Proceedings of the ASME 2010 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference
IDETC/CIE 2010
August 15 - 18, 2010, Montreal, Quebec, Canada

DETC2010-28813

MAKING THE MOST OUT OF SURROGATE MODELS: TRICKS OF THE TRADE

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ABSTRACT

Design analysis and optimization based on high-fidelity computer experiments is commonly expensive. Surrogate modeling is often the tool of choice for reducing the computational burden. However, even after years of intensive research, surrogate modeling still involves a struggle to achieve maximum accuracy within limited resources. This work summarizes advanced and yet simple statistical tools that help. We focus on four techniques with increasing popularity in the design automation community: (i) screening and variable reduction in both the input and the output spaces, (ii) simultaneous use of multiple surrogates, (iii) sequential sampling and optimization, and (iv) conservative estimators.

1 INTRODUCTION

Statistical modeling of computer experiments embraces the set of methodologies for generating a surrogate model (also known as metamodel or response surface approximation) used to replace an expensive simulation code [1]-[6]. The goal is constructing an approximation of the response of interest based on a limited number of expensive simulations. Although it is possible to improve the surrogate accuracy by using more simulations, limited computational resources often makes us face at least one of the following problems:

- Desired accuracy of a surrogate requires more simulations than we can afford.
- The output that we want to fit is not a scalar (scalar field) but a high-dimensional vector (vector field with several thousand components), which can be prohibitive or impractical to handle.
- We use the surrogate for global optimization and we do not know how to simultaneously obtain good accuracy near all possible optimal solutions.
- We use the surrogate for optimization, and when we do an exact analysis we find that the solution is infeasible.

This paper discusses sophisticated and yet straightforward techniques that address these four issues. We focus on (i) screening and variable reduction [7]-[11], (ii) use of multiple surrogates [12]-[14], (iii) sequential sampling and optimization [15], [16], and (iv) safe estimators under limited budget [17]-[19].

The remaining of the paper is organized as follows. Section 2 reviews the screening and dimension reduction techniques. Section 3 presents the use of multiple surrogates. Section 4 focuses on sequential sampling techniques. Section 5 presents the strategies for conservative surrogates. Finally, section 6 closes the paper recapitulating salient points and concluding remarks.

2 SCREENING FOR REDUCING THE NUMBER OF VARIABLES

2.1 Variable reduction in input space

As the number of variables in the surrogate increases, the number of simulations required for surrogate construction rises exponentially (curse of dimensionality). A question at this point is then the following: is it necessary to construct the response surface approximation in terms of all the variables? Some of the variables may have only a negligible effect on the response. Several techniques have thus been proposed for evaluating the importance of the variables economically. In the next few paragraphs we first provide a brief historical overview of methods that have been proposed in this context. Then we focus on a few techniques of particular interest in more detail.

A wide category of dimensionality reduction in input space is commonly referred to as variables screening. Among

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the simplest screening techniques are so called one-at-a-time (OAT) plans [20], which *evaluate* in turns the effect of changing one variable at a time. It is a very inexpensive approach, but it does not estimate interaction effects between variables. Variations of OAT screening that account for interactions have been proposed by Morris [21] and Cotter [22].

Another category of screening techniques are variance based. A simple, commonly used approach uses a k-level factorial or fractional factorial design followed by an analysis of variance procedure (ANOVA) [23]. The procedure allows identifying the main and interaction effects that account for most of the variance in the response. ANOVA can be carried out either using a reduced fidelity, computationally inexpensive model as has been recommended in [24]-[26], or using the high fidelity model as suggested in [27]. Note that using a reduced fidelity model is a common technique in variable screening, which will be illustrated again in the next paragraphs with global sensitivity analysis.

The iterated fractional factorial design (IFFD) method [28],[29] is another screening approach, designed to be economical for large number of variables (e.g. several thousands). The method assumes that only very few variables account for most of the variance in the response and calculates the main effects, quadratic effects and cross term effects for these significant variables based on a clustered sampling technique.

For additional details and applications on these and additional screening methods, such as Bettonvil's sequential bifurcation method [30], the reader can refer to [31]-[33] and the references therein. In the remainder of this subsection we will develop in more detail just a few techniques that we find of particular interest.

An approach gaining popularity for finding and eliminating variables that have negligible effects is Sobol's global sensitivity analysis (GSA) [34]. GSA is a variance-based approach that provides the total effect (i.e. main effect and interaction effects) of each variable, and thus indicates which ones could be ignored. The variances are usually computed using Monte Carlo simulation based on an initial crude surrogate (assumed to be accurate enough for screening). GSA was successfully applied to the piston shape design [35], the liquid rocket injector shape design [36], the bluff body shape optimization [37], and more recently to the optimization of an integrated thermal protection system [38], the design of high lift airfoil [39], the identification of material properties based on full field measurements [40] and stream flow modeling [41].

