Uncertainty and sensitivity analysis of functional risk curves based on Gaussian processes

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Abstract

A functional risk curve gives the probability of an undesirable event in function of the value of a critical parameter of a considered physical system. In several applicative situations, this curve is built using phenomenological numerical models which simulate complex physical phenomena. Facing to cpu-time expensive numerical models, we propose to use the Gaussian process model to build functional risk curve. An algorithm is given to provide confidence bounds due to this approximation. Sensitivity analysis of the model random input parameters on the functional risk curve is also studied. As important information is given by new sensitivity indices (called PLI) allowing to understand the effect of misjudgment on the input parameters' probability density functions.

1 INTRODUCTION

In industrial practice, the estimation of a functional risk curve is often required as a quantitative measure of a system safety. A functional risk curve gives the probability of an undesirable event in function of the value of a critical parameter of a considered physical system. The estimation of this curve sometimes relies on deterministic phenomenological computer models which simulate complex physical phenomena. Uncertain input parameters of this computer code are

modeled as random variables while one of its scalar output variable becomes the studied random variable of interest.

As it based on a probabilistic modeling of uncertain physical variables and their propagation through a numerical model, this problem can be directly related to the uncertainty management methodology in numerical simulation (de Rocquigny et al., 2008; Baudin et al., 2016). This methodology proposes a generic framework of modeling, calibrating, propagating and prioritizing uncertainty sources through a numerical model (or computer code). Indeed, investigation of complex computer code experiments has remained an important challenge in all domain of science and technology, in order to make simulations as well as predictions, uncertainty analysis or sensitivity studies (Fang et al., 2006; Smith, 2014). In this framework, the physical numerical model G just writes

$$Y = G(X) = G(X_1, \ldots, X_d) \ , \tag{1}$$

with $X \in \mathbb{R}^d$ the random input vector of dimension d and $Y \in \mathbb{R}$ a scalar model output.

However, standard uncertainty treatment techniques require many model evaluations and a major algorithmic difficulty arises when the computer code under study is too time expensive to be directly used. For cpu-time expensive models, one solution consists in replacing the numerical model by a mathematical approximation, called a response surface or a metamodel. Several statistical tools based on numerical design of experiments, uncertainty propagation efficient algorithms and metamodeling concepts will then be useful (Fang et al., 2006). In this paper, the Gaussian process regression (Rasmussen and Williams, 2006) is used as a metamodel technique (surrogate model of the computer code) and applied in the particular context of a functional risk curve as a quantity of interest. Indeed, numerous studies have shown that this interpolating model provides a powerful statistical framework to compute an efficient predictor of a deterministic computer code response (Marrel et al., 2008; Le Gratiet et al., 2016).

Associated to the estimation of the quantity of interest after the uncertainty propagation step, the sensitivity analysis step is performed to determine those parameters that mostly influence on model response (Saltelli et al., 2000). In particular, global sensitivity analysis methods take into account the overall uncertainty ranges of the input parameter (see Iooss and Lemaître (2015) for a recent review). Several works have focused on estimating global sensitivity indices (especially the variance-based ones, known as the Sobol' indices) using the Gaussian process model (Oakley and O'Hagan, 2004; Le Gratiet et al., 2014, 2016). In this paper, we propose new global sensitivity indices attached to the whole functional risk curve, while showing how to develop them with a Gaussian process model. We focus on a recently developed method, the Perturbed-Law based sensitivity Indices (PLI) of Lemaître et al. (2015), which seems promising in terms of efficiency and interpretation.

Two examples of functional risk curve largely used in some industrial safety practices are given in the following section. The third section describes the Gaussian process way to model and estimate a functional risk curve. The fourth section introduces the sensitivity indices based on probability density perturbations and their application on functional risk curve. A conclusion synthesizes this work.

2 MOTIVATING EXAMPLES

2.1 SEISMIC FRAGILITY CURVES

The "fragility curve" is a popular functional risk criterion, commonly used in many engineering fields (Pasanisi, 2014). It describes the probability that the actual damage to a structure exceeds a damage criterion, when the structure is assigned to a specified load intensity. For instance, the seismic fragility curve concerns systems subjected to earthquake, whose interest is of particular significance in nuclear safety studies.

