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Global Sensitivity Analysis Using an Auxiliary Variable Approach

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This paper develops a computational framework to assess the contribution of both aleatory and epistemic uncertainty sources towards the system response prediction. The probability integral transform is applied to distinguish and represent each uncertainty source explicitly, whether it is aleatory or epistemic. The resulting auxiliary variable facilitates building a deterministic function, so that global sensitivity analysis can be conducted to quantify the contribution of each uncertainty source in the prediction. The proposed framework is illustrated for two types of model inputs: random variable input and time series input, and this paper focuses more on the latter one which cannot be simply described by a probabilistic distribution. An autoregressive moving average (ARMA) model is chosen to represent the time series input due to its ability to capture both natural variability and epistemic uncertainty due to limited data.

Nomenclature

$\boldsymbol{\theta}_m$	=	set of model parameter
$\boldsymbol{X}$	=	vector of model inputs
ϵ_h	=	discretization error
$\delta(\boldsymbol{X})$	=	model discrepancy
$L(\boldsymbol{\theta}_m)$	=	likelihood function of $\boldsymbol{\theta}_m$
$f'(\boldsymbol{\theta}_m)$	=	prior distribution of $\boldsymbol{\theta}_m$
$\boldsymbol{\theta}_X$	=	distribution parameters
$\bar{X}$	=	constant term in the ARMA model
$\boldsymbol{\phi}$	=	coefficients of the AR model
$\boldsymbol{\theta}$	=	coefficients of the MA model
ϵ_t	=	random noise term at time t in the ARMA model
U	=	auxiliary variable
S	=	sensitivity index

I. Introduction

The uncertainty in system response is affected both by natural variability in the inputs and lack of knowledge or data (epistemic uncertainty). This paper focuses on assessing the contribution of each uncertainty source in the system response. Such sensitivity analysis is important for complicated systems where direct full-scale measurements of inputs and outputs may be sparse or impossible, and system response is predicted using computational models. Past work in uncertainty sensitivity analysis has mostly focused on aleatory inputs; this paper develops an approach to perform sensitivity analysis under both aleatory and epistemic uncertainties.

Consider a computational model $Y = F(\boldsymbol{\theta}_m; \boldsymbol{X})$ where $\boldsymbol{\theta}_m$ is a set of model parameters and $\boldsymbol{X}$ contains the model inputs. In case that this model is computationally expensive, we may use a surrogate model $S(\boldsymbol{\theta}_m; \boldsymbol{X})$ covering the domains of $\boldsymbol{\theta}_m$ and $\boldsymbol{X}$ to replace it. The surrogate models developed in the literature include polynomial response surface[1], polynomial chaos expansion[2], and Gaussian process model[3], etc. Due to limited training data, the output of a surrogate model can be stochastic, which brings uncertainty in the prediction. This paper uses the GP surrogate model.

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Before predicting the system response at a given model input $\boldsymbol{X} = \boldsymbol{x}$, the computational model needs two corrections due to: 1) the error in solving the computational model; 2) the model discrepancy between the computational model and the real physics. Additional prediction uncertainty is introduced if these corrections are stochastic. A common example for the first correction happens when the computational model is a finite element (FE) model and its solution has discretization error ϵ_h due to coarse mesh. The Richardson extrapolation (RE)[4] method computes the value of ϵ_h at a given model input and gives a deterministic correction to the FEA model. A method computing ϵ_h using Gaussian process (GP) model has also been developed[5] to overcome the limitations of Richardson extrapolation, and it gives a stochastic correction since the prediction of a GP model is a Gaussian distribution $\epsilon_h(\boldsymbol{X}) \sim N(\mu_h(\boldsymbol{X}), \sigma_h(\boldsymbol{X}))$ at fixed model input. The model discrepancy $\delta(\boldsymbol{X})$ in the second correction represents the difference between the computational model and the real system even if the computational model is solved correctly. The model discrepancy is input-dependent, and Kennedy and O'Hagan[6] represent it by another GP model; thus the correction due to model discrepancy is also stochastic at a given model input.

In the discussions above, the discretization error and model discrepancy depends on $\boldsymbol{X}$ rather than $\boldsymbol{\theta}_m$ since for the same system model inputs change over experiments while model parameters are unknown but fixed. The unawareness on the values of $\boldsymbol{\theta}_m$ brings the epistemic parametric uncertainty in model prediction. In this paper, Bayesian inference is used to quantify the epistemic uncertainty in $\boldsymbol{\theta}_m$. The Bayesian inference computes the posterior distribution of $\boldsymbol{\theta}_m$ as $f''(\boldsymbol{\theta}_m) \propto L(\boldsymbol{\theta}_m) f'(\boldsymbol{\theta}_m)$, where the likelihood function $L(\boldsymbol{\theta}_m)$ is constructed using observed data, and the prior distribution $f'(\boldsymbol{\theta}_m)$ reflects the subjective knowledge of the uncertainty in $\boldsymbol{\theta}_m$ before any observation. The resultant posterior distribution can be conveniently propagated to the system response prediction. Methods dealing with non-pairwise point data and interval data by Bayesian inference are also developed[7].

