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Probabilistic Sensitivity Analysis in Engineering Design using Uniform Sampling and Saddlepoint Approximation

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ABSTRACT

Sensitivity analysis plays an important role to help engineers gain knowledge of complex model behaviors and make informed decisions regarding where to spend engineering effort. In design under uncertainty, probabilistic sensitivity analysis (PSA) is performed to quantify the impact of uncertainties in random variables on the uncertainty in model outputs. One of the most challenging issues for PSA is the intensive computational demand for assessing the impact of probabilistic variations. An efficient approach to PSA is presented in this article. Our approach employs the Kolmogorov-Smirnov (KS) distance to quantify the importance of input variables. The saddlepoint approximation approach is introduced to improve the efficiency of generating cumulative distribution functions (CDFs) required for the evaluation of the KS distance. To further improve efficiency, optimized uniform samples are used to replace the direct Monte Carlo simulations for determining the cumulant generating function (CGF) in saddlepoint approximation. Efficient construction of a uniform design necessary to generate the "best" samples in a multidimensional space is presented. Our approach is illustrated with a structural design problem. It has the potential to be the most beneficial for high dimensional engineering design problems that involve expensive computer simulations.

INTRODUCTION

With the advance of computing technologies and numerical approaches, scientific and engineering disciplines have experienced tremendous growth in the use of sophisticated computer models to assist scientific investigation and engineering analysis and design. Engineers and scientists make use of the models to perform various tasks and decision-making by interrogating the models to predict behaviors of systems under different input variable settings. The typical input-output relationship represented by a computer model is expressed as follows.

$$Y = f(\mathbf{X}), \tag{1}$$

where $\mathbf{X} \in R^d$ are input variables, Y is an output or response variable representing product or system performance, and $f(\cdot)$ is the relationship function between inputs and the output. In complex engineering applications, $f(\cdot)$ typically does not have an analytic formula. In product development such as automobile, sophisticated engineering computer models are eminent. and important for various reasons.

As engineering design process becomes more complex because of ever increasing customer expectation toward product quality, deductive approach in design using physics-based models alone is inadequate, and variability information must be integrated into the decision process. The seminal work by Taguchi (1993) has been very influential in introducing the concept of robust design for which a product or system must be designed by choosing the right setting of "control" variables (variables that engineers choose to control) such that the "ideal function" is insensitive to noise factors (i.e., variations due to piece-to-piece, degradation over time, environment, load, system interactions). Complementary to the robust design view, the product or system must be designed with high reliability (i.e., low probability of failure). The later view is the subject in reliability-based design discipline (Du et al., 2004). The needs to address both robustness and reliability design necessitate the integration of probabilistic analysis with deterministic computer models. In this framework, the inputs to the computer

models are treated as random variables with assumed distributions.

The interest in the probabilistic analysis approach is to understand the probabilistic characteristics (e.g., mean, μ_Y, standard deviation, σ_Y, or probability distribution, p_Y) of the response variable, Y, due to the stochastic nature of input variables, $\mathbf{X}$. Unfortunately, in most practical situations, the above needs are not easy to meet because stochastic information of input variables is often imprecise, and acquiring such information can be a very expensive proposition. To remedy this problem, the sensitivity analysis approach is employed with intention to rank order or to assess the importance of random input variables among each other. Through this analysis - though the stochastic information of input variable may be imprecise, and thus the distribution of the response variability may not be fully trustworthy - one can still acquire useful information for engineering decision making such as to focus the effort to reduce the variation due to important variables, to gather more precise stochastic information for the important variables, or to eliminate insignificant variables thus to simplify further analysis.

Because the inputs to computer models can be numerous, probabilistic sensitivity analysis involves various integral analyses in a high dimensional space. Unfortunately, computer models in engineering such as computational fluid dynamics and finite element models are usually computationally intensive. Thus, exercising the model by means of Monte Carlo simulation is not practical and often prohibitive. Therefore, a computationally more efficient technique that requires much less number of samples than that of Monte Carlo technique is needed. To this end, we present an approximation approach using the Saddlepoint Approximation in combination with uniform design to reduce the sample size yet maintaining a reasonable accuracy. This paper has the following flow. Section 2 introduces the concepts of probabilistic design and sensitivity analysis. The saddlepoint approximation technique required to calculate the sensitivity analysis is discussed in Section 3. Efficient construction of uniform design necessary to generate the "best" samples to calculate the saddlepoint approximation is presented in Section 4. Section 5 illustrates the use of our method for an engineering application. Finally, the conclusion is presented in Section 6.

MAIN SECTION

2. PROBABILISTIC DESIGN AND SENSITIVITY ANALYSIS

In probabilistic design, the effects of input variability on product performance need to be addressed through rigorous variability analysis to prevent or to reduce the probability of failure occurrence or performance variation that leads to quality losses. The major task of probabilistic analysis is to obtain the probability distribution of the performance function (response) y given the distributions of the vector of random input variables **x**. For a given performance target requirement, $y \le Y$, the probability of the performance to meet the requirement can be calculated by a multi-dimensional integral,

$$P(Y \le y) = \int_{f(\mathbf{X}) \le y} \cdots \int p(\mathbf{x}) d\mathbf{x} \text{ ,} \qquad (2)$$

where $p(\mathbf{X})$ is the joint probability density function of random variables $\mathbf{X}$. The equality at the integration boundary $f(\mathbf{X}) = y$ is called the *limit-state*, separating between "acceptable" and "unacceptable" (or safe and failure) regions of input variable space. Obviously, due to the multi-dimensional integration and the nonlinear limit-state, the solution to Eq. (2) is analytically or numerically difficult to obtain; thus, Monte Carlo integration technique often becomes the method of choice. The solution is given by

$$P(Y \le y) = \frac{1}{n}\sum_{i=1}^{n} I(y_i) \quad \text{where} I(y_i) = \begin{cases} 1 \text{ for } y_i \le y \\ 0 \text{ otherwise} \end{cases}, \qquad (3)$$

where y_i is obtained by evaluating $f(x_i)$ and $\mathbf{x}_i = \{x_i^1, x_i^2, \ldots, x_i^d\}$ are random samples from independent and identical distributions (i.i.d), and *d* is the dimension or the number of input random variables.

