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The Use of Metamodeling Techniques for Optimization Under Uncertainty

Ruichen Jin, Xiaoping Du and Wei Chen

Abstract Metamodeling techniques have been widely used in engineering design to improve the efficiency in simulation and optimization of design systems that involve computationally expensive simulation programs. Many existing applications are restricted to deterministic optimization. Very few studies have been conducted on studying the accuracy of using metamodels for optimization under uncertainty. In this paper, using a two-bar structure system design as an example, various metamodeling techniques are tested for different formulations of optimization under uncertainty. Observations are made on the applicability and accuracy of these techniques, the impact of sample size, and the optimization performance when different formulations are used to incorporate uncertainty. Some important issues for applying metamodels to optimization under uncertainty are discussed.

Key words metamodeling – optimization under uncertainty

1 INTRODUCTION

When using computationally expensive simulation programs in engineering design, it becomes impractical to rely exclusively on simulation codes for the purpose of design optimization. A preferable strategy is to utilize approximation models which are often referred to as metamodels as they provide a "model of the model" (Kleijnen, 1987) to replace the expensive simulation model.

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A comprehensive review of metamodeling applications in mechanical and aerospace systems can be found in (Simpson, et al., 1997). A comparative study of various metamodeling techniques has been provided by Jin et al. (2000) using multiple modeling criteria and multiple test problems. While many existing works illustrate that the accuracy of using metamodels in locating the optimum solution is often sufficient, most of these applications are restricted to deterministic optimization. Some researchers have documented the use of metamodels in robust design applications where system variations are considered (Chen et al. 1996; Padmanabhan and Batill, 2000). Nevertheless, very few studies have been conducted on studying the accuracy of this approach for optimization under uncertainty. As one can predict that the accuracy for deterministic design optimization largely depends on whether a metamodel can capture the general (global) tendency of the design behavior, the accuracy for optimization under uncertainty also relies on how accurate the metamodel is in capturing the performance variations, which could be caused by small perturbations of design parameters. The knowledge on the accuracy of various metamodeling techniques in this context will be very valuable.

Our objective in this paper is to study the applicability and accuracy of various metamodeling techniques for optimization under uncertainty. Three representative techniques, the polynomial regression (PR) (Box, et al.; 1978; Myers and Montgomery, 1995), the Kriging method (KG) (Sacks, et al., 1989), and the method of radial basis function (RBF) (Hardy, 1971; Dyn, et al., 1986) are investigated. These methods are tested for different types of feasibility and objective function formulations in optimization models with the consideration of uncertainty. Through our investigations, we aim to answer the following questions: *Is metamodeling generally applicable for uncertainty propagation and optimization under uncertainty? What is the impact of sample size on the accuracy? Is there a particular optimization formulation (with consideration of uncertainty) more effective than the others when applying the metamodeling approach? Among the various metamodeling techniques, is there a technique superior to the others for optimization under uncertainty?* A two-bar structural design problem is utilized to help us answer these questions and demonstrate the various aspects involved.

2 THE TECHNOLOGICAL BASE

2.1 Incorporating Uncertainty in Engineering Design

It is generally recognized that uncertainty is inevitable at every stage of the life cycle development of a product. As an example, manufacturing variations could be considered as a contributing source of uncertainty in product design. Deterministic approaches do not consider the impact of such variations, and as a result, a design solution may be very sensitive to these variations. Moreover, deterministic optimization lacks the ability to achieve specified levels of constraint satisfaction (such as under reliability considerations). Therefore, a design based on the deterministic factor of safety may be risky or over-conservative.

Many approaches exist in the literature to incorporate uncertainty in a design formulation. Robust design (Taguchi, 1993), originally proposed by Japanese engineer G. Taguchi, is a method for improving the quality of a product through minimizing the effect of the causes of variation without eliminating the causes (Phadke, 1989). When using a nonlinear programming formulation for robust design (see, e.g., Parkinson et al., 1993; Sundaresan et al., 1993; Chen et al.1996; Su and Renaud, 1997), a robust design solution is obtained by making the trade-off between "optimizing the mean performance μ_y" and "minimizing the performance variance σ_y".

An alternative approach to incorporating uncertainty is through utility function optimization, where a utility function is used as an objective function to capture the risk attitude of designers under uncertainty. Decision-Based Design (DBD) is an emerging paradigm of engineering design that casts design into the framework of decision theory (Hazelrigg, 1998) and utilizes the approach of utility optimization. The preferred design option is chosen as the one that maximizes the expected utility U (Von Neumann and Morgenstern, 1953), which is the integration of the utility function $u(v)$ and the probability density function (PDF) $p(v)$, where v stands for the value measure such as the profit. When formulating robust design or decision-based design under the optimization framework, the feasibility of the constraints under uncertainty also needs to be considered. Feasibility under uncertainty is ensured by making the probability of the constraints being satisfied being greater than the user specified probability, a very similar concept as that used in reliability-based design (Rao 1992). In the work of Du and Chen (2000), several feasibility-modeling techniques are examined.

2.2 Optimization Formulations Under Uncertainty

By examining the optimization formulations under uncertainty in this section, we tend to identify the desired properties of the metamodeling approach to optimization under uncertainty. To start, a deterministic optimization model is stated in (1):

$$\begin{array}{ll} \text{Minimize} & F(\mathbf{x},\mathbf{q}) \\ \text{Subject to} & g_j(\mathbf{x},\mathbf{q}) \geq 0,\ j=1,2,...,J \\ & \mathbf{x_l} \leq \mathbf{x} \leq \mathbf{x_u}\,, \end{array} \tag{1}$$

where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ is a vector of design variables and $\mathbf{q} = [q_1, q_2, ..., q_m]^T$ is a vector of design parameters whose values are fixed as a part of the problem specifications. Both design variables and design parameters could be the contributing sources of variations. Consequently, the system performances $F(\mathbf{x},\mathbf{q})$ and $g(\mathbf{x},\mathbf{q})$ are random functions. For optimization under uncertainty, if only the mean and standard deviation (STD) of performance are used in constructing the objective function, such as the case in robust design, the objective function can be expressed as:

$$\text{Min or Max} \quad z[\mu_F(\mathbf{x},\mathbf{q}), \sigma_F(\mathbf{x},\mathbf{q})]\,. \tag{2}$$