So far, our discussion is limited to a given model input $\boldsymbol{X} = \boldsymbol{x}$ for prediction, and the prediction can be expressed as $Y = S(\boldsymbol{\theta}_m; \boldsymbol{x}) + \epsilon_h(\boldsymbol{x}) + \delta(\boldsymbol{x})$. The prediction Y is stochastic due to the uncertainty in the three terms on the right hand side. Practically, the distribution of Y at given $\boldsymbol{\theta}_m$ is first computed, and the unconditional or predictive distribution of Y can be obtained by:

$$f_Y(y) = \int f_Y(y|\boldsymbol{\theta}_m) f''(\boldsymbol{\theta}_m) \mathrm{d}\boldsymbol{\theta}_m \tag{1}$$

An important observation is that so far all the uncertainty sources in system prediction are epistemic: whenever the GP model or any other surrogate model is used to replace the computational model or represent error terms, its uncertainty can be reduced by using more training points; and the uncertainty in $\boldsymbol{\theta}_m$ can also be reduced by using more observed data. As their uncertainty reduced, the uncertainty in Y caused by these uncertainty sources also decreases.

The prediction of system response becomes more complicated if the model input $\boldsymbol{X}$ for prediction is not a fixed value but stochastic. This happens when the overall performance of the system covering the whole domain of model inputs is of interest. Both aleatory and epistemic uncertainties may contribute to the uncertainty in model inputs.

If a model input X is a random variable, its natural variability, which is aleatory, can be represented by a probability distribution (such as uniform or Gaussian distribution, etc.) with distribution parameters $\boldsymbol{\theta}_X$ (mean value and variance for Gaussian distribution). With a large number of observations of X, $\boldsymbol{\theta}_X$ can be precisely estimated by the techniques such the method of moments , and the method of maximum likelihood[8], etc. If only finite observations are available, there is uncertainty in the estimation of $\boldsymbol{\theta}_X$. This distribution parameter uncertainty is also referred as statistical uncertainty[8] or second-order uncertainty[9]. Therefore, the total uncertainty in model input X contains two parts: aleatory natural variability and epistemic distribution parameter uncertainty. Here we assume that the distribution type of X is known.

If the model input X is not a random variable but a time series, the prediction of system response Y requires the values of X over all the time steps. For instance, in fatigue damage diagnosis, the crack growth or fatigue life depends on the detailed load history[10], i.e., the value of load at each cycle or time step. In the context of linear-elastic fracture mechanics, the well-known Paris' law[11] and Wheeler's retardation model[12] are often used to predict the final crack length as a sequentially cumulative effect due to loading at each cycle. As the random variable input is represented by a probabilistic distribution, two types of time domain methods have been developed to model the time series input using observed data: cycle counting methods and random process methods. The cycle counting methods captures the natural variability of time series input, but ignore the epistemic uncertainty due to limited data. This paper applies a random process method, i.e., the autoregressive moving average (ARMA)[16] model to represent and simulate the time series input by including both aleatory and epistemic uncertainty.

The ARMA model is a combination of the autoregressive (AR) and moving average (MA) models. ARMA(p, q) model assumes that the input at current time step is a linear combination of 1) its past p values; and 2) the current and past q values of noises:

$$X_t = \bar{X} + \sum_{i=1}^{p} \phi_i X_{t-i} + \epsilon_t + \sum_{j=1}^{q} \theta_j \epsilon_{t-j} \quad (2)$$

where X_t and X_{t-i} are the inputs at time step t and time step $t-i$; $\boldsymbol{\phi} = \{\phi_1, \dots, \phi_p\}$ are the coefficients of the AR model; $\boldsymbol{\theta} = \{\theta_1, \dots, \theta_q\}$ are the coefficients of the MA model; $\bar{X}$ is a constant but not the mean value over time since the mean value is actually $\mu = \bar{X} / \sum_{i=1}^{p} \phi_i$; ϵ_t and ϵ_{t-j} are the random noise terms at time step t and time step $t-j$; all the random noise terms are independent and identically distributed normal variable $N(0, \sigma_\epsilon^2)$, and these noise terms represent the natural variability of the ARMA model.

To build an ARMA model, the values of its orders p and q are first identified by matching the sample autocorrelation function and sample autocorrelation function computed from observe time series data to the theoretical pattern of ARMA(p, q) model. The Ljung-Box Q statistic[17] can be used to measure the adequacy of the matching.