In the case of seismic risk assessment the load is usually expressed as a scalar characteristic of a seismic signal, typically the horizontal Peak Ground Acceleration (PGA), common choice in civil engineering. Several parameters and phenomena, distinct from the PGA, also influence the load: for each PGA value, the occurrence of the damage event is random. Then, the fragility curve may be interpreted as the cumulative distribution function of the "structural capability", i.e. the maximum load the structure under investigation can bear without damage (Zentner and Borgonovo, 2014; Damblin et al., 2014). Fragility curves are then useful tools in structural analysis as they provide a more complete information than the usual failure probability (established for a reference value of the load only).

In the standard practice, the assessment is made either following an approach entirely based on the expertise or by the statistical analysis of actually observed or simulated data. As actual damage data may be scarce due to the rarity of severe earthquakes liable to generate damages on highly safe structures, observations are generated by mock-up or (most often) numerical experiments.

2.2 PROBABILITY OF DETECTION CURVES

In several industries, the Probability Of Detection (POD) curve is a standard tool to evaluate the performance of Non Destructive Testing (NDT) procedures. The goal is to assess the quantification of inspection capability for the detection of harmful flaws for the inspected structure. For instance, new aeronautic regulations require for critical parts to perform appropriate damage tolerance assessments to address the potential for failure from material and manufacturing. This imposes enhanced expectations on POD sizing. Another example

is the eddy current non destructive examination process which is used to ensure integrity of steam generators tubes in nuclear power plants (Maurice et al., 2013; Browne et al., 2015). Experimental campaigns and simulations experiments are used in order to provide POD as a tool to the process qualification by the regulatory authorities.

In practice, high costs of the implementation of experimental POD campaigns combined with continuous increase in the complexity of configuration make them sometimes unaffordable. To overcome this problem, it is possible to resort to numerical simulation of NDT process. This approach has been called MAPOD for "Model Assisted Probability of Detection" (Thompson, 2008; Calmon, 2012).

More precisely, in the POD context, the problem is formulated as follow. Given a threshold $s > 0$, a flaw is considered to be detected when $Y > s$ with Y the signal amplitude and s a detection threshold. Therefore the one dimensional POD curve is denoted by:

$$\forall a > 0 \quad \mathrm{POD}(a) = P_X \left(G(a, X) > s \mid a \right) \ , \tag{2}$$

where a is the POD parameter of interest (for example the size flaw) and X are the other input parameters. When simulated experiments are used to build the POD, Y is a scalar output of a numerical model ($Y = G(a, X)$), where a is determined by its bounds and X is a random vector defined by its joint probability density function.

3 GAUSSIAN-PROCESS BASED FUNCTIONAL RISK CURVE ESTIMATION

Dealing with cpu-time expensive computer model, we use the Gaussian process regression (Sacks et al., 1989; Rasmussen and Williams, 2006). Let X be a random vector of influent and uncertain parameter inside the computer model $G(\cdot)$ and a be the parameter of interest (the abscissa of the functional risk curve). The prior knowledge on $G(a, X)$ is modeled by $Y(a, X)$ and defined as follows .

$$Y(a, X) = \beta_0 + \beta_1 a + Z(a, X), \tag{3}$$

where Z is a centered Gaussian process. We make the assumption that Z is second order stationary with variance σ^2 and a parametric covariance (for example the Matérn 5/2 parametrized by its lengthscale θ). Thanks to the maximum likelihood method, we can estimate the values of the so far-unknown parameters: $\beta_0, \beta_1, \sigma^2$ and θ (see for instance Marrel et al. (2008) for more details).

Gaussian process regression (also known as the kriging process) provides an estimator of $G(a, x)$ which is called the kriging predictor and written $\widehat{Y}(a, x)$. In addition to the kriging predictor, the kriging variance $\sigma^2_Y(a, x)$ quantifies

the uncertainty induced by estimating $Y(a,x)$ with $\widehat{Y}(a,x)$. The predictive distribution is given by $Y(a,x)$ conditioned by y^N:

$$\forall x \quad \left(Y(a,x) \mid y^N\right) \sim \mathcal{N}\left(\widehat{Y}(a,x), \sigma_Y^2(a,x)\right) \tag{4}$$

where $\widehat{Y}(a,x)$ (the kriging mean) and $\sigma_Y^2(a,x)$ (the kriging variance) can both be explicitly estimated.

