Stochastic Sensitivities across Scales and Physics

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ABSTRACT: The polynomial chaos expansions (PCE) provide stochastic representations of quantities of interest (QoI) in terms of a vector of standardized random variables that represent all uncertainties influencing the QoI. These uncertainties could reflect statistical scatter in estimated probabilistic model (of which the mean, variance, or PCE coefficients are but examples), or errors in the underlying functional model between input and output (e.g. physics models). In this paper, we show how PCE permit the evaluation of sensitivities with respect to all these uncertainties, and provide a rational paradigm for resource allocation aimed at model validation. We will demonstrate the methodologies on examples drawn across science and engineering.

1. INTRODUCTION

Sensitivity analysis aims at investigating the influence of small changes in independent parameters on system output. It has proven significant for ranking random inputs [1]. Traditionally, sensitivity approaches can be classified into three categories: variogram-based, regression-based, and variance-based methods. For instance, Sobol sensitivity analysis is a well-known variance-based approach [2]. In critical engineering applications, the sensitivity of probability density function (PDF) of the output to the additional information or additional numerical accuracy is relevant for resource risk assessment and management. These sensitivities are not readily attainable through standard sensitivity methods, and are developed in this paper.

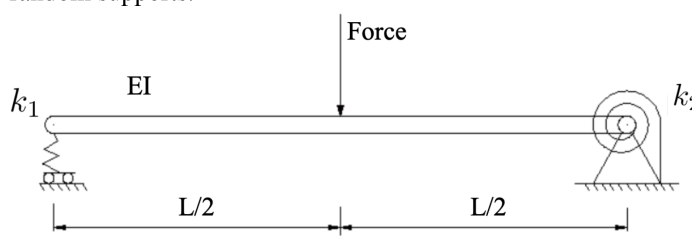
PCE is an uncertainty quantification method that has been widely used in many areas with demonstrated robustness and computational efficiency. PCE has already been integrated within a Sobol sensitivity framework for uncertainty ranking and computational cost mitigation [3,4]. These approaches, however, have come short of assessing the error propagation through the PCE representation to the output PDF.

In this paper, the sensitivity of PDF using PCE is investigated and demonstrated on a reduced probabilistic structural mechanics problem. The proposed approach provides a rigorous framework to simultaneously analyze the influence of modeling uncertainties, data uncertainties, and numerical errors, on the PDF of the predicted response. The object is to find: $\Delta f_X(x) = \sum_i \frac{\partial f_X(x)}{\partial P_i} \Delta P_i$, where $f_X(x)$ and $\Delta f_X(x)$ are, respectively, the PDF and change in PDF of the output, whereas P_i and ΔP_i refer, respectively, to the i^{th} statistical parameter of a random input and to its increment.

2. PHYSICAL MODEL

To provide insight into the proposed methodology, a simple structural mechanics problem is studied. The physical model characterizing the mid-span displacement X of a simply-supported beam with concentrated load acting in the middle is expressed as a function of $X = \chi(\boldsymbol{K})$, where the input $\boldsymbol{K} = (k_1, k_2, k_3, k_4)$ is a point of the random inputs in a four-dimensional vector space that characterize the linear spring instead of the pinned support, rotational spring instead of the roller suport, elastic modulus and beam span, respectively. Fig. 1 depicts the physical setup.

Figure 1: Schematic of the physical setup: Random beam on random supports.



The four random variables are assumed to be independent and to follow a beta distribution. Their statistical information is shown in Table 1 where the two shape parameters and lower and upper bounds in Beta distribution are denoted by a, b, q, r, respectively.

Table 1: Statistical parameters of Beta random inputs

$\boldsymbol{K}$	a	b	q	r
Linear spring k_1 (N*m)	2	2	350	650
Rotational spring k_2 (N*m/rad)	2	2	400	600
Bending stiffness k_3 (N/m*m)	2	2	80	186.67
Beam span k_4 (m)	2	2	0.216	0.264

The d-dimensional vector (d=4) of random parameters K is expressed as a mapping from a d-dimensional vector of standard Gaussian variables $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3, \xi_4)$. This mapping is obtained through the Rosenblatt transformation.

