ANALYTICAL VARIANCE-BASED GLOBAL SENSITIVITY ANALYSIS IN SIMULATION-BASED DESIGN UNDER UNCERTAINTY

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ABSTRACT

The importance of sensitivity analysis in engineering design cannot be over-emphasized. In design under uncertainty, sensitivity analysis is performed with respect to the probabilistic characteristics. Global sensitivity analysis (GSA), in particular, is used to study the impact of variations in input variables on the variation of a model output. One of the most challenging issues for GSA is the intensive computational demand for assessing the impact of probabilistic variations. Existing variance-based GSA methods are developed for general functional relationships but require a large number of samples. In this work, we develop an efficient and accurate approach to GSA that employs analytic formulations derived from metamodels. The approach is especially applicable to simulation-based design because metamodels are often created to replace expensive simulation programs, and therefore readily available to designers. In this work, we identify the needs of GSA in design under uncertainty, and then develop generalized analytical formulations that can provide GSA for a variety of metamodels commonly used in engineering applications. 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 constructed to calculate the multivariate integrals in GSA. The benefits of our proposed techniques are demonstrated and verified through both illustrative mathematical examples and the robust design for improving vehicle handling performance.

Key words: global sensitivity analysis, metamodeling, simulation-based design, uncertainty, analytical formulation, tensor basis product function

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Nomenclature

$p(\mathbf{x}) = p(x_1, x_2, ...x_M)$:	Joint probability density function (PDF)
M:	Number of variables
$p_i(x_i)$:	Individual (marginal) probability density function
$\phi_i(x_i)$:	Main effects in the ANOVA decomposition
$\phi_{i_1...i_s}(x_{i_1},...,x_{i_s})$:	Interaction effects in the ANOVA decomposition
$f_i(x_i)$, $f_{i_1 i_2}(x_{i_1}, x_{i_2})$ …:	Uncentered main and interaction effects
$V_{i_1...i_s}$:	Variance of $\phi_{i_1...i_s}(x_{i_1},...,x_{i_s})$
S_i:	Main sensitivity index (MSI) corresponding to x_i
$S_{i_1...i_s}$:	Interaction sensitivity index (ISI) corresponding to the interaction between x_{i_1}, x_{i_2}, …. and x_{i_s}
S_i^t:	Total sensitivity index (TSI) corresponding to x_i
$\widehat{\phi}_{\mathbf{U}_i}(\mathbf{x}_{\mathbf{U}_i})$, $\widehat{\phi}_{\mathbf{U}_1....\mathbf{U}_T}(\mathbf{x}_{\mathbf{U}_1}....\mathbf{x}_{\mathbf{U}_T})$:	Subset main effects and interaction effects
$\widehat{f}_{\mathbf{U}_i}(\mathbf{x}_{\mathbf{U}_i})$, $\widehat{f}_{\mathbf{U}_1....\mathbf{U}_T}(\mathbf{x}_{\mathbf{U}_1}....\mathbf{x}_{\mathbf{U}_T})$:	Subset uncentered main effects and interaction effects
$\widehat{S}_{\mathbf{U}_i}$, $\widehat{S}_{\mathbf{U}_{i_1}...\mathbf{U}_{i_s}}$, $\widehat{S}^t_{\mathbf{U}_i}$:	Subset main sensitivity index (SMSI), Subset interaction sensitivity index (SISI), and Subset total sensitivity index (STSI)
$\mathbf{x_D}$, $\mathbf{x_R}$:	Subset of design variables and noise variables
$\mu_y(\mathbf{x_D})$, $\sigma_y^2(\mathbf{x_D})$:	Response mean and Variance
S_i^r ($\widehat{S}_{\mathbf{U}}^r$):	Sensitivity index to measure the capability of a *design variable* x_i (or a design variable subset $\mathbf{x_U}$) to dampen response uncertainty
S_i^u ($\widehat{S}_{\mathbf{U}}^u$):	Sensitivity index to measure the capability of a *noise variable* x_i (or a noise variable subset $\mathbf{x_U}$) to reduce response uncertainty
$B_i(\mathbf{x})$:	Multivariate tensor-product basis function
$h_{il}(x_l)$:	Univariate basis function
N_b:	Number of multivariate basis functions
$C_{1,il}$, $C_{2,i_1 i_2 l}$:	Univariate integrals
ANOVA	Analysis of Variance
GSA	Global Sensitivity Analysis
ISI	Interaction Sensitivity Index
MSI	Main Sensitivity Index
SI	Sensitivity index
SISI	Subset Interaction Sensitivity Index
SMSI	Subset Main Sensitivity Index
TPBF	Tensor-Product Basis Functions

TSI	Total Sensitivity Index

1. INTRODUCTION

Sensitivity analysis has been widely used in engineering design to gain more knowledge of complex model behavior and help designers make informed decisions regarding where to spend the engineering effort. In deterministic design, sensitivity analysis is used to find the *rate of change* in the model output by varying input variables *one at a time* near a given central point, often called *local sensitivity analysis*. For design under uncertainty, sensitivity analysis is performed with436 1 Tct interaction effects of variables, but is seldom used to evaluate the nonlinear effect and the total effect (including linear, nonlinear main effects and interaction effects), information that is critical for ranking variable importance.

To extend the traditional ANOVA to GSA, a number of variance-based methods have been developed, including the Fourier Amplitude Sensitivity Test (FAST) (Saltelli, et al., 1999), correlation ratio (MacKay et al., 1999), various importance measures (Homma and Saltelli, 1996), Sobol's total effect indices (Sobol', 1993), etc. Reviews on different GSA methods can be found in Reedijk (2000), Helton (1993) and Chan et al. (1997). Similar to the concept as used in ANOVA, many of these methods decompose the total variance of an output to items contributed by various sources of input variations, and then derive sensitivity indices as the ratios of a partial variance contributed by an effect of interest over the total variance of the output. Nevertheless, most of these methods are developed for general functional relationships without consideration that acquiring sample outputs are resource (e.g., computationally) intensive. Therefore, the existing methods require a large number of samples or lengthy numerical procedures such as by employing Monte Carlo (Sobol', 1993) or lattice samplings (McKay et al., 1999 ; Saltelli et al., 1999). None of the existing GSA methods are analytical techniques which are expected to be more computationally efficient and accurate. *The efficiency is a major barrier of applying GSA for design problems that involve computationally expensive simulations*.

We note that in simulation-based design, to facilitate affordable design exploration and optimization, metamodels ("model of model") are often created based on computer simulations to replace the computationally expensive simulation programs (Chen et al. 1997). While it may be easy to identify the impact of input variations by simply inspecting the regression coefficients of a linear or a quadratic polynomial metamodel, it would be difficult to understand metamodels with sophisticated functional forms, such as radial basis function networks (Hardy, 1971; Dyn, et al., 1986), Kriging (Sacks, et al., 1989; Currin, et. al, 1991), etc., let alone when the input variations follow various probabilistic distributions. In this work, we develop an efficient and accurate approach to GSA that employs analytical formulations derived based on the metamodels, assuming that the accuracy of metamodels is satisfactory. The approach is especially applicable to simulation-based design because the information of metamodels is readily available to designers. Similar to many existing variance-based GSA methods, our method uses the concept of ANOVA decomposition for assessing the sensitivity indices. The proposed analytical approach eliminates the need of sampling which could be time-consuming even applied to metamodels. It also improves the accuracy by eliminating the random errors of statistical sampling (note that even a very sophisticated quasi-Monte Carlo sampling has a root mean square error of $O(n^{-3/2+\varepsilon})$, $\varepsilon > 0$ where n is the sample size (Owen, 1999)). In this work, we identify the needs of GSA in design under uncertainty, and then develop generalized analytical formulations that can provide GSA for a variety of metamodels, including those commonly used metamodels such as polynomial, Kriging, the Radial Basis Functions, and MARS (Friedman, 1991). Even though the function forms of these metamodels vary significantly, we show that all these models follow the form of *multivariate tensor-product basis functions* (TPBFs) for which the analytical results of univariate integrals can be constructed to calculate the multivariate integrals in GSA. Our paper is organized as follows. In Section 2, we lay out the mathematical background of GSA. The concepts of ANOVA decomposition and sensitivity indices are introduced. In Section 3, we identify the types of GSA for design under uncertainty and present our analytical approach to GSA. In Section 4, we verify and illustrate the advantages of our proposed techniques by mathematical and engineering examples. Section 5 is the closure of this paper.