If the utility optimization approach is employed, the objective function can be represented as:

$$\text{Max} \quad U = \int u(F)p(F)dF\,. \tag{3}$$

For achieving the feasibility of constraints under uncertainty, a general probabilistic feasibility formulation can be expressed as follows:

$$P[g_j(\mathbf{x},\mathbf{q}) \geq 0] \geq P_{oj},\ j=1,\cdots,J\,, \tag{4}$$

where P_{oj} is the desired probability for satisfying constraint j. To reduce the computational burden associated with the probabilistic feasibility evaluation, simplistic approaches are widely used in the literature. Assuming $g_j(\mathbf{x},\mathbf{q})$ is normally distributed, the constraint can then be written as:

$$\mu_{g_j} - k_j\sigma_{g_j} \geq 0\,, \tag{5}$$

where $k_j = \Phi^{-1}(P_{oj})$ and Φ^{-1} is the inverse function of the cumulative density function (CDF) of a standard normal distribution. This kind of constraints is also called moment matching formulation (Parkinson et al. 1993). For example, $k_j = 2$ stands for $P_{oj} = 0.9772$ and $k_j = 3$ means $P_{oj} = 0.9987$.

From (2) $\sim$ (5), we note that the accuracy of using the metamodeling approach to optimization under uncertainty highly depends on the accuracy in evaluating the following four functions: (a) the mean of performance μ_F, μ_{gi}; (b) the STDs of performance σ_F, σ_{gi}; (c) the probability of constraint feasibility $P[g_j(\mathbf{x},\mathbf{q}) \geq 0]$; and (d) the expected utility (3). While the accuracy in evaluating (a) should be very close to that is achieved from deterministic metamodels, the accuracy in evaluating (b), (c) and (d) are not necessary identical. It should also be noted that the ultimate interest of a designer is to identify a design solution that is close enough (especially in its performance space) to the one obtained using the original simulation program. In optimization, both the constraints and the objective have confounding contributions to an optimization solution. An empirical approach seems to be appropriate to help us achieve a better understanding on the applicability of using metamodeling techniques for optimization under uncertainty.

2.3 Metamodeling Techniques

The principal features of the three metamodeling techniques examined in our study are described in this section.

Polynomial Regression (PR)

The response surface methodology based on polynomial regression has been widely applied in engineering area because its easiness in implementation and interpretation. To fit a reasonable metamodel by polynomial regression, the sample size should be at least two or three times of the number of model coefficients. For a problem with n input variables, there are $(n+1)(n+2)/2$ coefficients for a quadratic polynomial model, $(n+1)(n+2)(n+3)/6$ coefficients for a cubic polynomial model, etc. However, it should be noted that with the number of input variables increasing, the cubic or higher order polynomial models could easily become unaffordable. In the example used in our paper, focus on the study of quadratic polynomial regression as it is more commonly used in the practice. We also present representative results from using the cubic polynomial model when the sample size is sufficient. A second-order polynomial model can be expressed as:

$$\widehat{y} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j \geq i}^{k} \beta_{ij} x_i x_j \qquad (6)$$

Kriging Method (KG)

A kriging model postulates a combination of a polynomial model and departures of the form:

$$\widehat{y} = \sum_{j=1}^{k} \beta_j f_j(\mathbf{x}) + Z(\mathbf{x}) \qquad (7)$$

where $Z(\mathbf{x})$ is assumed to be a realization of a stochastic process with zero mean and spatial correlation function given by

$$\mathrm{Cov}[Z(\mathbf{x_i}), Z(\mathbf{x_j})] = \sigma^2 R(\mathbf{x_i}, \mathbf{x_j}), \qquad (8)$$

where σ^2 is the process variance and R is the correlation. In this work, a constant term for $f_j(\mathbf{x})$ and a Gaussian correlation are used. Kriging method is extremely flexible in capturing nonlinear behavior because the correlation functions can be tuned by the sample data. However, the model construction process can be very time-consuming and fitting problems due to singularity have been observed when using kriging models.

Radial Basis Functions (RBF)

Radial basis functions (RBF) have been developed for scattered multivariate data interpolation (Dyn, et al., 1986). The method uses linear combinations of a radially symmetric function based on Euclidean distance or other such metric to approximate response functions. There exist many different kinds of radial basis function. The one used in our study follows a simple form, which can be expressed as:

$$\widehat{y} = \sum_{i} a_i \left\| x - x_{0i} \right\| \qquad (9)$$

where a_i is the coefficient of the expression and x_{0i} is the observed input. Radial basis function approximations have been shown to produce good fits to arbitrary contours of both deterministic and stochastic response functions (Powell, 1987).

3 THE EXAMPLE PROBLEM

3.1 Problem Description

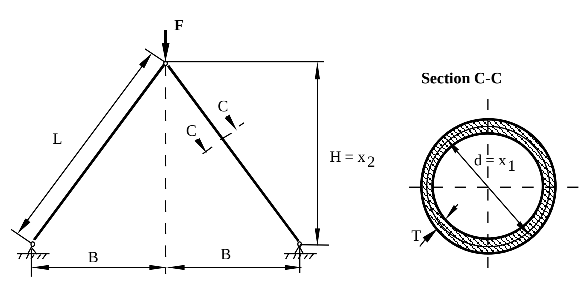
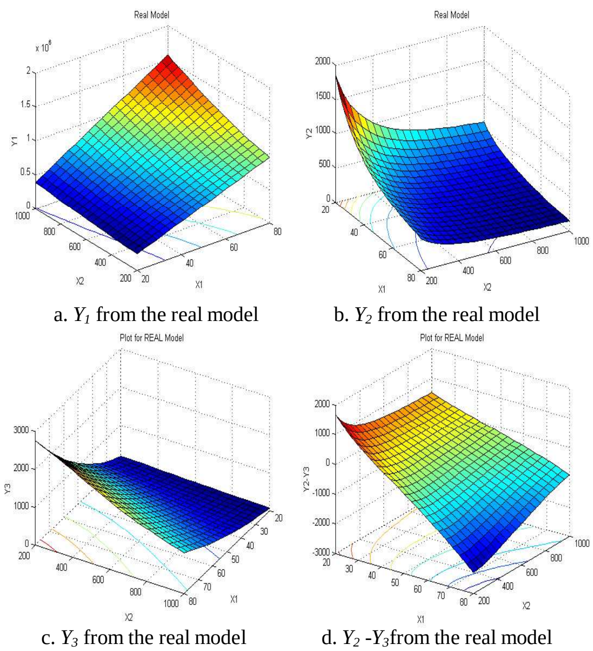


Fig. 1 The Two-bar Structure

A two-bar structure design problem is used as an example in our study. The two-bar design example is adopted from Geilen (Geilen, 1986). The purpose of this design problem is to find the values of two variables, i.e., d, nominal diameter of the cross section, and H, the height of the two bar structure, which can minimize the total volume V of the whole system. See the formulation below for details.

