

An extended polynomial chaos expansion for PDF characterization and variation with aleatory and epistemic uncertainties

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Abstract

This paper presents an extended polynomial chaos formalism for epistemic uncertainties and a new framework for evaluating sensitivities and variations of output probability density functions (PDF) to uncertainty in probabilistic models of input variables. An "extended" polynomial chaos expansion (PCE) approach is developed that accounts for both aleatory and epistemic uncertainties, modeled as random variables, thus allowing a unified treatment of both types of uncertainty. We explore in particular epistemic uncertainty associated with the choice of prior probabilistic models for input parameters. A PCE-based Kernel Density (KDE) construction provides a composite map from the PCE coefficients and germ to the PDF of quantities of interest (QoI). The sensitivities of these PDF with respect to the input parameters are then evaluated. Input parameters of the probabilistic models are considered. By sampling over the epistemic random variable, a family of PDFs is generated and the failure probability is itself estimated as a random variable with its own PCE. Integrating epistemic uncertainties within the PCE framework results in a computationally efficient paradigm for propagation and sensitivity evaluation. Two typical illustrative examples are used to demonstrate the proposed approach.

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1. Introduction

Dealing with uncertainty in model-based inference has been addressed with much attention in recent decades [1,2]. Uncertainty quantification (UQ) is the rational process of managing the interplay between data, models and decisions and involves steps of collecting data, constructing physics and probabilistic models, estimating their parameters, predicting quantities of interest, and updating the parameters of the models [3]. While Bayesian logic provides a rigorous foundation for updating model parameters, it is predicated on data being available for update. An assessment of the worth of information can be made prior to data acquisition by integrating over all possible data, within a Bayesian framework [4]. This approach is computationally prohibitive without considerable assumptions concerning the likelihood function [5]. This paper presents an alternative approach to assessing the significance of additional information concerning model parameters on the credibility of the probability density function of

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prediction variables. Additional information about the parameters is construed as modifying the parameters in the prior probability models (for instance, shape parameters in a Beta distribution, or coefficients in the PC model), while credibility of the PDF is interpreted as statistical scatter of the PDF, viewed as a statistic. In this paper, we construct a functional representation of the output PDF in terms of the uncertainty in the PDF of input parameters. We express this functional form in a polynomial chaos expansion, and use the directional sensitivities to quantify the effect of perturbing various statistical parameters from their current values.

Uncertain input parameters are usually modeled as random variables with specified prior models for their probability distributions. Estimating parameter values for these distributions is challenged, both numerically and conceptually, by model errors and measurement errors [6]. Insightful prior probabilistic models are important both as key ingredients of Bayesian updating and for the purpose of articulating prior knowledge in a useful format. Prior models are also crucial from a practical perspective, since in many settings data is not readily available, and prior models that are sufficiently robust to account for current knowledge are the only recourse for probabilistic inference. Emphasizing current knowledge, however, can hamper scientific discovery, and attempts to widen their scope have been pursued in the guise of epistemic uncertainty and model error [7]. Model parameters within each model class, when inferred from data, are typically described as random variables with a probabilistic structure that depends both on the model class and on the data. Sources of uncertainty can be generally classified into aleatory (or data) uncertainty and epistemic (or approximation) uncertainty [7]. Aleatory uncertainty typically refers to irreducible variabilities inherent in nature and is traditionally treated using random variables or random fields. Epistemic uncertainty, on the other hand, is usually reduced to within bounds, by acquiring more data and accordingly revising the predictive model. A variety of approaches focusing on modeling and propagating epistemic uncertainty has been proposed in the literature exploring both revisions to physics models and to uncertainty model for the parameters. For example, Helton J.C. represents epistemic uncertainty using evidence theory and implemented into Monte Carlo procedures [8]. Valdebenito M.A. applied intervening variables to quantify epistemic uncertainty based on the first-order Taylor expansion [9]. Jacquelin E. treated the uncertain inputs as random and fuzzy variables and the response is also described by fuzzy approach [10]. In this paper, we tackle the epistemic uncertainty associated with the choice of probabilistic model for input parameters.

The aleatory or epistemic nature of uncertainty is relative to the choice of predictive model, which includes both the physics and probabilistic models. Once these models have been selected, however, the aleatory/epistemic distinction becomes meaningful, and types are typically involved in any given problem. A common approach has been to segregate these two types of uncertainties and perform nested iterations, with aleatory analysis on the inner loop and epistemic analysis on the outer loop [11]. In this manner, the two types of uncertainties can be separated and easily traced. Specifically, each particular instance of the epistemic variables generates a response PDF based only on the aleatory uncertainties. The family of PDFs thus evaluated at many instances of the epistemic variables can be used to visualize the combined uncertainty in the response and further interpret the results using various statistical metrics. This paradigm, while conceptually simple, is computationally prohibitive. In this paper, we preserve the conceptually appealing uncertainty segregation for purposes of visualization and interpretation [12], and enhance its computational efficiency through novel stochastic polynomial chaos representations (PCE) that provide a uniform treatment of aleatory and epistemic uncertainties. PCE is an uncertainty quantification method that has been widely used in many areas across science and physics [13–16]. Conventionally, mostly dealing with aleatory uncertainty, PCE has demonstrated robustness and computational efficiency. As for epistemic uncertainty quantification applications, PCE has been applied in the context of multi-uncertainty modeling [17,18] and global sensitivity analysis [19]. Besides, PCE has been integrated within some frameworks as a surrogate model, including interval methods [9,20], fuzzy set theory [21], evidence theory [22].

A key idea in the present paper is to treat the coefficients in an aleatory PCE as random variables whose uncertainty encodes epistemic uncertainty, which is itself described as random variables independent of the aleatory ones. A PCE is then carried out relative to the epistemic variables. In view of the polynomial structure of PCE, this two-step expansion can be implemented as a single PCE in higher-dimension. This approach was already present in developing sampling distribution for PCE representations [23] and carrying out associated Bayesian updating [24–27]. In this work, the propagation of epistemic uncertainty to the PDF of the quantity of interest is assessed.