In robust design (Chen et al., 1996), engineers would like to minimize the variation of *y* which can be represented by a dispersion measure such as standard deviation, σ_Y, or quantile difference (Du et al., 2004), $\delta_y = y^{1-\alpha} - y^{\alpha}$, where α is a prespecified quantile (see Figure 1) with $y^{\alpha} = P^{-1}(\alpha)$ and $y^{1-\alpha} = P^{-1}(1-\alpha)$. The quantile difference measure may be more preferable than the standard deviation when the distribution of Y consists of significant higher moments (e.g., skewness and kurtosis).

The ability to calculate the distribution of y is needed for another important focus of probabilistic design: probabilistic sensitivity analysis (PSA) to quantify the impact of variability of input random variables on the variability of a model output. Results from PSA can be crucial to assist engineering design decisions, such as to help reduce the dimension of a design problem by identifying the probabilistically insignificant factors; to check the validity of a model structure and the assumptions made on the probability distributions of random inputs; to obtain insights about the design space and the probabilistic behavior of a model response; and to investigate the potential improvement on a probabilistic response by reducing the uncertainty in random inputs (Saltelli, 2000). If the interest is to study the effects of input variance on the output variance, variance-based method can be used to quantify the importance of input variables to an output (Saltelli,

2000). The variance-based method, however, will not be sufficient when the problem involves performance distributions with higher moments (Liu et al., 2004). In this situation, sensitivity analysis must include complete stochastic information of the distribution. Considering this need, in the following discussion, we employ Kolmogorov-Smirnov (KS) distance to quantify the importance of an input variable.

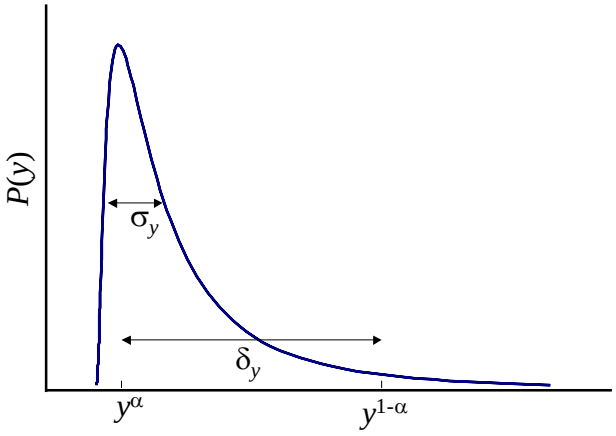

Figure 1. Measure of response variability.

The KS distance, d_{KS}, measures the difference between two cumulative distribution functions (CDF), P_1 and P_2, as follows,

$$d_{KS}(P_1,P_2)=\sup_y\left|P_1(y)-P_2(y)\right|,\quad y\in R. \qquad (4)$$

That is, the KS distance measures the maximum discrepancy between two distributions. In the context of sensitivity analysis, the KS distance can be used to quantify the main and total effects (i.e., the effect of a variable including all its interaction terms). The main effect of the *j*th variable, x^j, can be calculated as follows,

$$d_{KS}^{\,j}(P_0,P_j)=\sup_y\left|P_0\left(y\middle|\mathbf{x}\right)-P_j\left(y\middle|x^j\right)\right|,\quad y\in R, \quad (5)$$

where $P_0\left(y\middle|\mathbf{x}\right)$ is the CDF of y by including all variability of input variables where $P_j\left(y\middle|x^j\right)$is the CDF of y including only the variability of x^j and setting the rest of variables to constant values (e.g., their mean values). The smaller the value of $d_{KS}^{\,j}$ is, the closer $P_j\left(y\middle|x^j\right)$ is to $P_0\left(y\middle|\mathbf{X}\right)$, and the more dominant the variability of x^j is to define P_0; therefore, the smaller the value of $d_{KS}^{\,j}$ is, the more important the variable is to the distribution of response variable. The total effect of x^j including the effect of its interactions with other variables can be calculated as,

$$d_{KS}^{\sim j}(P_0,P_{\sim j})=\sup_y\left|P_0\left(y\middle|\mathbf{X}\right)-P_{\sim j}\left(y\middle|\mathbf{X}_{\sim j}\right)\right|,\quad y\in R, \quad (6)$$

where $\mathbf{x}_{\sim j}$ is the set of all variables excluding the variability of x^j (i.e., setting x^j to a constant value such as its mean) and correspondingly $P_{\sim j}\left(y\middle|\mathbf{X}_{\sim j}\right)$ is the CDF of y by excluding the variability of x^j. Thus, when x^j is the dominant variable then by excluding it, the discrepancy between the two distributions will be larger. In this case, the larger the $d_{KS}^{\sim j}$ value is, the more important x^j is. Based on the KS distance of the total effect, the importance of x^j can be ranked according to their order of importance.