Given
• Constant Parameters
Width of the structure:B=750mm; External Force:F=150kN;
Normal stress limit:s_{max}=400N/mm^2;
Elastic Modulus:E=210,000N/mm^2;
Thickness of the cross section:T=2.5mm
• Physical Relationships
Total Volume: $V = Y_1 = 2\pi T d\sqrt{B^2 + H^2}$;
Normal stress: $s = Y_2 = F\sqrt{B^2 + H^2}/2\pi T H d$;
Critical buckling stress: $s_{crit} = Y_3 = \pi^2 E(T^2 + d^2)/8(B^2 + H^2)$
Find
Nominal diameter of the cross section: $d = x_1$;
The height of the two bar structure: $H = x_2$
Subject to
• Constraints
Normal stress:$s \leq s_{max}$; Buckling stress:$s \leq s_{crit}$
• Bounds on the design variables
20mm$\leq d \leq$ 80mm; 200mm $\leq H \leq$1000mm
Objective
Minimize the total volume V

Fig. 2 The Two-bar Structure Design Formulation



a. Y_1 from the real model
b. Y_2 from the real model
c. Y_3 from the real model
d. Y_2 -$Y_3$from the real model

Fig. 3 Behavior of the Real Performance

The two-bar structure design is a very typical design problem that reflects the situation in most of the real world problems where the technical efficiency (the normal stress and the buckling stress constraints) and the economical efficiency (the volume objective) are conflicting. The three performance attributes in this example represent engineering behaviors with different orders of nonlinearity, which allows us to study the effectiveness of different metamodeling techniques. (Below x_1 and x_2 are used to denote the design variables d and H respectively; and Y_1, Y_2 and Y_3 are used to denote the performance attributes V, s and s_{crit} respectively.) From Fig. 3 and Physical Relationships in Fig. 2, it is noted that Y_1 is very close to linear and Y_2 is the most nonlinear function (the function decreases sharply when x_1 and x_2 are close to their lower bounds). It is also noted that $Y_2 - Y_3$ is nonlinear (Fig. 3d).

3.2 Formulations of Optimization under Uncertainty

The nature of the problem allows us test various optimization formulations under uncertainty. The width B is considered as the variation source of the problem: it is assumed to be normally distributed with mean value μ_B=750mm and STD σ_B=50mm. Three formulations of optimization under uncertainty, i.e. No 2, 3 and 4, are considered by taking the different forms of objective and constraint feasibility (see Table 1). All formulations have the same design variables and bounds as the deterministic model (formulation 1).

Table 1 Optimization Formulations: Objective and Constraints

No.	Objective	Constraints
1	Min.$f = Y_1$	$Y_2 \leq 400$ $Y_2 - Y_3 \leq 0$
2	Min.$f = \frac{\mu_{Y1}(x_1,x_2)}{\mu_{ideal}} + \frac{\sigma_{Y1}(x_1,x_2)}{\sigma_{ideal}}$	$(\mu_{Y_2} + 3\sigma_{Y_2})/400 \leq 1$ $P(Y_2 - Y_3 \leq 0) \geq 0.99$
3	Min.$f = \frac{\mu_{Y1}(x_1,x_2)}{\mu_{ideal}} + \frac{\sigma_{Y1}(x_1,x_2)}{\sigma_{ideal}}$	$(\mu_{Y_2} + 3\sigma_{Y_2})/400 \leq 1$ $\mu_{Y_2-Y_3} + 2.3264\sigma_{Y_2-Y_3} \leq 0$
4	Max.$f = U = \int u(Y_1)p(Y_1)dY_1$	$(\mu_{Y_2} + 3\sigma_{Y_2})/400 \leq 1$ $P(Y_2 - Y_3 \leq 0) \geq 0.99$

Both Formulations 2 and 3 are robust design models in which the weighted-sum approach is used to make the tradeoff between the mean and STD of Y_1(volume). m_{ideal} and σ_{ideal} , the best achievable optimal solutions of the mean and the STD of volume respectively, are identified by either minimizing the mean or minimizing the STD of volume for the given set of constraints. They are used to normalize the two aspects of robust design. The constraint feasibility is modeled differently in Formulations 2 and 3. In Formulation 2, constraint 1 is modeled using moment matching formulation with k=3. The second onstraint is expressed in the probabilistic form. In Formulation 3, both constraints 1 and 2 are expressed by the moment matching formulation. The k of the second constraint is set at 2.3264 corresponding to $P_0 = 0.99$ for normally distributed performance. Formulation 4 is a utility optimization model in which the objective is to maximize the expected utility U. Designer's risk attitude under uncertainty is captured by the utility function in (10), which is quadratic and stands for a risk averse attitude.

$$u(Y_1) = 1.2573 - 4 * 10^{-7} Y_1 - 9 * 10^{-14} * Y_1^2 \qquad (10)$$

The two constraints in Formulation 4 are modeled in the same way as that in Formulation 2. It has been discussed in Section 2 that the accuracy in optimization under uncertainty largely depends on the accuracy

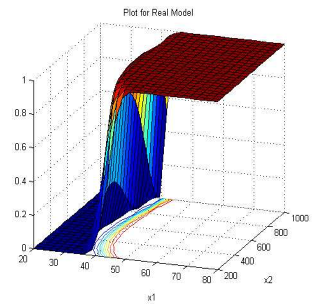


Fig. 4 Probability $P(Y_2 - Y_3 \le 0)$ from the Real Model

in predicting (a), (b), (c), and (d) functions ($2 \sim 5$). In this problem, they are evaluated as μ_{Y_1}, σ_{Y_1}, μ_{Y_2} , σ_{Y_2}, $\mu_{Y_2-Y_3}$, $\sigma_{Y_2-Y_3}$, $P(Y_2 - Y_3 \le 0)$, and the expected utility U. The probability of feasibility for $P(Y_2 - Y_3 \le 0)$ is plotted in Fig. 4 using Monte Carlo Simulations of the real models. It is noted that when the diameter of the cross section x_1 increases, $P(Y_2 - Y_3 \le 0)$ becomes higher. There exists a significant jump, where $P(Y_2 - Y_3 \le 0)$ increases dramatically in a narrow range of x_1 [36 46]mm. Beyond this range, the probability does not change much when x_1 varies. The impact of x_2 (the height of the two bar structure) on $P(Y_2 - Y_3 \le 0)$ is not significant. The irregular behavior of the constraint feasibility may cause difficulty when searching for the optimum solution.