Operationally, as new information is acquired, the probabilistic models (or parameters of these models, referred to herein as “statistical parameters”) of the input variables should be updated. As a result, the change in response

PDF resulting from the update in statistical input parameters, namely the sensitivity of response PDF with respect to statistical parameters of model inputs, is relevant for risk assessment, reliability analysis, model verification and validation. A simple idea is to treat the statistical parameters of input before and after update as two separate UQ problems and to solve them separately. This would entail two separate stochastic forward propagations of uncertainty each requiring significant computational resources, with no clear path for sharing the computational burden between the two tasks. This “sensitivity” relative to epistemic uncertainty is substantially more taxing, numerically, than standard sensitivity formulations [28,29]. This cost is the greater if the sensitivity of the PDF itself is sought, and not merely the sensitivity of the variance-based (or Sobol) and the moment-independent indices [30]. Recent works discussing the evaluation of sensitivity measures in multi-uncertainty problems include using the variance decomposition of the logarithm of the conditional failure probability [19], combining importance sampling and importance splitting methods with Sobol indices [31], and applying the Kriging method to compute conditional expectation of failure probability [32]. The aforementioned approaches are all based on conditional probabilities. In this paper, we construct a composite map from statistical parameters to PDF of QoI, by integrating a PCE of the QoI within a kernel density estimate (KDE) of that QoI’s PDF. We demonstrate the value of this map for both propagating epistemic uncertainty and evaluating PDF sensitivity relative to these uncertainties.

The objective of this work is thus twofold. First we provide a coherent framework to simultaneously model aleatory and epistemic uncertainties and propagate the influence of both uncertainties to the predicted response in a computationally efficient manner. Second, we develop a framework for efficiently evaluating the sensitivity of probability density functions (PDF) of output quantities relative to both aleatory and epistemic variables. The remainder of the paper is structured as follows. Section 2 reviews the conventional PCE approach and Section 3 presents the extended PCE approach that takes into account simultaneous aleatory and epistemic uncertainties. Section 4 describes the framework of quantifying the influence of aleatory and epistemic uncertainties on several response metrics. Section 5 applies the framework to an analytical and a numerical illustrative example. Section 6 presents the conclusions and some closing comments.

2. Polynomial chaos expansion

Let X represent a scalar QoI that can be expressed as a function of a vector $\mathbf{k} = \{k_1, \dots, k_d\}$ in $\mathbb{R}^d$ representing physical random parameters. The d -dimensional vector $\mathbf{k}$ is first expressed as a mapping from a d -dimensional vector $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_d\}$ of uncorrelated standard normal random variables using, for instance, the Rosenblatt transformation. The set $\boldsymbol{\xi}$ is referred to as the “germ” of the PCE. Expressing X as a function of $\boldsymbol{\xi}$ in the form $X(\boldsymbol{\xi})$ and representing $X(\boldsymbol{\xi})$ in an orthogonal polynomial expansion with respect to $\boldsymbol{\xi}$ yields the polynomial chaos expansion (PCE) of X relative to $\boldsymbol{\xi}$,

$$X(\boldsymbol{\xi}) = \sum_{|\boldsymbol{\alpha}| \leq p} X_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) \quad (1)$$

where $\{X_{\boldsymbol{\alpha}}\}$ are called PCE coefficients; p denotes the highest order in the polynomial expansion; $\boldsymbol{\alpha}$ is a d -dimensional multi-index, and $\{\psi_{\boldsymbol{\alpha}}\}$ denotes normalized multivariate Hermite polynomials that can be expressed in terms of their univariate counterparts as follows,

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{p=1}^d \psi_{\alpha_p}(\xi_p) = \prod_{p=1}^d \frac{h_{\alpha_p}(\xi_p)}{\sqrt{\alpha_p!}}, \quad \boldsymbol{\xi}, \boldsymbol{\alpha} \in \mathbb{R}^d \quad (2)$$

where, h_{α_p} represents the one-dimensional Hermite polynomial of order p . The collection of the multivariate polynomials forms an orthogonal set with respect to the multivariate Gaussian density function.

In order to emphasize its dependence on the PCE representation, we denote the realization of X synthesized from its PCE using sample $\boldsymbol{\xi}^{(i)}$ of $\boldsymbol{\xi}$ by,

$$X^{(i)} \triangleq X(\boldsymbol{\xi}^{(i)}, \{X_{\boldsymbol{\alpha}}\}) = \sum_{|\boldsymbol{\alpha}| \leq p} X_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{(i)}). \quad (3)$$

The PCE coefficients $X_{\boldsymbol{\alpha}}$ are estimated using quadrature approximations to multidimensional integrals as follows,

$$X_{\boldsymbol{\alpha}} = \sum_{q \in Q} X(\boldsymbol{\xi}^q) \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^q) w_q, \quad |\boldsymbol{\alpha}| \leq p, \quad (4)$$

where, Q is the set of sparse quadrature points, q is a quadrature node in Q and w_q is the associated weight. The quadrature level required to achieve a preset accuracy in approximating any X_α increases with the order of the associated polynomial, ψ_α . For a given polynomial order p and germ dimension d , the number of these PCE coefficients, denoted by N_c , is equal to,

$$N_c = \frac{(d+p)!}{d! p!}. \quad (5)$$

3. Extended polynomial chaos expansion for mixed aleatory and epistemic uncertainties

Clearly, the numerical value of X_α depends both on the mapping from $\mathbf{k}$ to X , and the mapping from ξ to $\mathbf{k}$. The former mapping encapsulates physics models and governing equations while the latter mapping describes the probabilistic model of the physical parameters $\mathbf{k}$, in a functional form that explicitly relates them to a set of independent Gaussian random variables ξ . Uncertainty in the probabilistic model of $\mathbf{k}$ is propagated into uncertainty about X through the composite map from $\mathbf{k}$ to ξ and ξ to X .

We introduce the m -dimensional vector $\mathbf{P} = \{P_1, \dots, P_m\}$ representing all the statistical parameters of the input random variables $\mathbf{k}$. These parameters are typically estimated based on a finite sample. Different estimation methods yield different probabilistic models for $\mathbf{P}$ with the Maximum Likelihood estimates (MLE) generally yielding an asymptotically (for large sample size) Gaussian distribution with variance that is inversely proportional to sample size. We represent the random vector $\mathbf{P}$ in a polynomial chaos decomposition relative to a new Gaussian germ ρ independent of ξ . Motivated by asymptotic results concerning MLE sampling distributions, we limit this PCE to a first order expansion, resulting in a Gaussian model for $\mathbf{P}$. We also assume a one-dimensional PCE representation for $\mathbf{P}$, imposing a strict dependence between the different P_i , making them all linear transformations of the same scalar random variable ρ . This statistical dependence between components of $\mathbf{P}$ is justified by the observation that experimental evidence that influences our estimate of any one of the P_i 's is likely to also affect our estimates of all other components of $\mathbf{P}$. We thus introduce ρ as a standard normal random variable independent of $\xi = \{\xi_1, \dots, \xi_d\}$, and express the parameters of the input PDFs, P_i , in the form,

$$P_i = \mu_{P_i} + \sigma_{P_i} \rho, \quad i = 1, \dots, N_P, \quad (6)$$

where μ_{P_i} is the mean of P_i , and σ_{P_i} its standard deviation. Also, N_P denotes the number of parameters from the set $\mathbf{P}$ that is presumed to be uncertain.

