Variance decomposition and global sensitivity for structural systems

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ABSTRACT

This paper applies the Sobol' decomposition of a function of many random variables to a problem in structural mechanics, namely the collapse of a two story two bay frame under gravity load. Prior to introduction of this example application, the Sobol' decomposition itself is reviewed and extended to cover the case in which the input random variables have Gaussian distribution. Then, an illustrative example is given for a polynomial function of 3 random variables.

In the structural example, the Sobol' decomposition is used to decompose the variance of the response, the collapse load, into contributions from the individual input variables. This decomposition reveals the relative importance of the individual member yield stresses in determining the collapse load of the frame. In applying the Sobol' decomposition to this structural problem the following issues are addressed: Calculation of the components of the Sobol' decomposition by Monte Carlo simulation; the effect of input distribution on the Sobol' decomposition; convergence of estimates of the Sobol' decomposition with sample size using various sampling schemes; the possibility of model reduction guided by the results of the Sobol' decomposition.

1. Introduction

One of the challenging issues in modern civil engineering analysis is the typically large number of random quantities defining the input and system parameters. This challenge arises in problems involving large structures such as tall buildings and those involving random and heterogeneous materials. One approach to making such problems tractable is to identify the most important sources of uncertainty and focus attention only on those dimensions of the input space.

Such a method is proposed here that uses the Sobol' decomposition [1], a global sensitivity analysis method. Sudret [2] demonstrated global sensitivity analysis using polynomial chaos expansion. Ghanem et al. [3] used stochastic model reduction for chaos representations, and, moreover, used stochastic model reduction by constructing a coarse-scale from a specified fine-scale whose probabilistic structure can be accurately determined [4]. Furthermore, one of the authors has applied dimension reduction techniques to problems in micromechanics [5–7].

Generally, there are two types of sensitivity analyses: regression-based methods and variance-based methods. Regression-based methods use a regression of the output on the input vector and variance-based methods decompose the variance of the output as a sum of contributions of each input variable. The variance-based techniques are sometimes called ANOVA techniques for ANalysis Of VAriance. The Sobol' decomposition is one of the family of ANOVA techniques. In this study the Sobol' decomposition is applied to two example response functions, one an analytic function used to demonstrate the calculations and to provide a template for interpreting the results, the second a realistic structural problem, in which the decomposition is used to analyze uncertainty in the collapse load of a building frame in which the individual members have random yield stress.

Before developing the example applications, the Sobol' decomposition and its properties are defined for the case when the input variables are uniform. This results in the simplest expressions for the terms of the decomposition. Section 2 presents the formal extension of the decomposition to the case in which the input variables are Gaussian. Following these introductory materials the paper proceeds to the two examples. Finally, it is shown that in addition to being a powerful tool for variance decomposition and sensitivity analysis, the Sobol' decomposition can provide guidance in model reduction procedures.

2. The Sobol' decomposition

This section presents the formulation of the Sobol' decomposition and its properties to make the current paper as self-contained

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as possible. More details about the assumptions and theory can be found in the original publications [1,2,8,9]. The Sobol' decomposition was originally developed for the analysis of functions of uniform random variables. Here the decomposition is extended and used for functions of Gaussian input variables. It should be noted that the Sobol' decomposition can be used for functions of variables with any distribution, however, uniform and Gaussian variables result in the most compact calculations. Use of uniform input variables results in simple calculations because the pdf is constant, and use of Gaussian input variables simplifies the calculations because the integrals of the Sobol' decomposition become expectations that are easily converted to the moments of a Gaussian variable, for which the numerical values are known. These expectations would not be so easy to calculate exactly if the inputs had, for example, beta or exponential distribution. After presenting the outline of the Sobol' decomposition for the uniformly distributed input variables, the formulation for the Gaussian case is presented.

2.1. Input variables with uniform distribution

Let the random vector $X \in K^n$ contain the random input and system parameters that are used to generate a response function $F(X)$. Here, X is restricted to contain independent components and have a joint density that is uniform on $K^n = \{X : 0 \le X_i \le 1, i = 1, \ldots, n\}$, the unit hypercube, and $F(X)$ is scalar. The Sobol' decomposition of $F(X)$ is given by

$$F(X) = F_0 + \sum_{1 \le i \le n} F_i(X_i) + \sum_{1 \le i < j \le n} F_{ij}(X_i, X_j) + \cdots$$
$$+ F_{12\ldots n}(X_1, \ldots, X_n) \tag{1}$$

which is a type of ANOVA-decomposition. In this expansion, the individual terms, called the Sobol' functions, can be calculated by integrating $F(X)$ according to

$$F_0 = \int_{K^n} F(x) \mathrm{d}x \tag{2}$$

$$F_i(X_i) = \int_{K^{n-1}} F(x_{\sim i}, X_i) \mathrm{d}x_{\sim i} - F_0 \tag{3}$$

$$F_{ij}(X_i, X_j) = \int_{K^{n-2}} F(x_{\sim ij}, X_i, X_j) \mathrm{d}x_{\sim ij} - F_i(X_i) - F_j(X_j) - F_0 \tag{4}$$

where $x_{\sim i}$ is the vector of dummy variables corresponding to all but the component X_i of the input random vector X, $\mathrm{d}x_{\sim i}$ means integration with respect to all variables except X_i and F_0 is the mean value of the response function. Similarly, higher order Sobol' functions can be calculated.

The decomposition depends on individual Sobol' functions being orthogonal in the sense that

$$\int_{K^n} F_{i_1,i_2,\ldots i_s}(x_{i_1}, x_{i_2}, \ldots x_{i_s}) F_{j_1,j_2,\ldots j_t}(x_{j_1}, x_{j_2}, \ldots x_{j_t}) \mathrm{d}x = 0 \tag{5}$$

when at least one of the subscripts on the two functions composing the integrand differs.