3.3 Examinations of Metamodels

The two design variables (x_1 and x_2) and the random variable B are used as input variables to construct metamodels for Y_1, Y_2 and $Y_2 - Y_3$. To study the impact of sample size, two sets of samples with different sizes are used, namely,
(1) Small Sample: 27 Latin Hypercube inner points + 8 corner points +1 center point, totally 36 points.
(2) Large Sample: 64 Latin Hypercube inner points +8 corner points +1 center point, totally 73 points.

The corner points are created using 2-level full factorial design for three variables. The inner points are chosen using Latin Hypercube design (McKay, et al., 1979) where the points are so selected that they are uniformly distributed for each dimension. Once the metamodels are created using polynomial regression, Kriging, and radial basis function, additional confirmation samples (20000 random points) are used to verify the accuracy of these metamodels. Two metrics, namely, R Square and Relative Maximum Absolute Error (RMAE) are used to measure the accuracy of metamodels. While R Square indicates overall accuracy (the larger the better), RMAE indicates local errors (the smaller the better). A good overall accuracy does not necessarily means a good local accuracy. The equations for R Square and RMAE are

Table 2 Accuracy of Metamodels

		RBF		Kriging		PR	
		R^2	RMAE	R^2	RMAE	R^2	RMAE
Small Sample	Y_1	0.9988	0.2760	0.9999	0.0018	0.9993	0.0878
	Y_2	0.9408	1.9764	0.9845	0.6946	0.8251	1.2630
	Y_2-Y_3	0.9928	0.6744	0.9964	0.5215	0.9744	0.4987
Large Sample	Y_1	0.9994	0.2460	0.9999	0.0041	0.9996	0.0903
	Y_2	0.9747	1.7729	0.9985	0.4488	0.9036	1.5027
	Y_2-Y_3	0.9957	0.6703	0.9998	0.1190	0.9832	0.6065

given in (11) and (12), respectively.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \widehat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \overline{y})^2} \tag{11}$$

where $\widehat{y}_i$ is the corresponding predicted value for the confirmation response y_i; $\overline{y}$ is the mean of y_i.

$$RMAE = \frac{\max(|y_1 - \widehat{y}_1| \,,\, |y_2 - \widehat{y}_2| \,,\, ..., |y_n - \widehat{y}_n|)}{\sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \overline{y})^2)}} \tag{12}$$

Table 2 shows the accuracy of each kind of metamodels. First, it is noted that the accuracy of Kriging is the best both in terms of R Square and in terms of RMAE. In terms of R Square, for Y_1, which is very close to linear, all methods have achieved a good accuracy - Kriging is the best while PR is slightly better than RBF; For Y_2, a highly nonlinear function, Kriging is the best while RBF is much better than PR; For $Y_2 - Y_3$, which is also nonlinear but not as much as Y_2, Kriging is still the best and RBF is better than PR. In terms of RMAE, in most cases, Kriging is far better than RBF and PR. It is interesting to note that although R Square of PR is worse than that of RBF, the local error of PR (RMAE) is less than that of RBF.

To make these more clear, the metamodels of Y_2 created using Kriging, RBF, and PR methods are shown in Fig. 5(b), (c) and (d) by varying x_1 and B and setting $x_2 = 600$ mm. We find that compared to the one from the real model (Fig. 5(a)), the metamodel from RBF is not so smooth as the real one. This is because RBF is an interpolation method and tends to over-fit the performance, which may lead to large local errors and increase the irregularity of the metamodel.

We also note that in most cases larger sample size leads to better overall accuracy of the metamodels (in terms of R Square). However, large sample size does not necessarily reduce local errors. It is noted that, for PR and RBF, in many cases, the RMAE for small sample is better than that for large sample. This is especially true for Y_2 and $Y_2 - Y_3$, which indicates that, for PR and RBF, increasing the sample size does not necessarily reduce local errors although it does improve the overall accuracy.

To verify the accuracy of metamodels for uncertainty analysis, the contour plots of μ_{Y_1}, σ_{Y_1}, μ_{Y_2} , σ_{Y_2}, $\mu_{Y_2-Y_3}$, $\sigma_{Y_2-Y_3}$, $P(Y_2 - Y_3 \le 0)$ and the expected utility U of Y_1

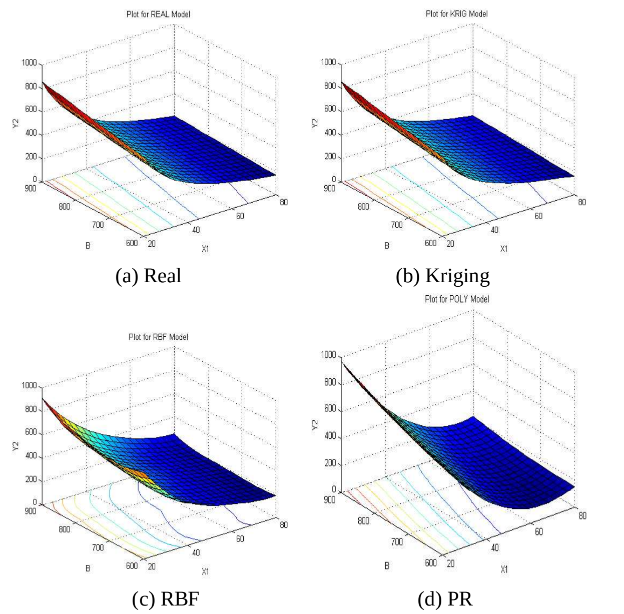


Fig. 5 Comparisons of Metamodels of Y_2 (Large Sample Size)

are studied. The plots are created over the design space (formed by x_1 and x_2) by taking B as the random variable with 20000 Monte Carlo samples. Part of them are provided in the appendix (Figs. 7-14, in Appendix).The comparison below is based on those contour plots.

It is noted that because Y_1 is not highly nonlinear, all three methods generate good approximations for the mean of Y_1 . Among them, KG is the most accurate (see Table 2). For the standard deviation of Y_1 , KG is again the best method based on the comparison of contours (See Fig. 7). This observation will be further verified through the optimization study presented later. The standard deviation from PR appears to be linear, which is due to its second-order polynomial form. As for RBF, there exist some twistings of the contours at the upper left corner of the design space where the standard deviation of Y_1 exceeds 29,000 mm^3, because RBF tends to over-fit a model.