In contrast to the cycle counting methods where the counting matrix is deterministic, epistemic uncertainty in building an ARMA model due to limited time series data can be captured by assuming the ARMA parameters – $\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, \sigma_\epsilon$ – as random variables. Non-informative uniform prior distributions may be assumed for each parameters. Bayesian inference updates the distributions of ARMA parameters using observed data. The likelihood function in Bayesian inference is[18]:

$$L\left(\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, p, q, \sigma_\epsilon\right) \approx (2\pi\sigma_\epsilon^2)^{-\frac{(n-p)}{2}} \exp\left(-\frac{1}{2\sigma_\epsilon^2} \sum_{t=p+1}^{n} \epsilon_t^2\right) \quad (3)$$

where $\epsilon_t = X_t - \bar{X} - \sum_{i=1}^{p} X_{t-i} - \sum_{j=1}^{q} \epsilon_{t-q}$ is the value of the noise term at time step t. Eq. (3) is an approximation in which ϵ_t is calculated from $t = p + 1$ and the values of the q initial error terms are arbitrarily fixed[18].

Thus, both issues of 1) identifying the uncertainty sources in the response prediction of an engineering system, and 2) classifying all the uncertainty sources into aleatory or epistemic uncertainty have been addressed, as shown in Table 1. It is observed that the uncertainties in model prediction are epistemic except for the natural variability in model input. The rest of this paper will focus on the overall objective of quantitatively assessing the contribution of each uncertainty source.

Table 1. Uncertainty sources in system response prediction

Variable/Error term	Variables	Uncertainty source	Aleatory/Epistemic
Solution approximation	$S(\boldsymbol{\theta}_m; \boldsymbol{X})$	Use of surrogate model	Epistemic
Solution approximation	$\epsilon_h(\boldsymbol{X})$	Discretization error	Epistemic
Model form error	$\delta(\boldsymbol{X})$	Discrepancy between math model and reality	Epistemic
Model parameter	$\boldsymbol{\theta}_m$	Limited calibration data	Epistemic
Random variable input	$\boldsymbol{\theta}_X$	Limited data on input variable	Epistemic
	X given $\boldsymbol{\theta}_X$	Input natural variability	Aleatory
Time series input by ARMA model	$\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, \sigma_\epsilon$	Limited time series data	Epistemic
	ϵ_t	Natural variability in time series input	Aleatory

In some cases a family of PDFs can distinguish the contributions of different uncertainty sources in prediction, shown in Figure 1. However, this is only a qualitative representation; while a quantitative assessment is needed to distinguish the contributions of multiple aleatory and epistemic uncertainty sources, and to guide activities to reduce the uncertainty in prediction.

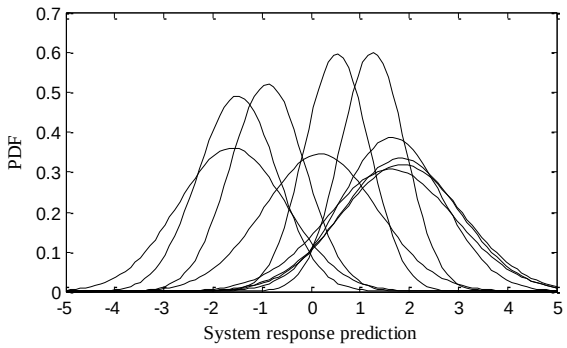


Figure 1. Family of PDFs

The discussions above leads to the main contribution of this paper, i.e., explicitly calculate the individual contribution of each uncertainty source towards the uncertainty in system response prediction. The methods of global sensitivity analysis[19] and auxiliary variable[20] are used for this purpose. In the following sections, Section II introduces the global sensitivity analysis briefly and explains the method of auxiliary variable in detail, and assesses the contribution of each uncertainty source in the case of random variable inputs. Section III extends this method to time series input. Section IV provides a numerical example with time series input.

II. Contribution assessment with random variable input

A. Global sensitivity analysis

The basic objective of sensitivity analysis is to assess the relative contribution of various model inputs to the uncertainty of model output. Global sensitivity analysis[19], which is needed for this assessment, requires a deterministic function $Y = F(\boldsymbol{X})$ where $\boldsymbol{X} = \{X_1, \dots, X_k\}$ is a vector containing all the model inputs. Here the model inputs are all random variables. The function is deterministic if a given realization of $\boldsymbol{X}$ gives to a single realization of Y. The importance of an input X_i is intuitively assessed by fixing it at a particular realization x_i and observing the conditional variance $V_{X_{\sim i}}(Y|X_i = x_i)$ where $X_{\sim i}$ represents all the inputs other than X_i. This conditional variance is a measurement of the importance of X_i, i.e., smaller $V_{X_{\sim i}}(Y|X_i = x_i)$ indicates greater importance of X_i. The dependence of this measurement on the position of X_i is removed by taking average of $V_{X_{\sim i}}(Y|X_i = x_i)$ over the distribution of X_i, and the result is denoted as $E_{X_i}(V_{X_{\sim i}}(Y|X_i))$, which can be simplified as $E(V(Y|X_i))$. Since the law of total variance proves that $V(Y) = E(V(Y|X_i)) + V(E(Y|X_i))$, a larger $V(E(Y|X_i))$ equally indicates a greater importance of X_i. Then a first-order sensitivity index is defined as:

$$S_i = \frac{V\big(E(Y|X_i)\big)}{V(Y)} \tag{4}$$

S_i is a number between 0 and 1 since $V(Y) \geq V(E(Y|X_i)) > 0$, and a higher value of S_i indicates more importance of X_i. $V(E(Y|X_i))$ is denoted as V_i in the following discussion.

The joint effect of X_i and X_j can be measured by $V_{ij}^c = V(E(Y|X_i, X_j))$. If X_i and X_j are uncorrelated, as V_i indicates the first-order effect by X_i alone, a second-order effect V_{ij} is defined to measure the interaction effect between X_i and X_j:

$$V_{ij} = V_{ij}^c - V_i - V_j \tag{5}$$

Similarly, higher-order effect is obtained by subtracting lower-order effect from the joint effect. Sobol's variance decomposition theorem[21] proved that if all the model inputs are uncorrelated, the sum of all the first-order and higher-order effects adds up to the total variance $V(Y)$:

$$V(Y) = \sum_i V_i + \sum_{i<j} V_{ij} + \sum_{i<j<m} V_{ijm} + \cdots + V_{12\dots k} \tag{6}$$

Dividing both sides of Eq. (7) by $V(Y)$, we get:

$$1 = \sum_i S_i + \sum_{i<j} S_{ij} + \sum_{i<j<m} S_{ijm} + \cdots + S_{12\dots k} \tag{7}$$

Eq. (7) defines the sensitivity index at each order, where the first-order index S_i is defined as shown in Eq. (4). S_i assesses the contribution of X_i by itself; and other higher-order indices (such as S_{ijm}) assess the contribution of the interaction of the inputs included in the subscripts (S_{ijm} measures the contribution of the interaction by X_i, X_j and X_m together).

The total effects index S_i^T for X_i is defined as the sum of all the terms in Eq. (7) including the index i, i.e., the total contribution of X_i by itself and through interaction with other inputs. The S_i^T can be computed as:

$$S_i^T = 1 - \frac{V\big(E(Y|X_{-i})\big)}{V(Y)} \tag{8}$$

An important observation is that the definition of the first-order index S_i only requires a deterministic function, so it is an informed choice whether the model inputs are correlated or not[22]. In contrast, Sobol's decomposition in Eq. (7) requires uncorrelated model inputs, so the total effects index S_i^T is only meaningful for uncorrelated model inputs[22].

B. Auxiliary variable and global sensitivity with random variable input

The auxiliary variable method was developed by Sankararaman and Mahadevan[20] to distinguish the contribution of aleatory natural variability and epistemic distribution parameter uncertainty in a random variable X. The distribution

of X is conditioned on the value of its distribution parameter $\boldsymbol{\theta}_X$, which has uncertainty denoted by distribution $f(\boldsymbol{\theta}_X)$. The conditional distribution of X is denoted as $f_X(x|\boldsymbol{\theta}_X = \boldsymbol{\theta}_X^*)$. Based on the probability integral transform theorem[23], random sampling from this conditional distribution is realized by two steps: 1) define a variable U_X of standard uniform distribution $U(0,1)$ and generate its sample u_X, which is taken as the CDF value of X, and 2) obtain a sample of X by inversing the conditional CDF function $\mathcal{F}_X(x|\boldsymbol{\theta}_X = \boldsymbol{\theta}_X^*)$, i.e.:

$$x = \mathcal{F}_X^{-1}\left(u_X \middle| \boldsymbol{\theta}_X = \boldsymbol{\theta}_X^*\right) \tag{9}$$

The sample of U_X and the sample of X has one-to-one mapping, i.e., the value of X has been determined once the value of U_X is decided. The same procedure is repeated for another realization of $\boldsymbol{\theta}_X$. Note that the distribution of U_X is independent with the realization of $\boldsymbol{\rho}$, thus the natural variability in X is represented by U_X.

This standard uniform random variable U_X, which is the CDF value of $f_X(x|\boldsymbol{\theta}_X = \boldsymbol{\theta}_X^*)$, is named as auxiliary variable. With U_X, Eq. (9) actually builds a deterministic function required by the global sensitivity analysis, since a sample of $\boldsymbol{\theta}_X$ and a sample U_X leads to a deterministic value of X. While the resultant sensitivity indices of $\boldsymbol{\theta}_X$ assess the contribution of epistemic distribution parameter uncertainty, the sensitivity index of U_X assesses the contribution of natural variability of X.

