Analytical Uncertainty Propagation via Metamodels in Simulation-Based Design under Uncertainty

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In spite of the benefits, one of the most challenging issues for implementing optimization under uncertainty, such as the use of robust design approach, is associated with the intensive computational demand of uncertainty propagation, especially when the simulation programs are computationally expensive. In this paper, an efficient approach to uncertainty propagation via the use of metamodels is presented. Metamodels, created through computer simulations to replace expensive simulation programs, are widely used in simulation-based design. Different from existing techniques that apply sample-based methods to metamodels for uncertainty propagation, our method utilizes analytical derivations to eliminate the random errors as well as to reduce the computational expenses of sampling. In this paper, we provide analytical formulations for mean and variance evaluations via a variety of metamodels commonly used in engineering design applications. The benefits of our proposed techniques are demonstrated through the robust design for improving vehicle handling. In addition to the improved accuracy and efficiency, our proposed analytical approach can greatly improve the convergence behavior of optimization under uncertainty.

Nomenclature

$\mathbf{x_R}$:	Random variables
$p_{\mathbf{R}}(\mathbf{x_R})$:	Joint probability density function (PDF) of random variables
$p_i(x_i)$:	Individual (marginal) probability density function
$\mu_y(\mathbf{x}), \sigma_y^2(\mathbf{x})$:	Response mean and Variance
$B_i(\mathbf{x})$:	Multivariate tensor-product basis function
$h_{il}(x_l)$:	Univariate basis function
N_b :	Number of multivariate basis functions
$C_{1,il}$, C_{2,i_1i_2l} :	Univariate integrals involved in analytical uncertainty propagation

1. INTRODUCTION

Development of efficient methods for uncertainty propagation has gained much attention in recent years due to the increasing awareness of the importance of nondeterministic optimization. By uncertainty propagation, we mean that the impact of input uncertainty on the variation of a model output (response) is studied. Despite the advancement of methods for uncertainty propagation, the rising fidelity of engineering analyses has significantly increased the computational expenses of simulation-based design and creates the barrier for applying nondeterministic optimization to real engineering design applications.

One difficulty with the conventional statistical approach to uncertainty propagation is that it relies heavily on the use of data sampling to generate probabilistic distributions of a system output. Monte Carlo simulation, a random simulation based approach is very expensive. Even reduced sampling techniques, like Latin Hypercube Sampling (Box et al. 1978) and Taguchi's orthogonal array (Phadke 1989), can still require a large amount of

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samples for complex systems. In practice, the mean-value based approximation methods (Parkinson, et al. 1993) that use Taylor series expansions to estimate the first two moments (mean and variance) of a system response have been used widely because of their simplicity. However, for nonlinear response functions, Taylor expansion is generally not sufficiently accurate (Wu, et. al, 1990), especially when the parameter uncertainty is large. In recent years, reliability analysis based approaches to uncertainty analysis have gained a lot of promises (Du and Chen 2003, Tu et al. 1999), where the concept of the *Most Probable Point* is utilized to generate the cumulative distribution function of a model output via a serial of limit state values. They generally provide better accuracy compared to mean-value based approximations and better efficiency compared to sampling-based methods. However, for problems that require expensive high-fidelity engineering analyses that may take hours or even days for a single simulation, the use of reliability analysis based methods is still not affordable.

Because the direct use of data sampling methods is very expensive, an alternative approach that is being widely considered is the use of metamodels to replace the expensive simulation models (Chen et al. 1997; Delaurentis and Mavris, 2000), either over the space of all variables or that of the random variables only. Data sampling is then performed using metamodels. Studies show that when samples are used to estimate the performance mean and variance in metamodel-based design optimization, the performance functions tend to be noisy causing problems for optimization convergence (Padmanabhan and Batill, 2000). Some of the metamodeling techniques such as Kriging (Sachs, et al., 1989) require more computational resources than the others (for example, polynomial response surfaces). Applying sample-based methods could still be inefficient for these relatively expensive matamodels in optimization under uncertainty

Our objective in this work is to develop an efficient approach to uncertainty propagation via the use of metamodels. Different from existing techniques that apply sample-based methods to metamodels, our method utilizes analytical derivations to reduce the computational expenses and to improve the accuracy by eliminating the random errors of statistical sampling. Our focus in this work is on deriving the first two moments (mean and variance) of a system response in optimization under uncertainty. Analytical formulations are provided for a variety of commonly used metamodels, such as the polynomial (Box et al. 1978), the Kriging (Sacks, et al., 1989; Currin, et. al, 1991), the Radial Basis Functions (Hardy, 1971; Dyn, et al., 1986), and the MARS (Friedman, 1991). We show that even though the function forms of these metamodels vary significantly, they all follow the form of multivariate tensor-product basis functions for which the analytical results of univariate integrals can be combined to evaluate the multivariate integrals in uncertainty propagation. Our paper is organized as follows. In Section 2, we lay out the general formulations for uncertainty propagation and introduce the concept of tensor-product basis functions. In Section 3, we provide detailed analytical derivations for various types of metamodels. In Section 4, we illustrate our approach and its advantages using the robust design for improving vehicle handing as an example. Section 5 is the closure of this paper.

2. MATHEMATICAL BACKGROUND

2.1 Formulations in Uncertainty Propagation

Various formulations are used for optimization under uncertainty. Robust Design (Chen et al., 1996) is a widely used paradigm where the emphasis is on improving the quality of a product through minimizing the effect of variation (noises) without eliminating the causes. A detailed comparison of various nonlinear programming based robust design formulations is provided in Du and Chen, 2002. As observed, the formulation selected is often a tradeoff between the accuracy required for uncertainty assessments, e.g., probability of constraint being feasibility, and the computational needs. In many practical applications, the first two moments of a performance distribution (mean and variance) are widely used to form a robust design objective and to assess the constraint feasibility under uncertainty.