Figs. 8 and 9 show the contours of the mean and the STD of Y_2. It is noted that since Y_2 is highly nonlinear, PR is not a good method to approximate the mean of Y_2. KG and RBF have very good accuracy for the mean of Y_2. However, due to the nonlinearity, all metamodeling techniques tested are not so accurate for approximating the STD (see Fig. 9). PR again linearizes the STD contours while RBF generates twisting curves. The curves from KG provide the best match with those from the real model. We have similar rankings for approximating the mean and the STD of $Y_2 - Y_3$, the expected utility U of Y_1. (Figs. 10 - 12)

From Fig. 13, it is noted that the probability contours $P(Y_2 - Y_3 \leq 0)$ from PR deviate quite a lot from the real contours, while those from KR is almost identical to the contours of the real function. Since the probability constraint limit is set at 0.99, the P =0.99 level curve is the most critical one. We find this particular level curve from the PR deviates towards the right side of the real position, which indicates a more conservative situation when the metamodels from PR are used. We can expect that the accuracy of metamodels will affect the feasibility of optimization solutions, especially if constraints are active at the solution.

All the contour plots created by using the small sample size are also examined. In terms of the accuracy in modeling means, probability, and the expected utility, although the accuracy from the large sample size is generally better than that from the small sample size, the impact of sample size is not distinctive. In terms of the accuracy in modeling the STDs, for Kriging, the accuracy from the large sample size is far better than that from the small sample size (See Figs. 9, 14); for RBF, however, in some regions, the accuracy from the small sample size is better than that from the large sample size; and for PR, we cannot draw a definite conclusion from the comparison.

In summary:

- Achieving accurate approximation for STD is more difficult than achieving accurate approximation for mean values.
- The second-order PR cannot capture the nonlinearity of the performance variations as the method linearizes the STD function, which can be mathematically verified.
- For the example problem, KR is the most accurate technique for both large and small sample sizes.
- Depending on the model behavior and the method used, larger sample size may not necessarily lead to better accuracy in estimating the performance variations.

The accuracy of using metamodels for optimization under uncertainty is examined in the coming section.

3.4 Optimization Results and Comparison

Because the optimization formulations 2 to 4 presented in Section 3.2 are sensitive to the starting point, six different starting points are used in our study. In the form of (x_1, x_2), these starting points can be written as: (70,900), (30,300), (70,300), (30, 900), (50,600), (40,500). The first four points are near to the corners of the design space and the last two are close to the optimum point for the deterministic formulation. The optimization results are provided in Table 4 (in Appendix), in which $x_1^*$and x_2^* is the best solution selected from all six optimization runs. All results reported are the so-called confirmed results where the $x_1^*$and x_2^* are used as the inputs of the real models to calculate the real values of objective f, constraints, mean μ_{Y_1}, and STD σ_{Y_1} of Y_1.

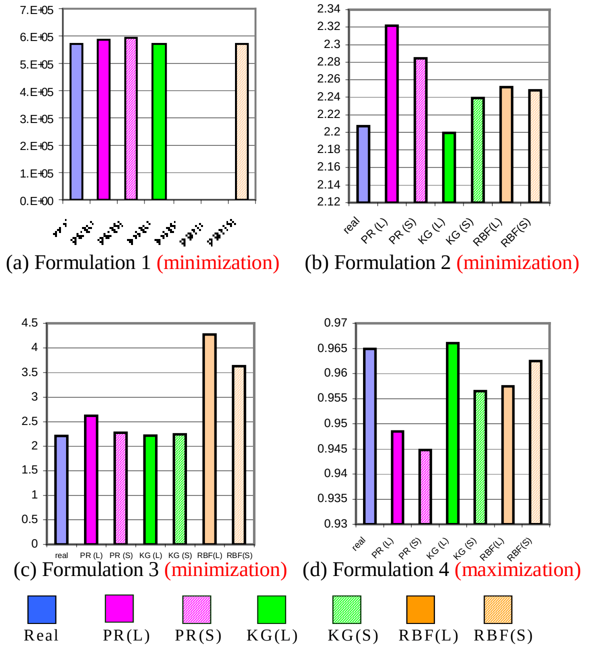


Fig. 6 Comparison of Confirmed Objective Function Values

Formulations 2 and 3 are robust design models where a smaller normalized f^* value is preferred. Formulation 4 is the utility optimization model where a larger f^* (expected utility) is preferred. The feasible rates of the optimization runs are also reported. A feasible solution means that the constraint violation is less than 0.005. The feasible rate is measured by the portion of runs that successfully locate feasible solutions before or after confirmation. It should be noted that a feasible solution before confirmation may not be feasible after confirmation, and vice versa.

Fig. 6 provides a graphical illustration of the relative difference between the achieved objective functions (note: formulation 1 3 is minimization and formulation 4 is maximization). In the figure, L and S stand for large and small sample sizes, respectively. From Table 4 and Fig. 6, we find that, overall, Kriging performs the best for all formulations of optimization under uncertainty (Formulations 2 to 4), not only because its solution is the closest to the real solution in both the design (x) and the performance (f) spaces, but also because its feasible rates after confirmation are very close to those before confirmation. This outcome matches with the accuracy examinations in Section 3.3. For deterministic optimization (Formulation 1), Kriging identifies a solution that is almost the same as the real one when large sample size is used for metamodeling. However, when the small sample size is used, after the confirmation test, the solution slightly violates the constraints and becomes infeasible.

The performance of RBF is ranked as the 2nd. RBF performs well for Formulations 2 and 4. However, for Formulation 1, when using large sample, no feasible solution is found after confirmation. For Formulation 3, the feasible solution obtained after confirmation is far from the real solution in the design space and much inferior in its performance. This is because although the solutions initially identified by the RBF model are very close to the real solution, they are found to be infeasible after confirmation due to the inaccuracy of the model in the neighborhood of the optimal solution, in particular the inaccuracy in predicting $\sigma_{Y_2-Y_3}$ (see Fig. 11). When using the PR, although the feasible rate is very high before and after confirmations, in most cases the solution is too conservative compared to using the metamodels from Kriging or RBF. It is interesting to note that for RBF, increasing the sample size actually deteriorates the optimization results for this particular example. For PR, with robust design formulations 2 and 3, the results identified using small sample size are better than those from large sample size.