Obtaining the functional risk curve $\Psi(a)$ consists in replacing $Y = G(a,X)$ by its Gaussian process metamodel (4) in (2). Hence we can estimate the value of $\Psi(a)$, for $a > 0$ from:

$$\Psi(a) = \mathbb{P}\left((Y(a,X) \mid y^N) > s|a\right). \tag{5}$$

Two sources of uncertainty have to be taken into account in (5): the first coming from the parameter X and the second coming from the Gaussian distribution in (4).

From (5), the following estimate for $\Psi(a)$ can be deduced:

$$\Psi(a) = \mathbb{E}_X\left[1 - \Phi\left(\frac{s - \widehat{Y}(a,X)}{\sigma_Y(a,X)}\right)\right], \tag{6}$$

where Φ is the standard Gaussian distribution function. This equation corresponds to the mean functional risk curve with respect to the Gaussian process metamodel. The expectation in (6) is estimated using a classical Monte Carlo integration procedure.

In order to estimate the uncertainty on the functional risk curve estimation, we start from its integral expression:

$$\begin{aligned} \Psi(a) &= P_X(y(a,X) > s|a) \\ &= \int 1_{y(a,x)>s} f(x)dx, \end{aligned}$$

where $f(x)$ if the joint probability density function (pdf) of X (independent on a). The first uncertainty source on $\Psi(a)$ comes from the numerical evaluation of the integral inside the $\Psi(a)$ definition. This evaluation is done by the Monte Carlo method:

$$\Psi(a) \approx \Psi_{MC}(a) = \frac{1}{n}\sum_{i=1}^{n} 1_{y(a,x^{(i)})>s}, \tag{7}$$

where $(x^{(i)})_{i=1,\ldots,n}$ is a sample of the random variable X. The size of this sample has to be large, then we replace the code by its Gaussian process approximation $Y(a,x)|y^N$:

$$\Psi_{MC}(a) \approx \Psi_{MC,PG}(a) = \frac{1}{n}\sum_{i=1}^{n} 1_{Y(a,x^{(i)})|y^N>s}. \tag{8}$$

Let us recall that $Y(a,x)|y^N$ is a Gaussian process that we know the mean and variance. To compute the integration error, the central limit theorem is used and gives for $n \to \infty$:

$$\begin{aligned} &\sqrt{n}\left(\Psi_{MC,PG}(a) - \Psi_{PG}(a)\right) \\ &\longrightarrow \mathcal{N}\left(0, \Psi_{PG}(a)(1-\Psi_{PG}(a))\right), \end{aligned}$$

where

$$\Psi_{PG}(a) = \int 1_{Y(a,x)|y^N > s}\, f(x)dx. \tag{9}$$

$\Psi_{PG}(a)$ corresponds to the functional risk curve for the process $Y(a,x)|y^N$. The algorithm consists in taking a large n in order to deal with a valid Gaussian approximation.

The second uncertainty source on $\Psi(a)$ estimation comes from the Gaussian process approximation. We simulate m realizations $(y^{(j)}(a,x))_{j=1,\dots,m}$ of $Y(a,x)|y^N$ in order to evaluate the variability of $\Psi_{MC,PG}(a)$ which comes from the Gaussian process approximation. We then compute:

$$\psi_{MC,PG,j}(a) = \frac{1}{n}\sum_{i=1}^{n} 1_{y^{(j)}(a,x^{(i)})>s}. \tag{10}$$

Therefore, for each $\psi^{(j)}_{MC,PG}(a)$, $j = 1,\dots,m$, we compute the Monte Carlo error thanks to the central limit theorem:

$$\psi^{(j)}_{PG}(a)) \sim \mathcal{N}\left(\psi^{(j)}_{MC,PG}(a), \Upsilon^{(j)}(a)\right), \tag{11}$$

where $\Upsilon^{(j)}(a) = \dfrac{\psi^{(j)}_{MC,PG}(a)\left(1-\psi^{(j)}_{MC,PG}(a)\right)}{n}$. $\psi^{(j}_{PG})(a)$ is the true value of the functional risk curve for the realization j of $Y(a,x)|y^N$.