3. REPRESENTATION OF SOLUTION: PCE

The mid-span displacement X depends on $\boldsymbol{\xi} \in \mathbb{R}^d$ through the Rosenblatt transform, and can thus be represented in a PCE decomposition of the form,

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

where $X_{\boldsymbol{\alpha}}$ and $\psi_{\boldsymbol{\alpha}}$ denote the PCE coefficients and PCE basis, respectively. Further, p denotes the highest order in the polynomial expansion, and $\boldsymbol{\alpha}$ is a d-dimensional multi-index. In order to emphasize their dependence on the PCE representation, we denote realizations of X synthesized from its PCE using the sample $\boldsymbol{\xi}^{(i)}$ of $\boldsymbol{\xi}$ by,

$$x(\boldsymbol{\xi}^{(i)}, X_{\boldsymbol{\alpha}}) = \sum_{\boldsymbol{\alpha}=0}^{P-1} X_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{(i)}). \tag{2}$$

The PC coefficients $X_{\boldsymbol{\alpha}}$ are calculated as quadrature approximations to multidimensional integrals as follows,

$$X_{\boldsymbol{\alpha}} = \sum_{q \in Q} X(\boldsymbol{\xi}^q) \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^q) w_q, \quad |\boldsymbol{\alpha}| \le p \,, \tag{3}$$

where, Q is the set of sparse quadrature points, q is a quadrature node in Q and w_q is the associated weight. The number of these coefficients, denoted by P, is given by $P = (d+p)!/(d!p!)$. Using a level 2 quadrature rule in dimension $d = 4$ reqsults in a set Q with $1,265$ quadrature nodes. In our present example, $d = 4$ and $p = 3$ with a resulting value of $P = 35$. Evaluating Eq. 3 at all quadrature nodes and organizing the results into matrix form yields, $\mathbf{X}_{\boldsymbol{\alpha}} = \boldsymbol{\Psi} \mathbf{X}^T \mathbf{w}_{\mathbf{q}}$, where, $\boldsymbol{\Psi}$, $\mathbf{X}$, $\mathbf{w}_q$ are 35×1265, 1×1265 and 1265×1 matrices, respectively.

4. REPRESENTATION OF PDF: KDE

Kernel Density Estimation (KDE) is used to build the probability density function (PDF). Let $f_X(x)$ denote the PDF of mid-span displacement computed by KDE using samples generated by PCE calculated by,

$$f_X(x) = \frac{1}{Nh} \sum_{i=1}^{N} K\left(\frac{x - x(\boldsymbol{\xi}^{(i)}, X_{\boldsymbol{\alpha}})}{h}\right) \tag{4}$$

where N is the number of PCE evaluations and $x(\boldsymbol{\xi}^{(i)}, X_{\boldsymbol{\alpha}})$ is a realization evaluated at a sample $\boldsymbol{\xi}^{(i)}$. The Gaussian kernel is used for K with the bandwidth h determined following Silverman's rule as $h = (4\sigma^5/3N)^{1/5}$, where σ is the standard deviation estimated from the N samples. Clearly, the centers $x(\boldsymbol{\xi}^{(i)}, X_{\boldsymbol{\alpha}})$ of the Gaussian mixture representation given by equation (4) depend on the PCE coefficients of X and we thus have a functional dependence between these coefficients and the PDF of X.

Thus, after the PC expansion of X has been evaluated we proceed as follows. We first generate $N = 10^6$ samples of Gaussian random variables $\boldsymbol{\xi}^{(i)}$, $i = 1, 2, ..., N$. We then evaluate the polynomial chaos expansion at each of these points using Eq. 2. We then form the sum in equation (4) to evaluate the PDF. We will next explore the sensitivity of the evaluations in this last step to perturbations in the PCE coefficients that could stem from a number of sources.