A different concept is based on grouping the variables into a smaller number by nondimensionalization. The Vaschy-Buckingham theorem [42]-[44] provides a systematic construction procedure of nondimnesional parameters and also guarantees that the parameters found are the minimum number of parameters (even though not necessarily unique) required for an exact representation of the given problem.

References [45]-[47] show that improved accuracy polynomial response surface approximations can be obtained by using nondimensional variables. This is mainly because, for the same number of numerical simulations, the generally much fewer nondimensional variables allow a fit with a higher order polynomial. Vignaux and Scott [46] illustrated this approach using statistical data from an automobile survey while Lacey and Steele [47] applied the method to several engineering case studies including a finite element (FE) based example.

Gogu et al. [48] managed to reduce the number of variables from eight to four by constructing the surrogate in terms of nondimensional variables for a vibration problem of a free plate. Venter and Haftka [49] achieved a reduction from nine to seven variables by using nondimensional parameters for FE analyses, modeling a mechanical problem of a plate with an abrupt change in thickness.

An even greater reduction in the number of variables is possible if nondimensionalization is combined with other screening techniques. Gogu et al. [50] achieved a reduction from fifteen to only two variables using a combination of physical reasoning, nondimensionalization and global sensitivity analysis for a thermal design problem for an integrated thermal protection system. Physical reasoning allowed formulating simplifying assumptions that reduced the number of variables from fifteen to ten. Nondimensionalization was then applied on the equations of the simplified problem reducing the number of variables to three nondimensional variables. Finally, global sensitivity analysis showed that one of the nondimensional variables had an insignificant effect thus leaving only two variablesfor the surrogate model.

A final variable reduction approach is important when designs of interest are confined into a reduced dimension (e.g. a plane in three dimensional space). If the input vectors (of dimension n) are all in a lower-dimensional subspace (of dimension k, with $k<n$), then using the initial input space for surrogate construction will lead to poor results due to numerical ill-conditioning. A reduced dimensional representation of the variables should then be used by expressing the initially n-dimensional input vectors in a basis of the corresponding k-dimensional subspace.

Principal components regression (PCR) is a technique developed to fit an approximation (e.g. polynomial) to the data in the appropriate sub-dimensional subspace ([51], Chapter 3). Mandel [52] has shown that the technique can be advantageous also when the variables-data is not strictly confined to a subspace, but the components outside of the subspace are relatively small. Rocha et al. [53] have recently shown that for the problem of fitting wing weight data of subsonic aircraft, PCR provides more accurate results compared to other fitting techniques (polynomial interpolation, kriging, radial basis function interpolation) due to its ability to account for the physical and historical trends buried within the input data.

The partial least squares [54] and sparse partial least squares [55] techniques have also been proposed as alternatives to principal component regression for reducing very high-dimensional data. These techniques have been notably used for fitting genomic data.

2.2 Dimensionality reduction in the output space

The question of a dimensionality reduction requirement in the output space poses itself less often than in the input space (that is, usually we want to have the minimal number of variables that controls a particular scalar field). For vector-based response, techniques that take into account correlation between components are available [56] and can in some cases

be more accurate than considering the components independently. For a relatively small dimension of the output vector, methods such as co-kriging [57] or vector splines [58] are available. However, these are not practical for approximating the high dimensional pressure field around the wing of an aircraft or approximating heterogeneous displacements fields on a complex specimen. These fields are usually described by a vector with thousands to hundreds of thousands components. Fitting a surrogate for each component is then time and resource intensive and might not take advantage of the correlation between neighboring points.

Principal components analysis (PCA), which we already touched upon in the previous section addresses this problem. PCA is also known as proper orthogonal decomposition (POD) or Karhunen-Loeve expansion, and it can be applied to achieve drastic dimensionality reduction in the output space (reductions from many thousands to less than a dozen coefficients are possible).

POD finds a low dimensional basis from a given set of *N* simulation samples. A field $\mathbf{U}$ within the sampling domain bounds is then approximated by

$$\mathbf{U} = \sum_{k=1}^{K} \alpha_k \mathbf{\Phi}_k = \sum_{k=1}^{K} \left\langle \mathbf{U}, \mathbf{\Phi}_k \right\rangle \mathbf{\Phi}_k \qquad (1)$$

where $\mathbf{U} \in \mathbb{R}^n$ is the vector representation of the field (e.g. pressure field, displacement field), $\left\{ \mathbf{\Phi}_k \right\}_{k=1..K}$ the basis vectors of the reduced-dimensional, orthogonal basis, and α_k the coefficients of the field in this basis (i.e. the orthogonal projection of the field onto the basis vectors).

This approach allows approximating the fields in terms of K POD coefficients α_k instead of n components of the vector $\mathbf{U}$. For additional details on the theoretical foundations of POD, the reader can refer to [59] and Chapter 1 of [60].