2. MATHEMATICAL BACKGROUND OF GSA

In this section, we first introduce the concept of ANOVA decomposition, which is foundational to the evaluation of sensitivity indices (SIs) in variation-based GSA. The SIs are defined next. An example is used to further explain the concept of GSA.

2.1 ANOVA Decomposition

The *global* sensitivity stands for the *global* variability of an output over the *entire range of the input variables* that are of interest and hence provides an overall view on the influence of inputs on an output as opposed to a local view of partial derivatives. With the concept of variance-based GSA, a function is decomposed through functional *Analysis of Variance* (ANOVA) (Sobol, 1993; Owen, 1992) into increasing order terms, i.e.,

$$f(x_1, x_2, ..., x_M) = f_0 + \sum_{i=1}^{M} \phi_i(x_i) + \sum_{i_1=1}^{M} \sum_{i_2=i_1+1}^{M} \phi_{i_1 i_2}(x_{i_1}, x_{i_2}) + ... + \phi_{1...M}(x_1, ..., x_M) . \qquad (1)$$

Let x_i (i=1,2,...,M) be independent random variables with probability density functions $p_i(x_i)$, the constant term f_0 is the mean of the $f(\mathbf{x})$:

$$f_0 = \int f(\mathbf{x}) \prod_{i=1}^{M} [p_i(x_i) dx_i] . \qquad (2)$$

It should be noted that the assumption of statistical independence of variables is used throughout this paper for the derivation of the proposed method. This assumption holds in many practical applications as contributions to multiple random variables often come from different, but independent sources, such as in structural design the random material properties due to material processing and the instability of load due to environment. If independent assumption among the random variables is warranted then the proposed approach provides significant computational advantage; otherwise, the Copula technique in Monte Carlo simulation have to be used. In practice, the real probabilistic distributions are often unknown or can not be practically defined with precision. Therefore, independent assumption is often used for the purpose of sensitivity analysis to conduct "what-if" analysis.

Based on Eqn. 2, a decomposition item depending on a single variable x_i, referred as the main effect, is obtained by averaging out all the variables except x_i and minus the constant item, i.e.,

$$\phi_i(x_i) = \int f(\mathbf{x}) \prod_{j \neq i} [p_j(x_j) d\mathbf{x}_j] - f_0 \ . \tag{3}$$

A decomposition item depending on two variables, referred as the second-order interaction, is obtained by averaging out all the variables except these two variables and minus their main effects as well as the constant item, i.e.,

$$\phi_{i_1 i_2}(x_{i_1}, x_{i_2}) = \int f(\mathbf{x}) \prod_{j \neq i_1, i_2} [p_j(x_j) dx_j] - \phi_{i_1}(x_{i_1}) - \phi_{i_2}(x_{i_2}) - f_0 \tag{4}$$

In general, a decomposition item depending on s variables (referred as s-order interaction) is obtained by averaging out all the variables except the s variables in concern and eliminating the items depending on any subsets of the s variables:

$$\phi_{i_1 \ldots i_s}(x_{i_1},\ldots,x_{i_s}) = \int f(\mathbf{x}) \prod_{j \neq i_1,\ldots,i_s} [p_j(x_j)dx_j] - \sum_{k=1}^{s-1} \sum_{j_1,\ldots,j_k \in (i_1,\ldots,i_s)} \phi_{j_1 \ldots j_k}(x_{j_1},\ldots,x_{j_k}) - f_0, \tag{5}$$

where $j_1 < j_2 \ldots < j_k$.

2.2 Variance Decomposition and Sensitivity Indices

By squaring and integrating Eq.1 and using the orthogonality feature of the decomposition terms in Eq.1, the variance V of f can be expressed as the summation of variances $V_{i_1 \ldots i_s}$ of $\phi_{i_1 \ldots i_s}$ (referred as partial variances),

$$V = \sum_{i=1}^{M} V_i + \sum_{i_1=1}^{M} \sum_{i_2=i_1+1}^{M} V_{i_1 i_2} + \ldots + V_{1,\ldots,M}, \tag{6}$$

where, $V = Var\{f(\mathbf{X})\} = \int f^2(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} - f_0^{\ 2}$, (7)

and $V_{i_1 \ldots i_s} = Var\{\phi_{i_1 \ldots i_s}(x_{i_1},\ldots,x_{i_s})\} = \int \phi^2_{i_1 \ldots i_s}(x_{i_1},\ldots,x_{i_s}) \prod_{j=i_1}^{i_s} [p_j(x_j)dx_j]$. (8)

In Eq.7, $\mathbf{x}$ stands of a vector of variables, the evaluation involves a multidimensional integration of the product of function f and density functions. With Eq. 6, the output variability of f (measured by variance) is decomposed into separate portions attributable to each input and interaction. A *global sensitivity index* is defined as a partial variance contributed by an effect of interest normalized by the total variance V, i.e.,

$$S_{i_1 \ldots i_s} = V_{i_1 \ldots i_s} / V. \tag{9}$$

A sensitivity index (S_i) corresponding to a single variable (x_i) is called *main sensitivity index* (MSI), and a sensitivity index corresponding to the interaction of two or more variables ($S_{i_1 \ldots i_s}$, $s \geq 2$) is called *interaction sensitivity index* (ISI). From Eq.6, it can be found easily that all the sensitive indices sum to 1, i.e.,

$$\sum_{s=1}^{M}\sum_{i_1<\ldots<i_s} S_{i_1\ldots i_s} = \sum S_i + \sum_{i_1<i_2} S_{i_1 i_2} + \ldots + S_{1\ldots M} = 1. \qquad (10)$$

To quantify the *total influence* of each individual variable induced by both its main effect and interactions with other variables, we can either sum all effects that involve the variable of interest or use the approach of 'freezing unessential variables' (Sobol, 1993). This is done by partitioning the variables into x_i and its complementary set $\mathbf{x}_{\sim i} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_M)$. The *total sensitivity index* (TSI) for variable x_i is given by

$$S_i^t = S_i + \widehat{S}_{i,\sim i} = 1 - \widehat{S}_{\sim i}, \qquad (11)$$

where $\widehat{S}_{i,\sim i}$ is the sum of all the $S_{i_1\ldots i_s}$ that involve the index i and at least one index from (1, ..., i-1, i+1, ..., M); $\widehat{S}_{\sim i}$ is the sum of all the $S_{i_1\ldots i_s}$ terms that do not involve the index i. For a three-variable model, the total effect of x_1, i.e., S_1^t is given by:

$$S_1^t = S_1 + S_{1,2} + S_{1,3} + S_{1,2,3} = 1 - (S_2 + S_3 + S_{2,3}). \qquad (12)$$