Given a response $y = f(\mathbf{x})$, where $\mathbf{x}$ are input variables that can be deterministic or stochastic (i.e., subject to randomness), associated with either design variables or noise variables, the response mean and variance are defined by:

$$\mu_y(\mathbf{x}) = \int f(\mathbf{x}) p_{\mathbf{R}}(\mathbf{x}_{\mathbf{R}}) d\mathbf{x}_{\mathbf{R}} , \tag{2.1}$$

$$\sigma_y^2(\mathbf{x}) = \int [f(\mathbf{x}) - \mu_y(\mathbf{x})]^2 p_{\mathbf{R}}(\mathbf{x}_{\mathbf{R}}) d\mathbf{x}_{\mathbf{R}}, \tag{2.2}$$

where **R** is the set of random variables. Here, it is assumed that the random variables are statistically independent, i.e., their joint probability density function (PDF) is a product of individual or marginal PDF of all variables, i.e., $p_{\mathbf{R}}(\mathbf{x}) = \prod_{l\in\mathbf{R}} p_l(x_l)$. Both the response mean and variance are functions of input variables **x**. When there are multiple random variables, the integrations in Eqs.1-2 involve multivariate integrals which are very computationally expensive. As introduced in Section 1, applying advanced sampling approaches directly to a model for uncertainty propagation is not practically feasible for problems with time-consuming model evaluations; random errors cannot be avoided even applied to easy-to-compute metamodels. We find that if a function can be expressed as a tensor-product basis function (c.f., Hastie, et al., 2001), then the analytical results of univariate integrals can be combined to evaluate the multivariate integrals in Eqs.2.1-2.2 for uncertainty propagation. As it will be disclosed later, most of the commonly used metamodels all follow the form of multivariate tensor-product basis functions for which the formulations of mean and variance can be analytically derived. The concept of tensor product basis function is first introduced next.

2.2 Tensor Product Basis Functions

A multivariate tensor-product basis functions $B_i(\mathbf{x})$ is defined as a product of *M* univariate basis functions $h_{il}(x_l)$, i.e.,

$$B_i(\mathbf{x}) = \prod_{l=1}^{M} h_{il}(x_l),\ i = 1,2,...,N_b\,. \tag{2.3}$$

For instance $B(\mathbf{x})=x_1x_2$ can be rewritten as $B(\mathbf{x})=h_1(x_1)h_2(x_2)$, where $h_1(x_1)= x_1$ and $h_2(x_2)= x_2$. Note here $h_{il}(x_l)$ could be equal to 1. Then a special category of functions, called tensor-product basis functions, can be defined as a linear expansion of these multivariate basis functions, i.e.,

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)]\,, \tag{2.4}$$

where a_i (i =0, 1,..., N_b) are constant coefficients. Many commonly used metamodels, i.e., polynomial regression model, MARS, RBF (with Gaussian basis functions), Kriging, can be expressed as tensor-product basis functions, with details shown in Sections 3.2-3.5.

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3. Analytical Formulations of Uncertainty Propagation via Metamodels

In this section, we first derive the generalized formulations for uncertainty propagation based on the concept of tensor product basis functions. We then illustrate the analytical derivations of function mean and variance for a set of commonly used metamodeling techniques.

3.1 Generalized UP Formulations in the Form of Tensor Product Basis Function

By substituting into Eq. 2.1 the expression of the tensor-product function (Eq.2.4), the performance mean as a function of input variable **x** can be written as:

$$\begin{aligned}\mu_y(\mathbf{x}) &= \int f(\mathbf{x}) \prod_{l\in\mathbf{R}} [p_l(x_l)dx_l] = \int \left\{ a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)] \right\} \prod_{l\in\mathbf{R}} [p_l(x_l)dx_l] \\ &= a_0 + \sum_{i=1}^{N_b} \left\{ a_i \prod_{l\in\mathbf{R}} [\int h_{il}(x_l) p_l(x_l) dx_l] \prod_{l\notin\mathbf{R}} h_{il}(x_l) \right\} \\ &= a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l\in\mathbf{R}} C_{1,il} \prod_{l\notin\mathbf{R}} h_{il}(x_l)],\end{aligned} \tag{3.1}$$

where, $C_{1,il}$ is the mean of the univariate basis function $h_{il}(x_l)$, i.e.,

$$C_{1,il} = \int h_{il}(x_l) p_l(x_l) dx_l\,. \tag{3.2}$$

Similarly, if we substitute into Eq.2.2 the expressions of $\mu_Y(\mathbf{x})$ (Eq.3.1) and the tensor-product function (Eq.2.4), we then derive the response variance as follows:

$$\begin{aligned}\sigma_Y^2(\mathbf{x}) &= \int \left\{ \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)] - \sum_{i=1}^{N_b} [a_i \prod_{l\in\mathbf{R}} C_{1,il} \prod_{l\notin\mathbf{R}} h_{il}(x_l)] \right\}^2 \prod_{l\in\mathbf{R}} [p_l(x_l)dx_l] \\ &= \int [\sum_{i=1}^{N_b} a_i \prod_{l=1}^{M} h_{il}(x_l)]^2 \prod_{l\in\mathbf{R}} [p_l(x_l)dx_l] - [\sum_{i=1}^{N_b} a_i \prod_{l\notin\mathbf{R}} C_{1,il} \prod_{l\notin\mathbf{R}} h_{il}(x_l)]^2 \\ &= \sum_{i_1=1}^{N_b} \sum_{i_2=1}^{N_b} \left\{ a_{i_1} a_{i_2} \prod_{l\in\mathbf{R}} (C_{1,i_1 l} C_{1,i_2 l}) \{ \prod_{l\in\mathbf{R}} [C_{2,i_1 i_2 l} / (C_{1,i_1 l} C_{1,i_2 l})] - 1 \} \prod_{l\notin\mathbf{R}} [h_{i_1 l}(x_l) h_{i_2 l}(x_l)] \right\}.\end{aligned} \tag{3.3}$$

It can be observed that both the mean and variance evaluations (Eqs.3.1 and 3.3) of a tensor product basis function depend on two common sets of quantities defined by univariate integrals, i.e., the mean of univariate basis function C_1 and the inner product of two univariate basis functions C_2, defined as:

$$C_{2,i_1 i_2 l} = \int h_{i_1 l}(x_l) h_{i_2 l}(x_l) p_l(x_l) dx_l \,. \tag{3.4}$$

Once the basis functions and the distributions of the variables are fixed, the values of C_1 and C_2 can be derived analytically and used to evaluate the response mean/variance at any given design settings (i.e., for given values of design input **x**). In the case that the distributions of several variables are changed, only the C_1 and C_2 corresponding to these variables need to be re-evaluated. In the following subsections we illustrate the derivations of C_1 and C_2 for various types of metamodels.

