 h as compared to 100 h); (3) the approximation process can help study the sensitivity of design variables, and thus give engineers insights to the problem; and (4) this method can handle both continuous and discrete variables.

Metamodel-Based Design Optimization (MBDO) Strategies. Three different types of strategies of MBDO can be found in the literature, as illustrated in Fig. 2. The first strategy (Fig. 2(*a*)) is the traditional sequential approach, i.e., fitting a global metamodel

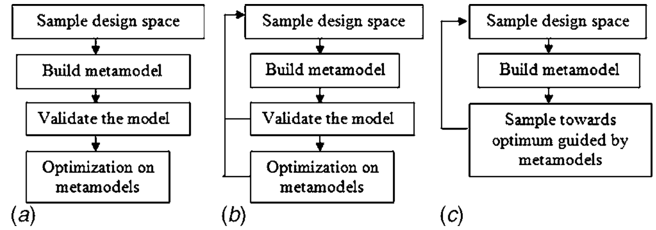

Fig. 2 MBDO strategies: (*a*) sequential approach; (*b*) adaptive MBDO; and (*c*) direct sampling approach

and then using the metamodel as a surrogate of the expensive function. This approach uses a relatively large number of sample points at the outset. It may or may not include a systematic model validation stage. If yes, the validation method might have to be cross validation. This approach is commonly seen in the literature [1,8,114]. The second approach (Fig. 2(*b*)) involves the validation and/or optimization in the loop in deciding the resampling and remodeling strategy. In Ref. [115], samples were generated iteratively to update the approximation to maintain the model accuracy. Osio and Amon [116] developed a multistage kriging strategy to sequentially update and improve the accuracy of surrogate approximations as additional sample points were obtained. Trust regions were also employed in developing several other methods to manage the use of approximation models in optimization [117,118]. Schonlau et al. [119] described a sequential algorithm to balance local and global searches using approximations during constrained optimization. Sasena et al. [120] used Kriging models for disconnected feasible regions. Knowledge was also incorporated in the identification of attractive design space [121]. Wang and colleagues developed a series of adaptive sampling and metamodeling methods for optimization, in which both the optimization and validation are used in forming the new sample set [45,46,111]. The third approach is recent and it directly generates new sample points towards the optimum with the guidance of a metamodel [37,38,122]. Different from the first two approaches, the metamodel is not used as a surrogate in a typical optimization process. The optimization is realized by adaptive sampling alone and no formal optimization process is called. The metamodel is used as a guide for adaptive sampling and therefore the demand on model accuracy is reduced. This method needs to be further tested for high-dimensional problems.

Global Optimization. A standard nonlinear optimization problem is usually formulated as

$$\begin{gathered} \min F(\mathbf{x}) \\ \text{S.T. } g_k(\mathbf{x}) \le 0, \quad (k=1,\ldots,K) \\ \mathbf{x} \in [\mathbf{x}_L, \mathbf{x}_U] \end{gathered} \tag{4}$$

where $\mathbf{x}=[x_1,x_2,\ldots,x_n]^T$ is a vector of design variable; and $\mathbf{x}_L$, $\mathbf{x}_U$ are the lower and upper bound vectors, respectively, which define the search range for each variable, and together define the design space. A typical metamodel-based optimization problem therefore becomes

$$\begin{gathered} \min \tilde{F}(\mathbf{x}) \\ \text{S.T. } \tilde{g}_k(\mathbf{x}) \le 0, \quad (k=1,\ldots,K) \\ \mathbf{x} \in [\mathbf{x}_L, \mathbf{x}_U] \end{gathered} \tag{5}$$

where the tilde indicates the metamodels for corresponding functions in Eq. (4).

Often a local optimizer is applied to Eq. (5) to search for the optimum. A limited number of methods have been developed for metamodel-based global optimization. One successful development was in Refs. [119,123], where the authors applied the Bayesian method to estimate a Kriging model, and then gradually identified points in the space to update the model and perform the optimization. Their method, however, has to preassume a continuous objective function and a correlation structure among sample points. A Voronoi diagram-based metamodeling method was proposed in which the approximation was gradually refined in ever smaller Voronoi regions and global optimum could be obtained [124]. Since the Voronoi diagram is from computational geometry, the extension of this idea to problems with more than three variables may not be efficient. Global optimization based on multipoint approximation and intervals was performed in Ref. [75]. Metamodeling was also used to improve the efficiency of genetic algorithms (GA) [125,126]. Wang and colleagues developed an adaptive response surface method (ARSM) for global optimization [45,111]. A so-called mode-pursuing sampling (MPS) method was developed [37], in which no existing optimization algorithm was applied. The optimization was realized through an iterative discriminative sampling process. MPS demonstrated high efficiency for optimization with expensive functions on a number of benchmark tests and design problems.