Once the reduced dimensional basis determined, one can construct surrogate models for each α_k ($k = 1 \ldots K$), based on the same N samples that were used for POD decomposition. It might seem surprising that, considering that n is equal to several thousands, K can be low enough to easily allow the construction of a surrogate model per POD coefficient, but successful applications have proven the applicability of the approach to various problems. This is due to the fact that variations even in complex fields can be controlled by physical phenomena exhibiting effects characterized by relatively low dimensionality.

This approach has been successfully applied to the multidisciplinary design optimization of an aircraft wing [61],[62]. The stream-flow field around the wing has been reduced using POD and surrogate models of the corresponding POD coefficients constructed. The method enabled cost-efficient fluid-structure interaction required for the multi-disciplinary design optimization. The initial application [61] was carried out on a two-dimensional wing model, where the variations in vectors of size $n = 70$ were reduced to only two POD coefficients. A subsequent study [62] applied the same approach to more realistic 3D wing models where the pressure fields around the wing (aerodynamics model) as well as for the wing displacement field (structural model) were reduced and approximated via this approach.

Another application of POD reduction combined with surrogate modeling concerned Bayesian identification of orthotropic elastic constants based on displacement fields on a plate with a hole [63]. Variations in displacement fields of about 5,000 pixels (i.e. vectors with 5,000 coefficients) were reduced to only four POD coefficients, containing enough information to perform the identification. Surrogate models of these POD coefficients were constructed, enabling a sufficient cost reduction for the Bayesian identification to be carried out, which requires expensive correlation information.

Note that PCA is a linear technique, in that the output is expressed as a linear combination of the basis vectors. Non-linear dimensionality reduction approaches have been developed for cases where linearity will not provide a sufficiently accurate approximation. Methods based on neural networks are relatively popular [64] and some applications include feature visualization [65], [66], image processing [67] and structural health monitoring [68].

3 MULTIPLE SURROGATES

The simultaneous use of multiple surrogates addresses two of the problems mentioned in the introduction:

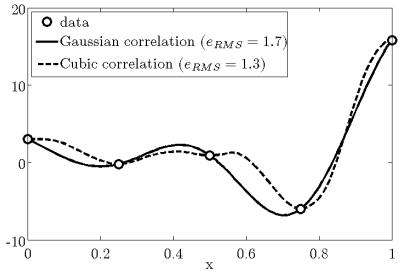
- Accurate approximation requires more simulations than we can afford by offering an insurance against poorly fitted models.
- Surrogate models for global optimization since different surrogates might point to different regions of the design space this constitutes at least a cheap and direct approach for global optimization.

3.1 How to Generate Different Surrogates

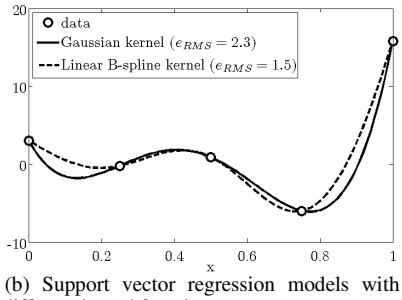
Most practitioners in the optimization community are familiar at least with the traditional polynomial response surface [23], [69], some with more sophisticated models such as kriging [70]-[72], neural networks [73]-[75], or support vector regression [76]-[78], and few with the use of weighted average surrogates [79]-[81]. The diversity of surrogate models might be explained by three basic components [82]:

1. Statistical modeling: for example, response surface techniques frequently assume that the data is noisy and the obtained model is exact. On the other hand, kriging usually assumes that the data is exact and is a realization of a Gaussian process.
2. Basis functions: response surfaces frequently use monomials. Support vector regression specifies the basis in terms of a kernel (many different functions can be used).
3. Loss function: the minimization of the mean square error is the most popular criteria for fitting the surrogate. Nevertheless, there are alternative measures such as the average absolute error (i.e., the L1 norm).

It is also possible to create different instances of the same surrogate technique. For example, we could create polynomials with different choice of monomials, kriging models with different correlation functions (see [83] for details), and support vector regression models with different kernel and loss functions (see [84] for details). Figure 1 illustrates this idea showing different instances of kriging and support vector regression fitted to the same set of points.



(a) Kriging surrogates with different correlation functions.



(b) Support vector regression models with different kernel functions.

Figure 1: Different surrogates models fitted to five data points of the function $y(x) = (6x-2)^2 \times \sin\left(2 \times (6x-2)\right)$ (adapted from [6]).

3.2 Comparison of Surrogates

The vast diversity of surrogates has motivated many papers comparing the performance among techniques. For example, Giunta and Watson [85] compared polynomial response surface approximations and kriging on analytical example problems of varying dimensions. They concluded that quadratic polynomial response surfaces were more accurate. However, they hedged that the investigation was not intended to serve as an exhaustive comparison between the two modeling methods. Jin et al. [86] compared different surrogate models based on multiple performance criteria such as accuracy, robustness, efficiency, transparency, and conceptual simplicity. They concluded that the performance of different surrogates has to do with the degree of nonlinearity of the actual function and the design of experiment (sampled points). Stander et al. [87] compared polynomial response surface approximation, kriging, and neural networks. They concluded that although neural nets and kriging seem to require a larger number of initial points, the three meta-modeling methods have comparable efficiency when attempting to achieve a converged result. Overall, the literature leads us to no clear conclusion. Instead, it confirms that the surrogate performance depends on both the nature of the problem and the sampled points.