As discussed above, probabilistic analysis including the sensitivity analysis requires numerous evaluations of ***f(x)*** to calculate the integral in (2). Note that, however, ***f(x)*** is represented by a complex computer model with nonlinear behavior and expensive to compute. Because the evaluation of $f(\mathbf{x})$ is expensive and $P(Y<y)$ is typically very large for a highly reliable product, Monte Carlo integration may not be a practical alternative. This computation difficulty has led to the development of various approximation methods using the linearization of limit state (Du and Sudjianto, 2004) which in some situations may not lead to satisfactory results. In Section 3, we propose an alternative method to the above problem.

3. SADDLEPOINT APPROXIMATION FOR PROBABILISTIC ANALYSIS AND SENSITIVITY ANALYSIS

3.1 REVIEW OF SADDLEPOINT APPROXIMATION

The Saddlepoint Approximation was introduced for approximating the probability density function (PDF) by Daniels (1954). Since then, the research and applications of Saddlepoint Approximations have vastly increased (e.g., Jensen, 1995).

Given a random variable Y with a density function $P(y)$, then the characteristic function of Y is

$$\xi(t)=\int_{-\infty}^{+\infty}e^{ity}\,p(y)\,dy, \qquad (7)$$

where $i=\sqrt{-1}$. The cumulant generating function (CGF) *K*(*t*) of y is defined as

$$K(t)=\log[\xi(t)], \qquad (8)$$

where *log* is the natural logarithm. The PDF of Y can be restored from $K(t)$ by the inverse Fourier transformation,

$$p(y)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ity}\xi(t)dt=\frac{1}{2\pi}\int_{-i\infty}^{+i\infty} e^{[K(t)-ty]}\,dt\,. \qquad (9)$$

The key idea of obtaining the PDF of Y is to accurately approximate the above integral through the concept of *saddlepoint* approximation. Simple formulae to calculate the PDF and CDF have been derived; consequently, their use is fairly straightforward. Daniels (1954) used the exponential power series expansion to estimate the integral in Eq. 9 as

$$p(y)=\left\{\frac{1}{2\pi K''(t_s)}\right\}^{\frac{1}{2}} e^{[K(t_s)-t_s y]}, \qquad (10)$$

where $K''(.)$ is the second order derivative of the CGF, and t_s is the saddlepoint, which is the solution to the equation at the point of interest, *y*.

$$K'(t)= y\,, \qquad (11)$$

where $K'(.)$ is the first derivate of the CGF. Lugannani and Rice (1980) provided a very concise formula to approximate CDF,

$$P(Y\le y)=\Phi(w)+\phi(w)\left(\frac{1}{w}-\frac{1}{v}\right)\,, \qquad (12)$$

where $\Phi(\cdot)$ and $\phi(\cdot)$ are CDF and PDF of the standard normal distribution, respectively,

$$w=\mathrm{sgn}(t_s)\left\{2\left[t_s Y-K(t_s)\right]\right\}^{1/2} \qquad (13)$$

and

$$v=t_s\left\{2K''(t_s)\right\}^{1/2}\,, \qquad (14)$$

where $\mathrm{sgn}(t_s)$ = +1, -1, or 0, depending on whether t_s is positive, negative or zero.

The Saddlepoint Approximation has several excellent features: (1) It yields extremely accurate probability estimation, especially in the tail area of a distribution; (2) it requires only the process of finding one saddlepoint without any integration; and (3) it provides estimations of the PDF and CDF simultaneously. In the following subsections, we will discuss how to combine Saddlepoint Approximations with simulation samples to conduct probabilistic sensitivity analysis.

3.2 ESTIMATION OF CDF BY SADDLEPOINT APPROXIMATIONS

As discussed in the preceding section, the use of Saddlepoint Approximation rests on the ability to estimate the CGF of a general performance function $y = f(\mathbf{x})$. In some situations, a proper approximation can be developed through a linearization process to approximate the CGF (Du and Sudjianto, 2004). However, in general, the empirical estimation of CGF using sample dataset may be necessary as follows.

- Generate n samples for the d input random variables, $\mathbf{X}=\left\{x_i^j\right\}, i=1,2,\ldots,n;\ j=1,2,\ldots,d$.
  Various sampling techniques are available for this purpose such as Monte Carlo random sample, Quasi Monte Carlo, lattice points, Latin Hypercube Sampling (LHS), and uniform design (Fang and Wang, 1994; Owen, 1997; Fang et al., 2000). The choice of sampling technique is crucial in probabilistic engineering design to achieve high accuracy of cumulant estimation while employing only limited sample size because of computationally expensive engineering models. In Section 4, we will discuss this step with a greater depth.
- Acquire outputs by applying the sample dataset to the engineering computer model. For the *i*th sample, $\mathbf{x}_i=\left(x_i^1, x_i^2, \cdots, x_i^d\right)$, the output of computer model is $Y_i = f(\mathbf{X}_i)$.
- Estimate cumulants of the response variable, *y*, based on the sample output. The first four cumulants are

$$\begin{cases} \kappa_1=\dfrac{s_1}{n} \\ \kappa_2=\dfrac{ns_2-s_1^2}{n(n-1)} \\ \kappa_3=\dfrac{2s_1^3-3ns_1s_2+n^2s_3}{n(n-1)(n-2)} \\ \kappa_4=\dfrac{-6s_1^4+12ns_1^2s_2-3n(n-1)s_2^2-4n(n+1)s_1s_3+n^2(n+1)s_4}{n(n-1)(n-2)(n-3)} \end{cases}, \qquad (15)$$

