REPORT DOCUMENTATION PAGE	Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
08-08-2011	Conference Proceeding	-

4. TITLE AND SUBTITLE	
Conservative Surrogate Model using Weighted Kriging Variance for Sampling-based RBDO	5a. CONTRACT NUMBER W911NF-09-1-0250
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 611102
6. AUTHORS Liang Zhao, K.K. Choi, Ikjin Lee, David Lamb, David Gorsich	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES	8. PERFORMING ORGANIZATION REPORT NUMBER
University of Iowa @ Iowa City Office of Sponsored Programs The University of Iowa Iowa City, IA 52242 -	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO 11. SPONSOR/MONITOR'S REPORT NUMBER(S) 56025-NS.27

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

In sampling-based reliability-based design optimization of practical complex engineering applications, the Monte Carlo simulation (MCS) for stochastic sensitivity analysis and probability of failure calculation is based on the prediction from the surrogate model for the performance functions. When the number of samples used to construct the surrogate model is small, the prediction from the surrogate model becomes inaccurate and thus MCS becomes inaccurate as well. Therefore, to count in the prediction error from the surrogate model and assure the obtained

15. SUBJECT TERMS

conservative surrogate model, dynamic Kriging method, weighted Kriging variance, corrected Akaike information criterion (AICc)

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Kyung Choi
UU	UU	UU	UU		19b. TELEPHONE NUMBER 319-335-5684

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Conservative Surrogate Model using Weighted Kriging Variance for Sampling-based RBDO

ABSTRACT

In sampling-based reliability-based design optimization of practical complex engineering applications, the Monte Carlo simulation (MCS) for stochastic sensitivity analysis and probability of failure calculation is based on the prediction from the surrogate model for the performance functions. When the number of samples used to construct the surrogate model is small, the prediction from the surrogate model becomes inaccurate and thus MCS becomes inaccurate as well. Therefore, to count in the prediction error from the surrogate model and assure the obtained optimum design from sampling-based RBDO does satisfy the probabilistic constraints, a conservative surrogate model is needed. In this paper, a conservative surrogate model is constructed using the weighted Kriging variance where the weight is determined by the relative change in the corrected Akaike information criterion (AICc) of the dynamic Kriging model. The proposed conservative surrogate model performs better than the traditional Kriging prediction interval approach because it does not generate unnecessary local optimum; and it performs better than the constant safety margin approach because it adaptively counts in the uncertainty of the surrogate model in the place that the samples are sparse. Numerical examples show that using the proposed conservative surrogate model for sampling-based RBDO is necessary to assure the optimum design satisfies the probabilistic constraints when the number of samples is limited.

Conference Name: 9th World Congress on Structural and Multidisciplinary Optimization

Conference Date: June 13, 2011

9th World Congress on Structural and Multidisciplinary Optimization
June 13 - 17, 2011, Shizuoka, Japan

Conservative Surrogate Model using Weighted Kriging Variance for Sampling-based RBDO

Liang Zhao[1], K.K. Choi[2], Ikjin Lee[3], David Lamb[4] and David Gorsich[5]

[1,2,3]Department of Mechanical & Industrial Engineering
College of Engineering
The University of Iowa
Iowa City, IA 52242, U.S.A.
Email: liazhao@engineering.uiowa.edu
kkchoi@engineering.uiowa.edu
ilee@engineering.uiowa.edu

[4,5]US Army RDECOM/TARDEC
Warren, MI 48397-5000, U.S.A.
david.lamb@us.army.mil
gorsichd@tacom.army.mil

1. Abstract
In sampling-based reliability-based design optimization of practical complex engineering applications, the Monte Carlo simulation (MCS) for stochastic sensitivity analysis and probability of failure calculation is based on the prediction from the surrogate model for the performance functions. When the number of samples used to construct the surrogate model is small, the prediction from the surrogate model becomes inaccurate and thus MCS becomes inaccurate as well. Therefore, to count in the prediction error from the surrogate model and assure the obtained optimum design from sampling-based RBDO does satisfy the probabilistic constraints, a conservative surrogate model is needed. In this paper, a conservative surrogate model is constructed using the weighted Kriging variance where the weight is determined by the relative change in the corrected Akaike information criterion (AICc) of the dynamic Kriging model. The proposed conservative surrogate model performs better than the traditional Kriging prediction interval approach because it does not generate unnecessary local optimum; and it performs better than the constant safety margin approach because it adaptively counts in the uncertainty of the surrogate model in the place that the samples are sparse. Numerical examples show that using the proposed conservative surrogate model for sampling-based RBDO is necessary to assure the optimum design satisfies the probabilistic constraints when the number of samples is limited.

2. Keywords: conservative surrogate model, dynamic Kriging method, weighted Kriging variance, corrected Akaike information criterion (AICc).

3. Introduction
In sampling-based RBDO, Monte Carlo simulation (MCS) is used to carry out both the probability of failure and the stochastic sensitivity analysis [1, 2]. To carry out MCS efficiently in complex engineering applications, a surrogate model is used to predict the performance function at the MCS samples. Zhao et al. [3] developed a dynamic Kriging method to accurately construct the prediction of the performance function for the MCS by using the genetic algorithm for the basis function selection and the generalized pattern search for the correlation parameter estimation. When the surrogate model is not accurate enough, new samples are sequentially inserted to improve the prediction accuracy [3]. However, inserting a large number of new samples sequentially may not be applicable when the samples are from the physical experiments or when the computational resource for simulation is limited. Therefore, the improvement of the surrogate model cannot be from the increase of the sample numbers. When applying the surrogate model for reliability-based design optimization when the number of samples is small, to assure the obtained optimum design can satisfy the probabilistic constraints, a conservative surrogate model is needed.

Picheny [4] used both safety margin and safety factor approaches to construct the conservative surrogate model and concluded that when the Kriging method is used, both methods provide similar performance in terms of the conservativeness and the accuracy. Hertog et al. [5] and Luna and Young [6] used the bootstrapping method to estimate the Kriging prediction interval to construct the conservative surrogate model. The bootstrapping variance is larger than the traditional Kriging prediction variance by considering the uncertainty from the correlation parameter in the Kriging method. However, the bootstrapping procedure is time-consuming and not applicable for high-dimensional problems. Viana et al. [7] used cross-validation to estimate the safety margin for the conservative surrogate model. While the cross-validation error is widely used to estimate the prediction error, this constant safety margin approach does not distinguish the prediction error at different sample locations and will yield an over-conservative surrogate model where the samples are aggregated around; and an under-conservative surrogate model where the samples are sparse.