The variance of $F(X)$, denoted by $D = \mathrm{var}[F(X)] = \int_{K^n} F^2(X)\mathrm{d}X - F_0^2$ can be decomposed according to

$$D = \sum_{1 \le i \le n} D_i + \sum_{1 \le i < j \le n} D_{ij} + \cdots + D_{12\ldots n} \tag{6}$$

$$D_i = \int_{K^1} F_i^2(x_i) \mathrm{d}x_i \tag{7}$$

$$D_{ij} = \int_{K^2} F_{ij}^2(x_i, x_j) \mathrm{d}x_i \mathrm{d}x_j. \tag{8}$$

Following the above definition of the partial variances, the Sobol' indices are defined as

$$S_i = \frac{D_i}{D} \tag{9}$$

$$S_{ij} = \frac{D_{ij}}{D}. \tag{10}$$

Higher order Sobol' indices can be calculated with a similar approach. A property of the Sobol' indices is

$$\sum_{1 \le i \le n} S_i + \sum_{1 \le i < j \le n} S_{ij} + \cdots + S_{12\ldots n} = 1. \tag{11}$$

2.2. Input variables with Gaussian distribution

The expressions of the previous subsection can be applied only when the input variables are uniform on the unit hypercube. In order to extend the definition to cases in which the input variables are non-uniform a new definition of the orthogonality of the Sobol' functions is required. This new definition comes from

$$\int_{\mathbb{R}^1} F_{i_1,i_2,\ldots,i_s}(x_{i_1}, x_{i_2}, \ldots, x_{i_s}) \phi_1(x_k) \mathrm{d}x_k = 0$$
$$\text{for } k = i_1, i_2, \ldots, i_s \tag{12}$$

where $\phi_1(x_k)$ is the Gaussian pdf. Due to Eq. (12), the summands have this notion of orthogonality to each other according to

$$\int_{\mathbb{R}^n} F_{i_1,i_2,\ldots,i_s}(x_{i_1}, x_{i_2}, \ldots, x_{i_s})$$
$$\times F_{j_1,j_2,\ldots,j_t}(x_{j_1}, x_{j_2}, \ldots, x_{j_t}) \phi_n(x) \mathrm{d}x = 0 \tag{13}$$

in which $\phi_n(X)$ is the n-dimensional Gaussian pdf. Then the following relationships are obtained using the Sobol' decomposition and the above conditions

$$\int_{\mathbb{R}^n} F(x) \phi_n(x) \mathrm{d}x = F_0 \tag{14}$$

$$\int_{\mathbb{R}^{n-1}} F(x_{\sim i}, X_i) \phi_{n-1}(x_{\sim i}) \mathrm{d}x_{\sim i} = (F_0 + F_i(X_i)) \phi_1(x_i) \tag{15}$$

$$\int_{\mathbb{R}^{n-2}} F(x_{\sim ij}, X_i, X_j) \phi_{n-2}(x_{\sim ij}) \mathrm{d}x_{\sim ij} = (F_0 + F_i(X_i) + F_j(X_j) + F_{ij}(X_i, X_j)) \phi_2(x_i, x_j). \tag{16}$$

The Sobol' functions can therefore be calculated by the following,

$$F_0 = \int_{\mathbb{R}^n} F(x) \phi_n(x) \mathrm{d}x \tag{17}$$

$$F_i(x_i) = \frac{\int_{\mathbb{R}^{n-1}} F(x_{\sim i}, X_i) \phi_{n-1}(x_{\sim i}) \mathrm{d}x_{\sim i}}{\phi_1(x_i)} - F_0 \tag{18}$$

$$F_{ij}(x_i, x_j) = \frac{\int_{\mathbb{R}^{n-2}} F(x_{\sim ij}, X_i, X_j) \phi_{n-2}(x_{\sim ij}) \mathrm{d}x_{\sim ij}}{\phi_2(x_i, x_j)} - F_0 - F_i(X_i) - F_j(X_j). \tag{19}$$

The second moments of the Sobol' functions are calculated by squaring the Sobol' decomposition equation and multiplying the squared formula by the joint density function and integrating it with respect to all the variables as follows,

$$\int_{\mathbb{R}^n} F^2(x) \phi(x) \mathrm{d}x$$
$$= \int_{\mathbb{R}^n} \left(F_0 + \sum_{s=1}^{n} \sum_{i_1 < i_2 < \cdots < i_s} F_{i_1,i-2,\ldots,i_s}(x_{i_1}, x_{i_2}, \ldots, x_{i_s}) \right)^2 \phi_n(x) \mathrm{d}x. \tag{20}$$

After expanding the right-hand side of Eq. (20) and considering

orthogonality, the expressions become

$$\int_{\mathbb{R}^n} F^2(x)\phi_n(x)\mathrm{d}x - F_0^2 = \int_{\mathbb{R}^1} F_1^2(x_1)\phi_1(x_1)\mathrm{d}x_1 + \int_{\mathbb{R}^1} F_2^2(x_2)$$

$$\times \phi_1(x_2)\mathrm{d}x_2 + \cdots + \int_{\mathbb{R}^2} F_{1,2}^2(x_1, x_2)\phi_2(x_1, x_2)\mathrm{d}x_1\mathrm{d}x_2 + \cdots, \quad (21)$$

thereby splitting Eq. (20) into variance terms

$$D = D_1 + D_2 + \cdots + D_{12} + \cdots D_{12\ldots n}. \quad (22)$$

After calculating the variances, the Sobol' indices can be calculated by the same approach presented in the previous subsection. The above derivations show that it is possible to apply the Sobol' decomposition to a system in which the input variables are Gaussian, rather than uniform. The key to extending the decomposition to the Gaussian case is a modified version of the orthogonality condition for the Sobol' functions, given in Eq. (13). The only difference between the orthogonality condition of Eq. (13) and that used when the input variables are uniform is that the Gaussian pdf $\phi_n(x)$ appears explicitly in the condition.

Therefore, by adopting a slightly altered form of the orthogonality condition it is possible to use this decomposition for response functions of Gaussian as well as uniform input variables.

The developments above show that the Sobol' decomposition can be applied to systems in which the input variables have Gaussian, rather than uniform distribution. Importantly, the calculations necessary to develop the decomposition do not become cumbersome when Gaussian input variables are considered because of the ease with which moments of the Gaussian distribution are calculated. In order to consider systems in which the input variables have non-uniform and non-Gaussian distribution all that is required is to replace the n-dimensional Gaussian pdfs $\phi_n(x)$ with the corresponding non-Gaussian pdfs. Although it is simple to adapt the formulation introduced above to the case where the input variables are non-uniform and non-Gaussian, exact calculations will in general be more difficult since the convenience of the easily obtained moments of the Gaussian distribution is lost. Furthermore, it is still required that the input variables be independent. If, however, the input variables are not independent, the required orthogonality condition, similar to that shown in Eq. (13), is not valid, and the decomposition cannot be constructed. One possibility to overcome this admittedly significant restriction would be to decorrelate, by an appropriate transformation, the vector of input variables, and then perform the decomposition on the decorrelated variables. This approach, however, may significantly distort the resulting Sobol' indices, and the Sobol' functions that depend on the decorrelated variables may not have any physical meaning. At this time, therefore, the conclusion is that the method cannot be applied with confidence to systems with correlated input variables.