While different metrics can be used to compare surrogates (such as the coefficient of determination R^2, the average absolute error, the maximum absolute error [86]-[89]) here, we will use the root mean square error e_{RMS}. The root mean square error e_{RMS} in a design domain D of volume V is given by

$$e_{RMS} = \sqrt{\frac{1}{V}\int_D \left(\hat{y}\left(x\right) - y\left(x\right)\right)^2 d\mathbf{x}} \quad , \tag{2}$$

where $\hat{y}\left(\mathbf{x}\right)$ is the surrogate model of the response $y\left(\mathbf{x}\right)$.

The integral of Eq. (2) can be estimated using numerical integration at test points. So, back to Figure 1, the e_{RMS} of a set of surrogates can greatly differ in terms of accuracy. As a result, it might be hard to point the best one for a given problem and data set.

3.3 Surrogate Selection

If only one predictor is desired, one could apply either selection or combination of surrogates [93]. Selection is usually based on a performance index that applies to all surrogates of the set (that is, a criterion that does not depend on the assumptions of any particular surrogate technique). In this case, the use of test points is a luxury and we usually have to estimate the accuracy of the surrogate based on the sampled data only. Because of that, cross validation (estimation of the prediction errors based on data points) is becoming popular[*].

A cross-validation error is the error at a data point when the surrogate is fitted to a subset of the data points not including this point. When the surrogate is fitted to all the other $p-1$ points, the process has to be repeated p times (leave-one-out strategy) to obtain the vector of cross-validation errors, $\mathbf{e}_{XV}$. Figure 2 illustrates computation of the cross-validation errors for a kriging surrogate. When the leave-one-out becomes expensive, the k-fold strategy can also be used for computation of the $\mathbf{e}_{XV}$ vector. According to the classical k-fold strategy [92], after dividing the available data (p points) into $p\,/\,k$ clusters, each fold is constructed using a point randomly selected (without replacement) from each of the clusters. Of the k folds, a single fold is retained as the validation data for testing the model, and the remaining $k-1$ folds are used as training data. The cross-validation process is then repeated k times with each of the k folds used exactly once as validation data.

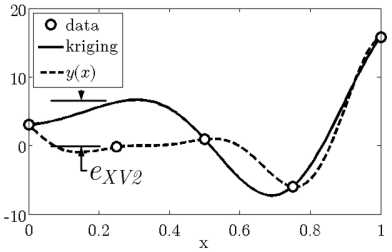


Figure 2: Cross-validation error at the second point of the five-point experimental design e_{XV_2}. The kriging model is fitted to the remaining four points of the function $y(x) = (6x-2)^2 \times \sin\left(2 \times (6x-2)\right)$.

The square root of the $PRESS$ value ($PRESS$ stands for prediction sum of squares) is the estimator of the e_{RMS}:

$$PRESS_{RMS} = \sqrt{\frac{1}{p}\mathbf{e}_{XV}{}^T\mathbf{e}_{XV}} \quad . \tag{3}$$

[*] Nevertheless, cross validation should be used with caution, since the literature has reported problems such as bias in error estimation [90], [91].

Since $PRESS_{RMS}$ is an estimator of the e_{RMS}, one possible way of using multiple surrogates is to select the model with best (i.e., smallest) $PRESS_{RMS}$ value [93]-[96]. Because the quality of fit depends on the data points, the surrogate of choice may vary from one experimental design to another.

Combining surrogates is based on the hope of canceling errors in prediction through proper linear combination of models. This is shown in Figure 3, in which the weighted average surrogate created using the four surrogates of Figure 1 has smaller e_{RMS} than any of the basic surrogates. Cross-validation errors can be used to obtain the weights via minimization of the integrated square error [81], [93]. Alternatively, the weight computation might also involve the use of local estimator of the error in prediction. For example, Zerpa et al. [97] presented a weighting scheme that uses the prediction variance of the surrogate models (available in kriging and response surface for example).

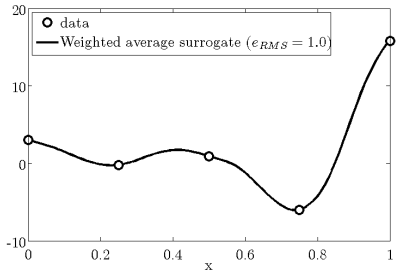


Figure 3: Weighted average surrogate based on the models of Figure 1.