Thus, X can be represented as a function of a new germ $\eta = \{\xi_1, \dots, \xi_d, \rho\}$, and is therefore denoted as $X(\eta)$. The extended polynomial expansion of X can thus be expressed as,

$$X(\eta) = \sum_{\substack{\gamma \in \mathbb{R}^{d+1} \\ |\gamma| \leq p}} X_\gamma \psi_\gamma(\eta), \quad \eta \in \mathbb{R}^{d+1} \quad (7)$$

where $\{X_\gamma\}$ denotes the PCE coefficients. Making use of Eq. (2), we can separate the dependence on ξ from the dependence on ρ , resulting in the following useful representation,

$$X(\eta) = X(\xi, \rho) = \sum_{\substack{\alpha \in \mathbb{R}^d, \beta \in \mathbb{R} \\ |\alpha| + |\beta| \leq p}} X_{\alpha\beta} \psi_\alpha(\xi) \psi_\beta(\rho), \quad \xi \in \mathbb{R}^d, \quad \rho \in \mathbb{R}, \quad (8)$$

with the subscript $\alpha\beta$ being a $d+1$ multi-index formed as the concatenation of α and β . It is consistent with common views [6–8,10,23–25] to construe dependence on ξ and ρ to represent, respectively, aleatory and epistemic uncertainties. Eq. (7) provides a joint and uniform representation of these two uncertainties in a single representation. It is worth mentioning that the extension of the foregoing to the case where each P_i is decomposed according to its own stochastic dimension ρ_i can be readily accommodated, with some increase in computational cost. This higher parameterization, however, is not necessarily more physical or more accurate. Indeed, all stochastic parameters can be viewed as depending on the same microstructure with the random parameter ρ identifying the particular microstructure being investigated. For instance, ρ could refer to such microstructure properties as the size of the largest impurity, or the magnitude of the largest contrast between elastic moduli, or the theoretical distance between upper and lower bounds on local elastic properties.. The linear dependence of P_i on ρ would then necessitate small sensitivity of the probabilistic parameters to perturbation in the microstructure. This linear dependence could be

relaxed by pursuing a higher-order PC expansion in Eq. (6). Our present formulation is restricted to capturing the influence of uncertainty in parameters of the input PDF, and does not account for model error which is a key component of epistemic uncertainty.

4. Quantification of aleatory and epistemic uncertainties

In Sections 4.1 and 4.2 we first introduce two key ingredients for constructing the composite map from input parameters to PDF of QoI and for evaluating sensitivities across this map. We then demonstrate the application of these tools to quantifying changes in these PDFs.

4.1. Representation of PDF: Kernel Density Estimation (KDE)

We will be mainly interested in quantifying the influence of input parameter uncertainties on the probability density function (PDF) of quantities of interest. We rely on Kernel Density Estimates (KDE) to represent these PDFs [33]. The PDF of X (the QoI), denoted by $f_X(x)$ and KDE of the PDF, denoted by $\hat{f}_X(x)$, can be expressed as,

$$f_X(x) \triangleq \hat{f}_X(x) = \frac{1}{Nh} \sum_{j=1}^N K\left(\frac{x - X^{(j)}}{h}\right) \quad (9)$$

where we recall that,

$$X^{(j)} = \sum_{|\gamma| \leq p} X_\gamma \psi_\gamma(\eta^{(j)}) . \quad (10)$$

The Gaussian kernel is used for K with its bandwidth h determined following Silverman's rule [34] as,

$$h = \left(\frac{4\sigma^5}{3N}\right)^{\frac{1}{5}} , \quad (11)$$

where σ is the sample standard deviation evaluated from the N samples. It should be noted that statistical properties of the KDE hinge on the samples being independently selected from the distribution of X . In our formulation, samples of $\eta \in \mathbb{R}^{d+1}$ are independently sampled from a $d+1$ -dimensional Gaussian distribution, and subsequently pushed through the PCE to yield samples of X . The sample thus collected does not necessarily, a-priori, follow the distribution of X . However, mean square convergence of PCE implies its convergence in distribution. Thus, provided the PCE of X is converged, samples collected from the PCE will adhere to the distribution of X .

4.2. Stochastic sensitivity measures

When considering the uncertainties of $P_i, i = 1, \dots, N_P$, as described in Eq. (6), the extended PCE as developed in Eq. (7) can be used and integrated with the KDE in Eq. (9), to result in,

$$f_X(x) = \frac{1}{Nh} \sum_{j=1}^N K\left(\frac{x - \sum_{|\gamma| \leq p} X_\gamma \psi_\gamma(\eta^{(j)})}{h}\right) , \quad \eta^{(j)} \in \mathbb{R}^{d+1} . \quad (12)$$

This expression for f_X involves summation over all $d+1$ stochastic dimensions (η) and does not therefore express dependence on any of them. In order to retain sensitivity with respect to the parameters $\mathbf{P}$, we make use of Eq. (8) and replace Eq. (12) by the following equation,

$$f_X(x, \rho) = \frac{1}{Nh} \sum_{j=1}^N K\left(\frac{1}{h} \left(x - \sum_{\substack{\alpha \in \mathbb{R}^d, \beta \in \mathbb{R} \\ |\alpha| + \beta \leq p}} X_{\alpha\beta} \psi_\alpha(\xi^{(j)}) \psi_\beta(\rho)\right)\right) , \quad \xi^{(j)} \in \mathbb{R}^d , \quad \rho \in \mathbb{R} \quad (13)$$