2.3. Application of the Sobol' decomposition

After calculation of the Sobol' indices, the variables which have greater contribution to the variance of the response can be identified by ranking the Sobol' indices. The series expansion can be truncated by eliminating those functions with correspondingly small Sobol' indices. This truncation results in a reduced order description of the response function. In general the integrals of the preceding sections cannot be calculated exactly, but must be estimated by numerical integration of the response function, often by Monte Carlo simulation. In this case the estimation of the higher order functions requires significantly more samples. It is therefore wise to first estimate the first order Sobol' functions and indices. If

$$\sum_{i=1}^{n} S_i \approx 1 \quad (23)$$

then it can be concluded that the higher order terms of the series have negligible contribution to the total variance, and can be neglected.

3. Classical gradient sensitivity analysis

The Sobol' decomposition has been introduced as a method for global sensitivity analysis. The emphasis here is on the global nature of the results obtained from the Sobol' decomposition, meaning that the Sobol' indices give a description of the importance of the individual input variables over their entire domain. The global sensitivity analysis provided by the Sobol' decomposition contrasts with point sensitivity analysis that provides a quantification of the importance of input variables at a single point in the input domain.

The standard formulation of a point sensitivity analysis is

$$R = \nabla F(X) \quad (24)$$

with componentwise approximations

$$R_i \approx \frac{F(X^{(0)} + I^{(i)}\epsilon) - F(X^{(0)} - I^{(i)}\epsilon)}{2\epsilon} \quad (25)$$

where $X^{(0)}$ is a vector often taken to be the mean value, but which in principle can be any point, and $I^{(i)}$ is a vector with components

$$I_k^{(i)} = \begin{cases} 0, & k \neq i \\ 1, & k = i \end{cases}, \quad (26)$$

and ϵ is a small increment. One important distinction between Sobol' and classical sensitivity is that the Sobol' decomposition detects interactions of input variables through the second and higher order terms, while classical sensitivity methods give only derivatives with respect to single variables.

4. Analytic example

This section presents a set of example calculations using the Sobol' decomposition in a case where an exact form of the response function is available. In engineering practice this will not often be the case, but here such an example is presented to clarify the method of calculation and application of the decomposition.

Let the response function be defined by polynomial

$$F(X_1, X_2, X_3) = X_1^2 + X_2^4 + X_1 X_2 + X_2 X_3^4 \quad (27)$$

with X_1, X_2 and X_3 independent and identically distributed variables defined by the standard normal distribution. It is emphasized at this point that this function is not meant to represent a physical system, but rather is chosen arbitrarily as an illustrative example.

A second version of this response function is defined to be

$$F(Y_1, Y_2, Y_3) = Y_1^2 + Y_2^4 + Y_1 Y_2 + Y_2 Y_3^4 \quad (28)$$

in which Y_1, Y_2 and Y_3 are independent and equal to $8Z_1 - 4$, $8Z_2 - 4$ and $8Z_3 - 4$ respectively with $Z \sim U(0, 1)$. The result of this transformation is that the variables Y_i are defined in $[-4, 4]$. This range is chosen so that the domain of the uniform input variables corresponds to the domain containing nearly the entire probability mass of the Gaussian input variables X_i.

Tables 1 and 2 show the Sobol' functions and Sobol' indices for the response functions given in Eqs. (27) and (28).

Many of the results presented in the tables can be interpreted by direct inspection of the response function itself. For example, X_3 and Y_3 do not appear in the response function in isolation, and therefore the first order Sobol' functions associated with these variables are zero. Furthermore, that S_2 is larger than S_1 is indicative of the higher order power on the variables X_2 and Y_2 in the response function. Finally, the nonzero values associated with S_{12}
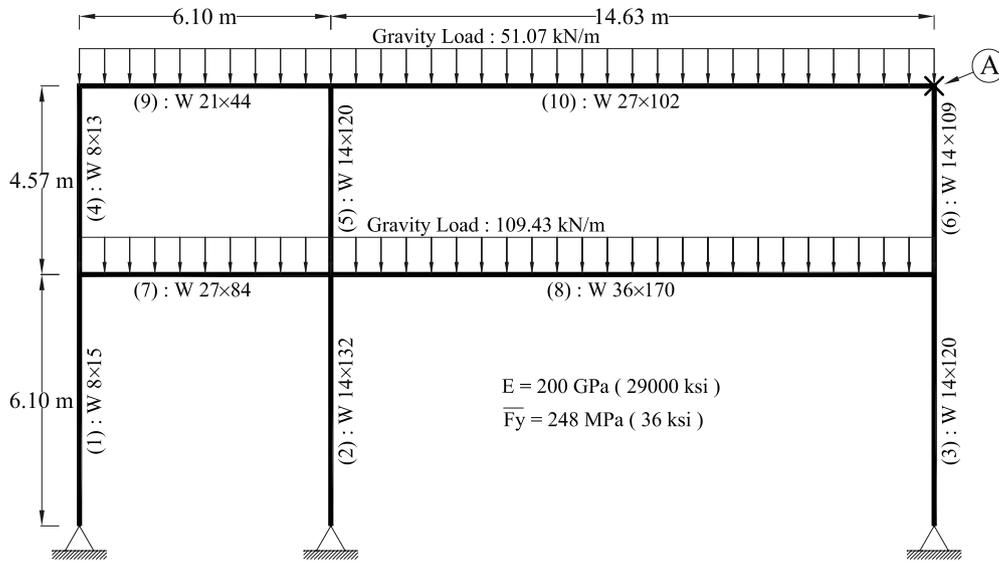
Fig. 1. Geometry, loading, and structural shapes of the UP36H frame used in the structural example [10].

Table 1
Sobol' functions derived from a polynomial response function with Gaussian and uniform input variables.

Sobol' functions	Uniform distributed input	Gaussian distributed input
F_0	56.53	4
F_1	$Y_1^2 - 5.33$	$X_1^2 - 1$
F_2	$Y_2^4 + 51.2Y_2 - 51.2$	$X_2^4 + 3X_2 - 3$
F_3	0	0
F_{12}	$Y_1 Y_2$	$X_1 X_2$
F_{13}	0	0
F_{23}	$Y_2 Y_3^4 - 51.2Y_2$	$X_2 X_3^4 - 3X_2$
F_{123}	0	0

Table 2
Sobol' indices derived from a polynomial response function with Gaussian and uniform input variables.

Sobol' indices	Uniform distributed input	Gaussian distributed input
S_1	0.0098	0.0005
S_2	0.5147	0.4281
S_3	0.0000	0.0000
S_{12}	0.0049	0.0007
S_{13}	0.0000	0.0000
S_{23}	0.4706	0.5708
S_{123}	0.0000	0.0000

and S_{23} capture the terms in the polynomial that involve products of more than one variable.

Despite overall similarity in the Sobol' indices obtained for Gaussian and uniform input variables, there are differences that highlight that the Sobol' decomposition not only captures global sensitivity, but also captures information about the probability density of the input variables. Specifically, S_2 is substantially higher for Gaussian than uniform input. This can be explained by observing that the variables X_2 and Y_2 appear in the response to the 4th power. Since the uniform variable Y_2 has significantly more probability mass at the extremes of its domain than does the Gaussian variable X_2 the importance of this 4th power term is accentuated and the corresponding Sobol' index is higher.