In this paper, a weighted Kriging variance is considered to construct a more accurate conservative surrogate model based the sample locations. To evaluate the importance from each sample and determine the weight for it, an accuracy measure of the surrogate model is needed first. Under the Kriging framework, the Akaike information criterion (AIC) [8] is a reliable indicator to assess the accuracy of the surrogate model. Hurvich and Tsai [9] proposed a corrected AIC (AICc) to correct the bias in AIC when the number of samples is small. Burnham and Anderson [10] recommended using AICc rather than AIC when the sample size is small and showed that the AICc converges to AIC as the number of samples increases. Martin and Simpson [11] compared the performance of the corrected AIC assessment with other methods and concluded that AICc provides the best accuracy assessment for surrogate model accuracy. In this paper, the AICc is used to assess the accuracy changes in the surrogate model during the cross-validation process, and an importance function value is assigned to each sample according to the relative changes in AICc of the surrogate model and the weight is also assigned to each sample according to the importance function values. Then a weighted Kriging variance is calculated based on the weight values for each sample. By applying this weighted Kriging variance, one can construct the conservative surrogate model for dynamic Kriging and use it for sampling-based RBDO to assure the obtained optimum design can satisfy the probabilistic constraint.

The remainder of this paper is organized in four sections. First, the backgrounds of the dynamic Kriging method, sampling-based RBDO, and the AICc are briefly summarized. Then, the weighted Kriging variance using the weight from the relative change in AICc is introduced to construct the conservative surrogate model. Third, the conservative surrogate model is applied to sampling-based RBDO and the optimum design is verified for the probabilistic constraint using numerical examples and compared with the results using the constant safety margin approach.

4. Background of the Dynamic Kriging Method, Sampling-based RBDO, and AICc

4.1 Dynamic Kriging Method

First consider a universal Kriging method. The outcomes are considered as a realization of a stochastic process, and the predicted values are derived by applying the stochastic process theory. Consider n sample points $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n]^{\mathrm{T}}$ with $\mathbf{x}_i \in \mathbf{R}^{\mathrm{nd}}$, and n responses $\mathbf{Y} = [y(\mathbf{x}_1), y(\mathbf{x}_2), ..., y(\mathbf{x}_n)]^{\mathrm{T}}$ with $y(\mathbf{x}_i) \in \mathbf{R}$. In the Kriging method, the responses at samples are considered as a summation of two parts as

$$\mathbf{Y} = \mathbf{F}\boldsymbol{\beta} + \mathbf{e} \tag{1}$$

The first part of the right-hand side of Eq. (1), $\mathbf{F}\boldsymbol{\beta}$, is considered as the mean structure of the response, where $\mathbf{F}=[\mathbf{f}(\mathbf{x}_i), i = 1,...,n]$ is a $(n \times K)$ design matrix, and $\mathbf{f}(x) = \left[f_k(\mathbf{x}), k = 1,...,K \right]$ represents the user-defined basis functions, which are usually in a simple polynomial form, such as $1, x, x^2, ...$. The second part of the right hand side in Eq. (1), $\mathbf{e} = [e(\mathbf{x}_1), e(\mathbf{x}_2), ..., e(\mathbf{x}_n)]^{\mathrm{T}}$, is a realization of the stochastic process $e(\mathbf{x})$ that is assumed to have zero mean and covariance structure $\mathbf{E}[e(\mathbf{x}_i)e(\mathbf{x}_j)] = \sigma^2 R(\boldsymbol{\theta}, \mathbf{x}_i, \mathbf{x}_j)$, where σ^2 is the process variance and $\boldsymbol{\theta}$ is the process correlation parameter. The optimal choice of $\boldsymbol{\theta}$ is defined as the maximum likelihood estimator (MLE), which is the maximizer of the likelihood function L, expressed as

$$L = \left(2\pi\sigma^2\right)^{-\frac{n}{2}} \left|\mathbf{R}\right|^{-\frac{1}{2}} \exp\left[-\frac{1}{2\sigma^2} (\mathbf{Y} - \mathbf{F}\boldsymbol{\beta})^{\mathrm{T}} \mathbf{R}^{-1} (\mathbf{Y} - \mathbf{F}\boldsymbol{\beta}) \right] \tag{2}$$

where $\mathbf{R}$ is the symmetric correlation matrix with i-j^{th} component $R_{ij} = R(\boldsymbol{\theta}, \mathbf{x}_i, \mathbf{x}_j),\ i, j = 1,...,n,$ and $\sigma^2 = \dfrac{1}{n}(\mathbf{Y} - \mathbf{F}\boldsymbol{\beta})^{\mathrm{T}} \mathbf{R}^{-1} (\mathbf{Y} - \mathbf{F}\boldsymbol{\beta})$ and $\boldsymbol{\beta} = \left(\mathbf{F}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{F}\right)^{-1} \mathbf{F}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{Y}$ are obtained from the generalized least square regression.

Under the general decomposition of Eq. (1), the objective is to predict the noise-free unbiased response at a new point of interest $\mathbf{x}$, expressed as

$$y_{krig}(\mathbf{x}) = \mathbf{f}^{\mathrm{T}}\boldsymbol{\beta} + \mathbf{r}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{Y} - \mathbf{F}\boldsymbol{\beta}) \tag{3}$$

where $\mathbf{r} = \left[R(\boldsymbol{\theta}, \mathbf{x}_1, \mathbf{x}), ..., R(\boldsymbol{\theta}, \mathbf{x}_n, \mathbf{x}) \right]^{\mathrm{T}}$. The prediction variance can be also obtained as

$$\sigma_p^2(\mathbf{x}) = \sigma^2 (1 + \mathbf{u}^{\mathrm{T}} (\mathbf{F}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{F})^{-1} \mathbf{u} - \mathbf{r}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{r}) \tag{4}$$

where $\mathbf{u} = \mathbf{F}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{r} - \mathbf{f}$.

