Probability of failure sensitivity with respect to decision variables

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Abstract This note introduces a derivation of the sensitivities of a probability of failure with respect to decision variables. For instance, the gradient of the probability of failure with respect to deterministic design variables might be needed in RBDO. These sensitivities might also be useful for Uncertainty-based Multidisciplinary Design Optimization. The difficulty stems from the dependence of the failure domain on variations of the decision variables. This dependence leads to a derivative of the indicator function in the form of a Dirac distribution in the expression of the sensitivities. Based on an approximation of the Dirac, an estimator of the sensitivities is analytically derived in the case of Crude Monte Carlo first and Subset Simulation. The choice of the Dirac approximation is discussed.

Keywords Probability of failure · Sensitivity · Decision variables

1 Introduction

In its most general form, a probability of failure is defined as:

$$P_f (z, \theta) = \int_{\Omega_f (z)} f_X (x|\theta) dx$$

where $z \in \mathbb{R}^n$ are decision variables (e.g., design variables) and $\theta \in \mathbb{R}^p$ are hyper-parameters of the joint probability density function (PDF) $f_X$ of the random variables $X \in \Omega$, with $\Omega$ the sampling space. $\Omega_f$ stands for the failure domain. Note that $\theta$ only influences the joint distribution while $z$ only influences the definition of the failure domain $\Omega_f$. Beyond reliability assessment, such a probability of failure also appears in Reliability-based Design Optimization (RBDO) (Youn et al. 2004; Aoues and Chateauneuf 2010) or in Uncertainty-based Multidisciplinary Design Optimization (UMDO) (Brevault et al. 2014).

When gradient-based techniques are used to solve RBDO or UMDO problems, the sensitivities of $P_f$ are needed (Zou and Mahadevan 2006; Lee et al. 2011; Lacaze and Missoum 2013). Sensitivities of $P_f$ with respect to $\theta$ have been derived for various reliability analysis techniques (Zou and Mahadevan 2006; Lebrun and Dutfoy 2009; Song et al. 2009; Dubourg et al. 2011). Sensitivities with respect to decision variables $z$ have also been derived for moment-based techniques such as the Reliability Index Approach (Bjerager and Krenk 1989) and the Performance Measure Approach (Nikolaidis et al. 2004). However, there are no derivations for sampling-based approaches (e.g., Crude Monte Carlo, Subset Simulation).

The difficulty stems from the dependence of the failure domain on the decision variables. In many approaches,
probabilities of failure are calculated based on a fixed failure domain. For methods involving the estimation of the gradient of the probability of failure, this has confined previous RBDO and current UMDO techniques to problems that exclude deterministic design variables. Sensitivities of the probability of failure with respect to deterministic variables would therefore substantially extend previous gradient-based RBDO techniques and offer new perspectives in UMDO.

The objective of this note is to propose a formulation of the sensitivity of the failure probability with respect to the decision variables \( z \). For this purpose, an analytical derivation based on the properties of the indicator function \( \mathbb{1} \) is proposed (Section 2). Estimators for the sensitivity using Crude Monte Carlo simulation and Subset Simulation (Section 3) are subsequently derived. In addition, the numerical implementation of the proposed formulation requires the approximation of a Dirac distribution (Section 4). In Section 5, the sensitivity estimates are compared to a case where the exact sensitivities are available. This section also discusses the choice of a parameter involved in the approximation of the Dirac distribution.

2 Sensitivity of \( P_f \) with respect to decision variables

In most applications, the failure domain is expressed as:

\[ \Omega_f(z) = \{ x | g(x, z) \leq 0 \} \tag{2} \]

where \( g \) is called the limit state function, which depends on random variables \( X \) and decision variables \( z \). This leads to another well known expression of the probability of failure:

\[ P_f(z) = \int_{\Omega} \mathbb{1}_{g(x,z) \leq 0} f_X(x) dx \tag{3} \]

For the sake of clarity and without loss of generality, \( \theta \) was omitted. According to the differentiation rules under the integral symbol using the theory of distributions (Schwartz 1957; Jones 1982), the sensitivity of \( P_f \) with respect to the variable \( z_k \) reads:

\[ \left. \frac{\partial P_f}{\partial z_k} \right|_z = \int_{\Omega} \left. \frac{\partial}{\partial z_k} \mathbb{1}_{g(x,z) \leq 0} f_X(x) dx \right|_z \]

\[ = \int_{\Omega} \left. \frac{\partial}{\partial z_k} \mathbb{1}_{g(x,z) \leq 0} f_X(x) dx \right|_z \]

From the theory of distributions, the derivative of the indicator function is:

\[ \frac{d\mathbb{1}_{y \geq 0}}{dy} = - \frac{d\mathbb{1}_{y < 0}}{dy} = \delta_y = \begin{cases} +\infty & \text{if } y = 0 \\ 0 & \text{otherwise} \end{cases} \tag{5} \]

where \( \delta \) is the Dirac distribution ("impulse"). Hence, (4) becomes:

\[ \left. \frac{\partial P_f}{\partial z_k} \right|_z = - \int_{\Omega} \frac{\partial g}{\partial z_k} \delta_{g(x,z)} f_X(x) dx \tag{6} \]

Note that (6) involves the derivative of \( g \). Such derivatives are always available if \( g \) is replaced by an approximation \( \tilde{g} \) such as a metamodel.