As discussed previously, one of the advantages of using the Sobol' decomposition is obtaining guidance in reducing the dimension of the domain of the response function. In this problem, according to Sobol' index values, the summation of S_2 and S_{23} is equal to 0.983 and 0.999 for uniform and Gaussian input respectively. This indicates that nearly all of the variance of the response can be represented by a function containing only X_2 and

the combination (X_2, X_3) or, for the uniform case, the variable Y_2 and the variable pair (Y_2, Y_3). Such a function can be obtained by truncating the Sobol' series representation of the response to be

$$F(X_1, X_2, X_3) \approx F(X_2, X_3) = F_0 + F_2(X_2) + F_{23}(X_2, X_3) \tag{29}$$

in which the appropriate Sobol' function should be used for the uniform and Gaussian cases. In the example application presented next, the accuracy of such a reduced dimension version of the response is investigated. This following example, for a practical problem of structural collapse, also illustrates the need for numerical integration by Monte Carlo simulation to obtain the Sobol' decomposition when an exact form of the response is not available.

5. Structural example

This section presents the application of the Sobol' decomposition to a practical problem in structural engineering, the collapse of a moment frame. The frame chosen for study here has been used extensively in previous studies of structural collapse [10] and reliability analysis [11]. In keeping with the nomenclature used in these previous studies, the frame is here called UP36H, and is shown in Fig. 1 with dimensions, element numbering, and the gravity load applied to the frame.

This frame is interesting for several reasons that make it suitable for an example application of the Sobol' decomposition. It is not symmetric so it fails in a lateral sidesway mode even when only gravity loads are applied. Moreover the failure mode and load is sensitive to even small changes in the yield stress of individual members. This feature of the response has already been observed in reliability studies of the frame [11].

In this problem the geometry and loading of the frame are constant, and uncertainty is introduced through the yield stresses of the individual members. These yield stresses are contained in a vector of input variables FY in which component FY_i is the yield stress of element i. The response is taken to be the load factor at collapse, that is, the multiplier applied to the loads shown in Fig. 1 to obtain the failure load. This load factor at collapse is denoted by S.

To obtain the response of the subject frame, a nonlinear collapse analysis is performed. Due to the asymmetry of the frame collapse occurs in a sidesway mode even under gravity load. The horizontal displacement of joint A, as labeled in the figure, is used to define
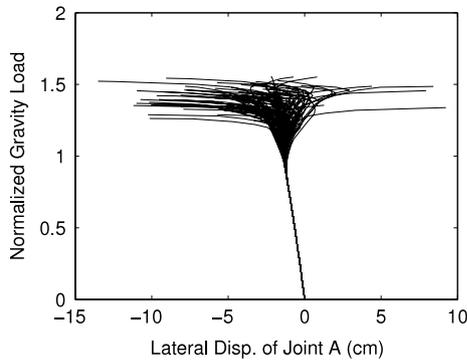
Fig. 2. Load–displacement traces for the collapse of the frame when the yield stress of the structural elements is random and independent with 10% coefficient of variation.
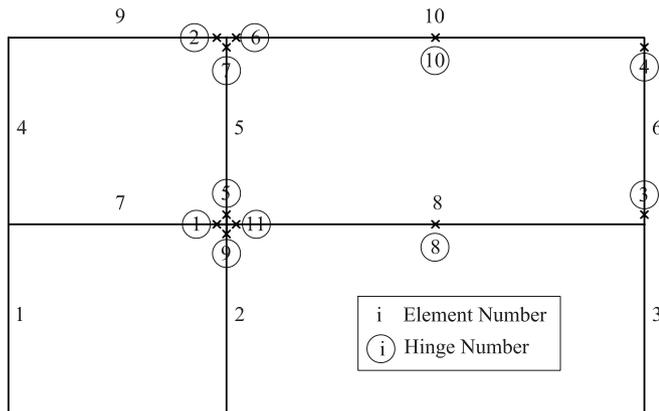
Fig. 3. Hinge sequence during the collapse of frame when all elements have yield stress of 248 MPa.

collapse of the structure. Fig. 2 shows load displacement traces for several realizations of frame UP36H. These traces show that lateral collapse is the failure mode, and that variation of the element yield stress does lead to significant qualitative and quantitative variation in the collapse mechanism. The uncertainty in the simulations shown in Fig. 2 is due to the member yield stresses FY_i being drawn from a uniform distribution on the interval (205, 291) MPa. More details about the modeling of input uncertainty is given in the next subsection.

When the yield stress in all members is set to the mean value of 248 MPa, plastic hinges form in the sequence shown in Fig. 3. As will be shown in the Sobol' analysis, there is a relationship between the locations of plastic hinging and the magnitude of the Sobol' indices.

5.1. Monte Carlo simulations

As mentioned above, the frame is analyzed for the two cases of uniform and Gaussian yield stress. In both cases, the yield stresses of the members are independent and identically distributed. For both cases, the mean value of the yield stress is assumed to be $E[FY_i] = 248$ MPa, and the coefficient of variation to be 0.10, consistent with the probability models used in previous reliability studies of the frame [11]. The probability models for the yield stress can therefore be compactly described by $FY_i \sim U(205, 291)$ MPa for the uniform case, and $FY_i \sim N(248, 24.8)$ MPa for the Gaussian case. The Gaussian model more closely represents the reality of property variation in structures, whereas the uniform model allows for simpler calculation of the Sobol' decomposition. Note that for formal calculations the Gaussian distribution should

be truncated at 0^+ so that non-physical negative yield stresses are not permitted. With the prescribed coefficient of variation of 0.10, however, the generation of negative yield stress does not occur in practice.

In addition to the two different probability models used for the yield stresses, two sampling schemes are used to generate realizations for use in the Monte Carlo simulation. A brute force (BF) sampling scheme is implemented for both the Gaussian and uniform models, and a Latin Hypercube (LH) scheme is implemented for the uniform model [12]. For the current example, with a 10 dimensional input space, and a response function that can be numerically evaluated for a given sample in a few seconds on a desktop computer, BF sampling is tractable and effective. As the dimension of the input space grows or the time required for individual function evaluations grows, however, BF sampling may become prohibitive. The LH sampling scheme is demonstrated here to show that it can provide accurate estimate of the components of the Sobol' decomposition with significantly less computational expense than with a BF scheme.