5. SENSITIVITY ANALYSIS

5.1 *Sensitivity of PDF to PCE coefficients*

The sensitivity of PDF to PCE coefficients denoted by $f_{X,\boldsymbol{\alpha}}(x)$ is given by,

$$f_{X,\boldsymbol{\alpha}}(x) = \frac{\partial f_X(x)}{\partial X_{\boldsymbol{\alpha}}}, \quad |\boldsymbol{\alpha}| \le p. \tag{5}$$

Taking the partial derivative of $f_X(x)$ with respect to $X_{\boldsymbol{\alpha}}$ and substituting into Eq. 5, results in,

$$f_{X,\boldsymbol{\alpha}}(x) = \frac{1}{Nh} \sum_{i=1}^{N} \frac{1}{h} \left[K\left(\frac{x - X(\xi^{(i)}, X_{\boldsymbol{\alpha}})}{h}\right)\right] \times \left(\frac{x - X(\xi^{(i)}, X_{\boldsymbol{\alpha}})}{h}\right) \psi_{\boldsymbol{\alpha}}(\xi^{(i)}), |\boldsymbol{\alpha}| \le p. \tag{6}$$

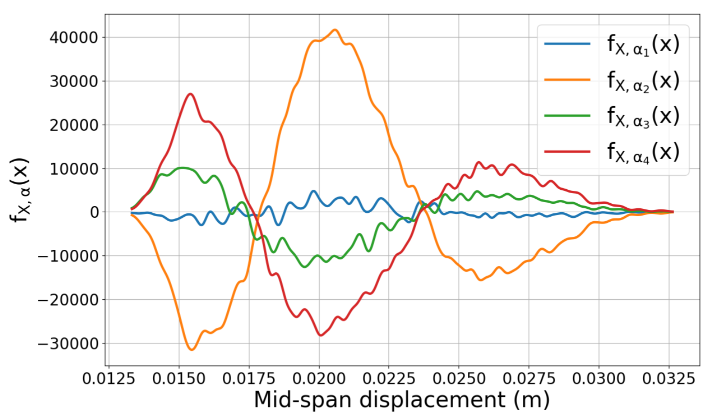


Figure 2: $f_{X,\boldsymbol{\alpha}}(x), |\boldsymbol{\alpha}| = 1$ (or $p = 1$)

Fig. 2 shows the results computed using Eq. 6 for $f_{X,\boldsymbol{\alpha}}(x)$, $|\boldsymbol{\alpha}| = 1$ as an example. The figure shows that the largest sensitivities in the first order ($p = 1$) are $f_{X,\boldsymbol{\alpha}_2}(x)$ and $f_{X,\boldsymbol{\alpha}_4}(x)$. Similarly, although the results are not shown for brevity, it is found that for $p = 2$, $f_{X,\boldsymbol{\alpha}_9}(x), f_{X,\boldsymbol{\alpha}_{11}}(x), f_{X,\boldsymbol{\alpha}_{14}}(x)$ are the dominant ones. For $p = 3$, $f_{X,\boldsymbol{\alpha}_{27}}(x), f_{X,\boldsymbol{\alpha}_{25}}(x), f_{X,\boldsymbol{\alpha}_{30}}(x)$ are the dominant sensitivities. For $p = 0$, there is $f_{X,\boldsymbol{\alpha}_0}(x)$ which is the mean, thus most sensitive among all $f_{X,\boldsymbol{\alpha}}(x)$. Moreover, the polynomial chaos of these dominant sensitivities are associated with either ξ_2 or ξ_4, as shown in Table 2.

Therefore, in this problem, the PDF of output is more sensitive to the PCE terms with respect to the inputs ξ_2 and ξ_4 associated with random rotational spring and random span.

5.2 *Sensitivity of change in PDF to change of statistical information of random variables*

When additional information is acquired, the statistics of the random inputs changes, and the values of the parameters shown in Table 1 are perturbed. We next investigate how these changes influence the PDF, in other words, we seek to evaluate the contributions to $\Delta f_X(x) = \sum_i \frac{\partial f_X(x)}{\partial P_i} \Delta P_i$.