In the dynamic Kriging method, the basis function set $\mathbf{f}(x)$ is no longer fixed. Instead, the optimal basis function set is decided by the given samples. First, a number of polynomial functions are considered as the candidate function. The highest order *P* of the polynomial is decided by $\binom{P}{nd+P} \le n-1$. A genetic algorithm is used to find the optimal subset of the basis function by minimizing the process variance σ^2. Second, a generalized pattern search algorithm is used to solve the problem that is maximizing Eq. (2). With these two steps carried out, the dynamic Kriging can generate a more accurate surrogate model than the traditional universal Kriging [3].

4.2 Sampling-based RBDO

The mathematical formulation of a general RBDO problem is expressed as

$$\begin{aligned} &\text{minimize} && \text{Cost}(\mathbf{d}) \\ &\text{subject to} && P[G_j(\mathbf{X})>0] \le P_{F_j}^{\text{Tar}}, \quad j=1,\cdots,nc \\ & && \mathbf{d}^{\text{L}} \le \mathbf{d} \le \mathbf{d}^{\text{U}}, \quad \mathbf{d}\in\mathbf{R}^{nd} \text{ and } \mathbf{X}\in\mathbf{R}^{nr} \end{aligned} \tag{5}$$

where $\mathbf{d}=\{d_i\}^{\text{T}}=\boldsymbol{\mu}(\mathbf{X}^{\mathbf{rv}})$, $i=1\sim nd$ is the design vector, which is the mean value of the *nd*-dimensional random variable vector $\mathbf{X}^{\mathbf{rv}}=\{X_1,\ X_2,\cdots,\ X_{nd}\}^{\text{T}}$; $\mathbf{X}=\{\mathbf{X}^{\mathbf{rv}},\mathbf{X}^{\mathbf{rp}}\}^{\text{T}}$ where $\mathbf{X}^{\mathbf{rv}}$ and $\mathbf{X}^{\mathbf{rp}}$ stand for the random design variable and random parameter components of the random input $\mathbf{X}$, respectively; $P_{F_j}^{\text{Tar}}$ is the target probability of failure for the j^{th} constraint; and *nc*, *nd*, and *nr* are the number of probabilistic constraints, design variables, and random variables plus parameters, respectively.

A reliability analysis for both the component and system levels involves calculation of the probability of failure, denoted by P_F, which is defined using a multi-dimensional integral as

$$P_F(\boldsymbol{\psi}) \equiv P[\mathbf{X}\in\Omega_F] = \int_{\mathbf{R}^{nr}} I_{\Omega_F}(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\psi})d\mathbf{x} = E\left[I_{\Omega_F}(\mathbf{X})\right] \tag{6}$$

where $\boldsymbol{\psi}$ is a vector of distribution parameters, which usually includes the mean (μ) and/or standard deviation (σ) of the random input $\mathbf{X}=\{X_1,\cdots,X_{nr}\}^{\text{T}}$; $P[\bullet]$ represents a probability measure; Ω_F is the failure set; $f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\psi})$ is a joint probability density function (PDF) of X; and $E[\bullet]$ represents the expectation operator. The failure set is defined as $\Omega_{F_j} \equiv \{\mathbf{x}: G_j(\mathbf{x})>0\}$ for component reliability analysis of the j^{th} constraint function G_j(x), and $\Omega_F \equiv \left\{\mathbf{x}: \bigcup_{j=1}^{nc} G_j(\mathbf{x})>0\right\}$ and $\Omega_F \equiv \left\{\mathbf{x}: \bigcap_{j=1}^{nc} G_j(\mathbf{x})>0\right\}$ for the series system and parallel system reliability analysis of *nc* performance functions, respectively. $I_{\Omega_F}(\mathbf{x})$ in Eq. (6) is called an indicator function and defined as

$$I_{\Omega_F}(\mathbf{x}) \equiv \begin{cases} 1, & \mathbf{x}\in\Omega_F \\ 0, & otherwise \end{cases} \tag{7}$$

In this paper, since the mean of X, $\boldsymbol{\mu}=\{\mu_1,\cdots,\mu_{nd}\}^{\text{T}}$ is used as a design vector, the vector of distribution parameters $\boldsymbol{\psi}$ is simply replaced with μ for the computation of the probability of failure in Eq. (6). Taking the partial derivative of probability of failure in Eq. (6) with respect to the i^{th} design variable μ_i yields

$$\frac{\partial P_F(\boldsymbol{\mu})}{\partial \mu_i} = \frac{\partial}{\partial \mu_i}\int_{\mathbf{R}^{nr}} I_{\Omega_F}(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\mu})d\mathbf{x} \tag{8}$$

and the differential and integral operators can be interchanged using the Leibniz's rule, giving

$$\begin{aligned} \frac{\partial P_F(\boldsymbol{\mu})}{\partial \mu_i} &= \int_{\mathbf{R}^{nr}} I_{\Omega_F}(\mathbf{x}) \frac{\partial f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\mu})}{\partial \mu_i} d\mathbf{x} = \int_{\mathbf{R}^{nr}} I_{\Omega_F}(\mathbf{x}) \frac{\partial \ln f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\mu})}{\partial \mu_i} f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\mu})d\mathbf{x} \\ &= E\left[I_{\Omega_F}(\mathbf{x}) \frac{\partial \ln f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\mu})}{\partial \mu_i}\right] \end{aligned} \tag{9}$$

since $I_{\Omega_F}(\mathbf{x})$ is not a function of μ_i. The partial derivative of the log function of the joint PDF in Eq. (8) with respect to μ_i is known as the first-order score function for μ_i and is denoted as

$$s_{\mu_i}^{(1)}(\mathbf{x};\boldsymbol{\mu}) \equiv \frac{\partial \ln f_{\mathbf{X}}(\mathbf{x};\boldsymbol{\mu})}{\partial \mu_i}. \tag{10}$$

To compute the probability of failure in Eq. (5) and the sensitivity of probability of failure in Eq. (8), statistical sampling such as the Monte Carlo simulation (MCS) at a given design needs to be applied to true responses, which is computationally very expensive and almost prohibited. Hence, instead of using true responses, which are usually obtained from computer simulations, surrogate models are used be implemented for the calculation of the probability of failure. To generate accurate surrogate models, this paper uses the dynamic Kriging method, which is discussed in the previous section.