5.2. Sobol' parameters evaluation

While the so-called curse of dimensionality applies to the size of the input domain, it also affects the estimation of the Sobol' functions from Monte Carlo simulations. If the number of samples required for an accurate estimate of the response function over its entire n_i-dimensional domain is $n_{s,total}$ then the number of samples required for accurate estimation of a Sobol' function of order p is approximately $\sqrt[n_i]{n_{s,total}}$. Thus, the number of samples needed for estimation of a Sobol' function grows rapidly with increasing order of the function. Recall that the order of the Sobol' function is the number of input variables upon which the Sobol' function depends, and should not be confused with, for example, the order of a polynomial. For example, the Sobol' function $F_{13}(x_1, x_3)$ is a second order function, regardless of what the actual form of the function is.

In practice, therefore, it is convenient to estimate all the first order Sobol' functions and indices from Monte Carlo simulations and calculate the sum

$$S^{(1)} = \sum_{i=1}^{n_i} S_i. \tag{30}$$

If $S^{(1)}$, the sum of all the first order Sobol' indices, satisfies the condition $1 - S^{(1)} < \epsilon$, where ϵ is some small number, perhaps 0.10, then all the higher order Sobol' indices must be negligible, and the set of first order Sobol' functions provides a nearly complete representation of the response.

Estimation of a first order Sobol' function from simulation data can be made by the following procedure that effectively involves projection of the simulation data onto one of the input coordinate axes. Denote by $\{I^{(j)}\}$ a set of intervals that completely covers the domain of X_i, one of the input variables. Let the center of each of these intervals be denoted by $X^{(j)}$, and let $\{X^{(j,k)}\}$ be the set of input vectors that satisfy $X_i \in I^{(j)}$, that is, whose i th component is in the j th interval dividing the input domain. This set of notations amounts to a binning of the Monte Carlo data according to the value of a single input variable. An estimate of the first order Sobol' function $f_i(X_i)$ is then obtained by the averaging operation

$$f_i(X^{(j)}) = \frac{\sum_{k=1}^{m_{ij}} F(X^{(j,k)})}{m_{ij}} \tag{31}$$

where m_{ij} is the number of input vectors satisfying $X_i \in I^{(j)}$ and $F(X^{(j,k)})$ is a response evaluation at input point $X^{(j,k)}$.
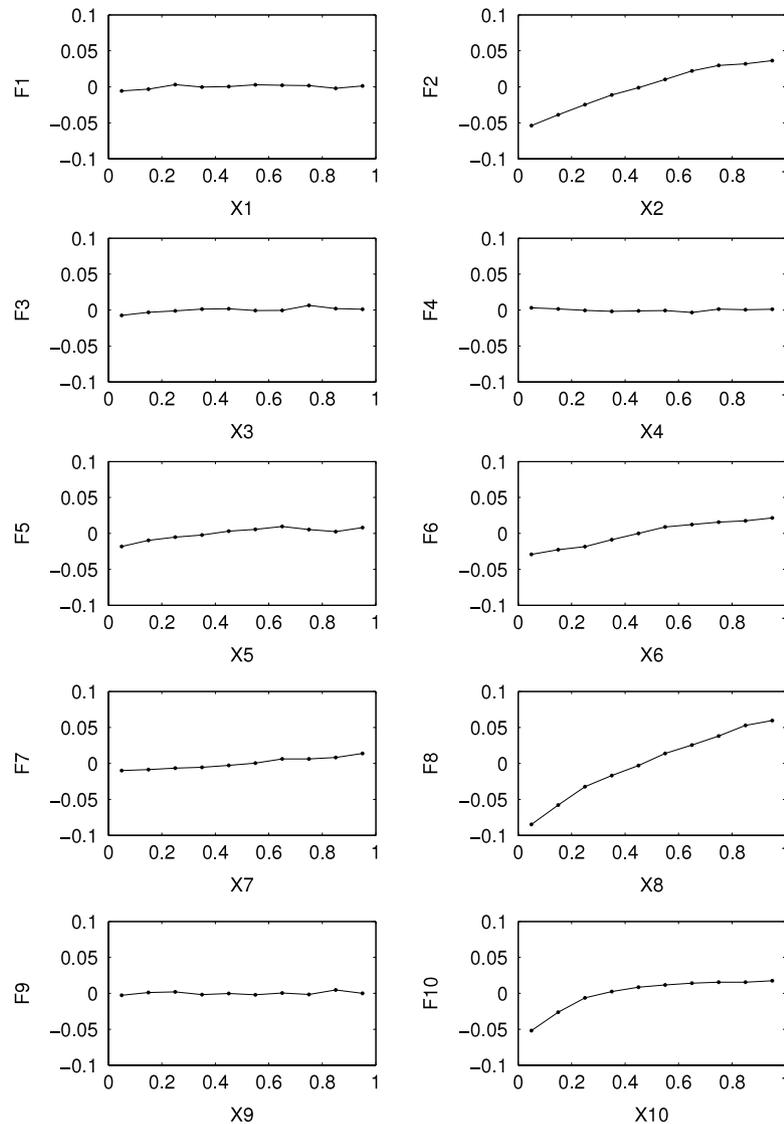
Fig. 4. Sobol' functions derived from BF simulation of the collapse of frame UP36H for uniform yield stresses.

Fig. 4 shows the ten first order Sobol' functions derived by BF sampling of the uniform input set $FY_i \sim U(205, 291)$. Note that the x-axis values in the figure have been scaled to be in the interval [0, 1], but that here $X_i = 0$ corresponds to $FY_i = 205$ MPa and $X_i = 1$ corresponds to $FY_i = 291$ MPa. If the variation of a Sobol' function surrounding its mean value is large then the influence of that variable on the response function is correspondingly large. For example, variation of F_8 surrounding its mean value is larger than that of F_1. Therefore, S_8 should be larger than S_1 which is confirmed by checking the results shown in Table 3. The first order Sobol' functions derived by LH sampling of the uniform input space and BF sampling of the Gaussian input space are qualitatively similar to those shown in Fig. 4, and are omitted for the sake of brevity.

Table 3 presents the comparison of the first order Sobol' indices for three kinds of analysis in this study. The results shown are based on 10 000 BF random samples of the uniform and Gaussian input spaces, and 800 LH samples of the uniform input space. The comparison is made to 10 000 BF samples because, based on the convergence study presented earlier, this number of samples provides very good estimates of the Sobol' indices. It should not be interpreted that 800 LH are equivalent to 10 000 BF samples, rather, LH sampling may give a substantially greater increase in simulation efficiency.

Table 3
Sobol' indices for the frame UP36H for three cases of input uncertainty and sampling method. (1) Uniform yield stresses and brute force Monte Carlo, (2) Uniform yield stresses and Latin Hypercube sampling, and (3) Gaussian yield stresses and brute force Monte Carlo.