3.2 Derivations via Polynomial Metamodels

All polynomial regression models can be transformed into the tensor product form. The most widely used second-order regression model is shown as:

$$f(\mathbf{x}) = \beta_0 + \sum_{i=1}^{M} \beta_i x_i + \sum_{i=1}^{M} \beta_{ii} x_i^2 + \sum_{i=1}^{M} \sum_{j=i+1}^{M} \beta_{ij} x_i x_j \,. \tag{3.5}$$

For the above model, for any $0 \le i, j \le M$ and $j \ne 0$, we define multivariate basis functions as

$$B_{(i,j)} = \begin{cases} x_j & i = 0 \\ x_j^2 & i = j \\ x_i x_j & i < j \end{cases} . \tag{3.6}$$

The univariate basis functions corresponding to variable x_l are:

$$h_{(i,j)l} = \begin{cases} 1 & \text{none of } (i,j) = l \\ x_l & \text{only one of } (i,j) = l \\ x_l^2 & \text{both of } (i,j) = l \end{cases} . \tag{3.7}$$

The polynomial model can be re-written as:

$$f(\mathbf{x}) = \beta_0 + \sum_{0\le i,j\le M, j\ne 0} \beta_{ij} B_{(i,j)} = \beta_0 + \sum_{0\le i,j\le M, j\ne 0} \beta_{ij} \prod_{l=1}^{M} h_{(i,j)l} \,, \tag{3.8}$$

where $\beta_{0j} = \beta_j$.

Based on Eqns. 3.2 and 3.4, the values of C_1 and C_2 are derived for the polynomial function, respectively as:

$$C_{1,(i,j)l} = \begin{cases} 1 & \text{none of } (i,j) = l \\ \int x_l p_l(x_l) dx_l = \mu_l & \text{only one of } (i,j) = l \\ \int x_l^2 p_l(x_l) dx_l = \mu_l^2 + \sigma_l^2 & \text{both of } (i,j) = l \end{cases} \tag{3.9}$$

$$C_{2,(i_1,j_1)(i_2,j_2)l}=\begin{cases}1 & \text{none of } (i_1,j_1,i_2,j_2)=l\\ \int x_l p_l(x_l)dx_l=\mu_l & \text{only one of } (i_1,j_1,i_2,j_2)=l\\ \int x_l^2 p_l(x_l)dx_l=\mu_l^2+\sigma_l^2 & \text{only two of } (i_1,j_1,i_2,j_2)=l\\ \int x_l^3 p_l(x_l)dx_l=\mu_{l,3}+3\mu_l\sigma_l^2+\mu_l^3 & \text{only three of } (i_1,j_1,i_2,j_2)=l\\ \int x_l^4 p_l(x_l)dx_l=\mu_{l,4}+4\mu_l\mu_{l,3}+6\mu_l^2\sigma_l^2+\mu_l^4 & \text{all of } (i_1,j_1,i_2,j_2)=l\end{cases} \quad (3.10)$$

Here, μ_l and σ_l^2 are the mean and variance of input variable x_l; $\mu_{l,n}$ (n = 3, 4) is the n^{th} centered moment of x_l, i.e., $\mu_{l,n}=\int (x_l-\mu_l)^n p(x_l)dx_l$. The values of μ_l, σ_l^2, $\mu_{l,3}$, and $\mu_{l,4}$ depend on the type of input distributions. For uniform distributions, we can derive $\sigma_l^2=\delta_l^2/3$, $\mu_{l,3}=0$, $\mu_{l,4}=\delta_l^4/5$; for normal distributions, we obtain $\mu_{l,3}=0$, $\mu_{l,4}=3\sigma_l^4$.

Noting that many items of C_1 and C_2 are equal to 1, we can further expand the mean (Eq. 3.1) and the variance (Eq. 3.2) as:

$$\mu_y(\mathbf{x})=\beta_0+\sum_{i\in\mathbf{R}}\beta_i\mu_i+\sum_{i\in\mathbf{R}}\beta_{ii}\sigma_i^2+\sum_{i\in\mathbf{R}}\sum_{j\in\mathbf{R},j\geq i}\beta_{ij}\mu_i\mu_j+\sum_{i\notin\mathbf{R}}(\beta_i+\sum_{j\in\mathbf{R}}\beta_{ij}\mu_j)x_i+\sum_{i\notin\mathbf{R}}\sum_{j\notin\mathbf{R},j\geq i}\beta_{ij}x_ix_j, \quad (3.11)$$

$$\sigma_y^2(\mathbf{x})=\sum_{i\in\mathbf{R}}\beta_{ii}^2(\mu_{i,4}-2\sigma_i^4)+\sum_{i\in\mathbf{R}}\sum_{j\in\mathbf{R},j\geq i}\beta_{ij}^2\sigma_i^2\sigma_j^2+\sum_{i\in\mathbf{R}}^{M}(\beta_i+\beta_{ii}\mu_i+\sum_{j\in\mathbf{R}}\beta_{ij}\mu_j+\sum_{j\notin\mathbf{R}}\beta_{ij}x_j)\beta_{ii}\mu_{i,3}$$
$$+\sum_{i\in\mathbf{R}}(\beta_i+\beta_{ii}\mu_i+\sum_{j\in\mathbf{R}}\beta_{ij}\mu_j+\sum_{j\notin\mathbf{R}}\beta_{ij}x_j)^2\sigma_i^2, \quad (3.12)$$

where $\beta_{ji}=\beta_{ij}$ if $i>j$.