From this double Monte Carlo method, we are able to compute the functional risk curve uncertainty due to the Gaussian process metamodel and due to the numerical integration process. Figure 1 illustrates the algorithm on a POD curve estimation in a NDT application (see section 2.2). A Gaussian process metamodel has been built on $N = 100$ numerical simulations of eddy current non destructive examination on steam generators tube (Browne et al., 2015). We visualize the confidence interval induced by the Monte Carlo (MC) estimation ($n = 10000$), the one induced by the Gaussian process approximation ($m = 3000$) and the total confidence interval (including both approximations: PG+MC).

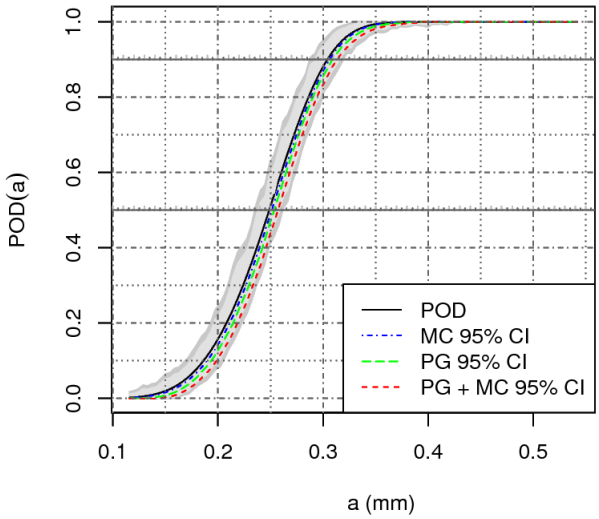

Figure 1: Example of functional risk curve estimated with a Gaussian process model. The present curve is a POD curve.

4 PERTURBED-LAW BASED SENSITIVITY INDICES

We propose now to quantify the impact, on the functional risk curve, of a perturbation of the input parameters pdfs by answering to the following question: "What would be the functional risk curve if the pdf of the ith input X_i had been modified?". In this approach, all the input parameters are modeled by random variables and their input probability densities are supposed to be uncertain. Let us remark that a negligible sensitivity index of an input will not allow to fix this input but just to say that its pdf has no influence on the functional risk curve.

We use the so-called Perturbed-Law based sensitivity Indices (PLI) measures recently introduced in Lemaître et al. (2015) (see also Borgonovo and Iooss (2016)). We start from the integral-form of the functional risk curve:

$$P_X\left(y(a,X) > s\right) = \int 1_{y(a,x)>s} f(x)\, dx,$$

where $f(x)$ is the joint pdf of X. Modifying the pdf $f_i(x_i)$ of X_i gives us $f_{i,\delta}(x_i)$, the perturbed pdf of X_i. After this perturbation, the functional risk curve, noticed $P_{X_i,\delta}(\cdot)$ instead of $P_X(\cdot)$, can be written as:

$$P_{X_i,\delta}\left(y(a,X) > s\right) = \int 1_{y(a,x)>s} \frac{f_{i,\delta}(x_i)}{f_i(x_i)} f(x)\, dx, \tag{12}$$

The PLI measures only consist in the comparison of the functional risk curves between and after the perturbation, and are defined by:

$$S_{i,\delta} = \begin{cases} \dfrac{P_{X_i,\delta}\left(y(a,X) > s\right) - P_X\left(y(a,X) > s\right)}{P_{X_i,\delta}\left(y(a,X) > s\right)} \\ \text{if} \quad P_{X_i,\delta}\left(y(a,X) > s\right) \geq P_X\left(y(a,X) > s\right), \\ \\ \dfrac{P_{X_i,\delta}\left(y(a,X) > s\right) - P_X\left(y(a,X) > s\right)}{P_X\left(y(a,X) > s\right)} \\ \text{if} \quad P_{X_i,\delta}\left(y(a,X) > s\right) < P_X\left(y(a,X) > s\right). \end{cases} \tag{13}$$

A negative $S_{i,\delta}$ means that the functional risk curve is smaller after the perturbation, while a positive $S_{i,\delta}$ means that the functional risk curve has increased. The estimation of $P_{X_i,\delta}\left(y(a,X) > s\right)$ is based on reverse importance sampling (Hesterberg, 1996). Asymptotical properties of the estimators give also some confidence intervals on the PLI measures.