The application of auxiliary variable can be easily extended to any variable whose distribution is conditioned on other variables. For the random variable $S(\theta_m; X), \epsilon_h(X)$ and $\delta(x)$ in Table 1 whose distribution is conditioned on the value of X and θ_m, auxiliary variables U_S, U_{ϵ_h} and U_δ can be introduce for each of them. In addition, auxiliary variable $\boldsymbol{U_X} = \{U_{X_1}, U_{X_2}, \dots, U_{X_n}\}$ is also introduced for each model input $X_i (i = 1 \text{ to } n)$. Thus a deterministic function suitable for global sensitivity analysis is built as:

$$Y = F\left(\boldsymbol{\theta}_X, \boldsymbol{\theta}_m, \boldsymbol{U_X}, U_S, U_{\epsilon_h}, U_\delta\right) \tag{10}$$

Note that no auxiliary variable is needed for $\boldsymbol{\theta}_X$ or $\boldsymbol{\theta}_m$ since their distributions are not conditioned on any other variables.

The flowchart in Figure 2 illustrates the application of Eq. (10). The resultant sensitivity indices of $\boldsymbol{\theta}_X$ assess the contributions of input parameter uncertainty in prediction; the indices of $\boldsymbol{\theta}_m$ assess the contributions of model parameter uncertainty; and the indices of auxiliary variables assess the contribution of the corresponding uncertainty sources, as shown in Table 1.

Note that Eq. (10) proposes a framework to assess the contribution of each uncertainty source with random variable input. If any uncertainty source is ignored in practice, this framework is still applicable by removing the corresponding variable in Eq. (10). For instance, if Richardson extrapolation is used to compute a deterministic discretization error and ignore the uncertainty in it, the auxiliary variable U_{ϵ_h} is not considered in Eq. (10).

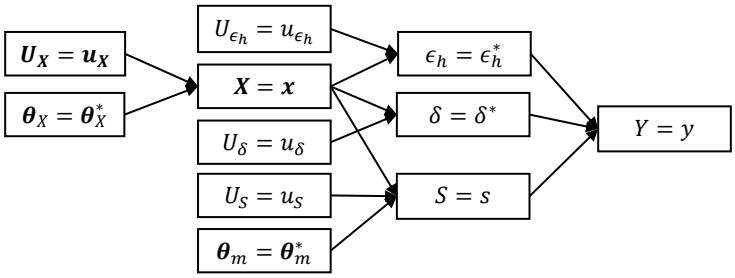


Figure 2. Deterministic function for random variable input

III. Contribution assessment with time series input

When time series input is represented using an ARMA model, the contributions of aleatory natural variability and epistemic model parameter uncertainty in the ARMA model towards the uncertainty in the prediction need to be assessed, in addition to the uncertainty sources considered in Eq. (10) . Here the auxiliary variable method is extended to assess the individual contributions of the uncertainty sources in the ARMA model. The deterministic function required by the global sensitivity analysis is:

$$Y = F\left(\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, \sigma_\epsilon, \boldsymbol{\theta}_m, U_S, U_{\epsilon_h}, U_\delta, U_\epsilon\right) \tag{11}$$

An evaluation of Eq. (11) is divided into six steps;

1. Generate a sample of the ARMA model parameters $\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, \sigma_\epsilon$ from their joint distribution. This joint distribution represents the epistemic parametric uncertainty in the ARMA model, and can be obtained by Bayesian inference using observed time series data.
2. Generate a sample of the physics model parameters $\boldsymbol{\theta}_m$.

3. Generate N_s time histories based on the samples of $\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, \sigma_\epsilon$ from Step 1. The difference between these time histories represents the natural variability in the ARMA model caused by the noise terms. By propagating each time history with the sample of $\boldsymbol{\theta}_m$through the stochastic surrogate model $S(\boldsymbol{\theta}_m; \boldsymbol{X})$, a family of N_s distributions can be constructed. Each distribution represents the effect of epistemic surrogate model uncertainty at a given time history, thus an auxiliary variable U_s is introduced to represent it; the spread of distributions is caused by different time histories thus represents the natural variability in the ARMA model, therefore another auxiliary variable U_ϵ is introduced to represent it.
4. A sample of U_s is generated to conduct CDF inversion at each distribution in the family of Step 3. The resultant N_s samples from the N_s distributions constitute a new distribution $f(S|U_S)$, representing the uncertainty in the surrogate model caused by the variation of N_s load histories (ARMA model natural variability). Then a sample of U_ϵ is generated to conduct CDF inversion at $f(S|U_S)$ to obtain a deterministic value of $S(\boldsymbol{\theta}_m; \boldsymbol{X})$.
5. If the discretization error $\epsilon_h(\boldsymbol{X})$ is stochastic (e.g., due to the use of a GP model) at a given time series input, each time history from Step 3 gives a distribution of discretization error, thus a family of N_s distributions can be constructed. An auxiliary variable U_{ϵ_h} is introduced to obtain a sample from each distribution and construct the distribution $f(\epsilon_h|U_{\epsilon_h})$. Since this uncertainty in the discretization error is also caused by the variation of the same N_s load histories, the same sample of U_ϵ from Step 4 is applied to conduct CDF inversion at $f(\epsilon_h|U_{\epsilon_h})$ and obtain a deterministic value of $\epsilon_h(\boldsymbol{X})$.
6. The same procedure as Step 5 is applied for $\delta(\boldsymbol{X})$ with auxiliary variables U_δ and U_ϵ, if $\delta(\boldsymbol{X})$ is stochastic for given time series input. As a family of N_s distributions are constructed, a sample of U_δ is used to obtain samples from each distribution and construct a distribution $f(\delta|U_\delta)$; the sample of U_ϵ gives a deterministic value of $\delta(\boldsymbol{X})$ by CDF inversion at $f(\delta|U_\delta)$.