  where $s_r, r=1,2,3,4,$ are the *r*th moment estimates from the sample of output

$$s_r=\sum_{i=1}^{n} y_i^r\,. \qquad (16)$$

  The empirical CGF is calculated based on series expansions of powers of *t*

$$K(t)=\log\xi(t)=\sum_{j=1}^{\infty}\kappa_j\frac{t^j}{j!}\,. \qquad (17)$$

- Calculate the saddlepoint solution. Since the empirical CGF in (17) is in a polynomial form, its first and second order derivatives can be derived

analytically. If the higher order terms (i.e., after the fourth cumulant) in Eq. (17) are omitted, Eq. (11) is expressed as

$$K'(t)=\kappa_1+\sum_{j=2}^{4}\kappa_j\frac{t^{j-1}}{(j-1)!}=y\,. \qquad (18)$$

Solving the above equation, we get the saddlepoint t_s. Then the PDF and CDF can be calculated using Eqs. (10) and (12), respectively.

4. EFFICIENT CONSTRUCTION OF UNIFORM SAMPLES

The efficiency of the saddlepoint approximation approach (Section 3) can be improved by replacing the Monte Carlo Simulation (MCS) with the Latin Hypercube Design (LHD) which produces more stable results and requires fewer samples than the MCS for the same accuracy for estimating statistics of a performance function (Olsson et al. 2003; Helton and Davis, 2003). To improve the multidimensional uniformity or called the space-filling property of the LHD, optimization can be employed to generate optimal LHDs based on certain optimality criteria representing the uniformity. Such type of optimized design is also called uniform design.

4.1 LATIN HYPERCUBE AND LOW DISCREPANCY SAMPLING

McKay et al. (1979) introduced the use of Latin Hypercube Sampling (LHS) for computer experiments. LHS stratifies each variable individually into equal intervals. Owen (1997) showed that for finite samples. LHS is never worse than Monte Carlo random samples. The measure of discrepancy that has been widely used in the Quasi Monte Carlo theory and uniform design is the star L_p-discrepancy (Fang and Wang, 1994). Hickernell (1998) explained the weakness of the L_p-discrepancy and proposed several alternatives, among which the centered L_2-discrepancy (CL_2) is the most attractive (Fang et al., 2000)

$$CL_2(\mathbf{X})^2=\left(\frac{13}{12}\right)^2-\frac{2}{n}\sum_{i=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|x_{ik}-0.5\right|-\frac{1}{2}\left|x_{ik}-0.5\right|^2\right)$$
$$+\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{k=1}^{m}\left(1+\frac{1}{2}\left|x_{ik}-0.5\right|+\frac{1}{2}\left|x_{jk}-0.5\right|-\frac{1}{2}\left|x_{ik}-x_{jk}\right|\right) \qquad (19)$$

A sample set, **X**, is called uniform if it has the minimum $CL_2(\mathbf{X})^2$. For the one-dimensional case, Fang et al. (2002) showed that the sample set with equidistant stratification (i.e., LHS) has the lowest discrepancy. For higher dimensional case, Fang et al. (2002) showed that LHS has better expected value of $CL_2(\mathbf{X})^2$ compared to that of Monte Carlo random samples:

$$E\left(CL_2(\mathbf{X}_{MC})\right)^2-E\left(CL_2(\mathbf{X}_{LHS})\right)^2=\left(\frac{13}{12}\right)^{d-1}\frac{d}{6n}\left(1-\frac{2d+11}{26n}\right)+O\left(n^{-3}\right) \qquad (20)$$

The advantage of LHS is more dramatic when the sample size is small and the dimension is large as shown in the figure below.

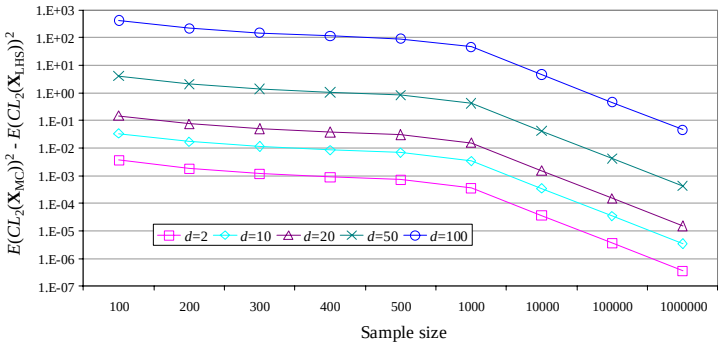

Figure 2. Difference between the expected value of CL2-discrepancy of Monte Carlo random sampling and LHS.

Combining the advantageous features of Quasi Monte Carlo and stratified sampling such as LHS, in this paper, we pursue to optimize LHS with respect to CL_2-discrepancy. That is, to arrive to optimal samples with LHS-type stratification which are uniformly distributed in the entire space and not only in the one-dimensional projection: the feature of *uniform design* (Fang, 2000). We employ an optimization approach to search for LHS that minimizes CL_2-discrepancy. Searching the optimal uniform designs, however, is a difficult optimization problem to solve. Several heuristic combinatorial optimization approaches have been proposed. The computational cost of the existing algorithms, e.g., the simulated annealing (SA) algorithm used by Morris and Mitchell (1995), the *columnwise-pairwise* (CP) algorithm by Ye, et al (2000), and the threshold accepting (TA) algorithm adopted by Fang, et al (2002) for constructing optimal LHD, is generally high. Ye, et al (2000) reported that generating an optimal 25×4 LHSs using CP could take several hours on a Sun SPARC 20 workstation. For a design as large as 100×10, the computational cost could be formidable. Motivated by reducing this computational cost, an efficient algorithm for constructing optimal experimental designs is developed and introduced in this section. This new algorithm significantly improves the computational efficiency as it cuts the computation time from hours to minutes and seconds. There are two major ideas behind this algorithm (Jin et al. 2004). One is on the use of an efficient global optimal search algorithm, named as the enhanced stochastic evolutionary (ESE) algorithm. The other is on the use of efficient methods for evaluating optimality criteria. Some details of the algorithm and results from comparative studies are provided in the following subsections.