3.3 Derivations via Kriging Model

The Kriging method is a widely used metamodeling technique due to its capability of capturing nonlinear behaviors. A Kriging model (Sacks, et al., 198; Currin, et al.,1999) with a constant global trend (i.e., Ordinary Kriging) can be written as:

$$f(\mathbf{x})=\hat\beta+\mathbf{r}(\mathbf{x})^T\mathbf{R}^{-1}(\mathbf{y}_0-\hat\beta)=\hat\beta+\mathbf{r}(\mathbf{x})^T\boldsymbol{\kappa}=\hat\beta+\sum_{i=1}^{N}\kappa_i r_i(\mathbf{x}), \quad (3.13)$$

where $\boldsymbol{\kappa}=\mathbf{R}^{-1}(\mathbf{y}_0-\beta)$ is a N×1 vector (N is the number of sample points) and κ_i is its i^{th} element. The Kriging model follows the form of a multivariate correlation function which can be defined to be a product of univariate correlation functions, i.e., $\rho(\mathbf{t},\mathbf{u})=\prod_{l=1}^{M}\rho_l(t_l,u_l)$, where ρ_l is the correlation function for l^{th} dimension. The correlation between $\mathbf{x}$ and a sample point $\mathbf{x}_i$, can be expressed as: $r_i(\mathbf{x})=\rho(\mathbf{x},\mathbf{x}_i)=\prod_{l=1}^{M}\rho_l(x_l,x_{il})$. Let $h_{il}(x_l)=\rho_l(x_l,x_{il})$, the Kriging model is then transformed into a tensor-product function:

$$f(\mathbf{x})=\hat\beta+\sum_{i=1}^{N}\kappa_i\prod_{l=1}^{M}h_{il}(x_l). \quad (3.14)$$

Many different one-dimensional correlation functions are used with Kriging metamodeling (see, e.g., Currin, et. al., 1991; Sacks, et. al., 1989). In this study, we focus on the commonly used Gaussian correlation function, with the expression of $h_{il}(x_l)=\exp\left[-\theta_l(x_l-x_{il})^2\right]$.

For uniform distributions of input variables, we can prove that (details are omitted here but can be found in Jin 2004):

$$C_{1,il} = \frac{1}{2\delta_l}\sqrt{\frac{\pi}{\theta_l}}\left\{\Phi(a_{il}\sqrt{2\theta_l}) - \Phi(b_{il}\sqrt{2\theta_l})\right\}, \tag{3.15}$$

$$C_{2,i_1i_2l} = \frac{1}{2\delta_l}\sqrt{\frac{\pi}{2\theta_l}}\exp\left[-\theta_l(x_{i_1l}-x_{i_2l})^2/2\right]\times\left(\Phi\left[\sqrt{\theta_l}(a_{i_1l}+a_{i_2l})\right]-\Phi\left[\sqrt{\theta_l}(b_{i_1l}+b_{i_2l})\right]\right), \tag{3.16}$$

where $a_{il} = \mu_l + \delta_l - x_{0il}$ and $b_{il} = \mu_l - \delta_l - x_{0il}$; $\Phi(.)$ stands for the CDF of standard normal distributions.

For normal distributions of input variables, it can be proved that:

$$C_{1,il} = \frac{1}{\sqrt{2\sigma_l^2\theta_l+1}}\exp[-\frac{\theta_l}{2\sigma_l^2\theta_l+1}(\mu_l - x_{il})^2], \tag{3.17}$$

$$C_{2,i_1i_2l} = \frac{1}{\sqrt{4\sigma_l^2\theta_l+1}}\exp\left\{-\frac{\theta_l}{4\sigma_l^2\theta_l+1}[(\mu_l-x_{i_1l})^2+(\mu_l-x_{i_2l})^2+2\sigma_l^2\theta_l(x_{i_1l}-x_{i_2l})^2]\right\}. \tag{3.18}$$

Substituting the expressions of C_1 and C_2 derived here (Eqns. 3.17 and 3.18) into the generalized formulations in Eqs.3.1 and 3.3, we then obtain the first and second moments in uncertainty propagation via Kriging models. The results evaluated by this analytical approach are generally highly accurate. However, if the correlation matrix **R** is ill-conditioned, large numerical errors could occur when σ_l, δ_l, or θ_l are very small. This is due to the loss of significant digits in the evaluation of $\prod_l [C_{2,i_1i_2l}/(C_{1,i_1l}C_{1,i_2l})]-1$ in Eqn. 3.3: when σ_l, δ_l, or θ_l are very small, $\prod_l [C_{2,i_1i_2l}/(C_{1,i_1l}C_{1,i_2l})]$ will be very close to 1 (e.g., if $\theta_l = 0$, then $C_{2,i_1i_2l} = C_{1,i_1l}C_{1,i_2l} = 1$); the subtraction of two nearly equal numbers would cause the canceling error. This canceling error will be largely magnified by the deteriorated accuracy of κ_i due to the ill-conditioned **R**. Numerical approaches to reduce the canceling errors can be found in Jin's (2004).