Note that Eq. (11) is as flexible as Eq. (10). The corresponding variable in Eq. (11) can be removed if any uncertainty source is ignored.

IV. Numerical examples

Figure 3. Cantilever beam

Crack growth analysis in the cantilever beam shown in Figure 3 is considered for illustration of the proposed methodology. Assume an edge crack of length 0.03 inch has been initiated at the top surface close to the wall, and this crack grows under the time series loading of N_t cycles imposed at the free end of the beam. The objective is to assess the contribution of each uncertainty source in the prediction.

Two crack growth models with different fidelities are established. In the lower fidelity model, a finite element model with coarse mesh (Figure 4) is built using the commercial software ANSYS to compute the stress intensity factor K_s under load P and crack length A. The crack growth is computed by Paris' law:

$$\frac{\mathrm{d}A^l}{\mathrm{d}N}(P, A) = C\Delta K_s^m \tag{12}$$

In Eq. (12), ΔK_s is the range of stress intensity factor at one cycle; C and m are known constants; $\mathrm{d}A^l/\mathrm{d}N$ is the crack growth rate, and its magnitude is equal to the predicted crack growth ΔA^l in one cycle. In this example, there is no reversal in the direction of the loading and the stress ranges from zero to a finite value. Thus the K_s computed by the finite element model is equal to ΔK_s used in the Paris's law.

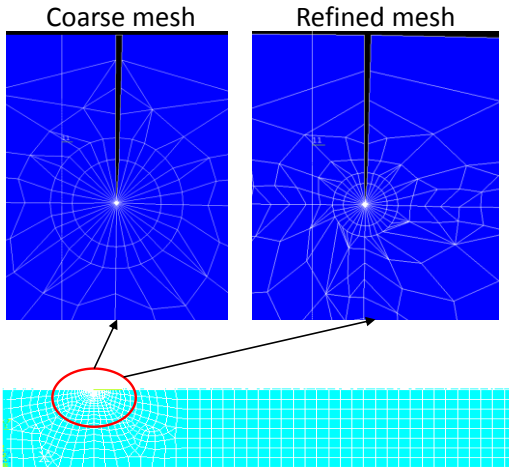


Figure 4. FEA model

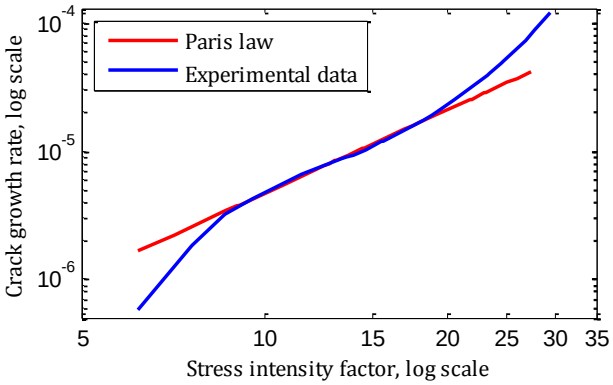


Figure 5. Paris law vs. Empirical curve

In the higher fidelity model, a finite element model with a finer mesh (Figure 4) is also built in ANSYS to compute ΔK_s. And the crack growth in one cycle $\Delta A^h\ (P, A)$ is not computed by Paris' law but based on an empirically observed curve (Figure 5) of crack growth rate vs. stress intensity factor range.

The difference between these two predictions is caused by two factors: 1) different stress intensity factors from the coarse mesh and fine mesh; 2) the deviation of Paris' law from the nonlinear part of the experimental data, which is shown in Figure 5. The first factor refers to model resolution, and the second factor refers to model fidelity.

