ECCOMAS European Congress on Computational Methods in Applied Sciences and Engineering

Sensitivity analysis of parametric uncertainties and modeling errors in generalized probabilistic modeling

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Motivation





Simulation-based design. Virtual testing. Parametric uncertainties. Modeling errors.

Multidisciplinary design. Multiple components.

Sensitivity analysis of parametric uncertainties, modeling errors, and multiple components in the context of generalized probabilistic modeling.

Outline

Motivation.

Outline.

Sensitivity analysis.

Generalized probabilistic modeling.

First illustration: parametric uncertainties and modeling errors.

Second illustration: multiple components.

Sensitivity analysis



The computational cost of stochastic methods can be lowered via the use of a surrogate model as a substitute for a numerical model or real tests.



There exist many types of sensitivity analysis.

Local sensitivity analysis:

- elementary effect analysis.
- differentiation-based sensitivity analysis.

- Global sensitivity analysis:
 - regression analysis.
 - variance-based sensitivity analysis,
 - correlation analysis,
 - methods involving scatter plots,
- ...

. . .

- Here, we focus here on global sensitivity analysis methods, which can help ascertain which sources of uncertainty are most significant in inducing uncertainty in predictions.
- References: [A. Saltelli et al. Wiley, 2008]. [J. Oakley and A. O'Hagan. J. R. Statist. Soc. B, 2004].

• Two statistically independent sources of uncertainty modeled as two statistically independent random variables X and Y with probability distributions P_X and P_Y :

 $(X,Y) \sim P_X \times P_Y.$

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 We assume that the relationship between the sources of uncertainty and the predictions is represented by a nonlinear function g:

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(X,Y)	Z = g(X, Y)	Z

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The probability distribution P_Z of the prediction is obtained as the image of the probability distribution $P_X \times P_Y$ of the sources of uncertainty under the function g:

$$Z \sim P_Z = (P_X \times P_Y) \circ g^{-1}.$$

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Sensitivity analysis:

• Is either X or Y most significant in inducing uncertainty in Z?

Least-squares-best approximation of function g with function of only one input:

Assessment of the significance of the source of uncertainty X:

$$g_X^* = \arg\min_{f_X^*} \iint |g(x,y) - f_X^*(x)|^2 P_X(dx) P_Y(dy).$$

• By means of the calculus of variations, it can be readily shown that the solution is given by $g_X^* = \int g(\cdot, y) P_Y(dy).$

In the geometry of the space of $P_X \times P_Y$ -square-integrable functions, g_X^* is the orthogonal projection of function g of x and y onto the subspace of functions of only x:



Expansion of function g in terms of main effects and interaction effects:

• Extension to assessment of significance of both sources of uncertainty X and Y:

$$g(x,y) = g_0 + \underbrace{g_X(x)}_{Y} + \underbrace{g_Y(y)}_{Y} + \underbrace{g_{(X,Y)}(x,y)}_{Y} ,$$

where

main effect of
$$X$$

main effect of Y

interaction effect of X and Y

$$g_0 = \iint g(x, y) P_X(dx) P_Y(dy),$$

$$g_X(x) = g_X^*(x) - g_0 = \int g(x, y) P_Y(dy) - g_0,$$

$$g_Y(y) = g_Y^*(y) - g_0 = \int g(x, y) P_X(dx) - g_0.$$

- Because they are obtained via orthogonal projection, the functions g_0 , g_X , g_Y , and $g_{(X,Y)}$ are orthogonal functions.
- The property that g_0 , g_X , g_Y , and $g_{(X,Y)}$ are orthogonal provides a link with other expansions, such as the polynomial chaos expansion.

Statistical point of view

Sensitivity indices = mean-square values of main effects and interaction effects:

• Quantitative insight into the significance of *X* and *Y* in inducing uncertainty in *Z*: $\iint |g(x,y) - g_0|^2 P_X(dx) P_Y(dy)$

$$= \underbrace{\int |g_X(x)|^2 P_X(dx)}_{=s_X} + \underbrace{\int |g_Y(y)|^2 P_Y(dy)}_{=s_Y} + \underbrace{\int \int |g_{(X,Y)}(x,y)|^2 P_X(dx) P_Y(dy)}_{=s_Y}.$$

Because g_X , g_Y , and $g_{(X,Y)}$ are orthogonal, there are no double product terms.