3.4 Derivations via Gaussian RBF Model

The Gaussian Radial Basis Function model (also called RBFN model) can be written as,

$$\hat{y}(\mathbf{x}) = \beta + \sum_{i=1}^{N_\phi}\lambda_i\varphi_i(\mathbf{x}), \tag{3.19}$$

where, $\varphi_i(\mathbf{x}) = \exp\left[-\frac{1}{2\tau_i^2}\sum_{l=1}^{M}(x_l - t_{il})^2\right] = \prod_{l=1}^{M}\exp\left[-\frac{(x_l - t_{il})^2}{2\tau_i^2}\right]$. If we define basis functions as $h_{il}(x_l) = \exp\left[-\frac{(x_l - t_{il})^2}{2\tau_i^2}\right]$, the RBF model is transformed into a tensor-product function:

$$f(\mathbf{x}) = \beta + \sum_{i=1}^{N_\phi}[\lambda_i\prod_{l=1}^{M}h_{il}(x_l)]. \tag{3.20}$$

Noting that the form of a Gaussian RBF model is similar to that of a Kriging model, except that the width τ_i is associated with each basis function instead of with each variable, the formulations can be derived in a similar way as shown in Section 3.3.

For uniform distributions of inputs, it can be proved that

$$C_{1,il} = \frac{\tau_i}{\delta_l}\sqrt{\frac{\pi}{2}}\left\{\Phi\left[(\mu_l + \delta_l - t_{il})/\tau_i\right] - \Phi\left[(\mu_l - \delta_l - t_{il})/\tau_i\right]\right\}, \tag{3.21}$$

$$C_{2,i_1i_2l} = \frac{a_{i_1i_2}}{\delta_l}\sqrt{\frac{\pi}{2}}\exp\left[-(t_{i_1l}-t_{i_2l})^2/(2\tau_{i_1}^2+2\tau_{i_2}^2)\right]\times\left(\Phi\left[(\mu_l+\delta_l-b_{i_1i_2l})/a_{i_1i_2}\right]-\Phi\left[(\mu_l-\delta_l-b_{i_1i_2l})/a_{i_1i_2}\right]\right), \tag{3.22}$$

where, $a_{i_1i_2} = \tau_{i_1}\tau_{i_2}/\sqrt{\tau_{i_1}^2+\tau_{i_2}^2}$ and $b_{i_1i_2l} = (\tau_{i_1}^2 t_{i_2l} + \tau_{i_2}^2 t_{i_1l})/(\tau_{i_1}^2+\tau_{i_2}^2)$.

For normal distributions of inputs, it can be proved that

$$C_{1,il} = \frac{1}{\sqrt{\sigma_l^2/\tau_l^2+1}}\exp[-(\mu_l - t_{il})^2/(2\tau_i^2+2\sigma_l^2)], \tag{3.23}$$

$$C_{2,i_1i_2j} = \frac{\tau_{i_1}\tau_{i_2}}{\sqrt{b_{i_1i_2l}}}\exp\left\{-\frac{1}{2b_{i_1i_2l}}[\tau_{i_2}{}^2(\mu_j - t_{i_1j})^2 + \tau_{i_1}{}^2(\mu_j - t_{i_2j})^2 + \sigma_j{}^2(t_{i_1j} - t_{i_2j})^2]\right\}, \quad (3.24)$$

where $b_{i_1i_2l} = \sigma_l{}^2(\tau_{i_1}{}^2 + \tau_{i_2}{}^2) + \tau_{i_1}{}^2\tau_{i_2}{}^2$.

3.5 Derivations via MARS Model

A MARS model is a weighted sum of tensor spline basis functions, i.e.,

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x}), \quad (3.25)$$

where the tensor spline basis functions are defined as tensor products of univariate truncated power functions:

$$B_i(\mathbf{x}) = \prod_{l\in\mathbf{K}_i}[s_{il}(x_l - t_{il})]_+^q . \quad (3.26)$$

If we define a set of univariate basis functions:

$$h_{il}(x_l) = \begin{cases} 1 & l \notin \mathbf{K}_i \\ [s_{il}(x_l - t_{il})]_+^q & l \in \mathbf{K}_i \end{cases}, \quad (3.27)$$

then the MARS model is transformed into a tensor-product function:

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b}[a_i \prod_{l=1}^{M} h_{il}(x_l)] . \quad (3.28)$$

The values of C_1 and C_2 can be evaluated respectively by:

$$C_{1,il} = \begin{cases} 1 & l \notin \mathbf{K}_i \\ s_{il}{}^q \int_{lb_1}^{ub_1}(x_l - t_{il})^q p_l(x_l)dx_l & l \in \mathbf{K}_i \end{cases}, \quad (3.29)$$

$$C_{2,i_1i_2l} = \begin{cases} 1 & l \notin \mathbf{K}_{i_1}, l \notin \mathbf{K}_{i_2} \\ C_{1,i_1l} & l \in \mathbf{K}_{i_1}, l \notin \mathbf{K}_{i_2} \\ C_{1,i_2l} & l \notin \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2} \\ (s_{i_1l}s_{i_2l})^q \int_{lb_2}^{ub_2}[(x_l - t_{i_1l})(x_l - t_{i_2l})]^q p_l(x_l)dx_l & l \in \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2} \end{cases} \quad (3.30)$$

where $ub_1 = \max(s_{il}\infty, t_{il})$, $lb_1 = \min(s_{il}\infty, t_{il})$, $ub_2 = \min[\max(s_{i_1l}\infty, t_{i_1l}), \max(s_{i_2l}\infty, t_{i_2l})]$ and $lb_2 = \max[\min(s_{i_1l}\infty, t_{i_1l}), \min(s_{i_2l}\infty, t_{i_2l})]$. If $lb_2 \geq ub_2$, then $C_{2,i_1i_2l} = 0$. While the formulations above are general enough to be applied to different *q*, in the following we focus on a commonly used setting, i.e., *q*=1.