2.3 Example of GSA

Considering the following second-order polynomial function:

$$f(\mathbf{x}) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2, \qquad (13)$$

where $\beta_1 = \beta_2 = \beta_3 = 1/100$, $\beta_4 = 1/10$, $\beta_{11} = 1$, and $\beta_{12} = 1$; each variable is uniformly distributed in [-1 1]. Based on the formulae in Eqs.1-11, the sensitivity indices are obtained as:

$$S_1=V_1/V=0.4371,\ S_2=S_3=V_2/V=1.639e\text{-}4,$$
$$S_4=V_4/V=1.639e\text{-}2,\ S_{12}=V_{12}/V=0.5462. \qquad (14)$$

Obviously, the sum of these indices is equal to 1. We note that the MSI (main sensitivity index) of x_1 (S_1) is influenced by the linear and quadratic coefficients (β_1 and β_{11}) of x_1; the MSIs of x_2, x_3, and x_4 are only related to the coefficients of linear terms because there are no nonlinear terms of these variables; the ISI (interaction sensitivity index) between x_1 and x_2 (S_{12}) is influenced by the coefficient β_{12}. Furthermore, the TSI (total sensitivity index) corresponding to x_1 can be obtained by $S_1^t = S_1 + S_{12} + S_{13} + S_{14} = 0.9835$. Likewise, the TSIs corresponding to x_2, x_3, and x_4 are 0.5463, 1.639e-4, and 1.639*e*-4 respectively. Based on the values of TSI, the variable importance with respect to their impact on the output variability is ranked following the sequence of x_1, x_2, x_3 (x_4). For this example, using MSIs or linear effects alone to rank the importance of variables would be misleading. It should be noted that as the sensitivity indices are (output) variance-based, they may enlarge the difference in significance between two variables. For instance, the ratio of the TSIs of x_1 and x_4 is close to 60, it means that the contribution to performance variance from x_1 is 60 times as that from $x_{1,}$ but it does not mean that x_1 is 60 times as important as x_4.

3. DEVELOPMENT OF ANALYTICAL FORMULATIONS OF GSA

The evaluations of sensitivity indices in Eqs.1-11 involve multivariate integrals which are very computationally expensive. Even though advanced sampling approaches have been developed for GSA as introduced in Section 1, they are not practically feasible for problems with time-consuming model evaluations. In this work, we develop an efficient and accurate approach to GSA that employs analytical formulations derived based on the metamodels, which are readily available in simulation-based design. In this section, we first introduce the concept of *subset decomposition* which will largely simplify the derivation of analytical formulations presented later. We then examine the special needs of GSA for design under uncertainty; the generalized GSA formulations are provided. Next, the concept of tensor product basis function is introduced. Using a polynomial model as an example, we illustrate how the GSA is conducted analytically by transforming a metamodel into the form of tensor product basis function. Due to the space limitation, our focus in this paper is on illustrating the idea and concept behind the proposed method. The details of derived formulae for the commonly used metamodeling techniques can be found in Jin (2004).

3.1 Subset Decomposition and Subset SIs

With subset decomposition, a variable set is divided into several subsets $\mathbf{x}_{\mathbf{U}_1}, \ldots, \mathbf{x}_{\mathbf{U}_T}$, and the function is decomposed into the effects related to these subsets. Assuming these subsets are statistically independent, then similar to the ANOVA decomposition for individual variables (Eq.1), we have:

$$f(\mathbf{x}) = f_0 + \sum \widehat{\phi}_{\mathbf{U}_i}(\mathbf{x}_{\mathbf{U}_i}) + \sum_{i_1=1}^{r} \sum_{i_2=i_1+1}^{r} \widehat{\phi}_{\mathbf{U}_{i_1}\mathbf{U}_{i_2}}(\mathbf{x}_{\mathbf{U}_{i_1}}, \mathbf{x}_{\mathbf{U}_{i_2}}) + \ldots + \widehat{\phi}_{\mathbf{U}_1 \ldots \mathbf{U}_T}(\mathbf{x}_{\mathbf{U}_1} \ldots \mathbf{x}_{\mathbf{U}_T}), \qquad (15)$$

where the symbol '$\widehat{\ }$' means that the decomposition items are related to subsets of variables. The definition of the decomposition item $\widehat{\phi}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}}$ is also similar to that of $\phi_{i_1 \ldots i_s}$ related to individual variables (Eq.2), except that subsets of variables $\mathbf{x}_{\mathbf{U}_{i_1}}, \ldots, \mathbf{x}_{\mathbf{U}_{i_s}}$ are used to replace individual variables $x_{i_1}, \ldots, x_{i_s}$. The variance of $f(\mathbf{x})$ is now decomposed into the sum of a set of subset variances,

$$V = \sum \widehat{V}_{\mathbf{U}_i} + \sum_{i_1<i_2} \widehat{V}_{\mathbf{U}_{i_1}\mathbf{U}_{i_2}} + \ldots + \widehat{V}_{\mathbf{U}_1 \ldots \mathbf{U}_T} \ . \tag{16}$$

The *subset sensitivity indices* are defined as the subset variance normalized by the total variance *V*, i.e.,

$$\widehat{S}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}} = \widehat{V}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}} / V \ . \tag{17}$$

A sensitivity index corresponding to one subset is called *subset main sensitivity index* (SMSI) and a sensitivity index corresponding to two or more subsets is called *subset interaction sensitivity index* (SISI). For instance, assuming there are totally three variables, grouped into two groups: $\mathbf{x}_{\mathbf{U}_1} = (x_1, x_2)$ and $\mathbf{x}_{\mathbf{U}_2} = (x_3)$, then,

$$\widehat{S}_{\mathbf{U}_1} = S_1 + S_2 + S_{1,2}, \ \widehat{S}_{\mathbf{U}_2} = S_3, \text{ and } \widehat{S}_{\mathbf{U}_1\mathbf{U}_2} = S_{1,3} + S_{2,3} + S_{1,2,3},$$

$$\widehat{S}^t_{\mathbf{U}_1} = S_1 + S_2 + S_{1,2} + S_{1,3} + S_{2,3} + S_{1,2,3} = 1 - S_3 \text{ and } \widehat{S}^t_{\mathbf{U}_2} = S_3 + S_{1,3} + S_{2,3} + S_{1,2,3} = 1 - S_1 - S_2 - S_{1,2}. \tag{18}$$

Subset decomposition provides a more generic form for ANOVA decomposition. One advantage with subset decomposition is that SISIs can be directly defined via a linear combination of a set of SMSIs. We can prove that the subset interaction effect $\widehat{\phi}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}}$ can be expressed as:

$$\widehat{\phi}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}} (\mathbf{x}_{\mathbf{U}_{i_1}}, \ldots, \mathbf{x}_{\mathbf{U}_{i_s}}) = \sum_{l=1}^{s} \sum_{j_1, \ldots, j_l \in (i_1, \ldots, i_s)} (-1)^{s-l} \widehat{\phi}_{\mathbf{U}_{j_1} + \ldots \mathbf{U}_{j_l}} (\mathbf{x}_{\mathbf{U}_{j_1}}, \ldots, \mathbf{x}_{\mathbf{U}_{j_l}}) \ , \tag{19}$$

where '+' means the combination of several subsets into a single subset. Correspondingly, the subset interaction variance $\widehat{V}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}}$ and SISIs $\widehat{S}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}}$ can be obtained by:

$$\widehat{V}_{\mathbf{U}_{i_1} \ldots \mathbf{U}_{i_s}} = \sum_{l=1}^{s} \sum_{j_1, \ldots, j_l \in (i_1, \ldots, i_s)} (-1)^{s-l} \widehat{V}_{\mathbf{U}_{j_1} + \ldots \mathbf{U}_{j_l}} \ , \tag{20}$$

$$\widehat{S}_{\mathbf{U}_{i_1}\ldots\mathbf{U}_{i_s}} = \sum_{l=1}^{s} \sum_{j_1,\ldots,j_l \in (i_1,\ldots,i_s)} (-1)^{s-l}\,\widehat{S}_{\mathbf{U}_{j_1}+\ldots\mathbf{U}_{j_l}} \,. \tag{21}$$

This property of subset decomposition will largely simplify the derivation of analytical formulations as only formulations related to SMSIs need to be derived. It also facilitates the study of the interaction between two groups of variables (e.g., groups of design and noise variables in design under uncertainty). The types of GSA in design under uncertainty are examined next.