Thus, the expansion of g (geometry) reflects a **partitioning of the variance** of Z into terms that are the variances of the main and interaction effects of X and Y (statistics), where:

 s_X = portion of the variance of Z that is explained as stemming from X,

 s_Y = portion of the variance of Z that is explained as stemming from Y.

Statistical point of view

By the conditional variance identity, we have

$$s_X = V\{E\{Z|X\}\} = V\{Z\} - E\{V\{Z|X\}\},\$$

$$s_Y = V\{E\{Z|Y\}\} = V\{Z\} - E\{V\{Z|Y\}\},\$$

so that s_X and s_Y may also be interpreted as expected reductions of amount of uncertainty:

 s_X = expected reduction of variance of Z if there were no longer uncertainty in X,

 s_Y = expected reduction of variance of Z if there were no longer uncertainty in Y.

In contrast to the expansion of g and the variance partitioning of Z, these expressions and these interpretations of s_X and s_Y remain valid even if X and Y are statistically dependent.

Example

Let us consider a simple problem wherein X and Y are uniform r.v. with values in [-1, 1],

$$X \sim \mathcal{U}([-1,1]),$$
$$Y \sim \mathcal{U}([-1,1]),$$

and the function g is given by

$$z = g(x, y) = x + y^2 + xy.$$

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To this expansion corresponds the variance partitioning

$$\sigma_Z^2 = s_X + s_Y + s_{(X,Y)},$$

$$\sigma_Z^2 = \frac{28}{45}, \quad s_X = \frac{1}{3} = 53.57\%\sigma_Z^2, \quad s_Y = \frac{8}{45} = 28.57\%\sigma_Z^2, \quad s_{(X,Y)} = \frac{1}{9} = 17.86\%\sigma_Z^2.$$

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Computation by means of a **stochastic expansion method**:

$$s_X \approx \sum_{\alpha \neq 0} c_{(\alpha,0)}^2,$$

$$s_Y \approx \sum_{\beta \neq 0} c_{(0,\beta)}^2, \quad \text{with} \quad g(x,y) = \sum_{(\alpha,\beta)} c_{(\alpha,\beta)} \varphi_{\alpha}(x) \psi_{\beta}(y).$$

Computation by means of **deterministic numerical integration**:

$$s_X \approx Q_X (|Q_Y g - Q_X Q_Y g|^2),$$

$$s_Y \approx Q_Y (|Q_X g - Q_X Q_Y g|^2).$$

Computation by means of **Monte Carlo integration**:

$$s_X \approx \frac{1}{\nu} \sum_{\ell=1}^{\nu} \left(g(x_\ell, y_\ell) - \frac{1}{\nu} \sum_{k=1}^{\nu} g(x_k, y_k) \right) \left(g(x_\ell, \tilde{y}_\ell) - \frac{1}{\nu} \sum_{k=1}^{\nu} g(x_k, \tilde{y}_k) \right),$$

$$s_Y \approx \frac{1}{\nu} \sum_{\ell=1}^{\nu} \left(g(x_\ell, y_\ell) - \frac{1}{\nu} \sum_{k=1}^{\nu} g(x_k, y_k) \right) \left(g(\tilde{x}_\ell, y_\ell) - \frac{1}{\nu} \sum_{k=1}^{\nu} g(\tilde{x}_k, y_k) \right).$$

References: [B. Sudret. Reliab. Eng. Syst. Safe., 2008], [Crestaux et al. Reliab. Eng. Syst. Safe., 2009], [I. Sobol. Math. Comput. Simulat., 2001], and [A. Owen. ACM T. Model. Comput. S., 2013].

Observation:

Most applications in the literature involve scalar-valued sources of uncertainty.

Opportunity:

The **concepts and methods** of global sensitivity analysis are **valid and useful more broadly** for stochastic process, random fields, random matrices, and other sources of uncertainty.

Generalized probabilistic modeling



Parametric uncertainties and modeling errors can present themselves.

- Types of probabilistic approach:
 - Parametric approaches capture parametric uncertainties by characterizing geometrical characteristics, boundary conditions, loadings, and physical or mechanical properties as random variables or stochastic processes.
 - Nonparametric approaches capture modeling errors (and possibly the impact of parametric uncertainties) by directly characterizing the model as a random model without recourse to a characterization of its parameters as random variables or stochastic processes.

In structural dynamics, Soize constructed a class of nonparametric models by characterizing the reduced matrices of (a sequence of) reduced-order models as random matrices.