Table 2: Polynomial chaos of dominant sensitivities

p	0	1	1	2	2
PCE basis	ψ_0	ψ_2	ψ_4	ψ_9	ψ_{11}
Polynomial chaos	1	ξ_2	ξ_4	$\xi_2^2 - 1$	$\xi_2\xi_4$
p	2	3	3	3	
PCE basis	ψ_{14}	ψ_{27}	ψ_{25}	ψ_{30}	
Polynomial chaos	$\xi_4^2 - 1$	$\xi_2^2\xi_4 - \xi_4$	$\xi_2^3 - 3\xi_2$	$\xi_2\xi_4^2 - \xi_2$	

Assume that because of additional data, the values of a and b are increased respectively by 50% and 10% for k_1, k_2, k_3, k_4, while q and r are unchanged. Let us denote this perturbation of information by $\Delta \boldsymbol{P} = \{\Delta P_i, i = 1,2...,8\}$ with the description of each P_i as shown in Table 3;

Table 3: Description of statistical information P_i

P_i	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8
Variable	k_1	k_1	k_2	k_2	k_3	k_3	k_4	k_4
Parameter	a	b	a	b	a	b	a	b
Value	3.0	2.2	3.0	2.2	3.0	2.2	3.0	2.2

5.2.1 *Derivation of important sensitivities*

In the previous section, we derived and studied the sensitivity of PDF to PCE coefficient, $\frac{\partial f_X(x)}{\partial X_{\boldsymbol{\alpha}}}$. Thus, the change in PDF can be expressed as

$$\Delta f_X(x) = \sum_{|\boldsymbol{\alpha}| \le p} f_{X,\boldsymbol{\alpha}}(x) \Delta X_{\boldsymbol{\alpha}}. \qquad (7)$$

It should be noted that perturbations to PCE coefficients are not only due to changes in P_i's but are also often associated with numerical errors inherent in any quadrature rule. We denote these errors by $\Delta X_{\boldsymbol{\alpha}}|_{L_j}$ where L_j refers to the j^{th} quadrature level used in the approximation. We also use the notation $\Delta X_{\boldsymbol{\alpha}}|_{L_j} = X_{\boldsymbol{\alpha}}|_{L_{j+1}} - X_{\boldsymbol{\alpha}}|_{L_j}$. Thus we finally have,

$$\Delta X_{\boldsymbol{\alpha}} = \sum_{i=1}^{8} \left. \frac{\partial X_{\boldsymbol{\alpha}}}{\partial P_i} \right|_{L_j} \Delta P_i + \Delta X_{\boldsymbol{\alpha}} \Big|_{L_j}. \qquad (8)$$

Thus, the sensitivity of a PCE coefficient to a statistical parameter $\frac{\partial X_{\boldsymbol{\alpha}}}{\partial P_i}|_{L_j}$ using a j^{th} level of quadrature, is given by,

$$\left. \frac{\partial X_{\boldsymbol{\alpha}}}{\partial P_i} \right|_{L_j} = \sum_{q \in Q} \left(\left. \frac{\partial X}{\partial P_i} \right|_{L_j} (\xi^q) \right) \psi_{\boldsymbol{\alpha}}(\xi^q) w_q \qquad (9)$$

and the sensitivity $\frac{\partial X}{\partial P_i}|_{L_j}(\xi^q)$ using j^{th} level quadrature is computed as,

$$\left. \frac{\partial X}{\partial P_i} \right|_{L_j} (\xi^q) = \frac{X(\boldsymbol{P}, \xi^q, L_j) - X(\boldsymbol{P} + \Delta P_i, \xi^q, L_j)}{\Delta P_i}, \qquad (10)$$

where $X(\boldsymbol{P_i}, \xi^q, L_j)$ is the solution evaluated using quadrature L_j, at quadrature node ξ^q, with statistical parameters $\boldsymbol{P}_i$.

5.2.2 *Results*

According to Eq. 7-10, the results of how the change of statistical information of k_1, k_2, k_3, k_4 influences the change of PDF of beam mid-span displacement are computed.