3.2 Types of GSA in Design under Uncertainty

In design under uncertainty, the variability of an output is caused by both the change of design variables and the uncertainty in noise variables. Based on subset decomposition, $f(\mathbf{x})$ can be expressed as,

$$f(\mathbf{x}) = f_0 + \widehat{\phi}_{\mathbf{D}}(\mathbf{x}_{\mathbf{D}}) + \widehat{\phi}_{\mathbf{R}}(\mathbf{x}_{\mathbf{R}}) + \widehat{\phi}_{\mathbf{DR}}(\mathbf{x}), \tag{22}$$

where $\widehat{\phi}_{\mathbf{D}}(\mathbf{x}_{\mathbf{D}})$ is the subset main effect of design variables $\mathbf{x}_{\mathbf{D}}$, $\widehat{\phi}_{\mathbf{R}}(\mathbf{x}_{\mathbf{R}})$ is the subset main effect of noise variables $\mathbf{x}_{\mathbf{R}}$, and $\widehat{\phi}_{\mathbf{DR}}(\mathbf{x})$ is the subset interaction effect between $\mathbf{x}_{\mathbf{D}}$ and $\mathbf{x}_{\mathbf{R}}$. The total variance of an output is decomposed into,

$$V = \widehat{V}_{\mathbf{D}} + \widehat{V}_{\mathbf{R}} + \widehat{V}_{\mathbf{DR}}\,. \tag{23}$$

The sensitivity indices obtained by normalizing the items in Eq. 23 allow designers to rank order the importance of design variables as well as noise variables. Studying the interactions between design and noise variables facilitates robust design (Phadke 1989), where the basic idea is to minimize the output uncertainty without eliminating the uncertainty source by adjusting the design variables. Here the sensitivity index $\widehat{S}_{\mathbf{DR}} = \widehat{V}_{\mathbf{DR}}/V$ can be used as a measure of the capability of design variables to desensitize the effect of noise variables. Similarly, the capability of a single design variable x_i to dampen the response uncertainty can be measured by a sensitivity index corresponding to the sum of interactions between x_i and all noise variables, defined as the sum of the ISIs involving x_i and at least one noise variable, i.e.,

$$S_i^r = \widehat{S}_{\mathbf{DR}} - \widehat{S}_{(\mathbf{D}-i)\mathbf{R}} = 1 - \widehat{S}_{\sim i} - \widehat{S}_{\mathbf{D}} + \widehat{S}_{\mathbf{D}-i}\,, \tag{24}$$

where $\mathbf{D}-i$ stands for an index subset containing all the indices in **D** except i.

Besides factor importance, it is also desirable to know the uncertainty elimination of which variable (or a set of variables) will lead to the most significant reduction of uncertainty of performance. Assuming that the uncertainty of a variable with index $i \in \mathbf{R}$ could be eliminated, then the uncertainty of the response is reduced by the value:

$$\Delta\sigma_{yi}{}^2 = Var[f(\mathbf{X})|\mathbf{x_D})] - Var[f(\mathbf{X})|\mathbf{x_D}, x_i)]. \tag{25}$$

If the values of design variables are not yet determined (e.g., in a prior-design stage), an uncertainty reduction measure averaged over the entire range of design variables, called *average uncertainty reduction*, can be used to evaluate the benefits of eliminating the uncertainty source. The average uncertainty reduction is evaluated by,

$$\overline{\Delta\sigma_{yi}{}^2} = V - \widehat{V}_{\mathbf{D}} - (V - \widehat{V}_{\mathbf{D}+i}) = \widehat{V}_{\mathbf{D}+i} - \widehat{V}_{\mathbf{D}} = V_i + \widehat{V}_{i\mathbf{D}}\,, \tag{26}$$

which is equal to the sum of the variance of the main effect of the noise variable x_i of interest and the variance of the subset interaction effect between x_i and design variable set $\mathbf{x_D}$. Correspondingly sensitivity index for uncertainty reduction, S_i^u, of variable x_i, is defined as:

$$S_i^u = \overline{\Delta\sigma_{yi}{}^2} / V = \widehat{S}_{\mathbf{D}+i} - \widehat{S}_{\mathbf{D}} = S_i + \widehat{S}_{i\mathbf{D}}\,. \tag{27}$$

3.3 Tensor Product Basis Functions

We find that if a function can be expressed as a tensor-product basis function (TPBF) (c.f., Hastie, et al., 2001), then the analytical results of univariate integrals can be constructed to evaluate the multivariate integrals required for GSA. A multivariate TPBF $B_i(\mathbf{x})$ is defined as a product of M univariate basis functions $h_{il}(x_l)$, i.e.,

$$B_i(\mathbf{x}) = \prod_{l=1}^{M} h_{il}(x_l),\ i = 1, 2, ..., N_b\,. \tag{28}$$

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 to represent a constant term. 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.,

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)]\,, \tag{29}$$

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 TPBFs, with details shown in Section 3.5.

3.4 Generalized Formulations for GSA

With subset decomposition shown in Section 3.1, all statistical quantities involved in GSA can be evaluated by two most fundamental quantities (Eqs.30-31). We name them as the *non-centered subset main effect* (or called conditional mean) and the *subset main variance*, respectively.

$$\widehat{f}_{\mathbf{U}}(\mathbf{x}_{\mathbf{U}}) = \int f(\mathbf{x}) \prod_{l \notin \mathbf{U}} [p_l(x_l) dx_l], \tag{30}$$

$$\widehat{V}_{\mathbf{U}} = \int [\widehat{f}_{\mathbf{U}}(\mathbf{x}_{\mathbf{U}}) - f_0]^2 \prod_{l \in \mathbf{U}} [p_l(x_l) dx_l], \tag{31}$$

where $\mathbf{x}_{\mathbf{U}}$ are a set of model input variables of interest. The quantity in Eq.30 is named as *non-centered* subset main effect because the constant item needs to be subtracted to evaluate the subset main effect, in the way similar to Eq.3.

Substituting into Eq.30 the expression of the tensor-product function (Eq.29), we write the non-centered subset main effect for $\mathbf{x}_{\mathbf{U}}$ as follows:

$$\begin{aligned} \widehat{f}_{\mathbf{U}}(\mathbf{x}_{\mathbf{U}}) &= \int \left\{ a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)] \right\} \prod_{l \notin \mathbf{U}} [p_l(x_l) dx_l] \\ &= a_0 + \sum_{i=1}^{N_b} \left\{ a_i \prod_{l \notin \mathbf{U}} [\int h_{il}(x_l) p_l(x_l) dx_l] \prod_{l \in \mathbf{U}} h_{il}(x_l) \right\} \\ &= a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l \notin \mathbf{U}} C_{1,il} \prod_{l \in \mathbf{U}} h_{il}(x_l)], \end{aligned} \tag{32}$$

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

$$C_{1,il} = \int h_{il}(x_l) p_l(x_l) dx_l \ . \tag{33}$$

The function mean f_0 can be directly obtained by using an empty subset $\mathbf{x}_{\mathbf{U}}$ (i.e., $\mathbf{U} = \varnothing$),

$$f_0 = a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} C_{1,il}] \,. \tag{34}$$