The predicted crack growth by the high fidelity model is assumed to be the true value, and the low fidelity model is used as the prediction model in subsequent analysis. The difference between ΔA^h and ΔA^l is taken as model discrepancy $\delta(P, A)$ to correct the prediction model. 25 values of $\delta(P, A)$ for different loads and crack lengths are computed to train a GP model for $\delta(P, A)$, which computes the model discrepancy at arbitrary load and crack length. Therefore the crack growth prediction at the i-th cycle by the corrected model is:

$$\Delta A_i^c(P_i, A_{i-1}) = \Delta A_i^l(P_i, A_{i-1}) + \delta(P_i, A_{i-1}) \tag{13}$$

The subscripts in Eq. (13) indicate the cycle number. P_i is the load at the i-th cycle, and A_{i-1} is the crack length after the $(i-1)$-th cycle. Note that $\delta(P_i, A_{i-1})$ in Eq. (13) is Gaussian distribution given by GP model, thus $\Delta A_i^c(P_i, A_{i-1})$ is also a Gaussian distribution $\Delta A_i^c \sim N(\Delta A_i^l(P_i, A_{i-1}) + \mu_\delta(P_i, A_{i-1}),\ \sigma_\delta^2(P_i, A_{i-1}))$, where $\mu_\delta(P_i, A_{i-1})$ and $\sigma_\delta^2(P_i, A_{i-1})$ are the mean value and variance of $\delta(P_i, A_{i-1})$.

The final crack length is predicted by applying Eq. (13) at each cycle sequentially and using $A_i = A_{i-1} + \Delta A_i^c$. Rigorously, the crack growth in each cycle is stochastic so the starting crack length for each cycle is also stochastic. But this stochastic starting crack length will make the application of Eq. (13) tedious. Since this numerical example is mainly used to illustrate the proposed framework of contribution assessment, the crack length prediction is simplified by assuming A_i at each cycle has a Gaussian distribution $N\left(\mu_{A_i}, \sigma_{A_i}^2\right)$ and:

$$\mu_{A_i} = \mu_{A_{i-1}} + \Delta A_i^l\left(P_i, \mu_{A_{i-1}}\right) + \mu_\delta\left(P_i, \mu_{A_{i-1}}\right)$$
$$\sigma_{A_i}^2 = \sum_1^i \sigma_\delta^2\left(P_i, \mu_{A_{i-1}}\right) \tag{14}$$

where $\mu_{A_0} = a_0 = 0.03$ inch. Eq. (14) actually takes the mean value of ΔA_i^c in Eq. (13) as the crack growth and assumes that the variance of A_i is the summation of σ_δ^2 over i cycles.

First the uncertainty in the final crack length A_{N_t} is from the time series input represent by an ARMA model, including the natural variability in ARMA model and the epistemic uncertainty in ARMA parameters. Second for a given time series input, the uncertainty in A_{N_t} is from $\sigma_{A_i}^2$ in Eq. (14), which is the summation of the variance of model discrepancy in each cycle. So the deterministic function required in global sensitivity analysis is:

$$A_{N_t} = F(\bar{X}, \boldsymbol{\phi}, \boldsymbol{\theta}, \sigma_\epsilon, U_\delta, U_\epsilon) \tag{15}$$

Eq. (15) does not include U_S and U_{ϵ_h} since their corresponding uncertainty sources are not considered in this example. The evaluation of Eq. (15) follow the steps in Section III.

Figure 6 shows a synthetic time history generated as observed data. The loading at each cycle includes a maximum value and a minimum value. Figure 6 only shows the minimum value at each cycle since the maximum values are assumed to be zero.

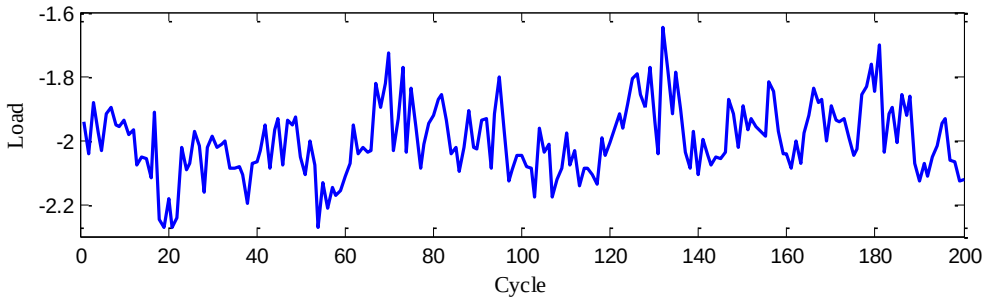


Figure 6. Synthetic time series data

An ARMA(2, 2) model is selected to model the time series input. The parameters of the ARMA(2, 2) model are $\bar{X}$, $\boldsymbol{\phi} = \{\phi_1, \phi_2\}$, $\boldsymbol{\theta} = \{\theta_1, \theta_2\}$ and σ_ϵ. Prior distributions are assumed for the ARMA model parameters, and posterior distributions are attained from Bayesian calibration using Markov Chain Monte Carlo (MCMC) sampling. The posteriors of some ARMA parameters were found to be highly correlated; for example, the correlation between ϕ_1 and ϕ_2 is -0.8. The correlation of ARMA parameters has a significant influence on assessing the contribution of each uncertainty source, which will be shown later.