In Lemaître et al. (2015), the numerical model is directly used to estimate the PLI measures by large Monte Carlo samples. We propose here to estimate the PLI measures by using the Gaussian process metamodel and integrating its error in the estimates. The mean functional risk curve that we consider is given by (6):

$$\Psi(a) = E_X\left[1 - \Phi\left(\frac{s - \widehat{Y}(a,X)}{\sigma_Y(a,X)}\right)\right] \tag{14}$$

$$= \int 1 - \Phi\left(\frac{s - \widehat{Y}(a,x)}{\sigma_Y(a,x)}\right) f(x)\, dx. \tag{15}$$

After the perturbation of the pdf of the ith input, the mean functional risk curve is given by:

$$\Psi_{i,\delta}(a) = \int 1 - \Phi\left(\frac{s - \widehat{Y}(a,x)}{\sigma_Y(a,x)}\right) \frac{f_{i,\delta}(x_i)}{f_i(x_i)} f(x)\, dx. \tag{16}$$

PLI measures are then given by:

$$S_{i,\delta}(a) = \begin{cases} \dfrac{\Psi_{i,\delta}(a) - \Psi(a)}{\Psi_{i,\delta}(a)} \\ \text{if} \quad \Psi_{i,\delta}(a) \geq \Psi(a), \\ \\ \dfrac{\Psi_{i,\delta}(a) - \Psi(a)}{\Psi(a)} \\ \text{if} \quad \Psi_{i,\delta}(a) < \Psi(a). \end{cases} \tag{17}$$

The last element of the PLI method is the definition of the perturbations $f_{i,\delta}(x_i)$. Lemaître et al. (2015) choose to perturb a statistical characteristic (for

example the mean, or the variance, or a quantile, ...) of X_i in order to be "as close as possible" to the initial pdf $f_i(x_i)$. The dissimilarity measure between $f_{i,\delta}(x_i)$ and $f_i(x_i)$, which contains the required properties, is the Kullback-Leibler divergence:

$$KL(f_{i,\delta}(x_i), f_i(x_i)) = \int_{-\infty}^{+\infty} f_{i,\delta}(x_i) \log \frac{f_{i,\delta}(x_i)}{f_i(x_i)} dx_i. \tag{18}$$

It implies that $f_{i,\delta}(X_i)$ and $f_i(X)$ have the same definition domain (as a consequence, the input domain bounds cannot be changed). The Kullback-Leibler divergence has the advantage to be easily minimized, in order to obtain explicit solutions for $f_{i,\delta}(X_i)$ for classical pdf (*e.g.* Gaussian).

Figure 2 gives some examples of perturbations for the uniform pdf on $[0, 1]$ (mean is 0.5 and variance is 1/12). Figure 3 gives some examples of perturbations for the standard Gaussian pdf (mean is 0 and variance is 1).

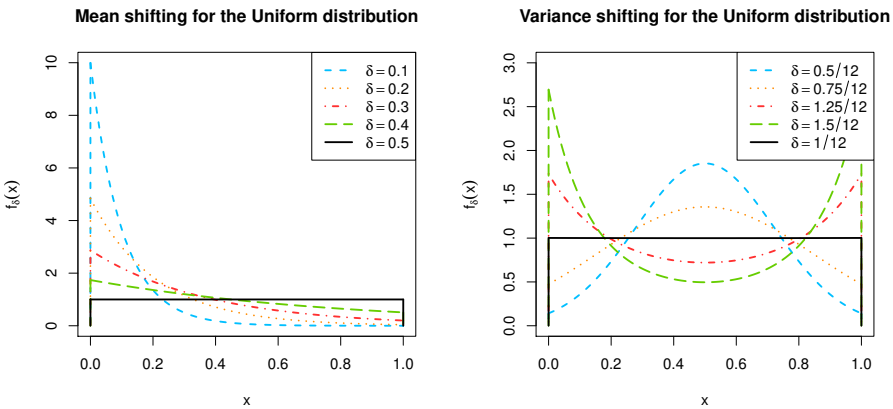

Figure 2: Examples of perturbations for the uniform pdf on $[0, 1]$. Left: the mean of the pdf is perturbed (δ is the new mean value). Right: the variance of the pdf is perturbed (δ is the new variance value).