By taking the directional derivative of $f_X(x, \rho)$ in Eq. (13) with respect to P_i , the sensitivity of the PDF to the statistical parameters of inputs, denoted by $f_{X, P_i}(x)$, is given by,

$$f_{X, P_i}(x, \rho) = \frac{\partial f_X(x, \rho)}{\partial P_i} = \sigma_{P_i} \frac{\partial f_X(x, \rho)}{\partial \rho} , \quad i = 1, \dots, N_P, \quad (14)$$

and substituting the KDE formulation in Eq. (13) into Eq. (14) results in,

$$f_{X,P_i}(x, \rho) = \frac{\sigma_{P_i}}{Nh^2} \sum_{j=1}^N \left[\frac{x - X(\eta^{(j)})}{h} K\left(\frac{x - X(\eta^{(j)})}{h}\right) \sum_{|\alpha|+\beta \leq p} X_{\alpha\beta} \psi_{\alpha}(\xi^{(j)}) \frac{\partial \psi_{\beta}(\rho)}{\partial \rho} \right], \quad i = 1, \dots, N_P \quad (15)$$

where we relied on the Gaussian form of the kernel. Eq. (15) provides a stochastic representation of the sensitivity of PDF with respect to probabilistic parameters in the input random variables. The sensitivity measure has the property that, for each value of ρ , the integral of f_X with respect to x is equal to zero.

4.3. Methods of quantifying the effect of aleatory and epistemic uncertainties on PDF of QoI

In this section, we investigate the influence on the response PDF of uncertainty in the parameters $\mathbf{P}$ characterizing the probability model of input parameters. We explore three different approaches to that end. The first approach is based on a finite difference scheme, the second one is based on a sensitivity analysis, and the third approach provides an explicit expression of the probability measure on the PDF induced by uncertainty in $\mathbf{P}$.

4.3.1. Finite difference approach

We consider information about the system contained in two distinct datasets that we label “original” and “new”. As above, we let N_P denotes the number of P_i treated as random variables, and we introduce $\mathbf{P}_o$ and $\mathbf{P}_n$ as the vectors of all P_i , ($i = 1, \dots, N_P$) values of the original and new datasets. We then pursue a PCE representation with each of these two sets of parameters, resulting in two distinct PDFs. Representing each of these two PDFs by a KDE relative to the same sample $\{X^{(i)}\}$, and taking the difference of the resulting two expressions yield the following representation for the change in PDF

$$\Delta f_X(x) = \frac{1}{Nh} \left[\sum_{i=1}^N K\left(\frac{x - X(\xi^{(i)}, \{X_{\alpha}^o\})}{h}\right) - \sum_{i=1}^N K\left(\frac{x - X(\xi^{(i)}, \{X_{\alpha}^n\})}{h}\right) \right]. \quad (16)$$

It should be mentioned that this approach does not take the uncertainties of the statistical parameters into account and does not involve any explicit modeling of $\mathbf{P}$. The approach does not therefore provide the facility to interpolate or extrapolate beyond the two datasets associated with $\mathbf{P}_o$ and $\mathbf{P}_n$. This approach is mentioned because of its simplicity and in order to provide a comparison with more advanced approaches described next. It is important to note that a rigorous probabilistic analysis as data is acquired should involve Bayesian update of model parameters. The result in this section, using a difference scheme, is meant to provide an assessment that is both easy and efficient to implement, while providing useful insight into the credibility of statistical inferences.

4.3.2. Stochastic sensitivity approach

Given our probabilistic model for P_i in accordance with Eq. (6), an interval for P_i can be associated with a pre-specified confidence level c_i . We note that this confidence level could be equally well have been specified on ρ . Denoting the upper and lower bounds of the associated confidence interval by u_i and l_i , respectively, permits us to express the precision of P_i as,

$$\Delta P_i = l_i - u_i, \quad i = 1, \dots, N_P, \quad (17)$$

which can be used to develop the induced precision on $f_X(x)$. Specifically, using Eq. (15) results in,

$$\Delta f_X(x, \rho) = \sum_{i=1}^{N_P} f_{X,P_i}(x, \rho) \Delta P_i. \quad (18)$$

Noting the recurrence equation for the derivative of univariate Hermite polynomials,

$$h'_n(x) = x h_n(x) - h_{n+1}(x), \quad (19)$$

and taking the mathematical expectation of the derivative of f_X relative to P_i , results in the following expression for the expected value of $\Delta f_X(x, \rho)$, where $\langle \cdot \rangle$ denotes the expectation operator,

$$\langle \Delta f_X(x, \cdot) \rangle = \sum_{i=1}^{N_P} \frac{\sigma_{P_i}}{N h^2} \sum_{j=1}^N \left[\frac{x - X(\eta^{(j)})}{h} K \left(\frac{x - X(\eta^{(j)})}{h} \right) \sum_{|\alpha| + \beta \leq p} X_{\alpha\beta} \psi_{\alpha}(\xi^{(j)}) \langle \rho \psi_{\beta}(\rho) \rangle \right] \Delta P_i. \quad (20)$$

The stochastic sensitivity approach considers the epistemic uncertainty that characterizes the uncertainty in the statistical parameters P_i .

The stochastic sensitivity approach requires the solution of a $(d + 1)$ -dimension problem while the difference-based method requires the solution of two independent d -dimensional problems.

4.4. Stochastic model for PDFs

A stochastic model for the PDF of X has already been developed in Eqs. (12) and (13). While these equations were used above to characterize sensitivity measures, in this section they are used to characterize confidence in estimates of failure probability. The extended PCE allows to separate the epistemic variable ρ from the aleatory variables ξ . Its PDF can be expressed in a more suggestive form than Eq. (13) as in,

$$f_X(x, \rho) = \frac{1}{N h} \sum_{j=1}^N K \left(\frac{x - \sum_{|\gamma| \leq p} X_{\gamma} \psi_{\gamma}(\xi^{(j)}, \rho)}{h} \right), \quad (21)$$

where $\psi_{\gamma}(\xi^{(j)}, \rho)$ indicates that the polynomial ψ_{γ} is evaluated at the sample where the first d components are specified by $\xi^{(j)}$, while the last $(d + 1)^{st}$ component remains as a free variable. It can be seen that Eq. (12) is the distribution of the family of PDFs generated by Eq. (21), marginalized over ρ .