Sobol' indices	Uniform dist. input (BF)	Uniform dist. input (LH)	Gaussian dist. input (BF)
S_1	0.002	0.008	0.003
S_2	0.203	0.196	0.162
S_3	0.003	0.010	0.004
S_4	0.001	0.018	0.001
S_5	0.016	0.037	0.021
S_6	0.069	0.068	0.058
S_7	0.013	0.015	0.009
S_8	0.463	0.458	0.423
S_9	0.001	0.020	0.003
S_{10}	0.104	0.107	0.154
$Sum =$	0.874	0.937	0.837

The results obtained by the three simulation schemes are generally similar to one another. Specifically, the rank ordering of the Sobol' indices is the same for all three cases, indicating that the yield stress of elements 8, 2, 10 and 6 are most important in determining the strength of the frame. Note that these are all
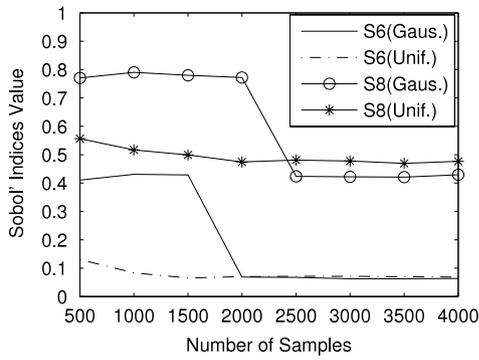
Fig. 5. Convergence of Sobol' indices S_6 and S_8 with increase in number of samples using brute force Monte Carlo on uniform and Gaussian input spaces.

elements in which hinges form in the collapse mechanism shown in Fig. 3. The total fraction of the variance captured by the first order functions is also similar, varying between 0.84 and 0.94. This indicates that for this problem higher order contributions to the Sobol' series are relatively small. From here forward the analysis focusses entirely on the first order functions.

Despite the overall similarity of the results, there are differences between the three sets of results. Differences between the BF and LH sampling of the uniform input space are simply a result of sampling uncertainty. Differences between the results for the uniform and Gaussian input spaces, however, show how the Sobol' decomposition captures information about input uncertainty in ways not possible with standard sensitivity analysis. For the Gaussian inputs, for example, members 2 and 10 make nearly equal contributions to the response uncertainty.

Particularly interesting are the cases in which the first order Sobol' functions show a nonlinear relationship between the input variable and the response. In such cases is where the results of a global sensitivity analysis will vary substantially from those of a classical sensitivity analysis. In this example, F_{10} and, to a lesser degree, F_8 show nonlinearity. The nonlinearity in F_{10} can be explained by reference to Fig. 3 which shows that the hinge at the middle of element 10 is one of the last to form. Therefore, at some value of the yield stress element 10 will stop participating in the collapse mechanism of the frame, and the corresponding Sobol' function will flatten, as is seen in Fig. 4. This change in the

collapse mechanism has been verified by simulation of the failure of the frame with the yield stress of element 10 set to a high value. This simulation, which is not shown here for brevity, shows that element 10 ceases to be part of the collapse mechanism when its yield stress is highly elevated.

5.3. Convergence of the Sobol' functions and indices

In the previous section an example Sobol' decomposition was shown that used BF sampling with 10,000 samples, and LH sampling with 800 samples. In this section it is shown that in both cases the number of samples used is sufficient to provide convergence of the results. The convergence study is performed on the Sobol' functions F_6 and F_8 and their corresponding indices S_6 and S_8. Fig. 5 shows the convergence of these Sobol' indices for BF sampling of the uniform and Gaussian input spaces. After 3000 samples convergence of the indices is observed.

One can immediately note that the convergence of the Sobol' indices for the Gaussian input space is not smooth, with seeming discontinuities in the estimated value of the Sobol' indices between about 1500 and 2500 samples. These anomalies in the convergence curves are caused by a phenomenon seen in Fig. 6 and Table 4. Concentrating on interval $I^{(1)}$, one can see from the table that, when the number of samples is 1500 and 2000, no sample points occur within this bin. This means that a correct estimate of the value of the Sobol' function F_8 is impossible in this interval, and results in the anomalous behavior observed in the top two frames of Fig. 6, where the Sobol' function itself has a large discontinuity near the left end of its domain. As soon as a single sample point is placed in $I^{(i)}$, however, which occurs between the 2000th and 2500th sample for F_8, the estimate of the Sobol' function improves dramatically as shown in the lower two frames of Fig. 6, and the corresponding Sobol' index converges rapidly to its correct value. A similar explanation is valid for the convergence behavior of S_6 in the Gaussian space, though the details are omitted here for brevity. This series of observations points to one of the shortcomings of performing numerical integration using BF samples in a Gaussian space, and indicates that estimation of the Sobol' functions could be dramatically improved by the implementation of more intelligent sampling techniques.

The reason for using the LH method is to achieve accurate estimation of the Sobol' functions using fewer samples than
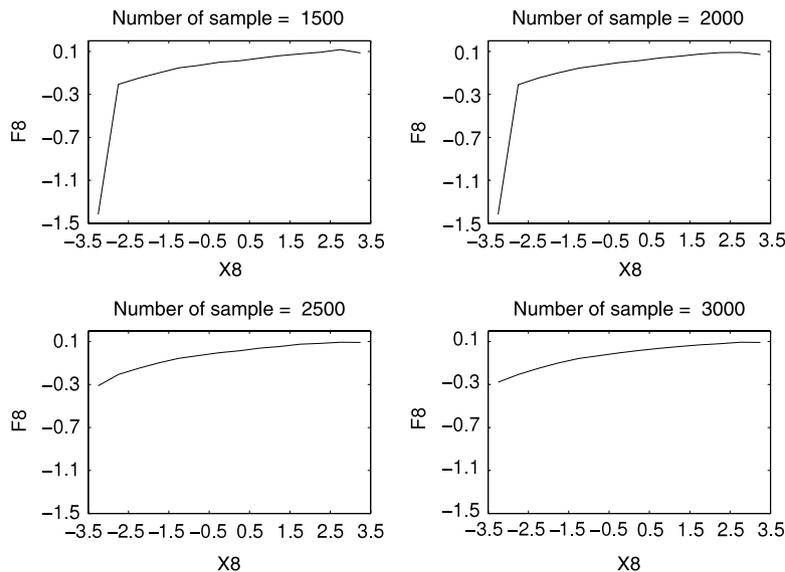
Fig. 6. Convergence of Sobol' function F_8 with increasing number of samples from a Gaussian input space.

Table 4
Number of samples in each interval $I^{(i)}$ for the calculation of S_8 from a Gaussian input space.