Denote the surrogate model obtained by the dynamic Kriging method for the constraint function $G_j(\mathbf{X})$ as $\hat{G}_j(\mathbf{X})$. Then, by carrying out the MCS using the conservative surrogate model $\hat{G}_j(\mathbf{X})$, the probabilistic constraints in Eq. (5) can be approximated as

$$P_{F_j} \equiv P[G_j(\mathbf{X}) > 0] \cong \frac{1}{M}\sum_{m=1}^{M} I_{\hat{\Omega}_{F_j}}(\mathbf{x}^{(m)}) \leq P_{F_j}^{\mathrm{Tar}} \tag{11}$$

where M is the MCS sample size, $\mathbf{x}^{(m)}$ is the m^{th} realization of $\mathbf{X}$, and the failure set $\hat{\Omega}_{F_j}$ for the surrogate model is defined as $\hat{\Omega}_{F_j} \equiv \left\{\mathbf{x} : \hat{G}_j(\mathbf{x}) > 0\right\}$. Sensitivity of the probabilistic constraint in Eq. (8) is obtained as

$$\frac{\partial P_{F_j}}{\partial \mu_i} \cong \frac{1}{M}\sum_{m=1}^{M} I_{\hat{\Omega}_{F_j}}(\mathbf{x}^{(m)})\, s_{\mu_i}^{(1)}(\mathbf{x}^{(m)};\boldsymbol{\mu}) \tag{12}$$

where $s_{\mu_i}^{(1)}(\mathbf{x}^{(m)};\boldsymbol{\mu})$ is obtained using Eq. (9).

4.3 Corrected Akaike information criterion (AICc)

AIC is originally proposed to evaluate the quality of a model in statistics based on the log-likelihood function [10]. It is a measure of the relative goodness of fit of a statistical model, and in general expressed as

$$AIC = 2k - 2\ln(L) \tag{13}$$

where k is the number of parameters in the statistical model and L is the maximized value of the likelihood function for the estimated model. In the Kriging framework discussed in Section 4.1, the k is the number of dimension of $\mathbf{X}$, which is nd, and L is the likelihood function as shown in Eq. (2). When the sample size is small, i.e., $n/k < 40$ (n is the number of sample), which is often the case in engineering problems, the corrected AIC (AICc) is used instead to provide an unbiased estimation, which is expressed as

$$AICc = AIC + \frac{2k(k+1)}{n-k-1} \tag{14}$$

5 Sampling-based RBDO Using Conservative Surrogate Model

5.1 Weighted Kriging Prediction Variance for Conservative Surrogate Model

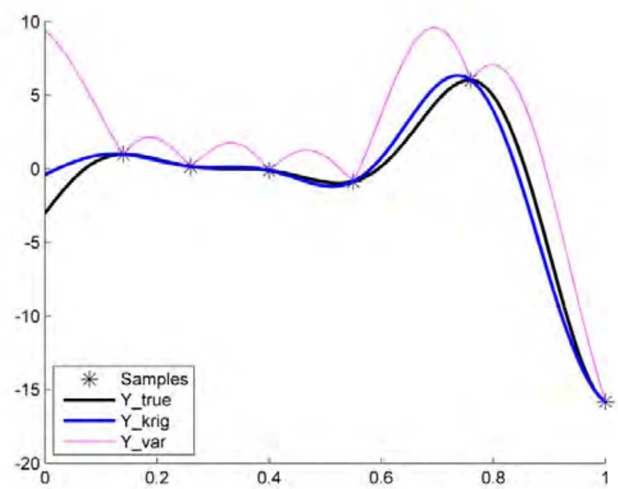
In Eq. (4), the Kriging prediction variance σ_p^2 is calculated, and the C% upper bound of the prediction interval is

$$y_{\mathrm{var}} = y_{\mathrm{krig}} + \Phi^{-1}\left(\frac{C}{100}\right)\sigma_p \tag{15}$$

where $\Phi^{-1}(\bullet)$ is the inverse CDF of the standard normal random variable. This prediction upper bound is usually used as the C% level conservative surrogate model for the Kriging method, and often it is considered as a variable safety margin approach for constructing the conservative surrogate model. Since the Kriging method is an interpolation method, the prediction variance σ_p^2 becomes zero at the sample point. As a result, the conservative surrogate model y_{var} is the same as the y_{krig} at the sample points. This interpolation property of the Kriging method causes trouble when the conservative surrogate model is used for an optimization problem. Consider a 1-D example,

$$\min\ y = -(6x-2)^2 \sin(12x-4) \quad x \in [0,1] \tag{16}$$

The function plot and the Kriging prediction using seven points are shown in Fig. 1.



wrong figure!!

Figure 1: 1-D problem with 7 samples

When the upper bound is used as the conservative surrogate model and for optimization, the optimum x could be easily converged to the sample points, which are the local minima of y_{var}. Therefore, this upper bound of the Kriging prediction interval is not applicable for optimization. Another constant safety margin approach is also often used for the conservative surrogate model [7], where the safety margin is decided based on the empirical CDF of the cross-validation error. In this constant safety margin approach, the conservative surrogate model is obtained by shifting the Kriging prediction to a certain amount and is often expressed as

$$y_{\text{xv}} = y_{\text{krig}} + e_{XV,\%C} \tag{17}$$

where $e_{XV,\%C}$ is the C percentile of the cross-validation error. This conservative surrogate model has the same discrepancy from the Kriging prediction regardless of the sample position. This raises the problem that the conservative surrogate model cannot count in the different uncertainty of the discrepancy due to different sample locations. Therefore, this constant safety margin approach may become over-conservative if the samples are dense and under-conservative if the samples are sparse. Consider the same example shown in Fig.1. If there is no sample at x = 0.76, the safety margin Eq. (17) is s = 1.454 and the conservative surrogate model is shown in Fig. 2. The conservative surrogate model is over-conservative in the region of [0, 0.55] and under-conservative in the region of [0.55, 1].