For uniform distributions of input variables, it can be proved that:

$$C_{1,il} = \frac{s_{il}}{2\delta_l}[\frac{x_l{}^2}{2} - t_{il}x_l]\Big|_{lb_{1a}}^{ub_{1a}} \quad (l \in \mathbf{K}_i), \quad (3.31)$$

$$C_{2,i_1i_2l} = \frac{s_{i_1l}s_{i_2l}}{2\delta_l}[\frac{x_l{}^3}{3} - \frac{(t_{i_1l} + t_{i_2l})x_l{}^2}{2} + t_{i_1l}t_{i_2l}x_l]\Big|_{lb_{2a}}^{ub_{2a}} \quad (l \in \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2}), \quad (3.32)$$

where $f(x)\big|_a^b = f(b) - f(a)$; $ub_{1a} = \min[ub_1, \mu_l + \delta_l]$ and $lb_{1a} = \max[lb_1, \mu_l - \delta_l]$; $ub_{2a} = \min[ub_2, \mu_l + \delta_l]$ and $lb_{2a} = \max[lb_2, \mu_l - \delta_l]$.

For normal distributions, it can be proved that:

$$C_{1,il} = s_{il}\{\frac{\mu_l - t_{il}}{\sigma_l}\Phi(\frac{x_l - \mu_l}{\sigma_l}) - \frac{1}{\sqrt{2\pi}}\exp[-\frac{(x_l - \mu_l)^2}{2\sigma_l{}^2}]\}\Big|_{lb_1}^{ub_1} \quad (l \in \mathbf{K}_i), \quad (3.33)$$

$$C_{2,i_1i_2l} = s_{i_1l}s_{i_2l}\{[\frac{(\mu_l - t_{i_1l})(\mu_l - t_{i_2l})}{\sigma_l} + \sigma_l]\Phi(\frac{x_l - \mu_l}{\sigma_l}) - \frac{x_l + \mu_l - t_{i_1l} - t_{i_2l}}{\sqrt{2\pi}}\exp[-\frac{(x_l - \mu_l)^2}{2\sigma_l^2}]\}\Big|_{lb_2}^{ub_2} \quad (l \in \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2}). \quad (3.34)$$

In the coming section, we demonstrate the advantages of the proposed method by applying it to an engineering design problem under the robust design concept.

4. Robust Design for Improving Vehicle Handling

We use the robust deign for improving vehicle handling, in particular preventing rollover of ground vehicles, as an example to illustrate the use of analytical uncertainty propagation (UP) in design under uncertainty. A topic related to the analytical UP is the analytical method for global sensitivity analysis (GSA) to study the impact of variations in input variables on the variation of a model output. The common underlying principle for both activities is to combine the analytical results of univariate integrals to evaluate the multivariate integrals that are associated with multvariate tensor-product basis functions (Jin et al. 2004). The details of the analytical approach to GSA are provided in Chen et al. 2004, but will not be repeated here. As applying GSA plays an important role in variable screening and building an accurate metamodel for further analytical UP in robust design, some of the results from GSA are highlighted here.

4.1 Problem Description and Variable Screening

Rollover of ground vehicles is one of the major causes of highway accidents in the United States (Mohemedshah and Council, 1997). To prevent vehicle rollover, we developed a robust design procedure (Chen, et al, 2001) to optimize vehicle and suspension parameters so that the design is not only optimal against the worst maneuver condition but is also robust with respect to a range of maneuver inputs. In our earlier work, the second-order polynomial function was created as the response surface model; factor importance was examined by checking the coefficients of the second-order polynomial function and screened based on the linear effects. In this work, our analytical techniques for GSA are applied to the same problem; the Kriging model is built and used for deriving analytical formulation for UP. Through comparisons, we illustrate the advantages of our newly developed methods.

The detailed description of the simulation program for studying the rollover behavior and the robust design formulation for preventing rollover can be found in (Chen, et al, 2001). In brief, the rollover simulation is the integrated computer tool ArcSim (Sayers and Riley, 1996) developed at the University of Michigan for simulating and analyzing the dynamic behavior of 6-axle tractor/semi-trailers. Without building the metamodel, the testing of an optimization scenario without robustness consideration takes at least five hours to converge (Michelena and Kim, 1998) on the Sun Ultra-1 workstation. When robustness considerations are introduced, the computational demand becomes more significant.

Table 1. Design Variables and Their Ranges

Variables	Description	Lower bound	Upper bound	Unit
HH1	Height of hitch above ground	51.20	76.80	in
KHX1	Hitch roll torsional stiffness	80000	120000	in-lb/deg
KT11	Axle 1 tire stiffness	5520.00	8280.00	lb/in
KT123	Axles 2 & 3 tire stiffness	5520.00	8280.00	lb/in
KT2123	Axles 4,5,& 6 tire stiffness	4139.20	6208.80	lb/in
LTS11	Distance between springs on Axle 1	30.40	45.60	in
LTS123	Distance between springs on Axles 2 & 3	30.40	45.60	in
LTS2123	Distance between springs on Axles 4,5 & 6	30.40	45.60	in
M11	Laden load for Axle 1	11540	17310	lbm
M123	Laden load for Axles 2 & 3	20358.40	30537.60	lbm
M2123	Laden load for Axle 4,5, & 6	16274.40	24411.60	lbm
SCFS11	Axle 1 spring stiffness scale factor	0.8	1.2	/
SCFS123	Axles 2 & 3 spring stiffness scale factor	0.8	1.2	/
SCFS2123	Axle 4,5 & 6 spring stiffness scale factor	0.8	1.2	/

Fourteen ArcSim input parameters corresponding to suspension and vehicle parameters are chosen as design variables (control factors) (see Table 1). The steering and braking parameters are taken as the noise factors to capture the range of maneuvering conditions (see Table 2). The level of braking (brake_level) is the amount of braking pressure applied. The level of steering (steer_level) is the angle the steering wheel is turned. The starting and ending times of braking defines when the driver starts and stops braking. The ending times of steering defines when the driver stops steering. A rollover metric (R) is used as the response for which the metamodel is created.

The rollover metric is defined as the square root of the integral of the square of the rollover angle in a 5-second period. If the rollover angle becomes greater than 45°, rollover will inevitably occur.