No. of sim.	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1500	0	10	20	64	128	245	290	282	219	140	59	29	8	5
2000	0	11	26	96	171	337	386	384	276	185	74	37	9	6
2500	1	13	32	114	228	416	489	472	360	222	88	45	10	8
3000	2	14	42	138	274	498	587	574	427	269	104	51	10	8
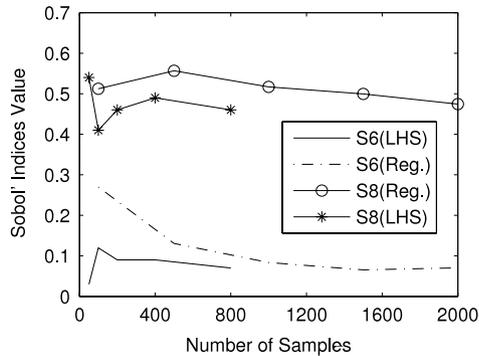
Fig. 7. Comparison of convergence of Sobol' indices S_6 and S_8 using brute force and Latin hypercube sampling on a uniform input space.

Table 5
Comparison between Sobol' global sensitivity indices and classical gradient sensitivities for frame UP36H.

Element	Sobol' indices	Sobol' index	Sensitivity	Normalized sensitivity
1	S_1	0.002	0.30	0.008
2	S_2	0.203	11.93	0.316
3	S_3	0.003	0.00	0.000
4	S_4	0.001	0.00	0.000
5	S_5	0.016	0.19	0.005
6	S_6	0.069	7.01	0.185
7	S_7	0.013	2.57	0.068
8	S_8	0.463	14.19	0.0375
9	S_9	0.001	0.31	0.008
10	S_{10}	0.104	1.30	0.034

required by the BF sampling method. In order to see how LH sampling is effective in this example, the convergence of Sobol' indices S_6 and S_8 is examined in the uniform input space using both BF and LH sampling. Fig. 7 shows this convergence and that LH sampling achieves an accurate result with roughly 400 samples as opposed to the approximately 2000 samples required for convergence using BF sampling.

5.4. Comparison between Sobol' analysis and classical sensitivity analysis

This section compares the global sensitivities obtained in the analysis described above to the results of a classical, gradient-based, sensitivity analysis in which the gradients of the response with respect to each of the input variables is computed using a finite difference approximation centered at the mean point of the input space. The comparison in this section is made for the uniform input space. A central finite difference approximation with each evaluation made by a nonlinear collapse analysis is used to obtain the gradient sensitivities. The comparison between the Sobol' global sensitivity and the gradient sensitivity results is shown in Table 5, in which the entries of the fifth column are the sensitivities normalized so that they sum to one. Although this normalization does not have a well-founded mathematical or physical justification, it allows easier comparison between the magnitude of the sensitivity and the magnitude of the Sobol' index.

The two approaches to sensitivity analysis give many similar results in this example, for example suggesting that the strength of elements 8 and 2 have significant effect on the collapse load, and that the strength of elements 3 and 4 are not important in determining the frame strength. One significant difference, however, is apparent in the result for element 10. The Sobol' global sensitivity analysis ranks the yield stress of element 10 as the fourth most important variable in determining the collapse load, and $S_{10} = 0.10$ is roughly 25% of the maximum sensitivity $S_8 = 0.46$. The point sensitivity results, however, rank the yield stress of element 10 as the fifth most important variable in determining the collapse load, and, more significantly, $R_{10} = 1.3$ is only 9% of the maximum sensitivity $R_8 = 14.19$. An analyst could reasonably conclude from the point sensitivity analysis that the yield stress of element 10 does not significantly affect the strength of the frame, whereas the Sobol' global sensitivity analysis shows that the strength can be significantly affected by the strength of element 10. It should be noted that the point sensitivity analysis could capture the significance of element 10 if a different point were chosen about which to center the estimate of the sensitivity. It may not be always possible to rationally choose the point at which to estimate sensitivity, and often the mean point of the input vector is used. While the Sobol' decomposition can detect the significance of element 10 in this case, estimation of the Sobol' indices requires a far greater number of samples than the point sensitivity analysis.

The difference in the global and point sensitivity results regarding element 10 stems from the nonlinear nature of the dependence of the frame strength on the strength of element 10. Fig. 4 shows this nonlinearity, and one can see that the variation over the entire domain of the function is much greater than would be concluded from observation of the gradient at the mean point of the input domain.

Despite this difference in the results, it should be noted that sensitivity analysis requires very few evaluations of the response function, and that there may also be times when it is advantageous to have an estimate of the sensitivity at a point rather than across the whole domain and that the point sensitivities can be computed with very few function evaluations.

5.5. Approximate response functions by truncation of the Sobol' series

In this section, another application of the Sobol' decomposition, dimension reduction, is presented. This dimension, or model, reduction is accomplished by truncating the Sobol' series in such a way that an approximation to the response function is constructed that depends on a reduced set of input variables. The truncation of the Sobol' series is guided by the values of the Sobol' indices, with only variables appearing in Sobol' indices above a threshold value being retained in the reduced model.

In the current example, an obvious truncation would include only the input variables corresponding to the yield stress of elements 2, 6, 8, and 10, which account, in only their first order forms, for 84% of the total response variance. This truncation would be applicable to the response function for both the uniform and Gaussian input spaces.

Figs. 8 and 9 show the Sobol' functions whose Sobol' indices exceed 0.05, namely F_2, F_6, F_8 and F_{10}, for uniform and Gaussian
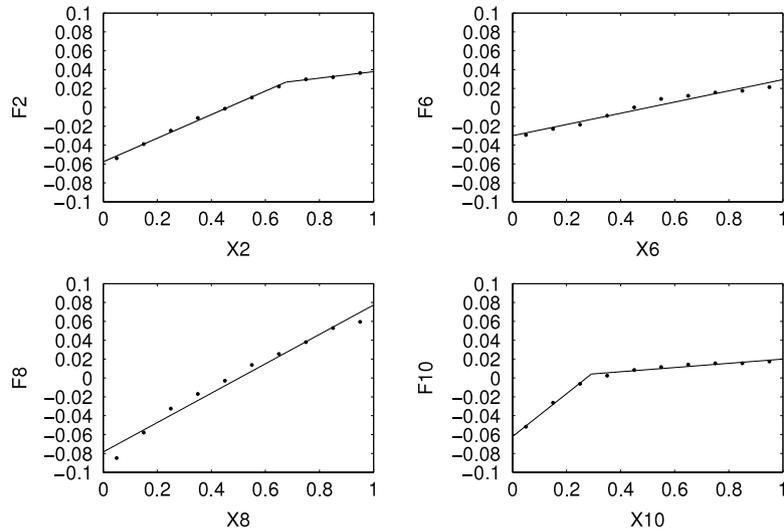
Fig. 8. Best bilinear fits to Sobol' functions derived from a uniform input space.
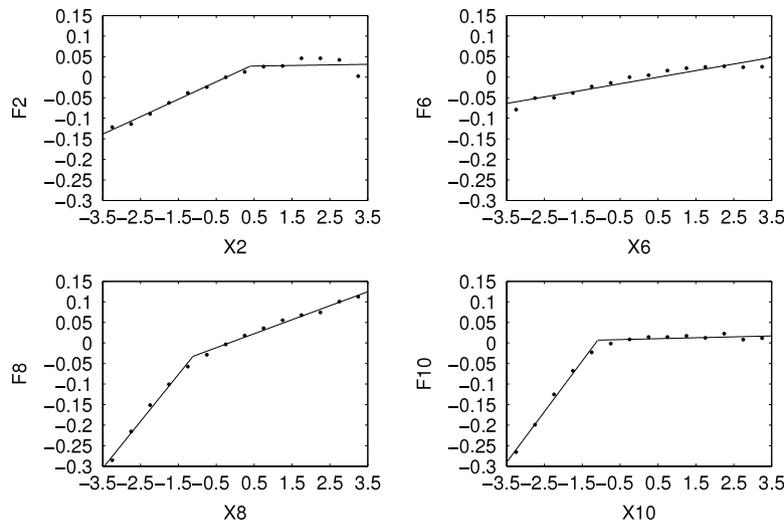
Fig. 9. Best bilinear fits to Sobol' functions derived from a Gaussian input space.