- Output-prediction-error approaches capture modeling errors (and possibly the impact of parametric uncertainties) by adding random noise terms to quantities of interest.
- Generalized approaches are couplings of parametric and nonparametric approaches.
- References: [C. Soize. Probab. Eng. Mech., 2000]. [C. Soize. Int. J. Num. Methods Eng., 2010].



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Nonlinear elasticity. [Capiez-Lernout et al. Comput. Methods Appl. Mech. Engrg., 2014].

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Viscoelasticity. [Capillon et al. Comput. Methods Appl. Mech. Engrg., 2016].

Deterministic model

FE model of linear dynamical behavior of dissipative structure:

$$[M(\boldsymbol{x})]\ddot{\boldsymbol{u}}(t) + [D(\boldsymbol{x})]\dot{\boldsymbol{u}}(t) + [K(\boldsymbol{x})]\boldsymbol{u}(t) = \boldsymbol{f}(t,\boldsymbol{x}),$$

where

x collects the parameters of the FE model, which may consist of material properties, loadings, geometrical characteristics, and so forth.

 $\boldsymbol{u} = (u_1, \ldots, u_m)$ is the (generalized) displacement vector,

f the (generalized) external forces vector,

and $[M(\boldsymbol{x})]$, $[D(\boldsymbol{x})]$, and $[K(\boldsymbol{x})]$ the mass, damping, and stiffness matrices.

Parametric probabilistic approach = probabilistic representation of uncertain parameters:

$$[M(\boldsymbol{X})]\ddot{\boldsymbol{U}}(t) + [D(\boldsymbol{X})]\dot{\boldsymbol{U}}(t) + [K(\boldsymbol{X})]\boldsymbol{U}(t) = \boldsymbol{f}(t, \boldsymbol{X}),$$

where

X is the probabilistic representation of the uncertain parameters, which may consist of random variables, stochastic processes, and so forth.

In order to obtain the probabilistic representation of the uncertain parameters, a suitable probability distribution must be assigned to the random variables or stochastic processes.

In stochastic mechanics, methods are available for deducing a suitable probability distribution from available information, such as methods dedicated to tensor-valued fields of material properties, methods dedicated to tensors in rigid-body mechanics, and methods dedicated to random loadings.

Generalized probabilistic model

Generalized probabilistic approach = enhancement of parametric probabilistic model by introducing in it a probabilistic representation of modeling errors.

Step 1: Associate with the parametric probabilistic model a **reduced-order probabilistic model**:

$$[M_n(\boldsymbol{X})]\ddot{\boldsymbol{Q}}(t) + [D_n(\boldsymbol{X})]\dot{\boldsymbol{Q}}(t) + [K_n(\boldsymbol{X})]\boldsymbol{Q}(t) = \boldsymbol{f}^n(t,\boldsymbol{X}),$$
$$\boldsymbol{U}^n(t) = [\Phi(\boldsymbol{X})]\boldsymbol{Q}(t),$$

where

 $[M_n(X)]$, $[D_n(X)]$, and $[K_n(X)]$ are the reduced mass, damping, and stiffness matrices, and $[\Phi(X)]$ the matrix collecting in its columns the reduction basis $\varphi_1(X)$, $\varphi_2(X)$, ..., $\varphi_n(X)$.

Such a reduced-order probabilistic model can be obtained, for instance, by solving the eigenvalue problem associated with the mass and stiffness matrices of the parametric probabilistic model,

$$[K(\boldsymbol{X})]\boldsymbol{\varphi}_{j}(\boldsymbol{X}) = \lambda_{j}(\boldsymbol{X})[M(\boldsymbol{X})]\boldsymbol{\varphi}_{j}(\boldsymbol{X});$$

in which case the reduced matrices of the reduced-order probabilistic are given by

$$[M_n(\boldsymbol{X})]_{ij} = \delta_{ij}, \quad [D_n(\boldsymbol{X})]_{ij} = \boldsymbol{\varphi}_i(\boldsymbol{X}) \cdot [D(\boldsymbol{X})] \boldsymbol{\varphi}_j(\boldsymbol{X}), \quad [K_n(\boldsymbol{X})]_{ij} = \lambda_i \delta_{ij}.$$

Step 2: represent the reduced matrices by using random matrices:

$$[\boldsymbol{M}_{n}(\boldsymbol{X})]\ddot{\boldsymbol{Q}}(t) + [\boldsymbol{D}_{n}(\boldsymbol{X})]\dot{\boldsymbol{Q}}(t) + [\boldsymbol{K}_{n}(\boldsymbol{X})]\boldsymbol{Q}(t) = \boldsymbol{f}^{n}(t,\boldsymbol{X}),$$
$$\boldsymbol{U}^{n}(t) = [\Phi(\boldsymbol{X})]\boldsymbol{Q}(t),$$