Figure 4 gives an example of a PLI-based sensitivity analysis on our NDT test case (see section 2.2) which aims to estimate POD curve and the associated sensitivity indices to its five physical input parameters (called E, ebav_1, ebav_2, h_{11} and h_{12}), the defect size a being fixed here at a given value. The input parameters pdfs are all uniform on $[0, 1]$. Their non-perturbed mean is then 1/2. Then, the mean of each input is modified in the range of $\delta \in [0.1, 0.9]$. For each δ value and each influent parameter, the graph 4 gives the PLI estimates $\hat{S}_\delta$. Large absolute value of $\hat{S}_\delta$ imply a large impact of the perturbation on the functional risk curve. Moreover, the sign of $\hat{S}_\delta$ indicates if the new probability has decreased (negative case) or has increased (positive case). Confidence intervals illustrated on the Figure 4 are obtained thanks to a Gaussian asymptotical

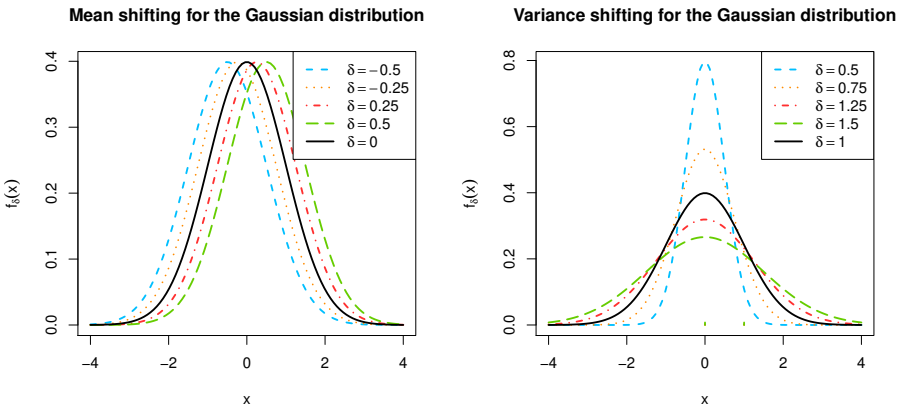

Figure 3: Examples of perturbations for the standard Gaussian pdf. Left: the mean of the pdf is perturbed (δ is the new mean value). Right: the standard-deviation of the pdf is perturbed (δ is the new standard-deviation value).

property of the estimates $\hat{S}_{i,\delta}$ (Lemaître et al., 2015). In Figure 4, one can see for instance that increasing the h_{12} input mean largely increases the functional risk curve, while decreasing the $ebav_1$ input mean largely decreases the functional risk curve. In contrary, perturbations of the E mean have no effect on the functional risk curve.

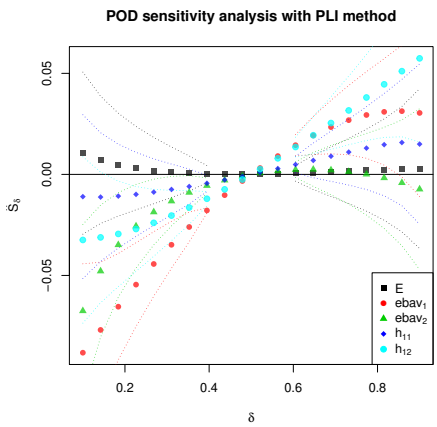

Figure 4: Graphical example for the PLI measures. The present study is on the POD curves.

In order to have a global view of the functional risk curve sensitivity for different defect sizes a, Figure 5 give the PLI graphs for each input, with varia-

tions of a and the δ perturbation. Clearly, the inputs ebav_1 and h_{12} have strong impacts on the functional risk curve, but especially in the $a < 0.3$ range. In contrary, the inputs E and h_{11} have no influence. These elements are key points for the engineers to understand the effects of the physical parameters on the POD curve. It is also an help for the presentation of the result before for the safety regulation.

5 CONCLUSION

In this paper, a Gaussian process metamodel has been used to build functional risk curves from numerical experiments. A functional risk curve gives the probability of an undesirable event in function of the value of a critical parameter of a considered physical system. In addition to the mean risk curve, the metamodel allows to obtain confidence bands via Gaussian process conditional simulations. Based on perturbation of the probability density functions of the model input variables, sensitivity indices (called PLI) of the model inputs on the functional risk curve are also proposed. They allow to understand the effect of misjudgment on the input parameters' probability density functions.