One important application of the foregoing ideas is to the characterization of failure probabilities, themselves, as random variables. In many applications, the failure probability P_f is defined as the probability of reaching or exceeding a critical threshold and is of great significance. This distribution is typically predicated on pre-specified probabilistic models for input parameters, and thus lends itself to the present analysis. To simplify the presentation, and without loss of generality, we assume a scalar description of the limit state in terms of a critical threshold for the QoI, denoted by X_c . The failure probability, P_f , is then given by the following integral,

$$P_f(\rho) = \int_{x \geq X_c} f_X(x, \rho) dx, \quad (22)$$

where we have explicitly expressed the dependence of P_f on the epistemic input uncertainty encoded in ρ . The PDF of P_f computed by KDE is expressed as,

$$f_{P_f}(x) = \frac{1}{N_{\rho} h_f} \sum_{j=1}^{N_{\rho}} K \left(\frac{x - P_f^{(j)}}{h_f} \right), \quad (23)$$

where N_{ρ} is the number of samples of ρ used in estimating the KDE, and $P_f^{(j)}$, $j = 1, \dots, N_{\rho}$ is the j th realization of failure probability evaluated at ρ^j . The Gaussian kernel is used for K with the bandwidth h_f determined following Silverman's rule as $h_f = (4\sigma_f^5/3N_{\rho})^{1/5}$, where σ_f is the standard deviation estimated from the N_{ρ} failure probability samples.

5. Illustrative numerical examples

In this section, two examples are investigated to demonstrate the proposed framework. Example I is a beam structure of which a closed-form expression for the QoI is known. Example II is a reinforced concrete wall of which the hysteresis analysis is performed using finite elements.

5.1. Example I: Beam structure

The beam structure is shown in Fig. 1. The model characterizes the mid-span displacement X_{mid} of the beam fixed by a linear spring and a rotational spring at each end, with concentrated load F acting in the middle of the

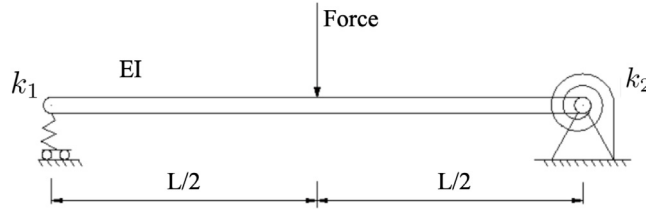


Fig. 1. Schematic of the physical setup for Example I: Random beam on random supports.

Table 1

Statistical parameters of random inputs for Example I.

Input variables	Distribution	a_o	b_o	a_n	b_n	q	r
Linear spring k_1 (N * m)	Beta	4	5	5	6	350	650
Rotational spring k_2 (N * m/rad)	Beta	4	5	5	6	400	600
Flexural stiffness EI (N/m * m)	Beta	4	5	5	6	80	186.67
Beam span L (m)	Beta	4	5	5	6	0.216	0.264

beam. The random inputs include the linear spring, rotational spring, flexural stiffness and beam span, which are denoted as k_1 , k_2 , EI and L , respectively. The four input variables are mutually independent and follow the Beta distributions. The vector of random statistical parameters $\mathbf{P}$ consists of the eight random variables $\mathbf{a}$ and $\mathbf{b}$. The mean value of $\mathbf{P}$ is taken equal to the values estimated from the original dataset, and the coefficient of variation of each entry in $\mathbf{P}$ is assumed to 5%. In order to explore the finite difference approach presented above, we assume that two datasets are made available to the analyst at two different occasions, yielding different parameters for the Beta distribution. These parameters can be estimated from the data using, for instance, a maximum likelihood approach. The distribution parameters are listed in Table 1 where, $\mathbf{a}_o$ and $\mathbf{b}_o$ are the vectors of two shape parameters of each input from the original dataset; $\mathbf{a}_n$ and $\mathbf{b}_n$ are the vectors of two shape parameters of each input from the new dataset; $\mathbf{q}$ and $\mathbf{r}$ are the vectors of the lower and upper bounds of each input and assumed to be the same in the two datasets. It can be shown from elementary mechanics of materials that mid-span displacement X_{mid} for this beam is given by,

$$X_{mid} = \frac{F}{16EI} \left[\frac{L^3}{3} - \frac{8EI k_2 L^3 + k_1 k_2 L^6}{16EI(k_2 + k_1 L^2)} + \frac{8EI k_1 L^2 - k_1 k_2 L^3}{2k_1 k_2 + 2k_1^2 L^2} \right]. \quad (24)$$

The PDF of X_{mid} using KDE based on the extended PCE as in Eq. (7) is shown in Fig. 2. A second order PCE was found to be sufficiently converged in the tail of the PDF to carry out the foregoing PDF sensitivity studies. Besides, to avoid the effect of noise from KDE on the tail of the PDF, the PDFs obtained from $N = 10^4, 10^5, 10^6$ are plotted in Fig. 2. It is found that 10^5 samples can give an accurate tail of the PDF and thus used in the remaining computation. Fig. 3 shows the family of PDFs computed from Eq. (13) at 1000 samples of ρ . As indicated previously, the PDF in Fig. 2 is just the distribution over the ensemble of PDFs for which samples are shown in Fig. 3.

Assuming failure is associated with $X_{mid} > 2.45$ cm, the distribution of the probability of failure (P_f) is obtained by evaluating P_f for each sample in Fig. 3, and plotting the PDF of the resulting values. The resulting PDF is shown in Fig. 4. Although confidence intervals for P_f can be easily synthesized from the PDF, more accurate decision analysis can be developed by relying on the full PDF.

The change in response PDF resulting from the change in the statistical parameters from $\mathbf{P}_o$ to $\mathbf{P}_n$ computed by the finite difference approach is shown in Fig. 5. Based on Fig. 5, the failure criterion of $X_{mid} = 2.45$ cm exhibits one of the largest sensitivities to changes in P_i in the tail region. The sensitivity plot in this figure tapers toward zero for larger values of displacement, consistent with the fact that P_i refers to the shape parameter of beta distributions rather than to its range. We thus observe, as expected, a deterministic upper bound on the mid-span displacement as the shape parameter varies over its range. On the other hand, given a 95% confidence level for ρ , the confidence intervals $[l_i, u_i]$ for each P_i , where $i = 1, \dots, N_p$ are computed to be [3.6, 4.4] for the shape parameters $\mathbf{a}$ and [4.51, 5.49] for the shape parameters $\mathbf{b}$. Thus, Fig. 6 shows the result computed by the stochastic sensitivity approach according to Eq. (18). The figure shows the statistical samples of the change in response PDF,