To accommodate in the reduced matrices a probabilistic representation of the modeling errors, the generalized probabilistic approach entails representing these reduced matrices as follows:

$$egin{aligned} & [oldsymbol{M}_n(oldsymbol{X})] = [L_M(oldsymbol{X})][oldsymbol{Y}_M][L_M(oldsymbol{X})]^{\mathrm{T}}, \ & [oldsymbol{D}_n(oldsymbol{X})] = [L_D(oldsymbol{X})][oldsymbol{Y}_D][L_D(oldsymbol{X})]^{\mathrm{T}}, \ & [oldsymbol{K}_n(oldsymbol{X})] = [L_K(oldsymbol{X})][oldsymbol{Y}_K][L_K(oldsymbol{X})]^{\mathrm{T}}, \end{aligned}$$

with $[L_M(X)]$, $[L_D(X)]$, and $[L_K(X)]$ the Cholesky factors of $[M_n(X)]$, $[D_n(X)]$, and $[K_n(X)]$.

Generalized probabilistic model

To assign a suitable probability distribution to the random matrices $[Y_M]$, $[Y_D]$, and $[Y_K]$, the generalized probabilistic approach uses the maximum entropy principle.

The probability distribution thus obtained is such that the mean values of $[Y_M]$, $[Y_D]$, and $[Y_K]$ are all equal to the identity matrix, that is,

$$E\{[\mathbf{Y}_{M}]\} = [I_{n}], \\ E\{[\mathbf{Y}_{D}]\} = [I_{n}], \\ E\{[\mathbf{Y}_{K}]\} = [I_$$

and the amount of uncertainty expressed in $[Y_M]$, $[Y_D]$, and $[Y_K]$ is tunable by free dispersion parameters δ_M , δ_D , and δ_K , respectively, defined by

$$\delta_{M} = \sqrt{E\{\|[\mathbf{Y}_{M}] - [I_{n}]\|_{\mathsf{F}}^{2}\}/\|[I_{n}]\|_{\mathsf{F}}^{2}},$$

$$\delta_{D} = \sqrt{E\{\|[\mathbf{Y}_{D}] - [I_{n}]\|_{\mathsf{F}}^{2}\}/\|[I_{n}]\|_{\mathsf{F}}^{2}},$$

$$\delta_{K} = \sqrt{E\{\|[\mathbf{Y}_{K}] - [I_{n}]\|_{\mathsf{F}}^{2}\}/\|[I_{n}]\|_{\mathsf{F}}^{2}}.$$

The dispersion parameters must be calibrated such that the amount of uncertainty expressed in $[Y_M]$, $[Y_D]$, and $[Y_K]$ reflects the significance of the modeling errors.

First illustration: parametric uncertainties and modeling errors



Parametric uncertainties and modeling errors present themselves.

Deterministic model

$$[H(\omega; \boldsymbol{x})] = [-\omega^2 M(\boldsymbol{x}) + i\omega D(\omega; \boldsymbol{x}) + K(\boldsymbol{x})]^{-1}.$$



$$[H(\omega; \boldsymbol{X})] = [-\omega^2 M(\boldsymbol{X}) + i\omega D(\omega; \boldsymbol{X}) + K(\boldsymbol{X})]^{-1},$$

where X = random field representation of shear and bulk moduli.



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$$\begin{split} [H(\omega; \boldsymbol{X}, \boldsymbol{Y})] &= [\Phi(\boldsymbol{X})][-\omega^2 \boldsymbol{M}_n(\boldsymbol{X}) + i\omega \boldsymbol{D}_n(\omega; \boldsymbol{X}) + \boldsymbol{K}_n(\boldsymbol{X})]^{-1} [\Phi(\boldsymbol{X})]^{\mathrm{T}}, \\ \text{where } \boldsymbol{Y} &= ([\boldsymbol{Y}_M], [\boldsymbol{Y}_D], [\boldsymbol{Y}_K]) \text{ with } \begin{cases} [\boldsymbol{M}_n(\boldsymbol{X})] = [L_M(\boldsymbol{X})][\boldsymbol{Y}_M][L_M(\boldsymbol{X})]^{\mathrm{T}}, \\ [\boldsymbol{D}_n(\omega; \boldsymbol{X})] = [L_D(\omega; \boldsymbol{X})][\boldsymbol{Y}_D][L_D(\omega; \boldsymbol{X})]^{\mathrm{T}}, \\ [\boldsymbol{K}_n(\boldsymbol{X})] = [L_K(\boldsymbol{X})][\boldsymbol{Y}_K][L_K(\boldsymbol{X})]^{\mathrm{T}}. \end{cases} \end{split}$$