Multiobjective Optimization (MOO). A metamodel-based multi-objective optimization problem can be defined as in Eq. (6).

$$\begin{gathered} \min \tilde{F}(\mathbf{x}) = \{\tilde{F}_1(\mathbf{x}), \ldots \tilde{F}_r(\mathbf{x})\} \\ \text{S.T. } \tilde{g}_k(\mathbf{x}) \le 0, \quad (k = 1, \ldots, K) \\ \mathbf{x} \in [\mathbf{x}_L, \mathbf{x}_U] \end{gathered} \tag{6}$$

where r number of objective functions are to be optimized with the tilde symbol indicates the metamodels.

Recent approaches to solve MOO problems with black-box functions were to approximate each single objective function or directly approximate the Pareto optimal frontier [127–130]. Wilson et al. [128] used the surrogate approximation in lieu of the computationally expensive analyses to explore the multiobjective design space and identify Pareto optimal points, or the Pareto set, from the surrogate. Li et al. [129] used a hyperellipse surrogate to approximate the Pareto optimal frontier for bi-criteria convex optimization problems. If the approximation is not sufficiently accurate, then the Pareto optimal frontier obtained using the surrogate approximation will not be a good approximation of the actual frontier. Recent work by Yang et al. [130] proposed the first framework managing approximation models in MOO. In the framework, a GA-based method was employed with a sequentially updated approximation model. It differed from Ref. [128] by updating the approximation model in the optimization process. The fidelity of the identified frontier solutions, however, was still built upon the accuracy of the approximation model. The work in Ref. [130] also suffered from the problems of the GA-based MOO algorithm, i.e., the algorithm had difficulty in finding frontier points near the extreme points (the minimum obtained by considering only one objective function). Shan and Wang recently developed a sampling-based MOO method in which metamodels were used only as a guide [38]. New sample points were generated towards or directly on the Pareto frontier.

Probabilistic Design Optimization. Probabilistic design optimization consists of both robust design optimization (RDO) and reliability-based design optimization (RBDO). Both types of probabilistic optimization problems have been intensively studied. A robust design optimization problem is usually formulated as follows [81]

$$\begin{gathered} \min \tilde{z}[\mu_F(\mathbf{x},\mathbf{q}), \sigma_F(\mathbf{x},\mathbf{q})] \\ \text{S.T. } \tilde{g}_k(\mathbf{x},\mathbf{q}) \le 0, \quad (k = 1, \ldots, K) \\ \mathbf{x} \in [\mathbf{x}_L, \mathbf{x}_U] \end{gathered} \tag{7}$$

where $\mathbf{q}=[q_1, \ldots, q_l]$ is a vector of design parameters whose values are fixed as a part of the problem specifications. Both design variables and parameters could be the contributing sources of variations. Therefore both the objective function $\mathbf{F}(\mathbf{x},\mathbf{q})$ and $g(\mathbf{x},\mathbf{q})$ are random functions. The commonly used objective is to minimize both the mean, μ, and variance, σ, of the objective function in robust design optimization. The tilde symbol, again, indicates the metamodel.

The other type is called reliability-based design optimization (RBDO), which focuses on achieving the feasibility of constraints under uncertainty

$$\begin{gathered} \min \tilde{F}(\mathbf{x},\mathbf{q}) \\ \text{S.T. } P[\tilde{g}_k(\mathbf{x},\mathbf{q})] \ge P_{0k}, \quad (k = 1, \ldots, K) \\ \mathbf{x} \in [\mathbf{x}_L, \mathbf{x}_U] \end{gathered} \tag{8}$$

where P_{0k} is the desired probability for satisfying constraint k. The use of metamodeling in RDO and RBDO is extensive. Instead of providing a detailed review of these areas, this work only summarizes works involving metamodeling with references to a few representative articles.