An example, coming from non destructive examination simulated experiments, shows the interest of the methodology on the probability of detection curves. Functional risk curves are used in many other engineering framework, e.g. in the seismic fragility assessment (as shown in section 2.1), in the evaluation of hydraulic works reliability submitted to extremely high water level (Pasanisi, 2014), ... These tools would be also useful in works aiming to separate effects of aleatory input variables and epistemic input parameters.

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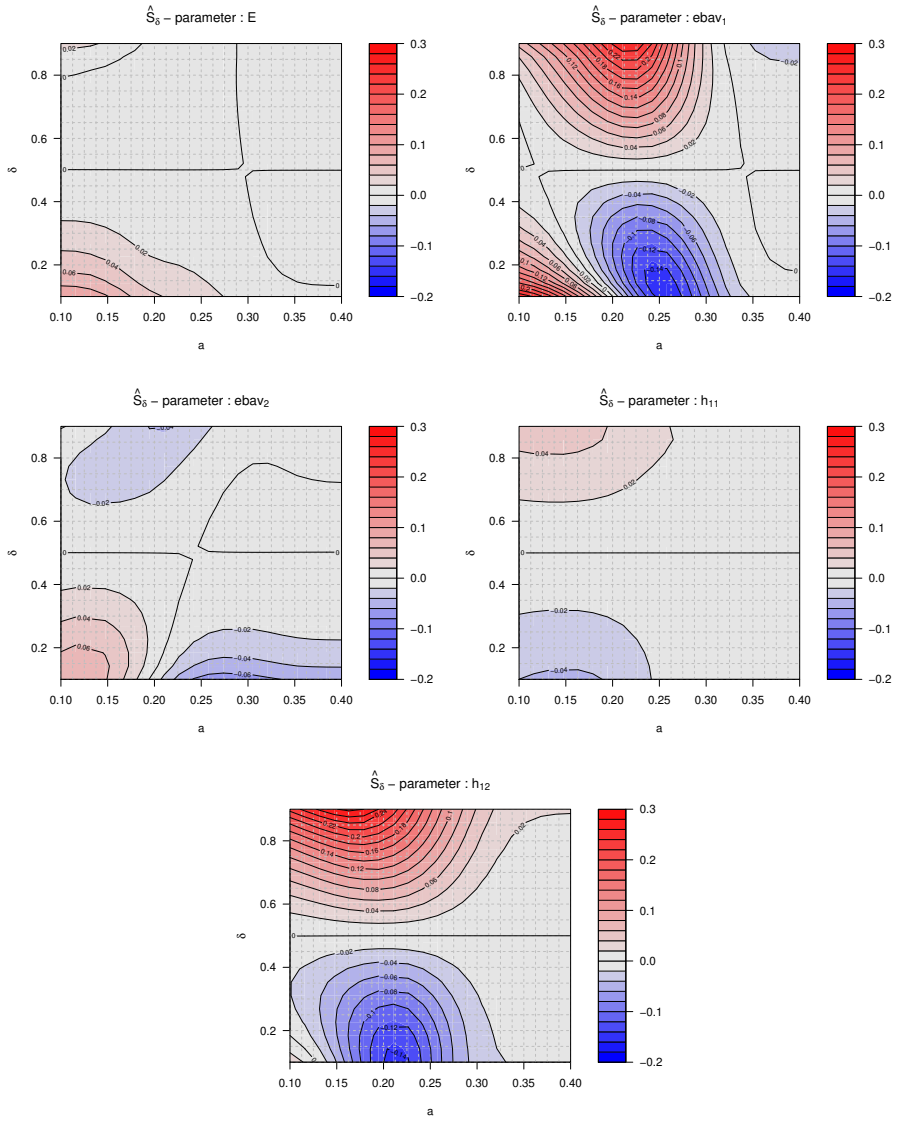

Figure 5: PLI measures on the POD curves for different perturbations on the pdf means and different values of a. $\delta = 0.5$ corresponds to the non perturbed case. The grey color corresponds to no change in the functional risk curve, while the red color (resp. blue) corresponds to an increase (resp. decrease) of the functional risk curve.

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