4.2 ALGORITHM FOR OPTIMIZING UNIFORMITY

The strategy to construct uniform LHS is summarized as follows,

1. Start from a randomly chosen LHS, $\mathbf{X_0}$;
2. Construct a new design (or a set of new designs) through *columnwise* operations on the current design;
3. Compute optimality criterion (e.g., the centered L_2 discrepancy criterion) value of the new design and decide whether to replace the current design with the new one.
4. Repeat steps 2 and 3 until a stopping criterion is met.

The *columnwise element-exchange* operations are used in the step 2 of the search to maintain the structure property of LHS. The element-exchange within a column interchanges two distinct elements in a column and guarantees to retain the LHS property. As shown in Figure 3 for a 5×4 LHS, after the element-exchange, the balance property of the 2nd column is retained, and the sample is still a LHS after the exchange.

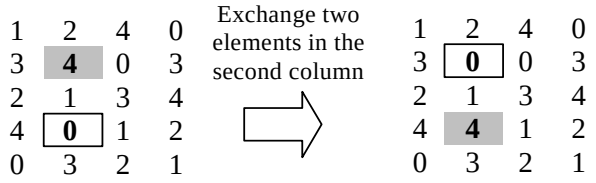

Figure 3. Element-exchange in a 5×4 LHS

In step 3 of the search process, a new sample set, $\mathbf{X}^{new}$, replaces the incumbent, X, if it leads to an improvement in terms of the criterion, i.e., CL2($\mathbf{X}^{new}$) < CL2(X). Otherwise, it will replace **X** with probability of $p(T, CL_2(\mathbf{X}^{new}), CL_2(\mathbf{X}))$ where T is a "threshold" of acceptance parameter. Several search algorithms have been applied to construct optimal design in the context of computer experiments. Principally, they differ in the strategy of threshold acceptance of $p(.)$ and T as follow:

Column Pair-wise (CP) algorithm (Li and Wu, 1997)

$$p\left(T, CL_2\left(\mathbf{X}^{\text{new}}\right), CL_2(\mathbf{X})\right) = \begin{cases} 1 & \text{for } CL_2\left(\mathbf{X}^{\text{new}}\right) - CL_2(\mathbf{X}) < T \text{ where } T = 0 \\ 0 & \text{otherwise} \end{cases} . \quad (21)$$

Threshold Acceptance (TA) algorithm (Winker and Fang, 1997)

$$p\left(T, CL_2\left(\mathbf{X}^{\text{new}}\right), CL_2(\mathbf{X})\right) = \begin{cases} 1 & \text{for } CL_2\left(\mathbf{X}^{\text{new}}\right) - CL_2(\mathbf{X}) < T^k \\ 0 & \text{otherwise} \end{cases} , \quad (22)$$

where T^k is a "threshold" parameter, initially set to $T^0 = T$ and will be monotonically reduced by some schedule $T^k = \alpha T$ where α $(0 \le \alpha \le 1)$ is a constant.

Simulated Annealing (SA) algorithm (Morris and Mitchell, 1995)

$$p\left(T, CL_2\left(\mathbf{X}^{\text{new}}\right), CL_2(\mathbf{X})\right) = \exp\left\{-\frac{1}{T^k}\left[CL_2\left(\mathbf{X}^{\text{new}}\right) - CL_2(\mathbf{X})\right]\right\} , \quad (23)$$

where T^k is also known as "temperature" parameter analogous to the physical process of annealing of solids which initially set to $T^0 = T$ and will be monotonically reduced by some cooling schedule $T^k = \alpha T$, where α $(0 \le \alpha \le 1)$ is a constant called *cooling* factor.

Enhanced Stochastic Evolutionary (ESE) algorithm (Jin et al., 2004)

$$p\left(T, CL_2\left(\mathbf{X}^{\text{new}}\right), CL_2(\mathbf{X})\right) = \begin{cases} 1 & \text{for } CL_2\left(\mathbf{X}^{\text{new}}\right) < CL_2(\mathbf{X}) \\ 1 - \frac{1}{T^k}\left[CL_2\left(\mathbf{X}^{\text{new}}\right) - CL_2(\mathbf{X})\right] & \text{for } CL_2\left(\mathbf{X}^{\text{new}}\right) - CL_2(\mathbf{X}) < T^k \\ 0 & \text{otherwise} \end{cases} , \quad (24)$$

where T^k is a "threshold" parameter, initially set to $T^0 = T$ and will be reduced or increased by some schedule $T^k = \alpha_1 T$ and $T^k = T / \alpha_2$ where α_j $(0 \le \alpha_j \le 1), j = 1,2$ are a chosen set of constants. The scheduling of the threshold value (reduced or increased) is adaptively determined by the history of the search results. Among the above strategies, the enhanced stochastic evolutionary (ESE) algorithm is the algorithm we recommend. It is adapted from the stochastic evolutionary (SE) algorithm (Saab and Rao, 1991). The algorithm uses a sophisticated combination of warming schedule and cooling schedule to control the threshold so that the algorithm can be self-adjusted during the search process. Details of the algorithm implementation can be found in Jin et al. (2004).