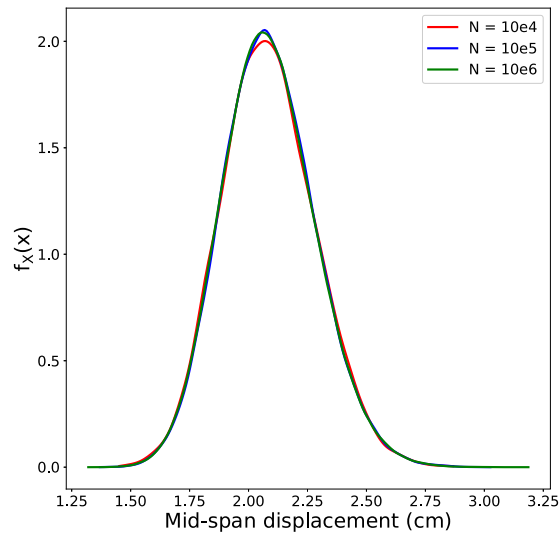


Fig. 2. PDF computed by KDE ($N = 10^4, 10^5, 10^6$) using extended PCE for Example I.

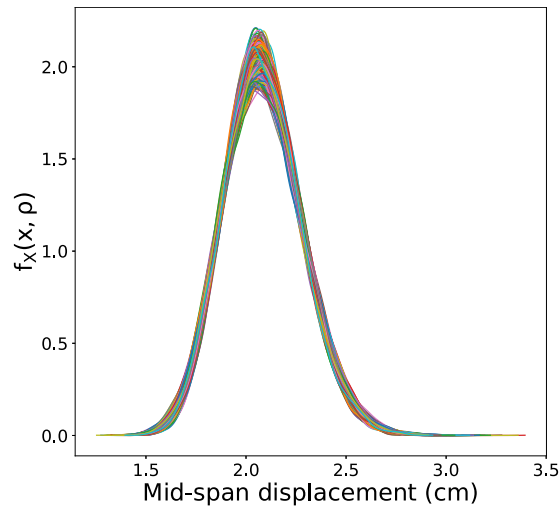


Fig. 3. The family of PDFs at 1000 realizations of ρ for Example I.

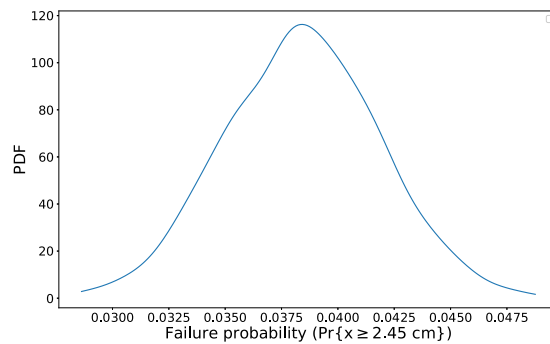


Fig. 4. PDF of failure probability that $X_{\text{mid}} \geq 2.45$ cm for Example I.

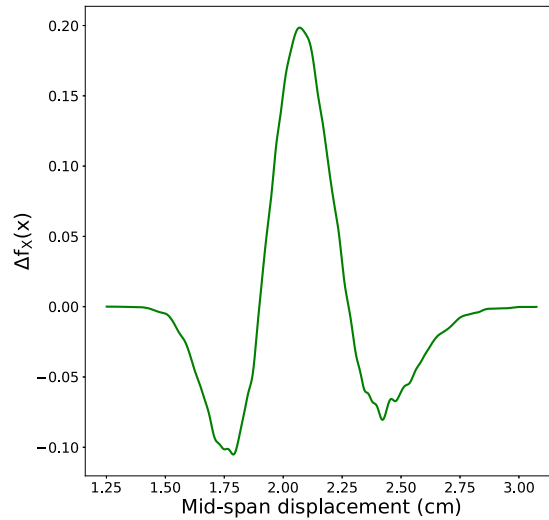


Fig. 5. Change in response PDF between P_0 and P_n by the finite difference method for Example I.

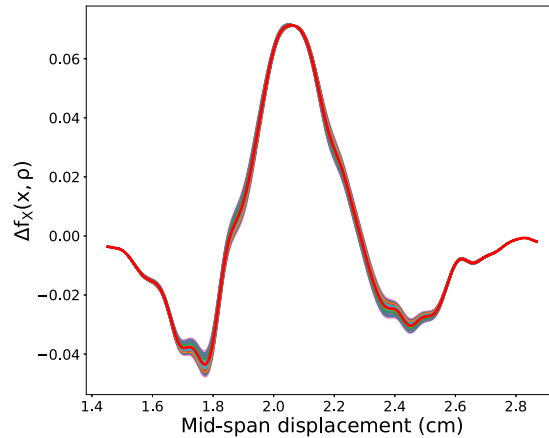


Fig. 6. Statistical samples (Eq. (18)) and their expectation (bold red; Eq. (20)) for change in response PDF with a 95% confidence interval of ρ by the stochastic sensitivity approach for Example I. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

as well as the expectation of these samples. The scatter in this sample is a reflection of the epistemic uncertainty about the probabilistic model of the input parameters. The shape of Δf_X using both the difference and the sensitivity methods is as expected with the largest difference near the mode and a change of sign before tapering off to zero. The net area under the curve is equal to zero. The change in PDF according to sensitivity is different from the change using finite difference which can be attributed to one or both of two factors. First, the derivative of the PDF with respect to P_i at each of the two datasets is quite different, leading to a discrepancy upon linearizing at either of the two datasets. Second, the values of P_i associated with the new dataset lie outside the confidence intervals just evaluated.

5.2. Example II: Reinforced concrete shear wall

It has been suggested that epistemic uncertainty is non-negligible in seismic analysis of structures [35] [36] [37]. To illustrate the proposed methodologies in this context, a reinforced concrete shear wall model is taken as an example in this study. This model comes from an experimental study [38]. Fig. 7 depicts the geometry, dimension and reinforcement of the shear wall.