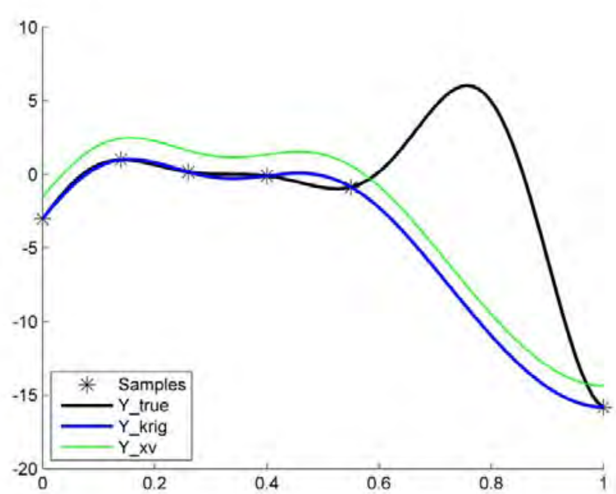


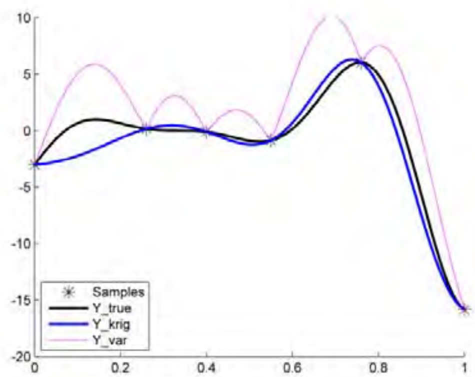
Figure 2: 1-D problem with 6 samples

According to the two examples discussed above, one can see that when a conservative surrogate model from the Kriging method is used for an optimization problem, a variable safety margin approach that has zero margin at the sample points is not desirable because it generates unnecessary local optima regions; whereas a constant safety margin may not be desirable because it does not count in the effect from the sample position. What is needed is a conservative surrogate model that uses a variable safety margin that does not generate local optima and counts in the effect from the sample position.

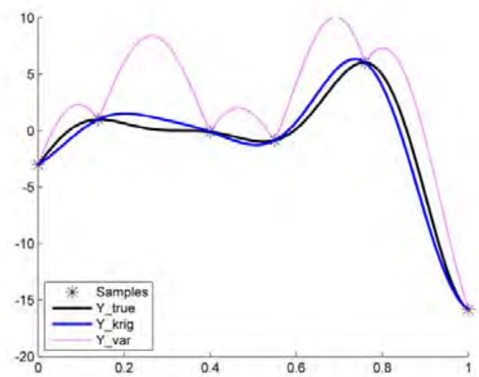
In this paper, a new conservative surrogate model that combines the variable safety factor approach from Eq. (15) and the constant safety margin approach from Eq. (17) is proposed. First, to count in the effect from the sample position, an importance measure for each sample is needed. In this paper, the AICc is chosen to quantify how important a sample is for the Kriging prediction. The importance function for sample x_i is defined as

$$\mathrm{Im}(x_i) = \left| \frac{AICc - AICc^{(-i)}}{AICc} \right|, \; i = 1, \ldots, n \tag{18}$$

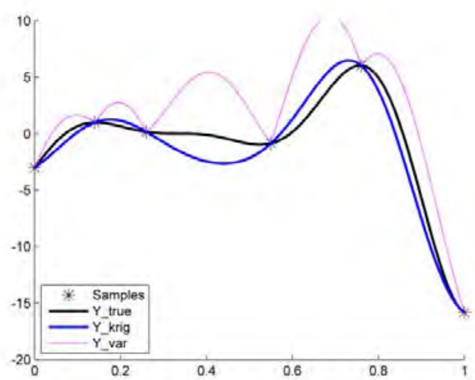
where $AICc$ is calculated using all n samples and $AICc^{(-i)}$ is calculated by omitting x_i. From Eq. (18), it shows that the larger $\mathrm{Im}(x_i)$ is, the more important x_i is. Consider the same example discussed above. Figs. 3(a)-(g) show the Kriging predictions when one of the samples is omitted, and the associated importance function values are shown in Fig. 3(h) as well. The sample point 6 at x = 0.76 is indeed around the highly nonlinear region, and its importance function value is the largest among all 7 samples. Therefore, this importance function by the relative change in *AICc* values can characterize how important one sample is for the Kriging prediction accuracy.



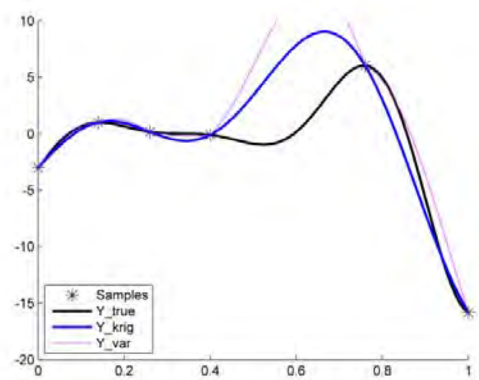
(a) Kriging prediction w/o sample #2



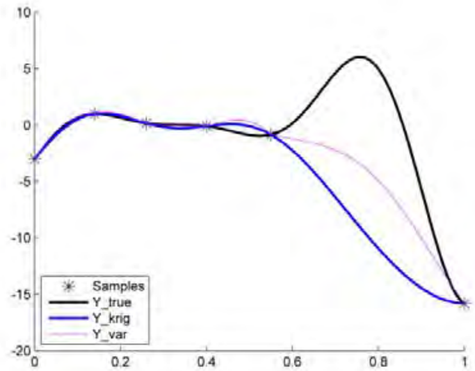
(b) Kriging prediction w/o sample #3



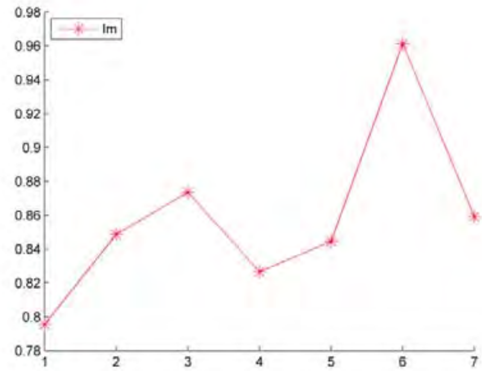
(c) Kriging prediction w/o sample #4



(f) Kriging prediction w/o sample #5



(g) Kriging prediction w/o sample #6



(h) Im(x) function values at each sample

Figure 3: Leave-one-out Kriging prediction

After the importance for each sample is calculated, to construct a weighted Kriging variance, a leave-one-out Kriging variance $\left(\sigma_p^2\right)^{(-i)}$ is calculated where the i^{th} sample x_{i} is omitted using Eq. (4), and then the weighted Kriging variance is expressed as

$$\sigma^2_{p,weighted} = \sum_{i=1}^{n} w(x_i)\left(\sigma_p^2\right)^{(-i)} \tag{19}$$

where the weight function is defined as

$$w(x_i) = \frac{1/\operatorname{Im}(x_i)}{\sum_{i=1}^{n} 1/\operatorname{Im}(x_i)} \tag{20}$$