$$\begin{split} [H(\omega; \boldsymbol{X}, \boldsymbol{Y})] &= [\Phi(\boldsymbol{X})][-\omega^2 \boldsymbol{M}_n(\boldsymbol{X}) + i\omega \boldsymbol{D}_n(\omega; \boldsymbol{X}) + \boldsymbol{K}_n(\boldsymbol{X})]^{-1} [\Phi(\boldsymbol{X})]^{\mathrm{T}}, \\ \text{where } \boldsymbol{Y} &= ([\boldsymbol{Y}_M], [\boldsymbol{Y}_D], [\boldsymbol{Y}_K]) \text{ with } \begin{cases} [\boldsymbol{M}_n(\boldsymbol{X})] = [L_M(\boldsymbol{X})][\boldsymbol{Y}_M][L_M(\boldsymbol{X})]^{\mathrm{T}}, \\ [\boldsymbol{D}_n(\omega; \boldsymbol{X})] = [L_D(\omega; \boldsymbol{X})][\boldsymbol{Y}_D][L_D(\omega; \boldsymbol{X})]^{\mathrm{T}}, \\ [\boldsymbol{K}_n(\boldsymbol{X})] = [L_K(\boldsymbol{X})][\boldsymbol{Y}_K][L_K(\boldsymbol{X})]^{\mathrm{T}}. \end{cases} \end{split}$$



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Identification

The dispersion parameters must be calibrated such that the amount of uncertainty expressed in $[Y_M]$, $[Y_D]$, and $[Y_K]$ reflects the significance of the modeling errors.



Generalized probabilistic model with $\hat{\delta}_M = \hat{\delta}_D = \hat{\delta}_K = 0.20$ (gray).

Because the problem is of high dimension, we compute the sensitivity indices by using Monte Carlo integration, whereby we assess the convergence as a function of the number of samples.



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Sensitivity analysis

$$\begin{split} \mathsf{V}\{\log|H_{jj'}(\omega; \boldsymbol{X}, \boldsymbol{Y})|\} &= s_{\boldsymbol{X}}(\omega) + s_{\boldsymbol{Y}}(\omega) + s_{(\boldsymbol{X}, \boldsymbol{Y})}(\omega),\\ s_{\boldsymbol{X}}(\omega) &= \mathsf{Var}_{\boldsymbol{X}}\big\{\mathsf{E}_{\boldsymbol{Y}}\{\log|H_{jj'}(\omega; \boldsymbol{X}, \boldsymbol{Y})|\big\}\big\},\\ s_{\boldsymbol{Y}}(\omega) &= \mathsf{Var}_{\boldsymbol{Y}}\big\{\mathsf{E}_{\boldsymbol{X}}\{\log|H_{jj'}(\omega; \boldsymbol{X}, \boldsymbol{Y})|\big\}\big\}. \end{split}$$



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Second illustration: multiple components

Stiffened panel with a hole.



Deterministic model

First few dynamical eigenmodes.





Mode 2 at 302.82 Hz.

After a component mode synthesis, we used the nonparametric probabilistic approach to introduce uncertainties in the submodels of the main panel and the stiffeners.



PDFs of the first and second eigenfrequencies.

Sensitivity analysis



Conclusion and acknowledgement

Global sensitivity analysis methods can help ascertain which sources of uncertainty are most significant in inducing uncertainty in predictions.

Although most applications in the literature involve scalar-valued sources of uncertainty, the concepts and methods of global sensitivity analysis are valid and useful more broadly for stochastic process, random fields, random matrices, and other sources of uncertainty.

Generalized probabilistic modeling approaches are hybrid couplings of parametric modeling approaches (to capture parametric uncertainties) and nonparametric probabilistic modeling approaches (to capture modeling errors).

We discussed global sensitivity analysis of generalized probabilistic models and demonstrated its application in two illustrations from structural dynamics.

Conclusion and acknowledgement

This presentation can be downloaded from our institutional repository:



http://orbi.ulg.ac.be.

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