Substituting into Eq.31 the expressions of f_0 (Eq.34) and the TPBF (Eq.28), we write the subset main variance for $\mathbf{x}_{\mathbf{U}}$ as follows:

$$\begin{aligned}\widehat{V}_{\mathbf{U}} &= \int\left\{\sum_{i=1}^{N_b}[a_i\prod_{l\notin\mathbf{U}}C_{1,il}\prod_{l\in\mathbf{U}}h_{il}(x_l)]-\sum_{i=1}^{N_b}(a_i\prod_{l=1}^{M}C_{1,il})\right\}^2\prod_{l\in\mathbf{U}}[p_l(x_l)dx_l]\\ &=\int\left\{\sum_{i=1}^{N_b}[a_i\prod_{l\notin\mathbf{U}}C_{1,il}\prod_{l\in\mathbf{U}}h_{il}(x_l)]\right\}^2\prod_{l\in\mathbf{U}}[p_l(x_l)dx_l]-[\sum_{i=1}^{N_b}(a_i\prod_{l=1}^{M}C_{1,il})]^2\\ &=\sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}\left\{a_{i_1}a_{i_2}\prod_{l\notin\mathbf{U}}(C_{1,i_1l}C_{1,i_2l})\prod_{l\in\mathbf{U}}\int h_{i_1l}(x_l)h_{i_2l}(x_l)p_l(x_l)dx_l\right\}-\sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}[a_{i_1}a_{i_2}\prod_{l=1}^{M}(C_{1,i_1l}C_{1,i_2l})]\\ &=\sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}\left\{a_{i_1}a_{i_2}\prod_{l=1}^{M}(C_{1,i_1l}C_{1,i_2l})\{\prod_{l\in\mathbf{U}}[C_{2,i_1i_2l}/(C_{1,i_1l}C_{1,i_2l})]-1\}\right\},\end{aligned} \tag{35}$$

where, C_{2,i_1i_2l} is the inner product of two univariate basis functions $h_{i_1l}(x_l)$ and $h_{i_2l}(x_l)$, i.e., $C_{2,i_1i_2l} = \int h_{i_1l}(x_l)h_{i_2l}(x_l)p_l(x_l)dx_l$. With $\mathbf{x_U} = \mathbf{x}$, we can directly obtain the variance of $f(\mathbf{x})$:

$$V = \sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}\left\{a_{i_1}a_{i_2}\prod_{l=1}^{M}(C_{1,i_1l}C_{1,i_2l})\{\prod_{l=1}^{M}[C_{2,i_1i_2l}/(C_{1,i_1l}C_{1,i_2l})]-1\}\right\}. \tag{36}$$

It can be observed that the above formulations (Eqs.32-36) 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. Once the forms of the basis functions and the distributions of the variables are defined, the values of C_1 and C_2 can be derived and used to evaluate all sensitivity indices for GSA.

3.5 Analytical GSA Formulations via Metamodels

Using the polynomial model and the Kriging model as examples, we illustrate in this section how to further expand the generalized analytical formulations in Section 3.4 for commonly used metamodels that follow the form of TPBFs. Detailed derivations of univariate integrals as well those for Gaussian radial basis function model and MARS model can be found in Jin 2004.

All polynomial regression models can be transformed into the tensor product form. Consider the most widely used second-order regression model,

$$f(\mathbf{x}) = \beta_0 + \sum_{i=1}^{M} \beta_i x_i + \sum_{i=1}^{M} \beta_{ii} x_i^2 + \sum_{i=1}^{M} \sum_{j=i+1}^{M} \beta_{ij} x_i x_j \,. \tag{37}$$

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

$$B_{(i,j)} = \begin{cases} x_j & i = 0 \\ x_j^2 & i = j \\ x_i x_j & i < j \end{cases} . \tag{38}$$

The univariate basis functions corresponding to variable x_l are:

$$h_{(i,j)l} = \begin{cases} 1 & \text{none of } (i, j) = l \\ x_l & \text{only one of } (i, j) = l \\ x_l^2 & \text{both of } (i, j) = l \end{cases} . \tag{39}$$

The polynomial model can be re-written as:

$$f(\mathbf{x}) = \beta_0 + \sum_{0 \le i, j \le M, j \ne 0} \beta_{ij} B_{(i,j)} = \beta_0 + \sum_{0 \le i, j \le M, j \ne 0} \beta_{ij} \prod_{l=1}^{M} h_{(i,j)l} \,, \tag{40}$$

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

The subset main effects/variances and the response mean/variance for a second polynomial regression model can be directly evaluated. The univariate integrals C_1 and C_2 are evaluated by, respectively:

$$C_{1,(i,j)l} = \begin{cases} 1 & \text{none of } (i, j) = l \\ \int x_l \, p_l(x_l) dx_l = \mu_l & \text{only one of } (i, j) = l \\ \int x_l^2 \, p_l(x_l) dx_l = \mu_l^2 + \sigma_l^2 & \text{both of } (i, j) = l \end{cases} \tag{41}$$

$$C_{2,(i_1,j_1)(i_2,j_2)l} = \begin{cases} 1 & \text{none of } (i_1, j_1, i_2, j_2) = l \\ \int x_l p_l(x_l) dx_l = \mu_l & \text{only one of } (i_1, j_1, i_2, j_2) = l \\ \int x_l^2 p_l(x_l) dx_l = \mu_l^2 + \sigma_l^2 & \text{only two of } (i_1, j_1, i_2, j_2) = l \\ \int x_l^3 p_l(x_l) dx_l = \mu_{l,3} + 3\mu_l \sigma_l^2 + \mu_l^3 & \text{only three of } (i_1, j_1, i_2, j_2) = l \\ \int x_l^4 p_l(x_l) dx_l = \mu_{l,4} + 4\mu_l \mu_{l,3} + 6\mu_l^2 \sigma_l^2 + \mu_l^4 & \text{all of } (i_1, j_1, i_2, j_2) = l \end{cases} \tag{42}$$

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 have $\sigma_l^2 = \delta_l^2 / 3$, $\mu_{l,3} = 0$, $\mu_{l,4} = \delta_l^4 / 5$; for normal distributions, we have $\mu_{l,3} = 0$, $\mu_{l,4} = 3\sigma_l^4$.

Furthermore, noting that many C_1 and C_2 are equal to 1, we can obtain the non-centered subset main effect (Eq.30) and the subset main variance (Eq.31) for GSA via the tensor product based polynomial function in Eq.40:

$$\hat{f}_{\mathbf{U}}(\mathbf{x}_{\mathbf{U}}) = \beta_0 + \sum_{i \notin \mathbf{U}} \beta_i \mu_i + \sum_{i \notin \mathbf{U}} \beta_{ii} \sigma_i^2 + \sum_{i \notin \mathbf{U}} \sum_{j \notin \mathbf{U}, j \geq i} \beta_{ij} \mu_i \mu_j + \sum_{i \in \mathbf{U}} (\beta_i + \sum_{j \notin \mathbf{U}} \beta_{ij} \mu_j) x_i + \sum_{i \in \mathbf{U}} \sum_{j \in \mathbf{U}, j \geq i} \beta_{ij} x_i x_j , \tag{43}$$

$$[\quad {}^2(\quad {}_{,4} \quad 2 \quad {}^4) \quad (\qquad {}_1 \qquad)^2 \quad {}^2 \quad (\qquad {}_1 \qquad) \quad {}_{,3}]$$

$$ {}^2 \quad {}^2 \quad {}^2 ,$$

$$, $$

Many different one-dimensional correlation functions could be used (see, e.g., Currin, et. al., 1991; Sacks, et. al., 1989). In practice, The Gaussian correlation function, $h_{il}(x_l) = \exp\left[-\theta_l (x_l - x_{il})^2\right]$ has become the most popular choice, where θ_l is the correlation coefficient.