The weight function decides how much the leave-one-out Kriging variance $\left(\sigma_p^2\right)^{(-i)}$ contributes to the total Kriging variance when x_{i} is missing according to the importance function value. Finally, the conservative surrogate model based on the weighted Kriging variance is

$$y_{con} = y_{krig} + \Phi^{-1}\left(\frac{C}{100}\right)\sigma_{p,weighted} \tag{21}$$

According to Eq. (19), one can see that when x_{i} is omitted, the leave-one-out Kriging variance $\left(\sigma_p^2\right)^{(-i)}$ would not become zero at x_{i}, and therefore the total Kriging variance would not be zero at x_{i} and indeed smoothes the conservative surrogate model eventually. On the other hand, since $\left(\sigma_p^2\right)^{(-i)}$ will be larger at the place where no sample is nearby, it will make the total weighted Kriging variance become variable among the entire domain. Consider the same example shown in Figs. 4 and 5. In Fig. 4, the lines labeled as Y_true , Y_krig , Y_xv , , Y_var and Y_con are the true response, the Kriging response, the conservative surrogate model using constant safety margin, the upper bound of Kriging prediction interval, and the conservative surrogate model using the weighted Kriging variance, respectively.

When all seven samples are used and the conservativeness is set to be 90%, the conservative surrogate model using the weighted Kriging variance is smoother than the upper bound of the Kriging prediction interval and closer to the true response than the conservative surrogate model using the safety margin. Moreover, if one important sample (i.e., $x = 0.76$ in this case) is missing, the conservative surrogate model using the weighted Kriging variance would have a larger discrepancy than the conservative surrogate model using the constant safety margin approach in the region of [0.55, 1] and a smaller discrepancy in the region of [0, 0.55], as shown in Fig. 5. These two cases indicate that the conservative surrogate model using the weighted Kriging variance can adaptively identify the conservativeness according to sample locations and provide a smooth surrogate model that does not change the optimum region of the original response function.

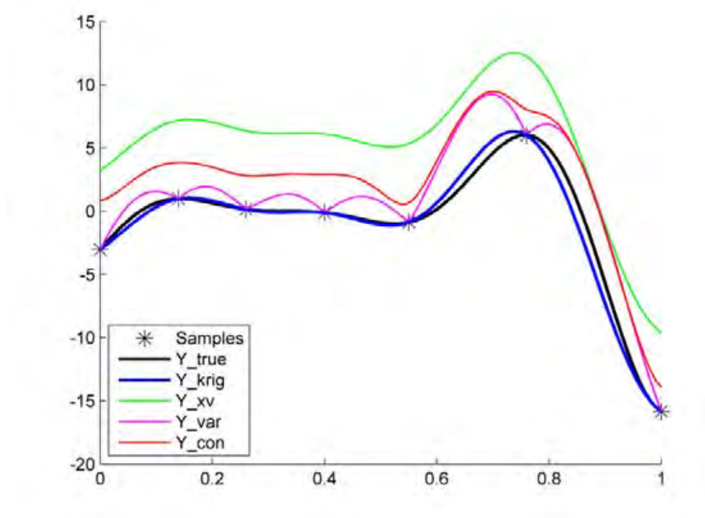


Figure 4: Conservative surrogate model using weighted Kriging variance (7 samples)

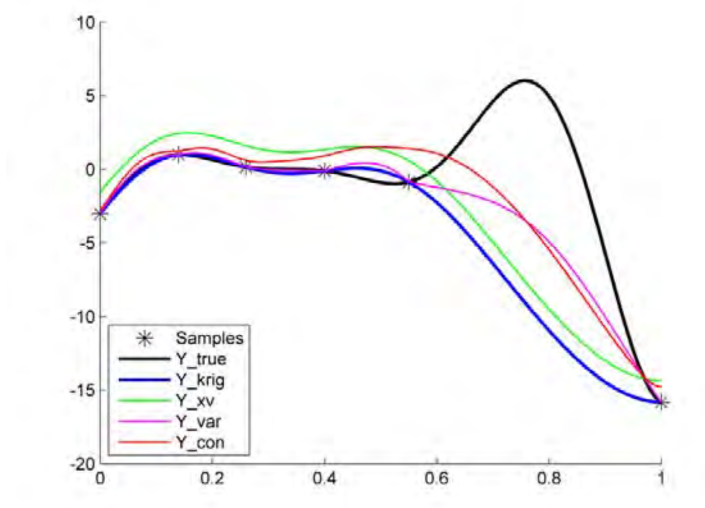


Figure 5: Conservative surrogate model using weighted Kriging variance (6 samples)

5.2. Sampling-based RBDO using the conservative surrogate model

When a limited number of samples is used to generate the surrogate model for MCS in sampling-based RBDO, to assure the optimal design can satisfied the probabilistic constraints, the surrogate models in Eqs. (11) and (12) need to be replaced by the conservative surrogate model. Therefore, the conservative surrogate model using the weighted Kriging variance from Eq. (21) is used to represent the original performance function. The formulation of sampling-based RBDO becomes

$$\begin{aligned} &\text{minimize} && \text{Cost}(\mathbf{d}) \\ &\text{subject to} && P[\hat{G}_j^c(\mathbf{X})>0] \le P_{F_j}^{\text{Tar}}, \quad j=1,\cdots,nc \\ & && \mathbf{d}^{\text{L}} \le \mathbf{d} \le \mathbf{d}^{\text{U}}, \quad \mathbf{d}\in\mathbf{R}^{nd} \text{ and } \mathbf{X}\in\mathbf{R}^{nr} \end{aligned} \tag{22}$$

where $\hat{G}_j^c(\mathbf{X})$ is the conservative surrogate model for representing performance function $G(\mathbf{X})$.