When studying the optimization performance of various formulations, it is noted that the feasible rates (before confirmation) for Formulations 1 and 3 are higher than those for Formulations 2 and 4, and the evaluation time is shorter. The difficulties in solving Formulations 2 and 4 are due to the use of probabilistic feasibility constraint (Table 1). As shown in Fig. 3, the function $P(Y_2 - Y_3 \leq 0)$ jumps significantly across the design space. This has imposed challenges in locating the optimum solution. When the moment matching formulations are used (Formulation 3), the constraint behavior is very smooth and the optimum solution can be easily located. We note from the optimization solutions from the real model that the results from Formulations 2 and 3 are very close, with that from Formulation 3 being slightly inferior. This is reasonable since actually Formulations 2 and 3 are not equivalent due to the nonlinearity of $Y_2 - Y_3$.

It is also observed from Table 4 that for RBF and PR, the feasible rates can be quite different before and after confirmations. This phenomenon is associated with the fact that the solutions for all formulations are all exactly at the constraint boundary. In that case, finding accurate optimization solutions using metamodels becomes more challenge. Due to the errors of metamodels at the neighborhood of constraint boundary, a feasible solution could become infeasible after confirmation. Because the RBF and PR models are not so accurate, in some cases, the feasible rate after confirmation is much less than that before confirmation. On one hand, it is important to confirm any results generated from the metamodels; on the other hand, it may be useful to tighten a constraint limit to compensate the errors of metamodels.

In terms of the computational efficiency, it is found that while Kriging is the most accurate for our example problem, it takes much more time to run the optimization program using this model compared to the other two methods. However, this time scale is still much smaller than that needed for using the computationally expensive simulations directly for optimization under uncertainty.

Table 3 The accuracy of Cubic Polynomial Model

		Kriging		PR(quadratic)		PR(cubic)	
		R^2	RMAE	R^2	RMAE	R^2	RMAE
Large Sample	Y_1	0.9999	0.0041	0.9996	0.0903	0.9999	0.0130
	Y_2	0.9985	0.4488	0.9036	1.5027	0.9722	0.7622
	Y_2-Y_3	0.9998	0.1190	0.9832	0.6065	0.9961	0.2525

4 DISCUSSIONS

By applying various metamodeling techniques to different formulations of the two-bar structure optimization under uncertainty, we have made some important observations on the applicability and accuracy of using metamodels for design uncertainty.

Regarding the accuracy of various metamodels, we find:

- For evaluating the performance variations due to the randomness in a system (uncertainty analysis), the accuracy for evaluating the mean of performance and the expected utility is close to that for evaluating the deterministic performance. On the other hand, the accuracy for evaluating the STD of performance and the probability of constraint feasibility largely depends on the capability of a metamodel in capturing the nonlinearity and variations of a behavior. Therefore, a metamodel that is acceptable for deterministic optimization may not be acceptable for optimization under uncertainty.
- The second-order polynomial regression model cannot capture the nonlinearity of the performance variations as the method linearizes the STD of a performance. In our study, the results obtained from PR are all over-conservative. Because the size of the example problem is very small, the large sample with 73 points is sufficient for a cubic polynomial regression. As shown in Table 3, it actually leads to better metamodels compared to the metamodels from quadratic polynomial regression. However, cubic polynomial metamodels are still not as good as those from kriging. From the contours plots for cubic polynomial regression (see Fig. 15), we can find there exist twisting in some local areas, which lead to large local errors in predicting parameters under uncertainty such as the standard deviation.
- For our example problem, Kriging method provides accurate approximations to both low-order and high-order nonlinear behaviors. It also provides accurate approximations to the STD of performance and the probability of constraint feasibility. This method appears to be superior to other techniques in our study.
- Although the radial basis function (RBF) method provides accurate metamodels of global performances, it failed to locate the accurate solution for a few formulations of optimization under uncertainty. This is because the method has the tendency to overfit the model which leads to increasing irregularity and larger local errors. Our earlier study (Jin et al., 2000) showed that RBF is very efficient for modeling irregular behaviors. Since the performances considered in our study are nonlinear but not irregular, RBF could still be potentially useful for those applications with irregular behaviors.
- It is noted that regression approaches, such as polynomial regression, are capable of smoothing a model behavior, while interpolation-based approaches, such as Kriging and RBF, are more sensitive to the numerical noises. Our analytical example does not address the issues related to numerical noises. It is anticipated that in the presence of large numerical noises a metamodeling technique that is both capable of smoothing the model behavior and capturing the nonlinear trend will be more appropriate than an interpolation-based technique that may mix the local nonlinearity with numerical noises.

In terms of using metamodels for constrained optimization formulations, it is discovered that the accuracy in modeling the constraint functions in the neighborhood of the constraint boundary is the most critical. Since optimal solution is often located at the boundary of constraints (including in optimization for uncertainty), less accurate metamodels for constraint functions may result in either risky or over-conservative solution. On the other hand, as long as the metamodel of the objective function approximates the general trend of performance correctly, it will lead to the right direction for optimization. To ensue feasible results after confirmation, it may be useful to tighten a constraint limit to compensate the errors of metamodels or to consider adaptive metamodeling procedures for getting more accurate results in the neighborhood of the constraint boundary.

Our study also illustrates that increasing the size of samples can improve the accuracy of the metamodels, but doesn't necessarily result in more accurate evaluations of performance variations and therefore better optimal solutions. Overall, Kriging is shown to be a robust metamodeling technique that performs well for both large and small sample sizes.

The type of formulation for optimization under uncertainty also has an impact on the computational efficiency of the optimization process. The moment matching formulation (only considering mean and STD) requires less random samples and is less sensitive to the starting point. The probabilistic formulation of constraint, on the other hand, requires larger random samples and more accurate metamodels, especially when the limit probability is close to 1.

The use of metamodeling techniques has shown to be promising for optimization under uncertainty. However, due to the computations involved in testing, our current study is only limited to a small-size analytical problem. Future research will be directed to larger-size complex engineering problems and the development of an adaptive metamodeling procedure for getting accurate results in the neighborhood of constraint boundary and obtaining "equivalent" (close enough) solutions in design under uncertainty.