4.3 EFFICIENT OPTIMALITY CRITERION CALCULATION

Let $\mathbf{Z} = \{z_i^j\}$ be the centered design matrix of **X**, i.e., $z_i^j = x_i^j - 0.5$. Let $\mathbf{C} = [c_{ij}]_{n \times n}$ be a symmetric matrix, whose elements are:

$$c_{ij} = \begin{cases} \frac{1}{n^2}\prod_{k=1}^{d}\frac{1}{2}(2 + |z_i^k| + |z_j^k| - |z_i^k - z_j^k|) & \text{if } i \ne j, \\ \frac{1}{n^2}\prod_{k=1}^{d}(1 + |z_i^k|) - \frac{2}{n}\prod_{k=1}^{d}(1 + \frac{1}{2}|z_i^k| - \frac{1}{2}z_i^{k2}) & \text{otherwise.} \end{cases} \quad (25)$$

Let $g_i = \prod_{k=1}^{d}(1 + |z_i^k|)$ and

$$h_i = \prod_{k=1}^{d}(1+\frac{1}{2}|z_i^k| - \frac{1}{2}z_i^{k\,2}) = \prod_{k=1}^{d}\frac{1}{2}(1+|z_i^k|)(2-|z_i^k|),$$

then,

$$c_{ii} = g_i / n^2 - 2h_i / n. \quad (26)$$

It can be proved easily that

$$CL_2(\mathbf{X})^2 = \left(\frac{13}{12}\right)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij} \quad . \quad (27)$$

From (33)-(35), the computational complexity to calculate the **C** matrix (and thus, CL_2) is $O(dn_2)$. Note, however, that each updating operation using columnwise element-exchanges for generating a new sample set, only involves two elements in the sample matrix. That is, with the element exchange operation, $x_{i_1}^k \leftrightarrow x_{i_2}^k$, only elements in i_1 and i_2 rows and i_1 and i_2 columns of **C** are changed. Considering this situation, we seek a more efficient CL_2 calculation after an element exchange without recalculating the entire **C** matrix. For any $1 \le j \le n$ and $j \ne i_1, i_2$, let

$$\gamma(i_1, i_2, k, j) = \\ (2+|z_{i_2}^k|+|z_j^k|-|z_{i_2}^k - z_j^k|)\big/(2+|z_{i_1}^k|+|z_j^k|-|z_{i_1}^k - z_j^k|) \quad ,(28)$$

then,

$$c_{i_1 j}' = c_{j i_1}' = \gamma(i_1, i_2, k, j) c_{i_1 j}, \quad (29)$$

and

$$c_{i_2 j}' = c_{j i_2}' = c_{i_2 j} / \gamma(i_1, i_2, k, j). \quad (30)$$

Let $\alpha(i_1, i_2, k) = (1+|z_{i_2}^k|)\big/(1+|z_{i_1}^k|)$ and

$\beta(i_1, i_2, k) = (2-|z_{i_2}^k|)\big/(2-|z_{i_1}^k|)$, then:

$$c_{i_1 i_1}' = \alpha(i_1, i_2, k) g_{i_1} / n^2 - 2\alpha(i_1, i_2, k)\beta(i_1, i_2, k) h_{i_1} / n, \quad (31)$$

and

$$c_{i_2 i_2}' = g_{i_2} / [n^2 \alpha(i_1, i_2, k)] - 2h_{i_2} / [n\alpha(i_1, i_2, k)\beta(i_1, i_2, k)] \quad . (32)$$

The new CL_2 can be computed by:

$$(CL_2^{\,2})' = \\ CL_2^{\,2} + c_{i_1 i_1}' - c_{i_1 i_1} + c_{i_2 i_2}' - c_{i_2 i_2} + 2 \times \sum_{1 \le j \le n,\, j \ne i_1, i_2} (c_{i_1 j}' - c_{i_1 j} + c_{i_2 j}' - c_{i_2 j}) \quad (33)$$

Now, the computational complexity of calculating CL_2 after an element exchange operation becomes $O(n)$, which is much less than $O(dn_2)$. This efficient updating calculation enables us to search larger size optimal samples.

4.4 EXAMPLE AND VERIFICATIONS

The search algorithm above can be used for optimizing various classes of designs of experiments, including but not limited to LHS, general balanced designs, Orthogonal Array with various optimization criteria other than Eqn.(19) (see Jin, 2004). Here we provide one example of optimal LHS based on the CL_2 criterion. As shown in Figure 4, before optimization, the initial LHS is a random LHS sample with good one-dimensional projective property but not so good space-filling property. After optimization, the projective property is maintained while the space filling property is much improved.

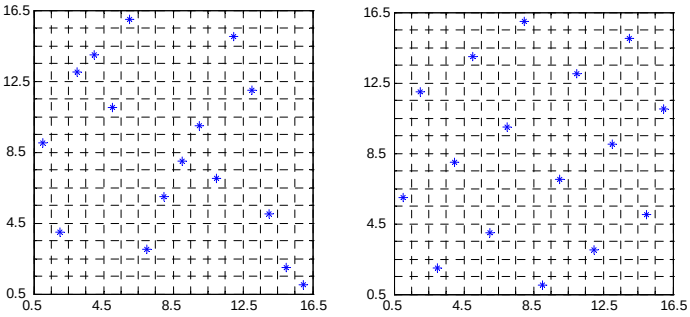

Figure4. LHS sample before and after optimization using CL2 Criterion.