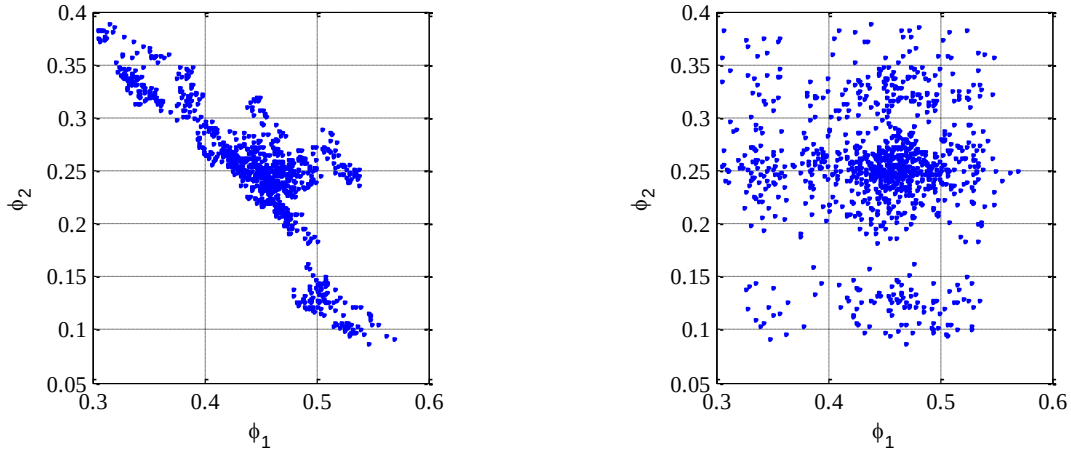
Two results of global sensitivity analysis are shown in Table 2. One result only uses the marginal distributions of the parameters and ignores the correlations, and another result correctly considers the correlations. Only the first-order indices are reported since the total effects indices are not applicable for correlated variables.

Table 2. Global sensitivity analysis results

	First-order indices	
	Correlation ignored	Correlation considered
$\bar{X}$	0.071	0.001
ϕ_1	0.269	0.008
ϕ_2	0.668	0.011
θ_1	0.000	0.003
θ_2	0.000	0.001
σ_ϵ	0.000	0.005
U_δ	0.001	0.642
U_K	0.001	0.004

The indices in Table 2 indicate the impact of ARMA parameter correlation in assessing the contribution of each uncertainty source. The result ignoring correlation misleads us to take ϕ_1 and ϕ_2 as the dominant factors, while actually their contribution reduces significantly when the correlation is considered. The reason for this overestimation can be revealed by the scatter plot in Figure 7: the scatter width of ϕ_1 and ϕ_2 is much narrower due to the correlation of -0.8 between them, so the uncertainty caused by them in the prediction is reduced significantly. The uncertainty in

model discrepancy represented by U_δ is the dominant uncertainty source. This means that more training points for the GP model of the model discrepancy are required to reduce the uncertainty in final crack length prediction.



(a) Correlation = -0.8 **(b) Correlation removed**

Figure 7. Scatter plot of ϕ_1 and ϕ_2

Conclusion

Various uncertainty sources arise at different steps in the prediction of the system response, including input variability, model parameter uncertainty, limited data, surrogate model uncertainty, and various model errors. These uncertainty sources are categorized as aleatory and epistemic uncertainty. Quantitative assessment of the contribution of each uncertainty source is needed to facilitate efforts to reduce prediction uncertainty by obtaining more information.

In this paper, the auxiliary variable method helps to include each uncertainty source explicitly in the global sensitivity analysis. Two types of model input are considered in this paper: random variable input and time series input. The random variable input can be described as a probabilistic distribution, so its epistemic uncertainty is represented by the distribution of its distribution type and parameters, and an auxiliary variable is introduced to represent its natural variability. The ARMA model is chosen to model the time series input in this paper. The ARMA parameter distributions represent the epistemic uncertainty in the time series input due to limited data, and an auxiliary variable is used to represent the natural variability in time series input. When considering model uncertainty sources, the auxiliary variable represents the epistemic uncertainty introduced by these sources. Thus the proposed approach has the flexibility to represent various types of uncertainty sources and include them in sensitivity analysis. This helps to prioritize uncertainty reduction activities such as testing and model refinement.

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