Fig. 3a shows the total effect of $\Delta \boldsymbol{P}$ on $\Delta f_X(x)$ and Fig. 3b shows the PDF's with respect to $\boldsymbol{P}$ and $\boldsymbol{P} + \Delta \boldsymbol{P}$. According to Eq. 7-8, the contribution of each $P_i, i = 1,2...,8$ to $\Delta f_X(x)$ can be expressed as

$$\Delta_i f_X(x) = \sum_{|\boldsymbol{\alpha}| \le p} f_{X,\boldsymbol{\alpha}}(x) \left. \frac{\partial X_{\boldsymbol{\alpha}}}{\partial P_i} \right|_{L_j} \Delta P_i, i = 1,2...,8. \qquad (11)$$

In addition, the change of PDF of output contributed by error from j^{th} quadrature can be expressed as:

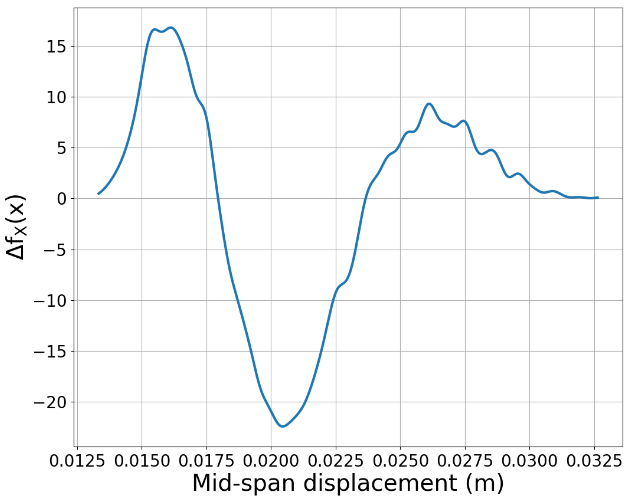
$$\Delta_{L_j} f_X(x) = \sum_{|\boldsymbol{\alpha}| \le p} f_{X,\boldsymbol{\alpha}}(x) \Delta X_{\boldsymbol{\alpha}}|_{L_j} \qquad (12)$$

Fig. 4 shows the results of $\Delta_i f_X(x), i = 1,2...,8$. It shows that: (1) For each random input, a contributes much more than b; (2) The contributions from a and b to PDF are in opposite phases; (3) The contribution from the four random inputs is ranked as: $k_2 > k_4 > k_3 > k_1$.

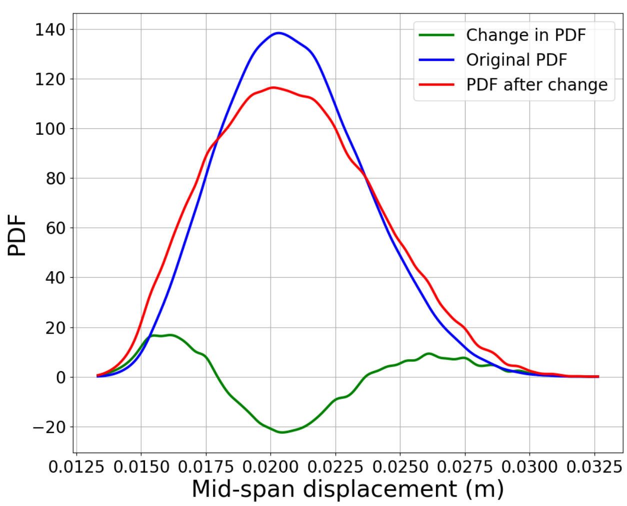
Fig. 5 shows the result of $\Delta_{L_2} f_X(x)$ which is the change in PDF of output induced by second level quadrature. Comparing $\Delta_{L_2} f_X(x)$ and $\Delta_i f_X(x)$ in Fig. 5 and Fig. 4, it shows that except for P_3 and P_7, the error from quadrature is quite significant compared with change of all other statistical information. In other words, the change of PDF of output can be not completely from the change of statistics of random inputs while the error in quadrature rules also has non-negligible contribution. The error from quadrature rules, however, is only significant for low levels of mid-span displacement and is insignificant when larger displacements are of interest.