Nevertheless, the advantages of combination over selection have never been clarified [98]. According to Yang [98], selection can be better when the errors in prediction are small and combination works better when the errors are large. Viana et al. [93] showed that while in theory the surrogate with best e_{RMS} can be beaten (via weighted average surrogate), in practice, the quality of information given by the cross-validation errors makes it very difficult. On top of that, they showed that the potential gains diminish substantially in high dimensions.

3.4 Multiple Surrogates in Optimization

A surrogate-based optimization cycle consists of choosing points in the design space (experimental design), conducting simulations at these points and fitting a surrogate (or maybe more than one) to the expensive responses. If the fitted surrogate satisfies measures of accuracy, we use it to conduct optimization. Then we verify the optimum by conducting exact simulation. If it appears that further improvements can be achieved, we update the surrogate with this new sampled points (and maybe zoom in on regions of interest) and conduct another optimization cycle.

In this scenario, it seems advantageous to use multiple surrogates. After all, one surrogate may be more accurate in one region of design space while another surrogate may be more accurate in a different region. The hope is that a set of surrogates would allow exploration of different portions of the design space by pointing to different candidate solutions of the optimization problem.

Examples of this approach can be found in the literature. For instance, Mack et al. [37] employed polynomial response surfaces and radial basis neural networks to perform global sensitivity analysis and shape optimization of bluff body devices to facilitate mixing while minimizing the total pressure loss. They showed that due to small islands in the design space where mixing is very effective compared to the rest of the design space, it is difficult to use a single surrogate to capture such local but critical features. Glaz et al. [99] used polynomial response surfaces, kriging, radial basis neural networks, and weighted average surrogate for helicopter rotor blade vibration reduction. Their results indicated that multiple surrogates can be used to locate low vibration designs which would be overlooked if only a single approximation method was employed. Samad et al. [100] used polynomial response surface, kriging, radial basis neural network, and weighted average surrogate in a compressor blade shape optimization of the NASA rotor 37. It was found that the most accurate surrogate **did not always** lead to the best design. This demonstrated that using multiple surrogates can improve the robustness of the optimization at a minimal computational cost. The use of multiple was found to act as an insurance policy against poorly fitted models.

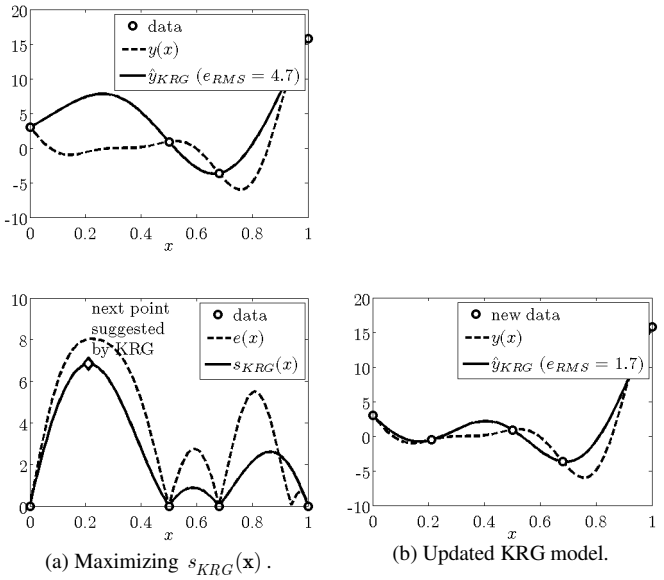
4 SEQUENTIAL SAMPLING AND OPTIMIZATION

Sequential sampling fits a sequence of surrogates with each surrogate defining the points that need to be sampled for the next surrogate. This can improve the accuracy for a given number of points, because points may be assigned to regions where the surrogate shows sign of poor accuracy. Alternatively, this approach may focus the sampling on regions of high potential for a single or multiple optima.

4.1 Sequential Sampling

In the literature [16], [101], [102], the word "sequential" is sometimes substituted by "adaptive" or "application-driven," and the word "sampling" is sometimes replaced by "experimental design," or "design of experiment". Usually, we will use of the uncertainty model associated with many surrogates to select new simulations. The uncertainty structure is present in surrogates such as polynomial response surface and kriging. Here, we give an example with kriging due to its popularity in the literature on computer experiments.

The basic sequential sampling approach uses finds the point in the design space that maximizes the kriging prediction error (here, we use the square root of the kriging prediction variance). Figure 4 illustrates the first cycle of the algorithm. Figure 4-(a) shows the initial kriging model and the corresponding prediction error. The maximization of the prediction error suggests adding $x = 0.21$ to the data set. The updated kriging model is shown in Figure 4-(b). There is a substantial decrease in the root mean square error, from 4.7 to 1.7. We can see that regions of high error estimates push exploration.



(a) Maximizing $s_{KRG}(\mathbf{x})$. (b) Updated KRG model.

Figure 4: Basic sequential sampling. Figure 4-(a) shows that the maximization of kriging prediction standard deviation, $s_{KRG}(\mathbf{x})$, suggests adding $x = 0.21$ to the data set. Figure 4-(b) illustrates the updated kriging (KRG) model after $x = 0.21$ is added to the data set.