For uniform distribution, we derive that (see Jin 2004)

$$C_{1,il} = \frac{1}{2\delta_l}\sqrt{\frac{\pi}{\theta_l}}\left\{\Phi(a_{il}\sqrt{2\theta_l}) - \Phi(b_{il}\sqrt{2\theta_l})\right\}, \tag{46}$$

$$C_{2,i_1i_2l} = \frac{1}{2\delta_l}\sqrt{\frac{\pi}{2\theta_l}}\exp\left[-\theta_l (x_{i_1l} - x_{i_2l})^2/2\right]\times\left(\Phi\left[\sqrt{\theta_l}(a_{i_1l} + a_{i_2l})\right] - \Phi\left[\sqrt{\theta_l}(b_{i_1l} + b_{i_2l})\right]\right), \tag{47}$$

where $a_{il} = \mu_l + \delta_l - x_{il}$ and $b_{il} = \mu_l - \delta_l - x_{il}$; $\Phi(.)$ stands for the CDF of the standard normal distribution; δ_l is the difference between upper bound and low bound of x_l.

For normal distributions, it can be shown that (see Jin 2004)

$$C_{1,il} = \frac{1}{\sqrt{2\sigma_l^2\theta_l + 1}}\exp[-\frac{\theta_l}{2\sigma_l^2\theta_l + 1}(\mu_l - x_{il})^2], \tag{48}$$

$$C_{2,i_1i_2l} = \frac{1}{\sqrt{4\sigma_l^2\theta_l + 1}}\exp\left\{-\frac{\theta_l}{4\sigma_l^2\theta_l + 1}[(\mu_l - x_{i_1l})^2 + (\mu_l - x_{i_2l})^2 + 2\sigma_l^2\theta_l(x_{i_1l} - x_{i_2l})^2]\right\}. \tag{49}$$

The Gaussian Radial Basis Function model (Hardy, 1971) can be written as,

$$f(\mathbf{x}) = \beta + \sum_{i=1}^{N_\phi}\lambda_i\varphi_i(\mathbf{x}), \tag{50}$$

where, $\varphi_i(\mathbf{x}) = \exp\left[-\frac{1}{2\tau_i^2}\sum_{l=1}^{M}(x_l - t_{il})^2\right] = \prod_{l=1}^{M}\exp\left[-\frac{(x_l - t_{il})^2}{2\tau_i^2}\right]$. τ_i is the width (also called radius) of a radial based function $\varphi_i(\mathbf{x})$; t_i is the center of the radial basis function and has elements t_{il}. If we define $h_{il}(x_l) = \exp\left[-\frac{(x_l - t_{il})^2}{2\tau_i^2}\right]$, then the RBF model is transformed into a tensor-product function:

$$f(\mathbf{x}) = \beta + \sum_{i=1}^{N_\phi}[\lambda_i \prod_{l=1}^{M} h_{il}(x_l)]. \quad (51)$$

Noting that the form of Gaussian RBF model is similar to that of Kriging model, except that the width τ_i is associated with each basis function instead of to each variable.

For uniform distributions, it is proved that

$$C_{1,il} = \frac{\tau_i}{\delta_l}\sqrt{\frac{\pi}{2}}\left\{\Phi\left[\left(\mu_l + \delta_l - t_{il}\right)/\tau_i\right] - \Phi\left[\left(\mu_l - \delta_l - t_{il}\right)/\tau_i\right]\right\}, \quad (52)$$

$$C_{2,i_1i_2l} = \frac{a_{i_1i_2}}{\delta_l}\sqrt{\frac{\pi}{2}}\exp\left[-(t_{i_1l} - t_{i_2l})^2/(2\tau_{i_1}^{\ 2} + 2\tau_{i_2}^{\ 2})\right]\times\left(\Phi\left[(\mu_l + \delta_l - b_{i_1i_2l})/a_{i_1i_2}\right] - \Phi\left[(\mu_l - \delta_l - b_{i_1i_2l})/a_{i_1i_2}\right]\right), \quad (53)$$

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, it is proved that

$$C_{1,il} = \frac{1}{\sqrt{\sigma_l^{\ 2}/\tau_l^{\ 2} + 1}}\exp[-(\mu_l - t_{il})^2/(2\tau_i^{\ 2} + 2\sigma_l^{\ 2})], \quad (54)$$

$$C_{2,i_1i_2j} = \frac{\tau_{i_1}\tau_{i_2}}{\sqrt{b_{i_1i_2l}}}\exp\left\{-\frac{1}{2b_{i_1i_2l}}[\tau_{i_2}^{\ 2}(\mu_j - t_{i_1j})^2 + \tau_{i_1}^{\ 2}(\mu_j - t_{i_2j})^2 + \sigma_j^{\ 2}(t_{i_1j} - t_{i_2j})^2]\right\}, \quad (55)$$

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

A MARS model (Friedman, 1991) can be viewed as is a weighted sum of tensor spline basis functions, i.e., $f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x})$, (56)

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

$$B_i(\mathbf{x}) = \prod_{l\in\mathbf{K}_i}\left[s_{il}(x_l - t_{il})\right]_+^q. \quad (57)$$

$\mathbf{K}_i = (k_{i1},...,k_{iJ_i})$ is the set of the indices of variables involved in the i^{th} multivariate basis function and J_i is the dimension of interaction (i.e., the number of different variables). t_{il} is a knot location corresponding to variable x_l. The exponent q is the order of the spline. The subscript '+' denotes the positive part of a function. The quantities s_{il} take on values ± 1, and indicate the right/left part of a function. If we define a set of univariate basis functions as

$$h_{il}(x_l) = \begin{cases} 1 & l \notin \mathbf{K}_i \\ \left[s_{il}(x_l - t_{il}) \right]_+^q & l \in \mathbf{K}_i \end{cases}, \tag{58}$$

then the MARS model is written in a tensor-product function as follows:

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} [a_i \prod_{l=1}^{M} h_{il}(x_l)]. \tag{59}$$

For uniform distributions, it is proved that:

$$C_{1,il} = \frac{s_{il}}{2\delta_l}[\frac{x_l^2}{2} - t_{il}x_l]\Big|_{lb_{1a}}^{ub_{1a}} \quad (l \in \mathbf{K}_i), \tag{60}$$

$$C_{2,i_1i_2l} = \frac{s_{i_1l}s_{i_2l}}{2\delta_l}[\frac{x_l^3}{3} - \frac{(t_{i_1l} + t_{i_2l})x_l^2}{2} + t_{i_1l}t_{i_2l}x_l]\Big|_{lb_{2a}}^{ub_{2a}} \quad (l \in \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2}), \tag{61}$$

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 is proved that:

$$C_{1,il} = s_{il}\{\frac{\mu_l - t_{il}}{\sigma_l}\Phi(\frac{x_l - \mu_l}{\sigma_l}) - \frac{1}{\sqrt{2\pi}}\exp[-\frac{(x_l - \mu_l)^2}{2\sigma_l^2}]\}\Big|_{lb_1}^{ub_1} \quad (l \in \mathbf{K}_i), \tag{62}$$

$$C_{2,i_1i_2l} = s_{i_1l}s_{i_2l}\{[\frac{(\mu_l - t_{i_1l})(\mu_l - t_{i_2l})}{\sigma_l} + \sigma_l]\Phi(\frac{x_l - \mu_l}{\sigma_l}) - \frac{x_l + \mu_l - t_{i_1l} - t_{i_1l}}{\sqrt{2\pi}}\exp[-\frac{(x_l - \mu_l)^2}{2\sigma_l^2}]\}\Big|_{lb_2}^{ub_2} \quad (l \in \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2}) \cdot \quad (63)$$

The detailed derivations of univariate integral results of RBF and MARS models can be found in Jin 2004.