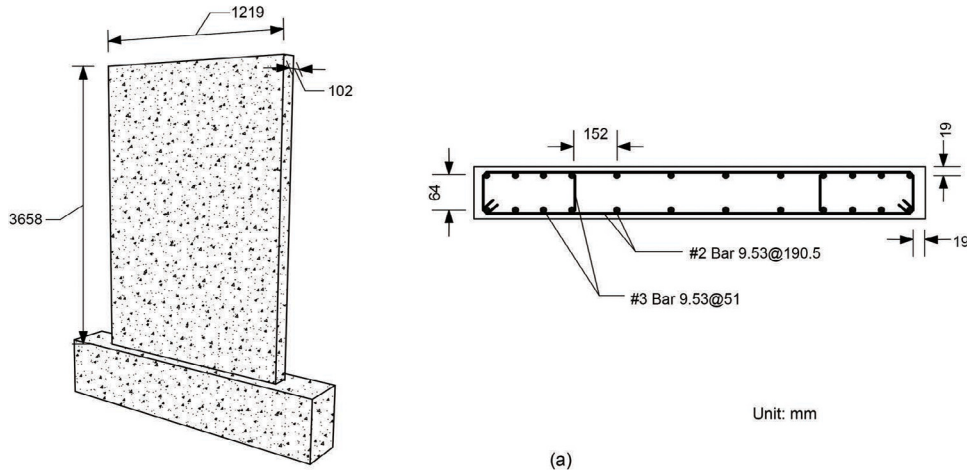


Fig. 7. Schematic of the physical setup for Example II: Reinforced concrete shear wall.

Table 2

Statistical parameters of random inputs for Example II.

Material	Input variable	Distribution	a_o^{SW}	b_o^{SW}	a_n^{SW}	b_n^{SW}	q^{SW}	r^{SW}
Concrete	Compressive strength f_c (in Pa)	Beta	2	2	2.4	2.3	3.91×10^7	5.29×10^7
Steel	Yielding strength f_y (in Pa)	Beta	2	2	2.4	2.2	3.40×10^8	4.60×10^8

There are two steps in the loading procedure. First, a constant axial load of 378 kN is applied on the top of the wall, followed by a cyclic lateral load achieved by controlling the displacement. The applied lateral drift consisted of a train of triangular pulses of alternating signs. Additional details of the setup and its loading are described elsewhere [38]. The purpose of the present analysis is to find the influence of the statistical parameters of mechanical properties of concrete and steel on the response PDF of the energy dissipated throughout the structure via hysteresis.

Some of the material properties are considered as random variables, including the concrete elastic modulus E_c , the concrete tensile strength f_r , the concrete compressive strength f_c and the steel yielding strength f_y . For concrete, E_c , f_r and f_c are of course correlated, but for simplicity they were regarded as fully correlated in this paper. According to the code ACI 318–19 [39], the relationships between these parameters are,

$$\begin{aligned} E_c &= 57,000\sqrt{f_c} \quad , \\ f_r &= 7.5\lambda\sqrt{f_c} \quad , \end{aligned} \quad (25)$$

where, the units are in psi. To calculate these concrete parameters, the f_c is sampled from a Beta distribution first and the f_r and E_c are then generated according to Eq. (25). The steel strength is also modeled as a Beta random input. The material properties input to the shear wall structure are listed in Table 2. where, in this shear wall hysteresis problem, a_o^{SW} and b_o^{SW} are the vectors of two shape parameters of each input from the original dataset; a_n^{SW} and b_n^{SW} are the vectors of two shape parameters of each input from the new dataset; q^{SW} and r^{SW} are the vectors of the lower and upper bounds of each input and assumed to be the same in the two datasets. Thus, in this example, the vector $\mathbf{P}$ of random parameters has four components consisting of the shape parameters a^{SW} and b^{SW} . The mean value of $\mathbf{P}$ is taken equal to the values estimated from the original dataset, and the coefficient of variation of each entry in $\mathbf{P}$ is assumed to 5%. The resulting $[l_i, u_i]$ interval, at the 95% confidence level, for each of the shape parameters is equal to [1.80, 2.20]. We also note, however, that parameters from the new dataset are outside this confidence interval.

We implement in Abaqus [40] a model that follows the theoretical development in Feng et al. [41] which features a multi-dimensional softened plasticity damage model. The steel material follows a Menegotto-Pinto model that includes strain-hardening, Baushinger effects and tension stiffening and a multi-layer shell element is used for the shear wall [41]. Additional material properties include the concrete Poisson's ratio, the steel elastic modulus and the steel hardening ratio which are deterministic inputs.

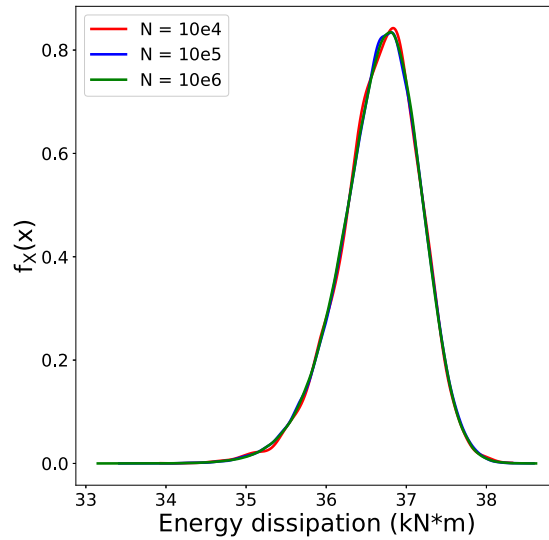


Fig. 8. PDF computed by KDE ($N = 10^4, 10^5, 10^6$) using extended PCE for Example II.

The response PDF of the energy dissipation using KDE based on the extended PCE is shown in Fig. 8. Again, convergence test is conducted by using $N = 10^4, 10^5, 10^6$ to avoid the effect of noise from KDE on the tail of the PDF, as shown in Fig. 2. $N = 10^5$ is found to give an accurate tail of the PDF and thus used in the final calculations. Then Fig. 9 shows the results of the family of PDFs computed at 1000 samples of ρ . Here again, a second order PCE was found to yield a converged PDF. Again, the PDF in Fig. 8 is just the distribution of the family of PDFs in Fig. 9. Postprocessing these results, the probability, P_f , of exceeding a threshold level of $37.5 X = 37.5$ kN m is shown in Fig. 10. We reiterate that the probability of failure is itself characterized as a random variable with a computed scatter that reflects its credibility for critical decision making. The change in response PDF due to the change in the statistical parameters from P_o to P_n computed by the finite difference approach is shown in Fig. 11. Here again we seek a value in the tail region of energy dissipation that exhibits significant sensitivity to fluctuations in P_i . We thus select a value of 37.5 kN m at which to evaluate sensitivities and variations in PDFs. On the other hand, given a 95% confidence level for ρ , the confidence intervals $[l_i, u_i]$ for each P_i , ($i = 1, \dots, N_p$) are computed and then ΔP is obtained. Thus, Fig. 12 shows the result from the stochastic sensitivity approach according to Eq. (18), as well as the expected value of change in PDF according to Eq. (20). The figure shows a statistical ensemble of these samples of change in PDF that reflects the epistemic uncertainty about the probabilistic parameters of the input variables. The same observations noted for the previous example while comparing $f_X(x)$ obtained using the two formalisms apply to the present example. There is a distinct difference in the shape of the scatter between this example and the previous one. In our definition of $\Delta f_X(x)$, the increments ΔP_i are deterministic. The scatter in Δf_X is thus due to the scatter in the sensitivities expressed in Eq. (15). The two examples clearly exhibit different dependence of the sensitivities on x and ρ , demonstrating the influence of the chaos coefficients of X on these sensitivities. The difference between Figs. 6 and 12 is mainly due to the contributions of higher order polynomials in ρ (Eq. (13)) in Example II while Example I is largely dominated by the first order polynomials in ρ . It is also noted that the scatter in the sensitivities does not mirror the scatter in the PDF, and that the sensitivity of the PDF varies considerably along its support.