Reliability assessment is the building block for RBDO. Metamodels are often used to approximate expensive constraint functions, or the limit state function. Some recent work included using IS together with metamodels [32,33]. Zou and colleagues developed a method, in which Monte Carlo simulation was only performed in a reduced region around the limit state [31]. Shan and Wang recently developed a more flexible discriminative sampling method with high efficiency and accuracy [39,122]. A novel concept, failure surface frontier (FSF), was also defined for reliability assessment [122]. FSF makes the accuracy of metamodeling less important, because in FSF-based reliability assessment, metamodels are mainly used as a guide of sampling.

Metamodels are commonly used as a surrogate of expensive processes; and probabilistic optimization processes are applied directly on the metamodels. Chen [9] applied metamodeling in robust design in her Ph.D. dissertation and from then on developed a series of methods in the field [56,131–133]. Booker continued on the surrogate management framework (SMF) [117] and applied it to reliability-based design [134]. These methods are implemented into Boeing's Design Explorer tool. Choi and his group has been very active in this area [135]. They started to look into using metamodels in support of RDO and RBDO.

Recently, Jin et al. performed a study on using metamodeling techniques for optimization when uncertainties were present [81]. It is found that a metamodel that is acceptable for deterministic optimization may not be acceptable for modeling the performance variations and the probability of constraint feasibility.

Multidisciplinary Design Optimization (MDO). MDO has been an intensively studied area, partially due to its broad definition. Its general formulation is as follows

$$\begin{gathered} \min F(\mathbf{x}_{cs}, \mathbf{y}) \\ \text{S.T. } \mathbf{y}_i = Y_i(\mathbf{x}_{cs}, \mathbf{x}_i, \mathbf{y}_{ci}), \quad i = 1, \ldots, s \\ g_k(\mathbf{x},\mathbf{y}) \le 0 \end{gathered} \tag{9}$$

where $\mathbf{y}$ is a state parameter output from its corresponding discipline; $\mathbf{y}_{ci}$ is a vector of state parameters output from other disciplines to disciplines i; $\mathbf{x}_i$ is a vector of disciplinary/local design variables; $\mathbf{x}_{cs}$ denotes a vector of system design variables; and vector $\mathbf{x}$ is the union of $\mathbf{x}_i$ and $\mathbf{x}_{cs}$. As compared with Eq. (4), MDO problems feature couplings between disciplines.

In real practice, MDO often involves a large number of design variables, computationally intensive function evaluations, and coupling between disciplinary functions. All these features of MDO make metamodeling an attractive tool to be included in MDO methodologies [4,11,136]. A detailed survey of MDO in aerospace was given in Ref. [136]. Golovidov et al. discussed in detail the strategies of using metamodeling in MDO via a commercial software tool iSight [137]. Batill et al. used metamodels in solving the coordination between design subspaces [138]. The use of metamodels in a current popular MDO methodology, Collaborative Optimization (CO), was archived in Ref. [139]. Wang et al. used metamodeling to guide sampling design solutions that satis-

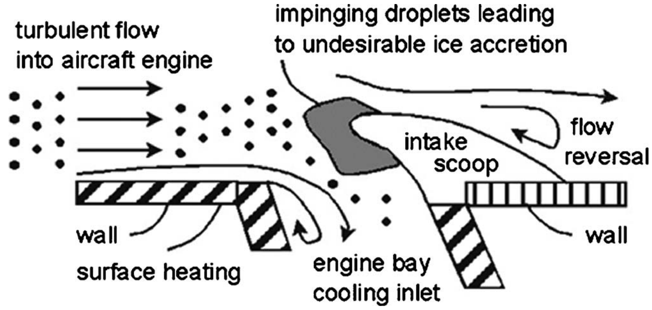

Fig. 3 Schematic of engine cooling bay inlet flow [144]

fied the coupling requirements between disciplines [140]. A metamodel-based approach was also developed to search for boundaries of coupled state parameters. With such boundaries, a coupled MDO problem can be reformulated with as an uncoupled problem and design engineers can have an enhanced understanding of the problem.