In Jin et al. (2004), the new algorithm is compared to existing techniques and found to be much more efficient in terms of the computation time, the number of exchanges needed for generating new designs, and the achieved optimality criteria. Specifically, it has cut the computation time from hours to minutes and seconds, which makes the just-in-time generation of relatively large size optimal samples possible. For the problems tested, we find that with the same number of exchanges, the optimal designs generated by ESE are generally better than those generated by Simulated Annealing (SA) and the columnwise-pairwise (CP) algorithm. To obtain a design statistically significantly better than those generated by SA and CP, ESE needs far less number of exchanges (typically around 1/6 ~ 1/2 of exchanges needed by SA or CP for small-sized designs and 1/33~1/4 of exchanges needed by CP for large-sized designs).

Through our comparative studies (Jin et al. 2004), it was discovered that the CL_2 criterion is much more efficient to evaluate than other optimality criteria such as MAXIMIN distance criterion (Morris and Mitchell, 1995) and the entropy criterion (Ye et al., 2000). For the

problems tested, the computing time for the MAXIMIN criterion is 2.3~3.0 times as much as that for the CL_2 criterion. The larger the size of an experimental design is, the more computational savings the method will make. For example, for 100x10 LHS, our new method for evaluating CL_2 criteria only requires 1/82.1 of the computation effort compared to re-evaluating the whole matrix.

As the global optimal samples may never be known, one way to access how good the optimal designs are by estimating the probability of a randomly generated LHS to be better than that of optimal samples, $P(CL_2(\mathbf{X}_{\text{random}}) \le CL_2(\mathbf{X}_{\text{opt}}))$. For the purpose of example, we generated 2×10^7 sets of 50×5 (n=50, d=5) LHS samples and calculate their CL_2 values. Figure 5 shows the empirical CDF of CL_2 values of random 50×5 LHSs. As we are only interested in the left tails of CDF curves (i.e., small CL_2 values), the right part of CDF curves have been truncated in the figure.

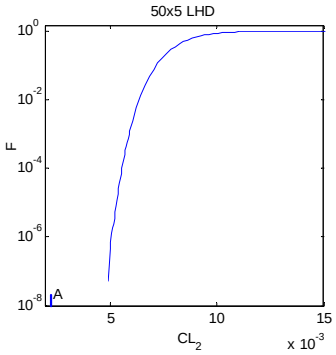

Figure 5. Empirical Cumulative Distribution of CL_2 values of random 50×5 LHSs

In this case, fitting a line through the points at the tail region, we estimated that $P(CL_2(\mathbf{X}_{\text{random}}) \le CL_2(\mathbf{X}_{\text{opt}})) \approx 10^{-19}$ where $CL_2(\mathbf{X}_{\text{opt}})$ = 0.002249. Similar observations were obtained for 100×10 LHSs. These indicate that the optimal designs constructed by ESE generally have significantly lower CL_2 values (better uniformity) than randomly generated LHSs.

5. APPLICATION

To illustrate the application, we present a simple example where the engineering model has an analytic form and thus computationally cheap. Typical real world engineering models do not have analytic forms and computationally much more expensive (see for example Ejakov, et al., 2004). Nevertheless, this example sufficiently demonstrates the use and the effectiveness of our proposed method. A composite beam with Young's modulus E_w and A *mm* wide by *B mm* deep by *L mm* long, has an aluminum plate with Young's modulus E_a and a net section *C mm* wide by *D mm* high securely fastened to its bottom face, as shown in Fig. 6. Six external vertical forces, P_1, P_2, P_3, P_4, $P5$ and P_6 are applied at six different locations along the beam, L_1, L_2, L_3, L_4, L_5, and L_6. The allowable tensile stress is S.

In this problem, there are twenty random variables as follows,

$$\mathrm{X} = [\mathrm{X}_1, ..., \mathrm{X}_{20}]^{\mathrm{T}} =$$

$$[A, B, C, D, L_1, L_2, L_3, L_4, L_5, L_6, L, P_1, P_2, P_3, P_4, P_5, P_6, E_a, E_w, S]^T$$

Details of these random variables are given in Table 1.

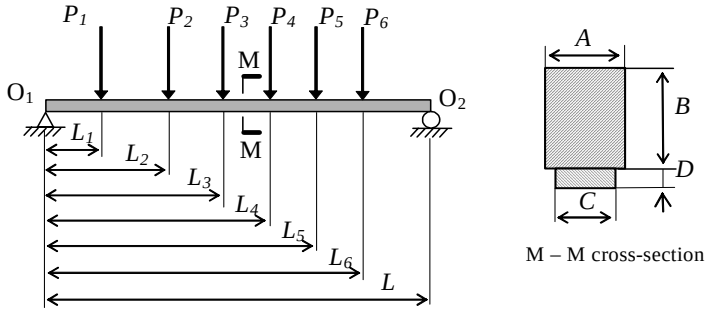

Figure 6. A Composite Beam with 20 random variables.