6. CONCLUSIONS

Sensitivity analysis based on part of output statistics (e.g. variance) cannot provide a comprehensive description of the response in an engineering application. On the other hand, PCE has shown its efficiency and accuracy in the area of stochastic computational mechanics. Therefore, sensitivity of the complete PDF of response with respect to the uncertainties in the inputs data is proposed using PCE. Moreover, the error induced by quadrature is very significant to take into account, especially in complex applications where high quadrature level is needed. The methodology is demonstrated in this paper on a reduced model from structural mechanics. The perturbation to the model induced by updating the statistics of input parameters is propagated through the surrogate model and its influence on the PDF of the response is investigated. Error caused by quadrature rules is quantified. The ranking of importance of random inputs is obtained and is found to be reflected in the PCE coefficients. Three important sensitivities: $\frac{\partial X}{\partial P_i}|_{L_j}(\xi^q)$, $\frac{\partial X_\alpha}{\partial P_i}|_{L_j}$, $\frac{\partial f_X(x)}{\partial X_\alpha}$ are derived which jointly can be used to investigate the propagation of uncertainty in inputs statistics to the complete PDF of output, capturing error from quadrature rules. These sensitivities could also be useful for other general sensitivity analysis using PCE in the future.



(a) Change in PDF of output resulting from change of statistical information of inputs



(b) Comparison of PDF of output before and after change of $\Delta \boldsymbol{P}$

Figure 3: Influence of change of statistics of inputs on PDF of output

The PDF-based sensitivity analysis methodology presented in this paper will be further demonstrated during the presentation on a the development of hazard maps for tsunami run-up and on the design under uncertainty of a scramjet.

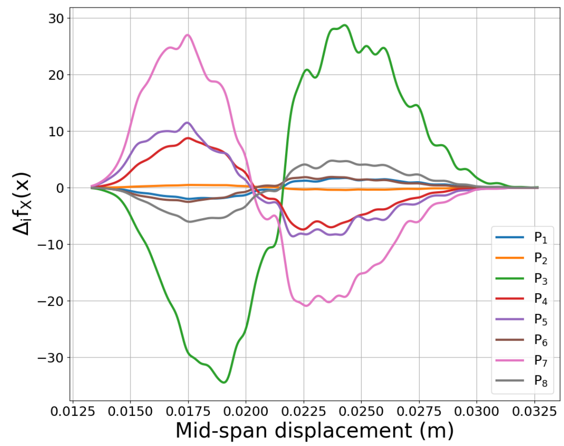


Figure 4: $\Delta_i f_X(x)$ contributed from each $P_i, i = 1, 2..., 8$

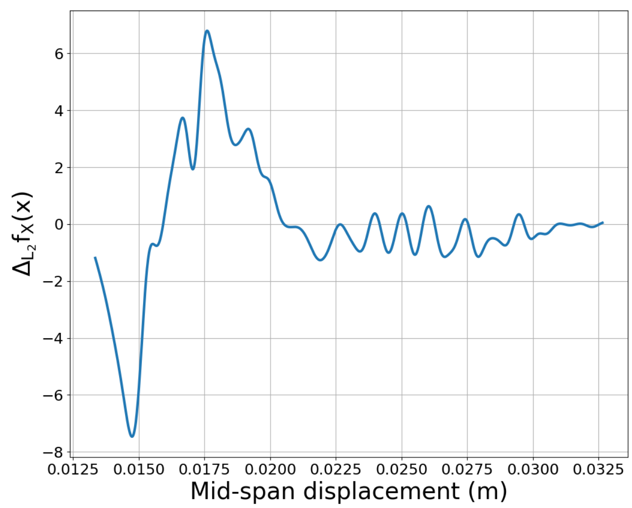


Figure 5: $\Delta_{L_2} f_X(x)$ contributed from $\Delta X_\alpha|_{L_2}$

7. REFERENCES

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