Jin et al. [16] reviewed various sequential sampling approaches (maximization of the prediction error, minimization of the integrated square error, maximization of the minimum distance, and cross validation) and compared them with simply filling of the original design (one stage approach). They found that the performance of the sequential sampling methods depended on the quality of the initial surrogate (i.e., there is no guarantee that sequential sampling will do better than the one stage approach). Kleijnen and Van Beers [101] proposed an algorithm that, after the first model is fitted, iterates by placing a set of points using a space filling scheme and then choosing the one that maximizes the variance of the predicted output (variance of the responses taken from cross validation of the original data set). In a follow up, Van Beers and Kleijnen [102] improved their approach to account for noisy responses. In the works of Kleijnen and Van Beers, an improved kriging variance estimate [103] is used and that might be a reason for better results.

Recent developments in sequential sampling are exemplified by refs. [104]-[107]. Rai [104] introduced the qualitative and quantitative sequential sampling technique. The method combines information from multiple sources (including computer models and the designer's qualitative intuitions) through a criterion called "confidence function." The capabilities of the approach were demonstrated using various examples including the design of a bi-stable micro electro mechanical system. Turner et al. [105] proposed a heuristic scheme that samples multiple points at a time based on non uniform rational B-splines (NURBs). The candidate sites are generated by solving a multi-objective optimization problem. The effectiveness of the algorithm was demonstrated for five trial problems of engineering interest. Gorissen et al. [106] brought multiple surrogates to adaptive sampling. The objective is to be able to select the best surrogate model by adding points iteratively. They tailored a genetic algorithm that combines automatic model type selection, automatic model parameter optimization, and sequential design exploration. They used a set of analytical functions and engineering examples to illustrate the methodology. Rennen et al. [107] proposed nested designs. The idea is that the low accuracy of a model obtained might justify the need of an extra set of function evaluations. They proposed an algorithm that expands an experimental design aiming maximization of space filling and non-collapsing points.

4.2 Optimization-driven Sequential Sampling

Surrogate-based optimization has been a standard technology for long time [108]. Traditionally, the surrogate replaces the expensive simulations in the computation of the objective function (and its gradient, if that is the case). Yet, Jones et al. [15] added a new twist by using both prediction and prediction variance of the kriging model to help selecting the next point to be sampled in the optimization task. They introduced the efficient global optimization (EGO) algorithm, which we will briefly describe here (for complete description see [14], [15], and [109]).

EGO starts by fitting a kriging model for the initial set of data points. After that, the algorithm iteratively adds points to the data set in an effort to improve upon the present best sample y_{PBS}. In each cycle, the next point to be sampled is the one that maximizes the expected improvement

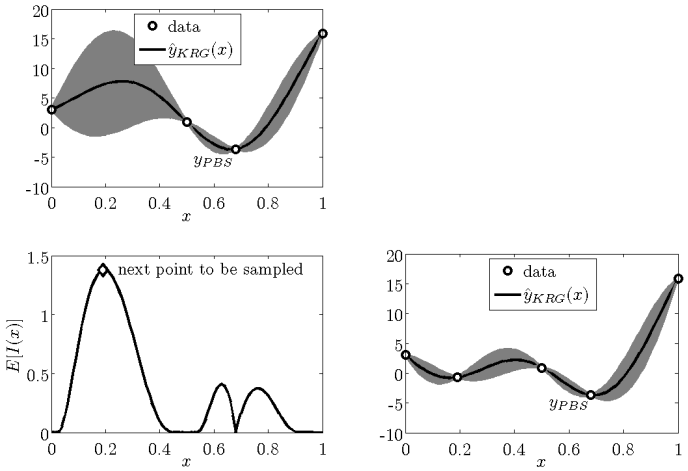
$$E\left[I(\mathbf{x})\right] = s(\mathbf{x})\left[u\Phi(u) + \phi(u)\right], \quad u = \left[y_{PBS} - \hat{y}(\mathbf{x})\right] / s(\mathbf{x}), \tag{4}$$

where $\Phi(\cdot)$ and $\phi(\cdot)$ are the cumulative density function (CDF) and probability density function (PDF) of a normal distribution, $\hat{y}(\mathbf{x})$ is the kriging prediction; and $s(\mathbf{x})$ is the prediction standard deviation (here estimated as the square root of the prediction variance $s^2(\mathbf{x})$). See [70]-[72] for details about the kriging predictior $\hat{y}(\mathbf{x})$ and its prediction variance $s^2(\mathbf{x})$.

Unlike methods that only look for the optimum predicted by the surrogate, EGO will also favor points where surrogate predictions have high uncertainty. After adding the new point to the existing data set, the kriging model is updated (usually without going to the costly optimization of the correlation parameters). Figure 5 illustrates the one cycle of the EGO algorithm. Figure 5-(a) shows the initial kriging model and the corresponding expected improvement. The maximization of $E\left[I(\mathbf{x})\right]$ adds $x = 0.19$ to the data set. In the next cycle, EGO uses the updated kriging model shown in Figure 5-(b).