4. VERIFICATION AND ENGINEERING EXAMPLES

4.1 Verification Example

We consider here a four-variate function,

$$f(\mathbf{x}) = 1 + \exp\{-2[(x_1 - 1)^2 + x_2^2] - 0.5(x_3^2 + x_4^2)\} + \exp\{-2[x_1^2 + (x_2 - 1)^2] - 0.5(x_3^2 + x_4^2)\} \quad (64)$$

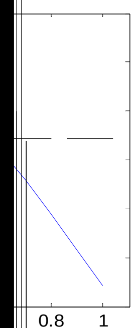
where $0 \le x_1, x_2, x_3, x_4 \le 1$, x_i follows the uniform distribution. The uniform distribution is chosen so that the GSA provides the effects of each individual variable across the whole range formed by its lower and upper bounds. The above function has the form of a Kriging model, in which the correlation coefficients θ_1 and θ_2 are equal to 2 and the correlation coefficients θ_3 and θ_4 are equal to 0.5. Therefore, the Kriging metamodel provides an exact fit of the original function. The results of using the analytical GSA are expected to be the same as the exact solutions. Due to the symmetric feature in this function, x_1 and x_2 , x_3 and x_4 should have the same influence on $f(\mathbf{x})$, respectively.

The main effects and second-order interactions obtained using the analytical formulations derived for Kriging model are graphically shown in Figures 1 and 2, respectively. In the following, '$x_1(x_2)$' means x_1 and x_2 are mutually replaceable since the effects are the same; the same with '$x_3(x_4)$'. From the figures, it is observed that the main effect of $x_3(x_4)$ is much larger than that of $x_1(x_2)$; the interaction between x_1 and x_2, however, is much larger than that between $x_1(x_2)$ and x_3 (x_4) and that between x_3 and x_4.

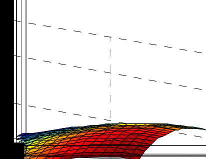
[redacted] Eq.52. The nonlinearity of [redacted] of MSI and TSI (S_i, S_{Ti}) [redacted] the following relationships [redacted]

[redacted] (65)

[redacted] Carlo samples are both [redacted] the analytical results, it is [redacted] $x_1(x_2)$ are very large due to [redacted]; on the other hand, the TSI [redacted] involving $x_3(x_4)$ are [redacted] we learned from Figs 1, 2.



[redacted]



[redacted]

Different sizes of Monte Carlo random samples are tested and compared to the analytical results. We observe that for this particular function tested, Monte Carlo method is inaccurate with relatively small sample size (i.e.,1000). With a large sample size (100,000), the results from Monte Carlo improve; however, due to estimation errors, some of the results from the sampling method are still not accurate. For example, results from all sampling tests show that TSI for x_4 is smaller than MSI, which is impossible as total effect should always be larger than or equal to main effect. We conclude from this verification example that our proposed analytical method can avoid random errors associated with sampling methods. The results from our method are expected to be the most accurate since they are analytically derived.

Table 1 Comparison of Main/Total Sensitivity Indices

			$(S_1,\ S_1^t)$	$(S_2,\ S_2^t)$	$(S_3,\ S_3^t)$	$(S_4,\ S_4^t)$
Analytical Method			(0.0033,0.5798)	(0.0033,0.5798)	(0.2063,0.2220)	(0.2063,0.2220)
Monte Carlo Method	**Sample Size**	100,000	(0.0208,0.5820)	(0.0089,0.5838)	(0.2126,0.2235)	(0.2326,0.2216)
		10,000	(0.0787,0.5809)	(0.0518,0.5835)	(0.2115,0.2245)	(0.2845,0.2232)
		1,000	(0.2448,0.6119)	(0.3761,0.6167)	(0.4844,0.2225)	(0.2814,0.2467)

As discussed in Section 3.2, the information offered by GSA can be used for various aspects to guide design under uncertainty. In the context of robust design, a sensitivity index $\widehat{S}_{\mathbf{U}}^r$ can be used to measure the capability of a set of design variables $\mathbf{x_U}$ to desensitize the effect of noise variables on the output uncertainty; on the other hand, a sensitivity index $\widehat{S}_{\mathbf{U}}^r$ can be used to measure the impact of eliminating all noise variable(s) $\mathbf{x_U}$ to reduce the output uncertainty. All sensitivity indices for design under uncertainty can be obtained based on SMSIs. For instance, the sensitivity index S_1^r can be calculated by: $S_1^r = 1 - \widehat{S}_{(3,2,4)} - \widehat{S}_{(1,3)} + S_3$. The values of the sensitivity indices are shown in Table 2.

Table2 Sensitivity Indices for Design Under uncertainty

Sensitivity indices for robust design			Sensitivity indices for uncertainty reduction	
S_1^r	S_3^r	$\widehat{S}_{(1,3)}^r$	S_2^u	S_4^u
0.5764	0.0156	0.5806	0.5683	0.2105

Since the interaction between the subsets of design and noise variables is significant, i.e., $\widehat{S}_{(1,3)(2,4)} = \widehat{S}_{(1,3)}^r = 0.5806$, it means that adjusting the design variables could considerably desensitize the effect of noise variables for this model. In particular, the capability of the design variable x_1 to dampen output uncertainty could be considerable since S_1^r is large. From the values of S_2^u and S_4^u in the table, it is observed that reducing the uncertainty source in the noise variable x_2 will have a larger impact than reducing that in the noise variable x_4.

4.2 Vehicle Handling Problem

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 proposed analytical techniques for GSA are applied to the same problem. Through comparisons, we illustrate the advantages of our newly developed methods.

Problem Definition

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

Development of the Kriging Metamodel and GSA

To reduce the problem size, screening experiments are first performed to identify the critical variables. A 200×19 (200 runs for 19 variables) optimal LHD (Jin et al. 2003) is generated for the screening experiments. A kriging metamodel of rollover metric is created over all the design variables and noise variables. When implementing the GSA, uniform distributions are used for all design variables over the whole design range defined by lower and upper bounds; distributions defined in Table 4 are taken as the input for noise variables. By using uniform distributions we assume that the chance of taking a specific value is equal across the whole range of a variable. Thus the GSA provides the effects of each individual variable over its range for the purpose of screening.

Table 3. 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	/

Table 4. 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

As shown in Fig. 3, the total sensitivity index (TSI), which takes into account not only the contribution of main effects of a variable but also the contribution of interactions between variables, is used for ranking the importance of different variables. From Fig. 3, it is evident that the eight design variables listed as ‘Rest’ as a whole contribute merely 0.001% of the variability in the metamodel in terms of subset TSI ($\widehat{S}^{t}_{\mathbf{Rest}} \approx 1.0e-5$). In addition, the interactions between these eight design variables and the noise variables are also negligible ($\widehat{S}^{r}_{\mathbf{Rest}} \approx 1.6e-6$).

Based on these observations, 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. Table 5 shows the importance ranking of the top 11 variables in terms of TSI and the sensitivity indices of main effects (MSI). It is noted that for this problem, the two rankings are not the same. For instance, MSI of M123 is negligible, while its TSI is considerably large. In our earlier study (Chen et al. 2001), ANOVA based study of main effects was used to reduce the size of the problem, where M123 is considered as unimportant. We believe that the TSI better reflects the whole contribution of a variable to a response and should be used in screening.