Table 1. Random Variables of the Beam Reliability Problem

Var#	Var	Mean value	Standard deviation	Distribution type
1	A	100 mm	0.2 mm	Normal
2	B	200 mm	0.2 mm	Normal
3	C	80 mm	0.2 mm	Normal
4	D	20 mm	0.2 mm	Normal
5	L1	200 mm	1 mm	Normal
6	L2	400 mm	1 mm	Normal
7	L3	600 mm	1 mm	Normal
8	L4	800 mm	1 mm	Normal
9	L5	1000 mm	1 mm	Normal
10	L6	1200 mm	1 mm	Normal
11	L	1400 mm	2 mm	Normal
12	P1	20 kN	4 kN	Extreme Type l
13	P2	20 kN	4 kN	Extreme Type l
14	P3	15 kN	2 kN	Extreme Type l
15	P4	15 kN	2 kN	Extreme Type l
16	P5	15 kN	2 kN	Extreme Type l
17	P6	15 kN	2 kN	Extreme Type l
18	Ea	70 GPa	7Gpa	Normal
19	Ew	8.75 GPa	1 Gpa	Normal
20	S	27 MPa	2.78 MPa	Normal

The maximum stress occurs in the middle cross-section M-M and is given by

$$\sigma = \frac{\left[\frac{\sum_{i=1}^{6} P_i(L-L_i)}{L} L_3 - P_1(L_2-L) - P_2(L_3-L_2)\right]\left[\frac{0.5AB^2 + \frac{E_a}{E_w}DC(B+D)}{AB+\frac{E_a}{E_w}DC}\right]}{\left\{\begin{array}{l}\frac{1}{12}AB^3 + AB\left\{\left[\frac{0.5AB^2 + \frac{E_a}{E_w}DC(B+D)}{AB+\frac{E_a}{E_w}DC}\right] - 0.5B\right\}^2 \\ + \frac{1}{12}\frac{E_a}{E_w}CD^3 \\ + \frac{E_a}{E_w}CD\left\{0.5D + B - \left[\frac{0.5AB^2 + \frac{E_a}{E_w}DC(B+D)}{AB+\frac{E_a}{E_w}DC}\right]\right\}^2\end{array}\right\}} \quad (34)$$

The response model is defined as the difference between the stress σ and the allowable stress (strength) *S* as below,

$$y = g(x) = S - \sigma \ . \tag{35}$$

The probability of failure p_f is defined by the probability of the strength less than the stress, i.e.,

$$p_f = \Pr(S - \sigma < 0) \tag{36}$$

Since there is no analytic solution for (36), we employed relatively large size Monte Carlo samples (n = 1,000,000) as a reference for comparison. From this Monte Carlo sample set, we found that $p_f = 2.45\times10^{-4}$. The saddlepoint approximation with an optimal LHS of n = 500 produces $p_f = 2.397 \times10^{-4}$. Accordingly, the probabilistic sensitivity (i.e., total sensitivity) is obtained with optimized LHS of n =500 using Eq. 6. The results are summarized in Figure 7.

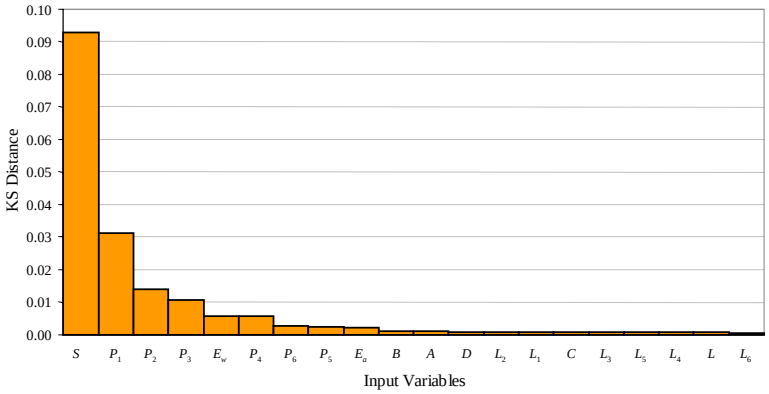

Figure 7. KS distance and ranking of input random variables.

From the chart, it is noted that the most important variable is the material strength, S (about 50% of the output variation is due to this variable). This is in agreement with an observation of Eq. (35) and the variability information in Table 1. The other important variables include P_1, P_2, P_3, E_w, and P_4.

CONCLUSION

A comprehensive uniform sample-based approach to probabilistic analysis and sensitivity analysis is presented in this work. The efficiency of the probabilistic sensitivity analysis is enhanced from several aspects.

First, the saddlepoint approximation approach is used to improve the efficiency as well as the accuracy for probabilistic analysis when generating the whole cumulative density functions to evaluate the importance of random input variables. The accuracy is maintained because the saddlepoint approximation yields extremely accurate probability estimation, especially in the tail area of a distribution. The approach is also efficient as it requires only the process of finding one saddlepoint without any integration and provides estimations of PDF and CDF simultaneously.

Second, for implementing the saddlepoint approximation approach, the uniform samples are used to replace the intensive Monte Carlo simulations. A combination of Latin Hypercube Sampling (LHS) and low discrepancy criterion known as uniform design is employed by optimizing the uniformity of samples in multidimensional space. Given that for finite samples LHS is never worse than Monte Carlo random samples, the advantages of using optimal LHS is more dramatic when sample size is small and the dimensionality is large.

Third, an efficient algorithm is developed for constructing the uniform designs. The new algorithm employs both an enhanced global search algorithm and a method for efficient evaluation of the uniformity criterion. The proposed algorithm to calculate CL_2 criterion cuts the computation time of other existing algorithms in this area from hours to minutes and seconds. That is, optimizing uniform designs using the CL_2 criterion is much more efficient to evaluate than other optimality criteria. The statistical tests indicate that the optimal designs constructed by our proposed algorithm have significantly better uniformity than randomly generated LHSs.

We demonstrated the utility of the proposed framework using an engineering example. In this paper, we use KS distance as the sensitivity measure. If desired, one may employ other sensitivity measures such as Kullback-Leibler divergence. This is subject to future research.

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