Since the work of Jones et al. [15], EGO-like algorithms have attracted much attention from the scientific community (e.g., [14], and [109]-[113]). In the follow up of [15], Jones [109] provided a detailed study on the ways that surrogate models can be used in global optimization (from the simple use of the prediction to the elaborated EGO algorithm). Forrester and Keane [14] provided an extended and modern review, which also includes topics such as constrained and multi-objective optimization. Ginsbourger et al. [110], Villemonteix et al. [111], and Queipo et al. [112] share the common point of proposing alternatives to the expected improvement for selection of points. Ginsbourger et al. [110]

extended both the expected improvement and the probability of improvement as infill sampling criteria allowing for multiple points in each additional cycle. However, they also mention the high computational costs associated with this strategy. Villemonteix et al. [111] introduces a new criterion that they called "conditional minimizers entropy" with the advantage of being ready to use in noisy applications. Queipo et al. [112] focused on the assessment of the probability of being below a target value given that multiple points can be added in each optimization cycle (this strategy is more cost-efficient than the expected improvement counterpart). Finally, Viana et al. [113] proposed using multiple surrogates that optimize the expected improvement (see Eq. (4)) as a way of generating multiple points in each additional cycle. Preliminary results showed that their approach is a cheap and efficient way of generating multiple points per cycle.



(a) Maximizing $E[I(\mathbf{x})]$. (b) Updated KRG model.

Figure 5: Cycle of the Efficient Global Optimization (EGO) algorithm. Figure 5-(a) shows that the maximization of the expected improvement, $E[I(\mathbf{x})]$, suggests adding $x = 0.19$ to the data set. Figure 5-(b) illustrates the updated kriging (KRG) model after $x = 0.19$ is added to the data set.

5 BEING SAFE UNDER LIMITED BUDGET

In constrained optimization (constraints being surrogate models) or in reliability-based design optimization (limit state composed by surrogate models), it can happen that after running the optimization the solution turns out to be infeasible due to surrogate errors. This section is devoted to approaches that either (i) use conservative constraints so that the optimization is pushed to the feasible region; or (ii) make the limit state more accurate near the boundary between of the feasible domain.

5.1 Conservative Surrogates

Usually, surrogate models are fit to be unbiased (i.e., the error expectation is zero). However, in certain applications, it might be important to safely estimate the response (e.g., in structural analysis, the maximum stress must not be underestimated in order to avoid failure). One of the most widely used methods for conservative estimation is to bias the prediction response by additive or multiplicative constants (termed safety margin and safety factors, respectively) [114]-[116]. The choice of the constant is often based on previous knowledge of the problem. However, the practice is fairly recent for surrogate-based analysis.

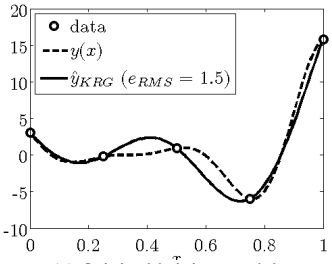
One way of improving the how conservative the surrogate (i.e. the conservativeness of a surrogate[†]) is to require it to conservatively fit the data points (e.g refs. [117] and [118]). Another way is to use the prediction interval given by the weighted least square surrogate model as a safeguard against surrogate error [119]. However, these approaches do not allow tuning in the level of desired conservativeness. In their previous work (see refs. [120] and [121]), authors explored and compared different approaches to design conservative surrogate models. They are summarized in Table 1. Picheny et al. [120] found that there was no clear advantage of the one specific method over the simple use of safety margin to bias the surrogate model. However, the safety margin approach lacked a basis for selecting its magnitude. Viana et al. [19] proposed a method for design the safety margin based on cross-validation errors.

Table 1: Methods for creating conservative surrogates. Adapted from [120].

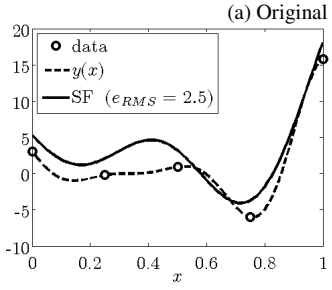
Method	Principle
Biased fitting	The surrogate is constrained to be above the training points
Constant safety factor	The surrogate response is multiplied by a constant
Constant safety margin	A constant is added to the surrogate response
Indicator kriging	The estimate is a percentile
Error distribution	Error distribution is used to build confidence intervals

Figure 6 illustrates two of the techniques shown in Table 1. Consider a conservative prediction, one that overestimates the actual response. Figure 6-(a) shows that the original kriging model (fit to be conservative 50% of the time) would present a root mean square error of 1.5. Figure 6-(b) and (c) are conservative surrogates designed for 90% conservativeness (here, we consider overestimation as being conservative). Figure 6-(b) shows that by using safety margin, we shift the surrogate up and that would lead to a root mean square error of 2.5 (i.e., loss in accuracy of 67%). Figure 6-(c) illustrates what happens with the error distribution approach. Here, the root mean square error would be 2.9 (i.e., loss in accuracy of 97%).