6. Concluding remarks

A framework is proposed in this paper to quantify mixed aleatory and epistemic uncertainties and to evaluate their influence on the probability density functions of various quantities of interest. The epistemic uncertainty is modeled as random variables which are integrated with the aleatory variables into the extended PCE, thus realizing a single-stage efficient quantification of both type of uncertainties. The sensitivity of response PDF with respect to the statistical parameters of input variables is expressed through a combination of KDE and extended PCE,

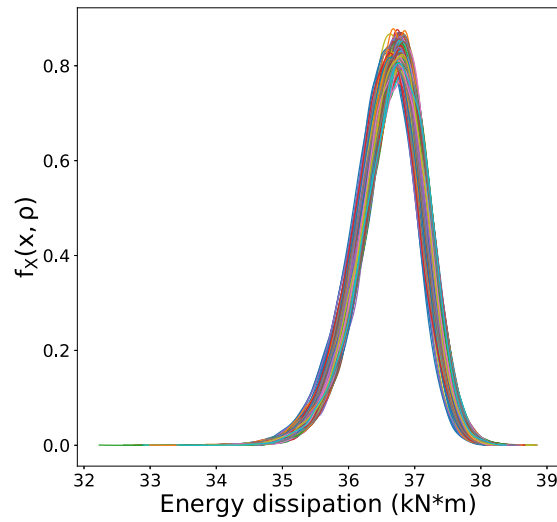


Fig. 9. The family of PDFs at 1000 realizations of ρ for Example II.

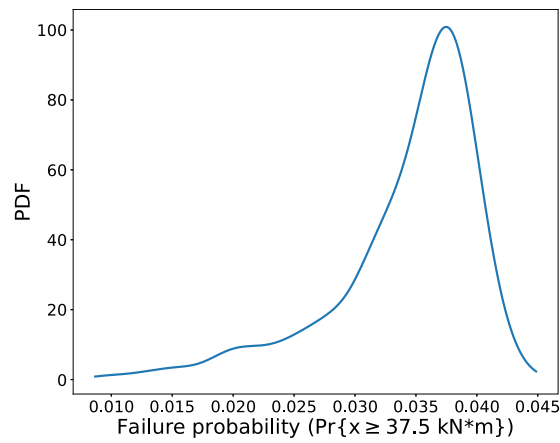


Fig. 10. PDF of failure probability that $X \geq 37.5$ kN*m for Example II.

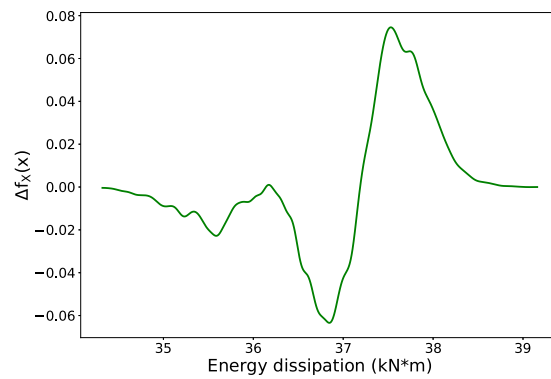


Fig. 11. Change in response PDF between P_0 and P_n by the finite difference method for Example II.

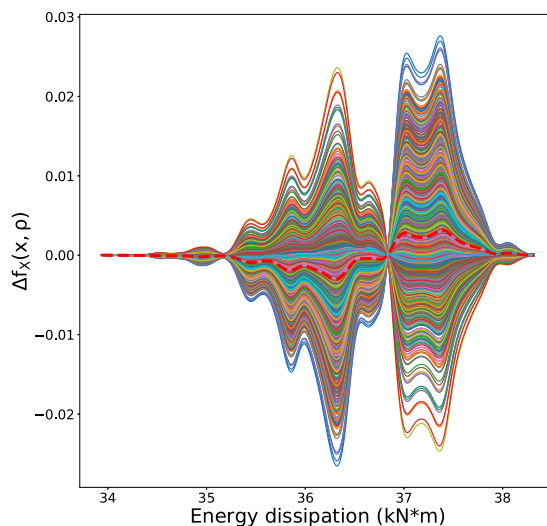


Fig. 12. Statistical samples (Eq. (18)) and their expectation (dashed bold red; Eq. (20)) for the change in response PDF with a 95% confidence interval of ρ by the stochastic sensitivity approach for Example II. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

thus allowing for a straightforward post-processing of the extended PCE to determine the sensitivity of PDF to epistemic variables, with little additional computational effort. Based on the result of the extended PCE, several metrics including the family of PDFs and the distribution of the failure probability are investigated to provide interpretations to the response from different angles. Based on the significant variation of the sensitivities along the support of the PDF, we deduce that the acquisition of additional observations, aimed at shaping the statistical parameters, should take into account which portion of the support is expressed by the relevant decisions.

If the statistical parameters $\mathbf{P}$ are estimated according to the MLE arguments, then their asymptotic distribution will be Gaussian. However, in the small data case, the distribution of $\mathbf{P}$ will generally depend on the dataset. As a potential extension of this work, one could replace Eq. (6) with a higher-order PCE to account for more general form of the density function. In this case, the development in Section 4.3.2 will have to be modified, while the development in Sections 4.4 and 4.3.1 will remain valid.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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