6. Numerical Example

6.1 2-D RBDO Problem with Highly Nonlinear Constraint Functions

Consider a 2-D RBDO problem with three probabilistic constraints, expressed as

$$
\begin{aligned}
&\text{minimize} \quad \text{Cost}(\mathbf{d}) = -\frac{(d_1+d_2-10)^2}{30} - \frac{(d_1-d_2+10)^2}{120} \\
&\text{subject to} \quad P(G_j(\mathbf{X}(\mathbf{d}))>0) \le P_{F_j}^{\text{Tar}} = 2.275\%, \quad j = 1 \sim 3 \\
&\qquad \mathbf{d}^L \le \mathbf{d} \le \mathbf{d}^U, \quad \mathbf{d} \in \mathbf{R}^2 \text{ and } \mathbf{X} \in \mathbf{R}^2
\end{aligned} \tag{23}
$$

where three constraints functions are

$$
\begin{aligned}
G_1(\mathbf{X}) &= 1 - \frac{X_1^2 X_2}{20} \\
G_2(\mathbf{X}) &= -1 + (Y-6)^2 + (Y-6)^3 - 0.6 \times (Y-6)^4 + Z \\
G_3(\mathbf{X}) &= 1 - \frac{80}{X_1^2 + 8X_2 + 5}
\end{aligned} \tag{24}
$$

where $\begin{Bmatrix} Y \\ Z \end{Bmatrix} = \begin{bmatrix} 0.9063 & 0.4226 \\ 0.4226 & -0.9063 \end{bmatrix} \begin{Bmatrix} X_1 \\ X_2 \end{Bmatrix}$ and are drawn in Fig. 6. The distribution and design domain for each variable are shown in Table 1. The initial design point is $\mathbf{d}^0$ = [5 5].

Table 1: Properties of Random Variables

Random Variables	Distribution	$\mathbf{d}^{\mathbf{L}}$	$\mathbf{d}^{\mathbf{0}}$	$\mathbf{d}^{\mathbf{U}}$	Standard Deviation
X_1	Normal	0.0	5.0	10.0	0.3
X_2	Normal	0.0	5.0	10.0	0.3

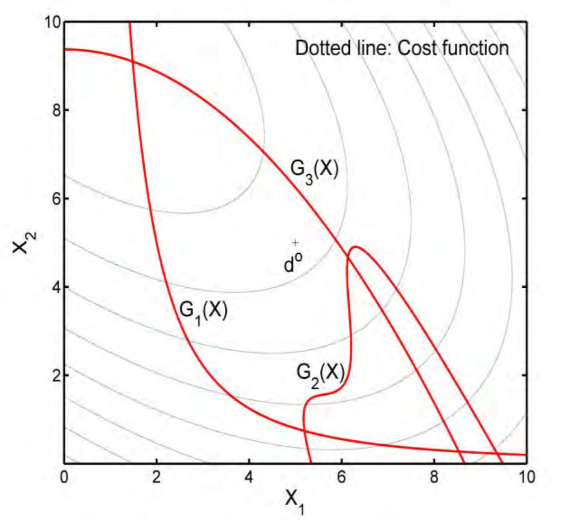


Figure 6: Cost and constraint functions plot

It is worth mentioning that there is no need to construct the conservative surrogate model from the initial design point. In the proposed RBDO process, the deterministic design optimization is carried out first. The RBDO process starts from the deterministic optimum thereafter. The conservative surrogate model will be constructed for the RBDO process only. In this example, the deterministic optimum is $\mathbf{x}$ = [5.19, 0.74] (which is the magenta cross in Fig. 7), and the number of samples in the local window is fixed to 10 samples from the Latin hypercube sampling method. Since 10 samples may not be enough to construct the accurate surrogate models, the conservative surrogate models using the proposed weighted Kriging variance from Eq. (21) are generated for two active constraints G_1 and G_2. For comparison study, the conservative surrogate models using the constant safety margin from Eq. (17) are also generated. The sampling-based RBDO is carried out using these two different conservative surrogate models, and the optimum designs are compared in Table 2 and plotted in Fig. 7. The C% level is set to be 90% in this example.

In Fig. 7, it can be seen that the surrogate model from the dynamic Kriging model itself, which is the blue line, underestimates the true response and results in danger for the obtained optimum design **d** = [4.7432, 1.5391] (blue cross in Fig. 7) as the probability of failure for G_2 is 2.4992%, which is larger than the target probability of failure 2.275%, as shown in Table 2. Therefore the conservative surrogate model is indeed necessary for counting in the uncertainty from the surrogate model and assuring that the optimum design can satisfy the probabilistic constraints. By using the weighted Kriging variance for the conservative surrogate model, which is the red line in Fig.7, the obtained RBDO optimum design is **d** = [4.7020, 1.5801], which is the red cross in Fig. 7, and the cost function value, the probability of failure for G_1, and the probability of failure for G_2 are -1.8956, 2.0654%, and 1.6313%, respectively. As a comparison, the constant safety margin approach gives a more conservative optimum design **d** = [4.6510, 1.6205] (the green cross in Fig. 7) where the probability of failure for G_1 and G_2 are 1.8354% and 0.9455%, respectively; and the cost function value is -1.8783. From the results in Table 2, one can see that the conservative surrogate model using the weighted Kriging variance can assure the optimum design satisfying the probabilistic constraints and has a better optimum design in terms of cost function compared to the conservative surrogate model using the constant safety margin approach.