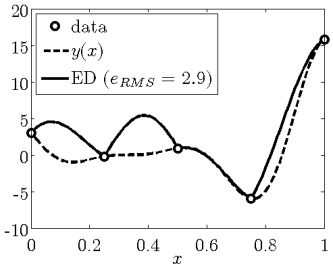
[†] There are different measures of the conservativeness of a surrogate (e.g., the average error or the maximum non-conservative error). For convenience, we use the percentage of conservative errors (we consider positive errors as being conservative).



(a) Original kriging model.



(b) Conservative kriging via safety margin.



(c) Conservative kriging via error distribution

Figure 6: Conservative surrogates via safety margin and error distribution (consider overestimation as being conservative). Figure 6-(a) shows the original kriging model (fit to be conservative 50% of the time). Figure 6-(b) and (c) are conservative surrogates designed for 90% conservativeness. Conservativeness comes with the price of loss in accuracy.

5.2 Accurate Approximation of the Limit State

One alternative to the use of conservative surrogates is the improvement of the surrogate model near the boundary between the feasible and infeasible domains (i.e., improved accuracy for target values of the actual function). Recent developments on direction employ sequential sampling. Audet et al. [122] and Picheny et al. [123] looked at the issue of better characterizing the function of interest at around target values (of the function). Audet et al. [122] used the expected violation (concept similar to the expected improvement) to make the surrogate of the constraint function more accurate along the boundaries of the feasible/unfeasible region. Picheny et al. [123] proposed a modified version of the classical integrated mean square error criterion by weighting the prediction variance with the expected proximity to the target level of response. The method showed substantial reduction of error in the target regions, with reasonable loss of global accuracy. Bichon et al. [124] discussed how to formally apply the ideas behind EGO to the reliability-based optimization (RBDO) problem. They present details about the effcient global reliability analysis (EGRA) method including the expected violation and feasibility functions and how EGRA deals with different formulations of the RBDO problem.

6 CONCLUDING REMARKS AND FUTURE RESEARCH

In this paper, we have summarized four methodologies that allow smarter use of the sampled data and surrogate modeling. We discussed (i) screening and variable reduction, (ii) simultaneous use of multiple surrogates (iii) sequential sampling and optimization, and (iv) conservative surrogates. Our understanding is that:

- Screening and variable reduction: is an efficient step for reducing the cost of the surrogate's construction, with drastic dimensionality reductions being possible. Some approaches such as non-dimensionalization or principal component regression can at the same time improve the accuracy of the approximations.
- Multiple surrogates: is attractive because no single surrogate works well for all problems and the cost of constructing multiple surrogates is often small compared to the cost of simulations.
- Sequential sampling and optimization: is an efficient way of making use of limited computational budget. Techniques make use of both the prediction and the uncertainty estimates of the surrogate models to intelligently sample the design space.
- Safe estimators under limited budget: research has been providing tools for design of conservative surrogates. Here, there are also benefits in using multiple surrogates. Recent developments also embrace sequential sampling for constrained and reliability-based design optimization.

We would like to point topics of future research:

- Screening and variable reduction: (a) automatic construction of non-dimensional parameters governing the partial differential equations, and (b) generalization of principal orthogonal decomposition alleviating the sampling needs (and if possible working directly on the partial differential equations).
- Multiple surrogates: (a) resource allocation of simulators with tunable fidelity (either in the traditional variable fidelity framework or seeing low fidelity samples as "noisy" samples), and (b) investigation of the benefits multiple surrogates on sequential sampling and reliability-based optimization, (c) visualization and design space exploration (since different surrogates might be more accurate in different regions of the design space).
- Sequential sampling and optimization: (a) development of variable fidelity approaches, (b) measurement (and reduction) of the influence of the surrogate accuracy on the method, and (c) combined use of space-filling and adapted strategies for increased robustness.
- Safe estimators under limited budget: (a) combined use of conservative predictions and sequential strategies in order to increase accuracy in the regions near the optimum (reducing change of overdesign or failure), and (b) design for the life cycle, meaning integration of data gathered along the design life cycle of the product in the redesign (e.g., incorporating the effects of possible future tests in redesign).

Finally, complexity and in some cases the lack of commercial software may hinder these techniques from popularity in the near term. So, we believe that it is very beneficial the investments in packages and learning tools together with ongoing scientific investigation.

ACKNOWLEDGEMENTS

Authors would like to acknowledge support from the AFOSR under the grant FA9550-09-1-0153, the ANR under the grant ANR-09-COSI-005, and NSF under the grant CMMI-0856431.

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