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Appendix

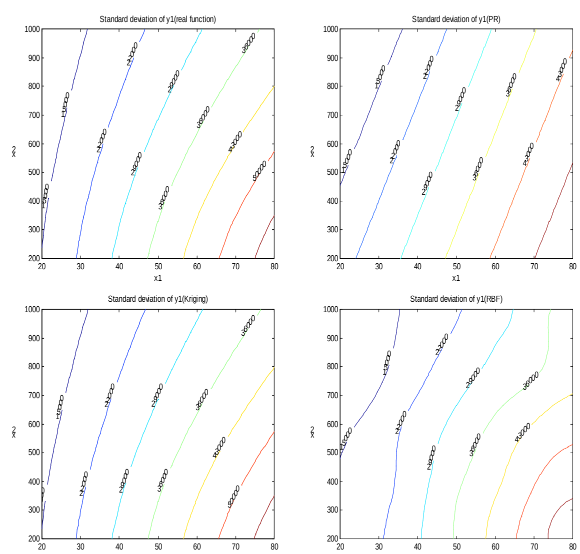

Fig. 7 STD of Y_1 (large sample size)

Table 4 Optimization Results

		Real Model	PR		Kriging		RBF	
			Large Sample	Small Sample	Large Sample	Small Sample	Large Sample	Small Sample
Formulation 1	x_1^*(mm)	37.877	38.906	38.909	37.842	N/A	N/A	37.982
	x_2^*(mm)	608.89	590.11	614.41	610.84	N/A	N/A	604.48
	f^*(mm^3)	574763	583225	592561	574924	N/A	N/A	574707
	Feasible Rate (B.C.)	6/6	6/6	6/6	6/6	6/6	6/6	6/6
	Feasible Rate (A.C.)	6/6	6/6	6/6	6/6	0/6	0/6	6/6
Formulation 2	x_1^*(mm)	41.583	43.589	43.171	41.457	41.958	42.455	42.320
	x_2^*(mm)	628.11	963.098	688.37	635.63	651.33	640.96	615.55
	f^*	2.2070	2.32164	2.2844	2.1993	2.2391	2.2516	2.2479
	$\mu_{Y_1}^*$(mm^3)	639437	836316	690815	640657	655137	658391	645437
	$\sigma_{Y_1}^*$(mm^3)	25062	21061	25003	24863	24904	25373	25717
	Feasible Rate (B.C.)	5/6	4/6	4/6	5/6	5/6	5/6	4/6
	Feasible Rate (A.C.)	5/6	1/6	1/6	5/6	5/6	1/6	4/6
Formulation 3	x_1^*(mm)	41.813	49.245	43.049	41.837	42.253	79.927	68.546
	x_2^*(mm)	673.10	600.24	831.61	661.98	642.42	1000	893.81
	f^*	2.2139	2.6186	2.2764	2.2163	2.2406	4.2710	3.6338
	$\mu_{Y_1}^*$(mm^3)	662342	743780	757768	657866	655876	1570310	1257110
	$\sigma_{Y_1}^*$(mm^3)	24464	30226	22669	25658	25227	37715	34646
	Feasible Rate (B.C.)	6/6	6/6	6/6	6/6	6/6	6/6	6/6
	Feasible Rate (A.C.)	6/6	1/6	6/6	6/6	6/6	2/6	1/6
Formulation 4	x_1^*(mm)	41.514	43.492	43.096	41.353	41.892	42.044	41.604
	x_2^*(mm)	629.63	632.36	662.13	629.90	653.88	644.07	637.20
	f^*	0.9649	0.9485	0.9448	0.9661	0.9565	0.9575	0.9625
	$\mu_{Y_1}^*$(mm^3)	639018	670653	677733	636647	655207	653342	643591
	$\sigma_{Y_1}^*$(mm^3)	24996	26139	25323	24894	24823	25075	24925
	Feasible Rate (B.C.)	5/6	4/6	2/6	6/6	4/6	4/6	5/6
	Feasible Rate (A.C.)	5/6	4/6	3/6	5/6	4/6	3/6	5/6

Note: B.C. stands for Before Confirmation, A.C. stands for After Confirmation and N/A means No feasible solutions after Confirmation.

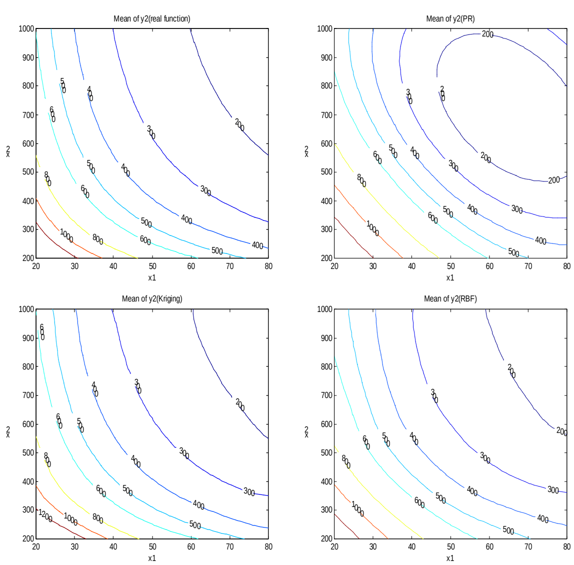

Fig. 8 Means of Y_2 (large sample size)

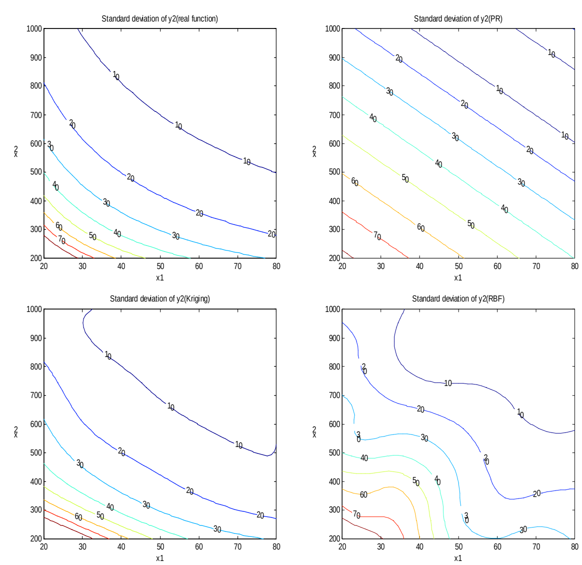

Fig. 9 STD of Y_2 (large sample size)