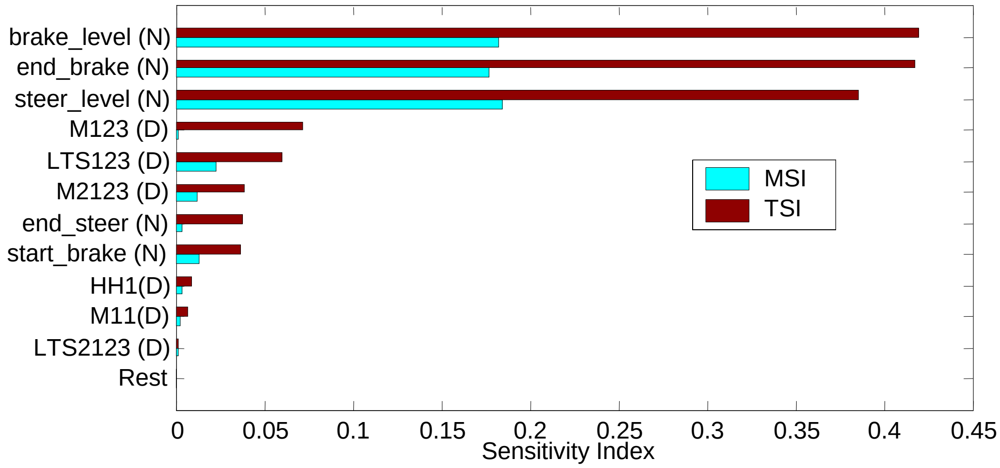


Figure 3. Sensitivity Indices of 19 Variables (D-Design Variable, N-Noise Variable)

Table 5. Importance Ranking of the Variables

Importance Ranking	TSI	MSI
1	brake_level	steer_level
2	brake_end	brake_level
3	steer_level	brake_end
4	M123	LTS123
5	LTS123	brake_start
6	M2123	M2123
7	steer_end	steer_end
8	brake_start	HH1
9	HH1	M11
10	M11	LTS2123
11	LTS2123	M123

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. 2001). The Kriging model obtained for the reduced set of 11 variables is used to refine the ranking of variable importance and to interpret the response behavior. Fig. 4 illustrates the contribution (to the variability of rollover metric) of the subset main effect of noise variables, the subset main effect of design variables, and the subset interaction between the two groups. It is found that the subset interactions are not negligible, which is a desired feature in robust design. Table 6 shows the sensitivity indices S_i^r for all the interactions between one design variable and *all noise variables*. From the table, we observe that the capability of M123 to dampen the output uncertainty is larger than other design variables. This further confirms the importance of keeping variable M123 in robust design.

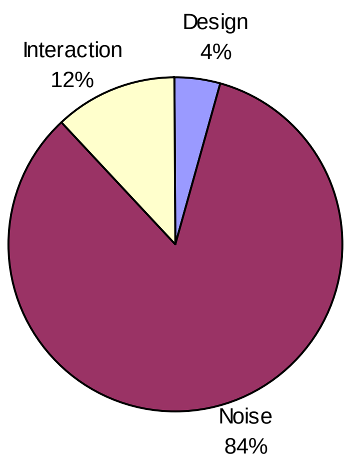


Figure 4. Subset Contributions of Noise, Design Variables, and Interactions

Fig. 5 shows the main effect of each variable on the rollover metric (all the variables are normalized). Main effects of noise variables, in particular, brake_level, end_brake and steer_level, are very significant and nonlinear. Figs. 6 and 7 show respectively the interactions between design variable M123 and the noise variables start_brake and end_brake. Based on the robust design concept, these interactions may lead to a reduction in variability of rollover metric incurred by noise variables. For instance, from Figs. 6

and 7, it is found that choosing the low bound of M123 will lead to smaller variability caused by start_brake and end_brake.

Table 6. Interactions between One Design Variable and All Noise Variables

	HH1	**LTS123**	**LTS2123**	**M11**	**M123**	**M2123**
S_i^r	2.078e-2	3.170e-2	2.211e-2	1.643e-2	3.914e-2	7.549e-3

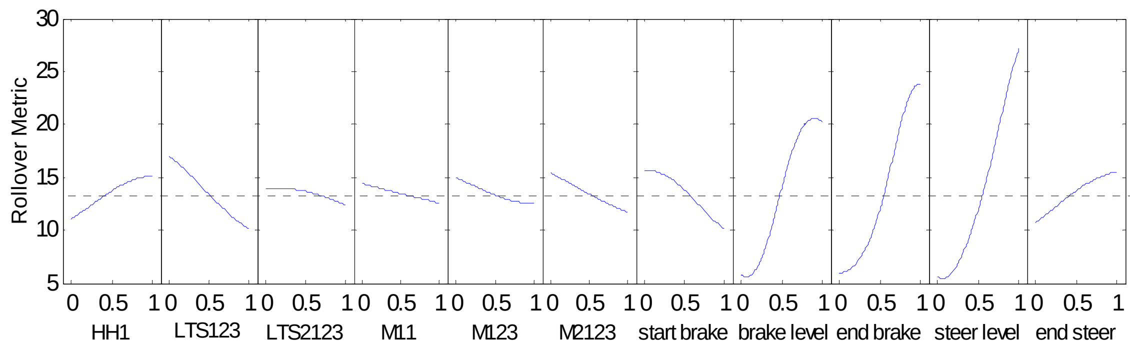
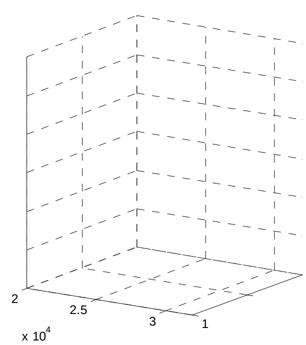


Figure 5. Main Effects of Variables (on Rollover Metric)



presented in this paper for GSA is used for deriving analytical formulations of mean and variance in uncertainty propagation to facilitate efficient robust design. It is found that the robust design achieved is far better than the results obtained in our earlier work (Chen et al. 2001). Besides the reason 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 use of the proposed GSA method has helped provide more accurate assessments of design performance and it variance while the problem size is also reduced. The GSA method used in this work has identified M123 as a critical variable through the total sensitivity index. Chen's et al.' earlier study, however, failed to identify M123 as an important variable because a quadratic response model was created for the screening purpose, and only the linear main effects were used in ranking variable importance due to the limitation of the classical ANOVA analysis.

5. CLOSURE

The fundamental contribution of this work is the development of analytical techniques for assessing the global sensitivity and performance distribution characteristics via the use of metamodels in simulation-based design under uncertainty. We discover 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 GSA (global sensitivity analysis). We identify the needs of GSA in design under uncertainty and further derive the generalized analytical formulations as well as the metamodel specific analytical formulations.

Our other contribution is the introduction of variable subset decomposition in GSA which transforms the evaluations of subset interaction sensitivity indices into a combination of subset main sensitivity indices. In particular, the decomposition of control and noise variable sets provides a powerful tool to facilitate insightful construction of robust design.

Using both mathematical examples and an engineering problem, we demonstrate that compared to the existing sampling based approaches to variance-based GSA, our approach provides more accurate as well as more efficient GSA results, assuming that the accuracy of metamodels is satisfactory. The techniques are especially useful for design applications that require computationally expensive simulations. The knowledge obtained though global sensitivity analysis 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 make informed decisions in product design with the consideration of uncertainty, a step beyond traditional sensitivity analysis in deterministic design.

As a part of our research effort, the same idea presented in this paper has been used for deriving analytical formulations for uncertainty propagation, in particular, the assessments of mean and variance of a model output in robust design (Chen et al. 2004). Results show that the use of the analytical approach significantly reduces the random errors associated with the sampling approach and greatly facilitates the convergence of optimization for robust design. Future work in this area will involve the consideration of the dependence of the variability of input variables and alternative GSA measures that evaluate the impact of variables not only by the influence on the variance but also on the whole probabilistic distribution of a model output.

ACKNOWLEGEMENT

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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