Table 2. Noise Variables and Their Ranges

Variable	Distribution	Lower Bound	Upper Bound	Unit
brake_level	Uniform	70	120	psi
start_brake	Uniform	1.02	1.38	sec
end_brake	Uniform	1.53	2.07	sec
steer_level	Uniform	60	100	deg
end_steer	Uniform	2.16	3.24	sec

Based on the observations obtained from global sensitivity analysis (Chen et al. 2004), it is decided to use the 11 relatively important variables in subsequent procedures and freeze the eight relatively unimportant variables at their nominal values. It is also found that three noise variables, i.e., brake_level, end_brake, and steer_level, play very significant roles in the variability of the response. With the knowledge of variable importance, an additional 400 sample runs are applied in a sequential manner to build the Kriging model for the reduced set of 11 variables. The R square value of the metamodel is at around 0.8 after confirmation. Previous experience has shown that this problem is very nonlinear and it is difficult to obtain a metamodel with a very high accuracy (Chen et al., 2001; Jin et al. 2000).

4.2 Robust Design Optimization

The design for preventing vehicle rollover under a range of maneuver conditions is modeled using the robust design formulation as shown in Fig. 8. Note that the design variables here are the reduced set of design variables after screening.

Given

- Distribution of noise factors**:** start_brake, brake_level, end_brake, steer_level, and end_steer (Table 2)
- Kriging Model for the rollover metric

Find

Vehicle Parameters: HH1, LTS123, LTS2123, M11, M123, M2123

Satisfy

M11 + 2M123 + 3M2123 = Constant

(The total sum of the laden loads needs to be maintained as a constant.)

Boundaries of the variables

Maximize

Robust Design Metric

$C_{dk} = (URL-\mu_y)/3\sigma_y$

y – rollover metric; *URL* – the critical roll over condition.

Figure 1. Robust Design Formulation

The design capability index C_{dk}, which measures the portion of the range of designs that satisfies the ranged design requirement, is used as the robust design metric for improving vehicle handling performance. *URL* is the upper requirement limited, i.e., the critical rollover condition, which is set as 45 deg-sec$^{1/2}$ in this study. Statistically, the use of 3σ implies that when C_{dk} reaches 1, 99.865% of the performance distribution conforms to the requirements, assuming that the performance is normally distributed.

Using the developed analytical techniques for uncertainty propagation (for assessing mean μ_y and STD σ_y), in particular based on the Kriging model in this case, we obtain the solutions to the robust design formulation in Fig. 1. The baseline design and the robust design, together with the confirmed values of μ_y, σ_y, and C_{dk} (evaluated from the results of 40 optimal LHS runs constructed for noise variables while fixing the design variables at their solutions) are shown in Table 3. Graphical representations of the probability (based on the simulation results) of the rollover of the baseline design and the robust design from our method are presented in Figs. 2 and 3. It is noted that while for the baseline design, the probability of rollover is more than 12% (see Fig. 2); for the robust design obtained by using our methods, no rollover occurs (see Fig. 3). The standard deviation of rollover metric for baseline, i.e., 18.29, is much higher than those obtained from robust design formulation (3.15 for using our methods). In particular, we observe that the distribution of rollover metric for the robust design is much farther away from the critical rollever condition. Thus, we conclude that the robust design optimization has resulted in improved vehicle handling performance.

Table 3. Solution of Robust Design

	Baseline Design	Robust Design	Robust Design in Chen et al (1999)
HH1*	64.0	51.2	51.2
LTS123*	38.0	45.6	45.6
LTS2123*	38.0	45.6	45.6
M11*	14425.0	17310.0	17310.0
M123	25448.0	30108.4	25448.0
M2123*	20343.0	16274.4	24411.6
KHX1*	1000000	1000000	1200000
KT11	6900.0	6900.0	5520.0
KT123	6900.0	6900.0	5520.0
KT2123*	5174.0	5174.0	4139.2
LTS11*	38.0	38.0	30.4
SCFS11*	1	1	1.2
SCFS123	1	1	0.8
SCFS2123	1	1	0.8
μ_y	14.63	5.74	9.27
σ_y	18.29	3.15	15.22
C_{dk}	0.554	4.159	0.783

Note: The first six variables are the reduced set of design variables in our study. The variables with '*' are the reduced set of design variable in the study of Chen et al (1999).

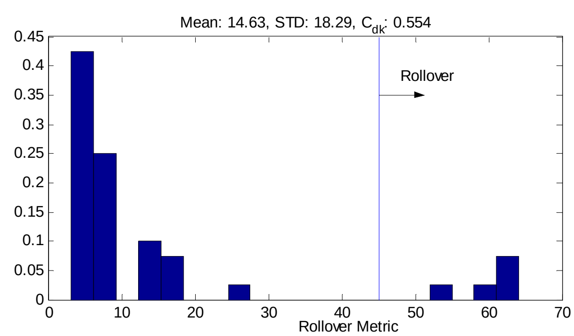

Figure 2. Rollover Metric Distribution for Baseline Design

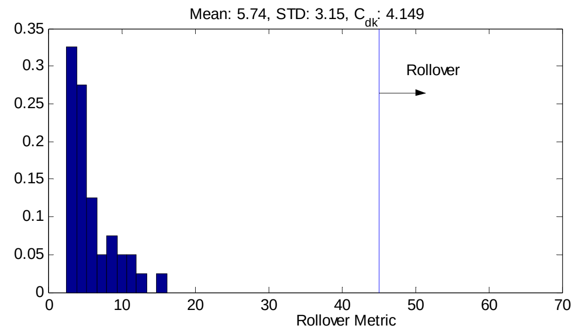

Figure 3. Rollover Metric Distribution for Robust Design

Table 3 also provides the robust design obtained in our earlier study (Chen et al, 1999). It is noted that the robust design achieved in this study is far better than the robust design result reported in the earlier work. Indeed, the robust design procedure used in the earlier study fails to find a robust design with a C_{dk} large than 1 and rollover occurs with probability close to 5% (Chen et al, 1999). For this reason, in the earlier study, the range of maneuver condition was reduced to obtain a more desirable robust design. Specifically, the range of the three most significant noise variables, i.e., brake_level, end_brake and steer_level, was reduced by 30% to achieve a robust design with C_{dk} equal to 2.559. Nevertheless, even with this noise reduction, the robust design obtained is still not as good as the robust design obtained in this study. Furthermore, the significantly better robust design solution is obtained in this study with less number of simulations (720 in total including the simulation employed in screening, creating metamodel, and confirmation versus 756 in earlier study).