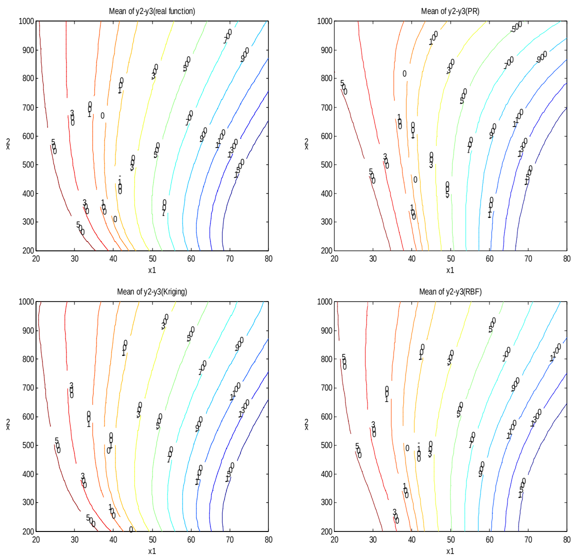

Fig. 10 Means of $Y_2 - Y_3$ (large sample size)

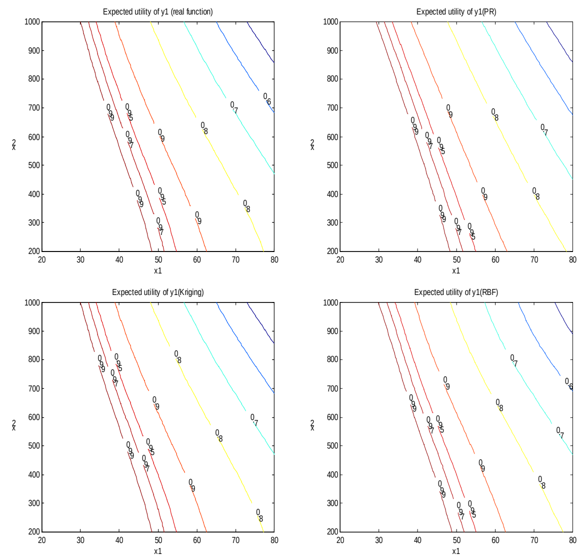

Fig. 12 Expected Utility of Y_1 (large sample size)

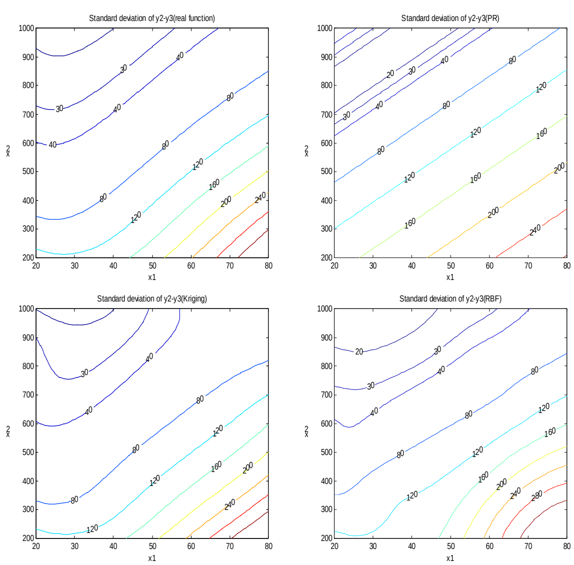

Fig. 11 STD of $Y_2 - Y_3$ (large sample size)

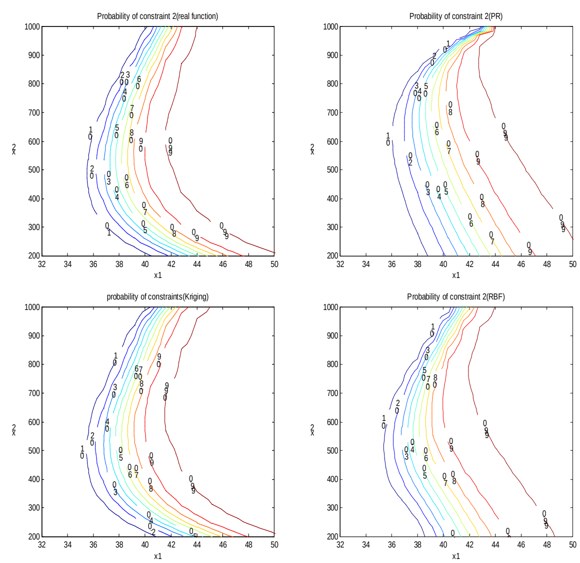

Fig. 13 Probability of Constraint Satisfaction (large sample size)

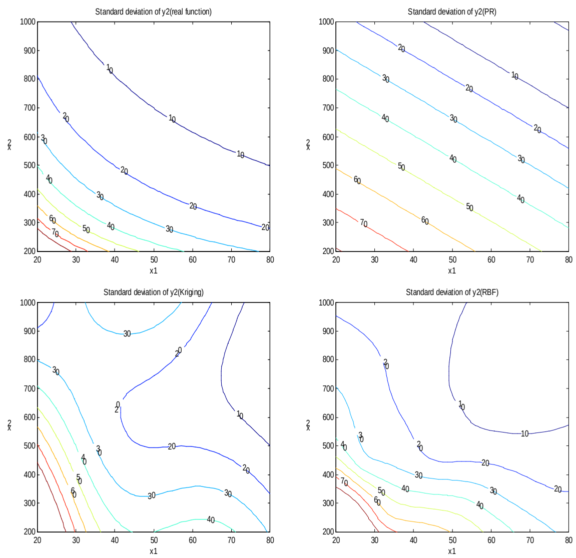

Fig. 14 STD of Y_2 (small sample size)

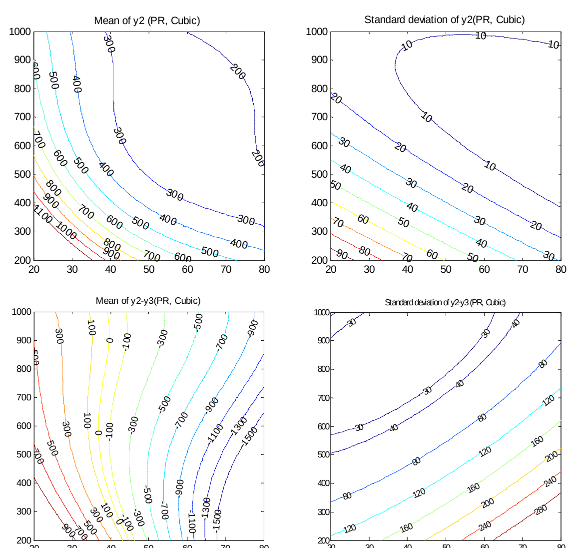

Fig. 15 Mean and Standard Deviation for Y_2 and $Y_2 - Y_3$ by Using Cubic Polynomial Metamodel