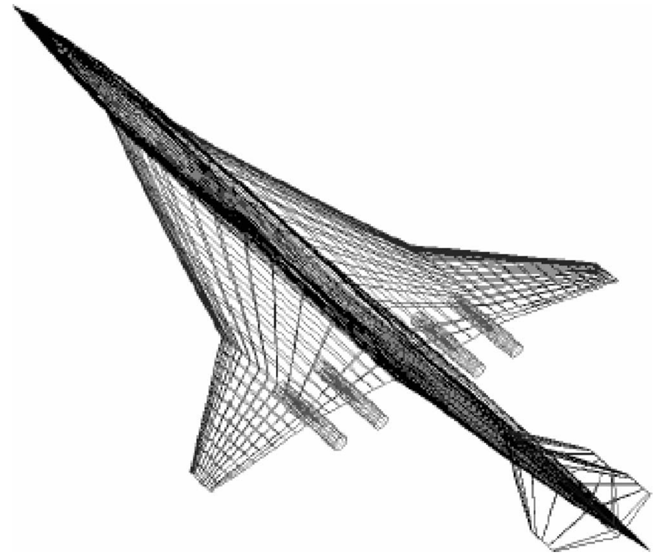

Fig. 4 A typical HSCT configuration [147]

Applications and Tools

A wide spectrum of applications of metamodeling and MBDO was documented in the literature. More than half a century ago, there was an aircraft jet engine inlet design involving 11 variables and five responses that used a 12 point Plackett-Burman design [141]. Otto et al. [142,143] applied Bayesian validated surrogates in the optimization of air foil and trapezoidal ducts. Golovidov et al. [137] built a global metamodel for an oil tanker design with six inputs, 14 outputs, and 50 function evaluations for each of the disciplinary analysis, hydrodynamics, and structural analysis. Wang et al. [144] applied the ARSM for the shape design of an air intake scoop for a helicopter's engine cooling bay (see Fig. 3). To reduce ice buildup on the intake scoop, the scoop shape is optimized with certain additional heat added to the scoop. Both heat transfer and air flow finite element models were built. The optimization involves 5 inputs and 45 function evaluations to reach the global optimum. Automotive crashworthiness has been intensively studied with special sessions in recent ASME Design Engineering Technical Conferences. Yang et al. [145] presented an example with 9 input variables, 11 output responses, and only 33 sample points to fit global metamodels for crashworthiness analyses. Gu [1] compared the accuracy of different metamodels for crashworthiness studies. Recent work documented crash-related design problems of 2, 11, and 20 variables [146]. The design of HSCT was also studied by many researchers [2,147] (see Fig. 4). Metamodeling was also applied to fuel cell component and system design [38,148], electronic packaging [116], engine bearings [149], and fixture configuration [114].

Current tools with MBDO capabilities are listed as follows. To avoid commercialism, readers are referred to individual URLs to learn about each tool.

1. Commercial tools:
   - iSight, by Engineous Software, Inc. (http://engineous.com/products.htm);
   - Optimus, by Neosis Solutions NV (http://www.noesis.be) and built into LMS Virtual.Lab optimization (http://www.lmsintl.com/simulation/virtuallab/optimization)
   - VisualDOC, by Vanderplaats Research and Development, Inc. (http://vrand.com/);
   - ModelCenter, by Phoenix Integration (http://www.phoenix-int.com/products/ModelCenter.php);
   - MARS, by Salford System (http://www.salford-systems.com/) and
   - LS-OPT, by Livermore Software Technology Corporation (http://www.lstc.com/)
2. Public domain tools:
   - DAKOTA, written in C++ by Sandia National Laboratories, is publicly available and under continuous development (http://endo.sandia.gov/DAKOTA/).
3. In-house tools:
   - Design explorer, by Boeing Company, commercially available through Phoenix Integration; and
   - PEZ System, General Electric Company.

Challenges and Future Development

Though intensive research on metamodeling and MBDO has been carried out and success has been achieved through numerous applications, some major research challenges remain to be overcome.