inputs respectively. The points in the figure are obtained by applying Eq. (31) to 10 000 BF simulations. The solid lines are linear or bilinear regressions to these data that are used to construct approximate analytic response functions.

Tables 6 and 7 show the slope and intercept of the lines in regression for uniform and Gaussian inputs respectively. An approximate response function is

$$F \approx F_0 + F_2 + F_6 + F_8 + F_{10}. \tag{32}$$

The accuracy of the response function depends both on the truncation chosen and the regressions chosen to represent the individual Sobol' functions. To quantify the accuracy of the approximate response function, the normalized standard deviation (NSD),

$$NSD = \sqrt{\dfrac{\displaystyle\sum_{i=1}^{10\,000} (F_{response} - F_{predict})^2}{\displaystyle\sum_{i=1}^{10\,000} (F_{response}) - (mean(F_{predict}))^2}} \tag{33}$$

is used. The NSD should be interpreted as a combination of regression and truncation error. To investigate the relative magnitude

Table 6
Parameters of best bilinear fits to Sobol' functions derived from a uniform input space with $F_0 = 1.419$.

Line specification	F_2	F_6	F_8	F_{10}
First line slope	0.125	0.060	0.156	0.228
First line intercept	−0.058	−0.030	−0.079	−0.062
Second line slope	0.034	0.060	0.156	0.022
Second line intercept	0.004	−0.030	−0.079	−0.002

Table 7
Parameters of best bilinear fits to Sobol' functions derived from a Gaussian input space with $F_0 = 1.417$.

Line specification	F_2	F_6	F_8	F_{10}
First line slope	0.043	0.016	0.114	0.123
First line intercept	0.010	−0.008	0.095	0.142
Second line slope	0.001	0.016	0.034	0.002
Second line intercept	0.026	−0.008	0.005	0.009

of the regression and truncation errors, the NSD can be compared with the Sobol' truncation error defined by

$$Sobol'\ Error = 1 - \sum_{i=1}^{m} S_{k_i} \tag{34}$$
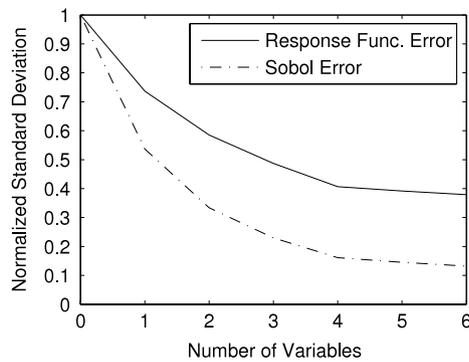
Fig. 10. Reduction in normalized standard deviation error with inclusion of additional terms in the truncated Sobol' decomposition of the uniform input space.
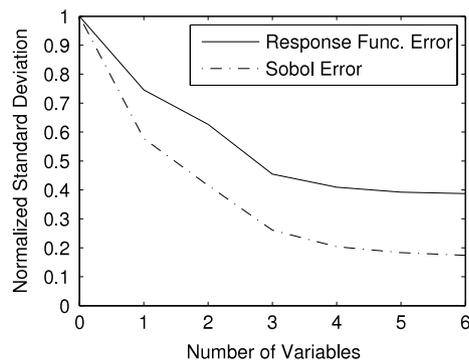
Fig. 11. Reduction in normalized standard deviation error with inclusion of additional terms in the truncated Sobol' decomposition of the Gaussian input space.

in which m is the number of variables retained in the approximate response function and $\{S_{k_i}\}$ are the indices of the included variables. The NSD is comparable to the Sobol' error because both of them are based on the standard deviation, but the Sobol' error represents only the truncation error. Therefore the difference between the Sobol' error and the NSD represents the regression error.

The NSD and the Sobol' error are calculated for an approximate response function with 1 to 6 variables retained in order of descending Sobol' index. Figs. 10 and 11 show the NSD and Sobol' errors in terms of number of variables for uniform and Gaussian inputs respectively. They show that the accuracy increases only moderately after the inclusion of the fourth variable. The Sobol' error shown in the figure is an approximation of the true truncation error since the Sobol' error in this example is obtained from BF simulation rather than exact calculations. This example study demonstrates that a reasonable characterization of the response of this frame could be obtained by a function depending on only four of the ten input variables.

6. Conclusion

As a preliminary to the example applications, the Sobol' decomposition of a function of many random variables is introduced and it is shown how it can be applied to functions with non-uniform input variables.

Two example applications, one for an exact response function and one for the problem of the collapse of a structural frame are presented. In each case, the Sobol' decomposition is used to decompose the variance of the response into components stemming from uncertainty in individual input variables. In the structural example the collapse load is the response considered and the yield stresses of the 10 individual members are the input variables. For the structural example Monte Carlo simulation is used to compute the components of the Sobol' decomposition and it is shown that significant increase in the rate of convergence of the estimates of the Sobol' functions can be obtained by implementing appropriate sampling algorithms such as Latin Hypercube sampling.

Through the examples it is demonstrated that the distribution of the input variables can have subtle but important effects on the variance decomposition and that the Sobol' decomposition, a global sensitivity analysis method, can provide insight into uncertainty not available from standard sensitivity analysis. Finally, it is shown how the Sobol' indices provide information that can lead to a model reduction procedure that delivers an approximate response function that retains reasonably predictive accuracy while substantially reducing the dimension of the domain on which the response function is defined.

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