Several factors have contributed to the improved robust design solution obtained by the proposed techniques in this work. One major reason is that the Kriging model created based on space-filling sample points in this study is much more accurate than the quadratic response surface model created based on ad hoc sampling approach in the earlier work: The $PRESS\text{-}R^2$ of quadratic metamodel, which estimates the prediction capacity and has similar meaning as the R^2_{CV}, is merely 0.504, while the R^2_{CV} of the metamodel in this study is 0.792. Furthermore, the global sensitivity analysis method used in this work has identified M123 as a critical variable through TSI due to its strong interactions with noise variables. Chen's et al.' earlier study, however, fails to identify M123 as an important variable because a quadratic response model was created for the screening purpose, only the linear part of main effect was used in ranking variable importance. One more reason behind the improved robust design solution is that in this study, analytical uncertain propagation is used, which provides more accurate evaluation of performance mean and variance than the 3-level full factorial design (243 sample points) approach used in Chen et al's work.

To further illustrate the benefits of using analytical UP compared to applying Monte Carlo samples to the metamodel, we illustrate in Figs. 4-7 a comparison between the response mean and response variation obtained from these two methods, respectively. The pictures show the results from the analytical method and the Monte Carlo method (1000 random sample points), when all the design variables except M123 and LTS 123 are fixed at their nominal values. From the figures, it is observed that the Monte Carlo results for both mean and STD are very noisy, which will cause serious convergence problem in the process of optimization. We tested with different starting points for using Monte Carlo samples for UP in the optimization process. In all cases, the optimizer fails to converge. Furthermore, the Monte Carlo method is far more expensive than analytical method. For instance, the evaluation of 21×21grid points in the graphs takes 139 seconds for Monte Carlo method, while it takes only 38 seconds (PIII 650MHZ, MATLAB) when using the proposed analytical method.

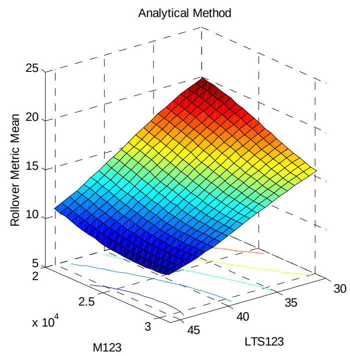

Figure 4. Mean of Rollover Metric by Analytical Method

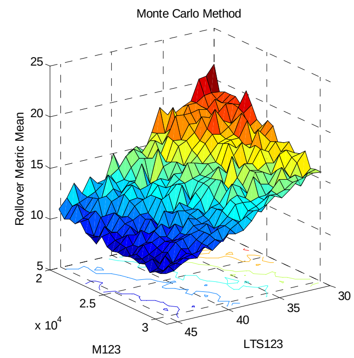

Figure 5. Mean of Rollover Metric by Monte Carlo Method

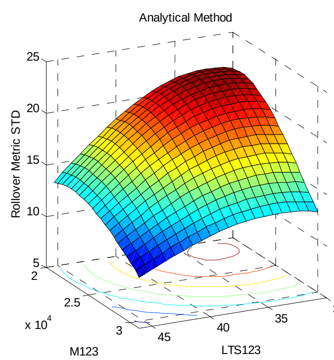

Figure 6. STD of Rollover Metric by Analytical Method

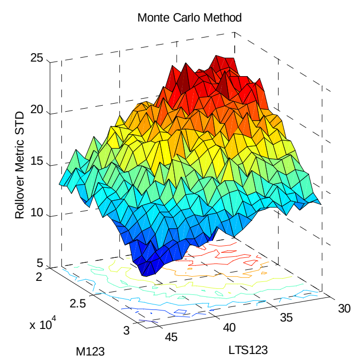

Figure 7. STD of Rollover Metric by Monte Carlo

5. Closure

The fundamental contribution of this work is the development of analytical techniques for assessing the mean and variance of a model output via the use of metamodels in simulation-based design under uncertainty. We illustrate that the commonly used metamodels such as polynomial, Kriging, the Radial Basis Functions, and MARS all follow the form of multivariate tensor-product basis functions for which the analytical results of univariate integrals can be combined to evaluate the multivariate integrals in uncertainty propagation.

Through the example problem, we demonstrate that compared to the existing sampling based approaches to uncertainty propagation, our approach provides more accurate as well as more efficient uncertainty propagation results. The techniques are especially useful for design applications that require computationally expensive simulations, where the metamdoels are often readily available to designers. Analytical uncertainty propagation reduces the noises associated with sampling methods and greatly facilitates the convergence of robust design optimization.

As a part of our research effort, the same idea presented in this paper has been used for deriving analytical formulations for global sensitivity analysis (Chen et al. 2004). The knowledge obtained though global sensitivity analysis (Saltelli et al. 1997) offers insights into the model behavior, provides guidance in reducing the problem size, and helps to identify sources for variance reduction. Overall, they help designers to make informed decisions in product design with the consideration of uncertainty. Future work in this area will involve the consideration of the dependence of the variability of input variables and higher moments in uncertainty propagation.

Acknowledgments

The support from Ford URP (University Research Program) and NSF grant DMI0335877 is greatly acknowledged. We are grateful for the Arcsim program provided by the Automotive Research Center (ARC) at University of Michigan.

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