Large-Scale Problems. It is widely recognized that when the number of design variables is large, the total computation expense for metamodel-based approaches makes the approaches less attractive or even infeasible [2]. As an example, if the traditional CCD and a second-order polynomial function are used for metamodeling, the minimum number of sample points is $(n+1)(n+2)/2$, with n being the number of design variables. Therefore, the total number of required sample points increases exponentially with the number of design variables. Therefore, a well-known problem is the so-called "curse of dimensionality" for metamodeling. There seems to be a lack of research on large-scale problems, and many questions are not answered or even addressed. For example, what are the characteristics of a large-scale problem? Are there special models and sampling schemes that best suit large-scale problems [150]? Is decomposition the necessary path to solve the large-scale problem? What is the best decomposition strategy then? Is decomposition always feasible? What are the visualization techniques so that high-dimensional data are comprehensible? How does visualization help metamodeling for high-dimensional problems? It seems that the limitation for large-scale problems is the most prominent problem in MBDO. New metamodeling techniques for large-scale problems, or simple yet robust strategies to decompose a large-scale problem, are needed.

Flexible Metamodeling. Recent research seems to be moving towards developing more flexible and generic metamodeling approaches. Metamodels of variable fidelity across the entire or subdomains of design spaces have been integrated to increase overall efficiency [151]. Metamodeling of multiple responses from a single simulation was also developed [152]. Sahin and Diwekar [153] used reweighting to update a kernel density estimator when new sample points were obtained. The metamodeling process was not repeated, and thus the efficiency of metamodeling was improved [153]. Recalibrated composite approximation models were also used in support of optimization [154]. The extended RBF method allows the user to choose the best RBF model from many alternatives that all interpolate the sample points [68].

Currently metamodeling is mostly used for approximating the design variables and their performances, which are often used as an output of the "black-box" functions. It would be beneficial to have a model of gradient of the performance function, a model of curvatures, and so on. In the case of uncertainties, it might be helpful to have a metamodel of standard deviation to help probabilistic design optimization [81]. Moreover, it would be even better if such a metamodel of certain function property can be derived from the metamodel of the performance function. Therefore, new innovative metamodel forms may be invented for this purpose. Second, if engineers have *a priori* knowledge about a computation intensive process, how can this knowledge be categorized, represented, and incorporated in metamodeling [155]? Third, studies on metamodels and metamodeling techniques for problems with mixed discrete and continuous variables are lacking. Finally, when models of different fidelity are used to generate sample points for metamodeling, if a metamodel is proved to be accurate for a low fidelity model, can it be tuned for a higher fidelity model? In the field of electrical engineering, a method called space mapping [156] was developed, which built a connection between low and high fidelity models. Another situation is when the "black-box" function is slightly altered, for example, a constant is changed due to the change of operating condition. Can we have a mechanism to fine tune the existing metamodel to adapt to such a change?

Intelligent Sampling. Current sampling schemes for metamodeling focus on the initial sampling in order to achieve certain space filling properties. As a matter of fact, if the function to be approximated is considered as a "black box," the best initial sample size will remain to be a mystery. Without knowing the best sample size, the distribution of the sample points becomes less important. Therefore, the subtle differences between various space filling sampling methods may not deserve so much attention. The focus on sampling, in our opinion, should shift to how to generate a minimum number of sample points intelligently so that the metamodel reflects the real "black-box" function in areas of interest. This statement implies that the sampling process is iterative and ought to be progressive, which is reflected in some recent work [157,158]. Though there are methods on iterative sampling as reviewed before, more "intelligent" sampling schemes need to be developed to further advance the metamodeling techniques.

Uncertainty in Metamodeling. Metamodeling can be used to filter noises in computer simulation [159]. On the other hand, the uncertainty in metamodels brings new challenges in design optimization. For constrained optimization problems, if both constraint and objective functions are computation expensive and metamodeling is applied, it is found that the constrained optimum is very sensitive to the accuracy of all metamodels [46]. Mathematically rigorous methods have to be developed to quantify the uncertainty of a metamodel, only based on which metamodel-based probabilistic optimization and constrained optimization can be confidently performed.

Summary

This work provides an overview of the metamodeling techniques and their application to support engineering design optimization. Research and development in metamodeling are categorized according to the needs of design engineers: model approximation, design space exploration, problem formulation, and support of optimization. Challenges and future developments are also discussed. It is hoped that this work can help researchers and engineers who are just starting in this area. Also it is hoped that this work will help current researchers and developers by being a reference and inspiration for future work.

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