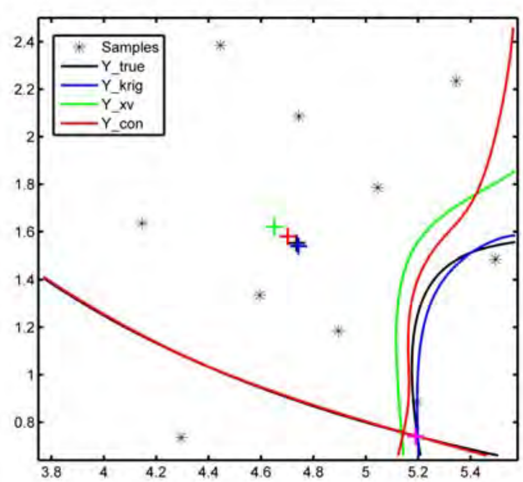


Figure 7: Different conservative surrogate models and optimum designs

Table 2: Optimum designs from different surrogate models and the probability of failure at the optimum

Methods		Cost	Optimum Design	MCS (5M)	
				P_{F_1}, %	P_{F_2}, %
Surrogate Model	Dynamic Kriging	-1.9136	4.7432, 1.5391	2.3256	2.4992
	Constant Safety Margin	-1.8783	4.6510, 1.6205	1.8354	0.9455
	Weighted Kriging Variance	-1.8956	4.7020, 1.5801	2.0654	1.6313
Analytical		-1.9079	4.7351, 1.5518	2.2715	2.2633

When using the surrogate model for sampling-based RBDO, the sample profile may affect the result as well. A good sample profile for dynamic Kriging may end up having a better surrogate model. Therefore, to investigate whether the proposed weighted Kriging variance for the conservative surrogate model has a stable performance, a statistical study is carried out. In this statistical study, 50 sets of 10-LHS samples are generated. For each sample set, the sampling-based RBDO is carried out using both the weighted Kriging variance approach and the constant safety margin approach. The comparison for cost function value and the probability of failure at the optimum are shown in Table. 3.

Table: 3 Cost function and probability of failure at optimum design (50 trials)

Methods	Cost (Median)	P_{F_1}, % (Median)	P_{F_2}, % (Median)	# of Violation G_1	# of Violation G_2
Dynamic Kriging	-1.9164	2.2982	2.3232	1	28
Constant Safety Margin	-1.8809	1.9002	0.9519	0	1

Weighted Kriging Variance	-1.8981	2.1352	1.6287	0	3

In Table 3, when using the dynamic Kriging method itself, the optimum designs violate the probabilistic constraint G_2 28 times out of 50 trials. It shows that the dynamic Kriging prediction either underestimates the true response or overestimates the true response at a rough 50% chance for each way. By using the weighted Kriging variance for the conservative surrogate model, the obtained optimum designs violate the probabilistic constraint G_2 three times. As a comparison, if the constant safety margin is used for the conservative surrogate model, the number of violations for G_2 is 1 time out of 50 trials. Constraint G_1 is not violated in both conservative surrogate modeling cases due to its linearity. The median cost function value at the optimum (which is -1.8809) using the constant safety margin is larger than the one by using the weighted Kriging variance, which is (-1.8981). It is worth mentioning that since the conservativeness level in this example is set to be 90%, both the constant safety margin approach and the weighted Kriging variance approach satisfy the conservativeness. However, the weighted Kriging variance approach provides a better optimum in terms of the cost function value.

7. Conclusion

When applying the surrogate model for optimization problems, the conservative surrogate model using the upper bound of the Kriging prediction interval is not desirable because it generates multiple local optimums at the sample points. The conservative surrogate model using the constant safety margin does not distinguish the uncertainty of the surrogate model at different sample locations, and often the obtained optimum becomes over-conservative where samples are dense and under-conservative where samples are sparse. A weighted Kriging variance using the changes in AICc of the Kriging model to quantify the importance from each sample point is proposed to construct a conservative surrogate model that does not generate unnecessary local optimum and distinguishes the uncertainty of the surrogate model at different sample locations. By applying the weighted Kriging variance for the conservative surrogate model in the sampling-based RBDO problem, the obtained optimum satisfies the probabilistic constraints at the conservativeness level and achieves a better optimum in terms of cost function value compared with the optimum using the constant safety margin.

8. Acknowledgement

Research is supported by the Automotive Research Center, which is sponsored by the U.S. Army Tank Automotive Research, Development and Engineering Center (TARDEC) and Army Research Office (ARO).

9. References

[1] I. Lee., K.K. Choi., Y. Noh., L. Zhao., and D. Gorsich., “Sampling-Based Stochastic Sensitivity Analysis Using Score Functions for RBDO Problems With Correlated Random Variables,” *Journal of Mechanical Design*, 021003-3, Vol. 133, 2011.

[2] I. Lee., K.K. Choi., and L. Zhao., “Sampling-Based RBDO Using the Dynamic Kriging (D-Kriging) Method and Stochastic Sensitivity Analysis,” *Submitted to Structural and Multidisciplinary Optimization*, 2011.

[3] L. Zhao., K.K., Choi., and I. Lee., “A Metamodeling Method Using Dynamic Kriging for Design Optimization,” *accepted by AIAA Journal*, 2011.

[4] V. Picheny., “Improving Accuracy and Compensating for Uncertainty in Surrogate Modeling,” Ph.D Dissertation, Univ. of Florida, Gainesville, FL, 2009.

[5] D. Hertog., J. Kleijnen., and A. Siem., “The correct Kriging variance estimated by bootstrapping,” *Journal of the Operational Research Society*, Vol. 57, pp. 400-409, 2006.

[6] S.D. Luna and A. Young., “The bootstrap and Kriging Prediction Intervals,” *Scandinavian J Stat*, Vol. 30, pp. 175-192, 2003.

[7] F.A.C. Viana, V. Picheny, and R.T. Haftka, "Using cross validation to design conservative surrogates," *AIAA Journal*, Vol. 48, No.10, pp. 2286-2298, 2010.

[8] H. Akaike., “A new look at the statistical model identification,” *IEEE Transaction on Automatic Control*, Vol. 19, No. 6, pp. 716-723, 1974.

[9] C.M. Hurvich., and C.L. Tsai, “Regression and Time Series Model Selection in Small Samples,” *Biometrika*, Vol. 76, pp. 297-307, 1989.

[10] K.P. Burnham and D.R. Anderson., “Model Selection and Multimodel Inference: A Practical Information-Theoretic Approach,” Springer, 2002.

[11] J. Martin., and T.W. Simpson., “Use of Kriging Model to Approximate Deterministic Computer Models,” *AIAA Journal*, Vol. 43, No. 4, pp. 853-863, 2005.