3 Sensitivity estimators

In practice, the integrals involved in (3) and (6) are intractable. In order to evaluate the integral in (3), sampling-based techniques are typically used. The so-called Crude Monte Carlo (CMC) estimator is defined as:

\[ P_f(z) \approx \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{g(X^{(i)}, z) \leq 0} \tag{7} \]

where \( X = \{ X^{(1)}, \ldots, X^{(N)} \} \) is a CMC sample of size \( N \) distributed according to \( f_X \). From (6), the CMC estimator of \( \left. \frac{\partial P_f}{\partial z_k} \right|_z \) is:

\[ \left. \frac{\partial P_f}{\partial z_k} \right|_z \approx - \frac{1}{N} \sum_{i=1}^{N} \frac{\partial g}{\partial z_k} \bigg|_{X^{(i)}, z} \delta_{g(X^{(i)}, z)} \tag{8} \]

However, in the case of a rare event, CMC simulations are intractable. For this reason, a wide variety of variance reduction techniques have been introduced over the years (Rubinstein and Kroese 2011). Among them, the Subset Simulation (SubSim) (Au and Beck 2001; Song et al. 2009) derives a small probability of failure as a product of larger conditional ones. Specifically, given a failure domain \( \Omega_f \), let \( \Omega_{f_0} \equiv \Omega \supset \Omega_{f_1} \supset \cdots \supset \Omega_{f_m} \equiv \Omega_f \) be a decreasing sequence of \( m+1 \) failure domains where:

\[ \Omega_{f_i}(z) = \{ x | g_i(x, z) \leq 0 \} \quad \forall i = \{1, \ldots, m\} \tag{9} \]

(3) can be expressed as:

\[ P_f(z) = \prod_{i=1}^{m} P_{f_i}(z) \tag{10} \]
where:

\[ P_{f_i}(z) = \int_{\Omega} \mathbb{I}_{g_i(x,z) \leq 0} f_X(x) \, dx \]  

and for all \( i = 1, \ldots, m \):

\[ P_{f_i}(z) = \int_{\Omega} \mathbb{I}_{g_i(x,z) \leq 0} q_{i-1}(x|\Omega_{f_i-1}(z)) \, dx \]  

with \( q_{i-1}(x|\Omega_{f_i-1}(z)) \) the conditional auxiliary PDF associated with the failure domain \( \Omega_{f_i}(z) \) defined as Song et al. (2009).

\[ q_{i-1}(x|\Omega_{f_i-1}(z)) = \frac{\mathbb{I}_{g_{i-1}(x,z) \leq 0}}{\prod_{j=1}^{i-1} P_{f_j}(z)} f_X(x) \]  

Therefore:

\[ P_{f_i}(z) = \int_{\Omega} \mathbb{I}_{g_i(x,z) \leq 0} \prod_{j=1}^{i-1} P_{f_j}(z) f_X(x) \, dx \]  

Based on SubSim, the sensitivity of \( P_f \) is:

\[ \frac{\partial P_f}{\partial z_k} \bigg|_z = P_f(z) \sum_{i=1}^{m} \frac{1}{P_{f_i}(z)} \frac{\partial P_{f_i}}{\partial z_k} \bigg|_z \]  

For the first SubSim sub-domain, we have:

\[ \frac{\partial P_{f_1}}{\partial z_k} \bigg|_z = -\int_{\Omega} \frac{\partial g_1}{\partial z_k} \delta_{g_1(x,z)} f_X(x) \, dx \]  

and for any subsequent step \( i > 1 \):

\[ \frac{\partial P_{f_i}}{\partial z_k} \bigg|_z = \int_{\Omega} \frac{\partial}{\partial z_k} \left[ \mathbb{I}_{g_i(x,z) \leq 0} \prod_{j=1}^{i-1} P_{f_j}(z) \right] f_X(x) \, dx \]  

\[ = -\int_{\Omega} \frac{\partial g_i}{\partial z_k} \delta_{g_i(x,z)} \prod_{j=1}^{i-1} P_{f_j}(z) f_X(x) \, dx \]  

\[ - \frac{\partial}{\partial z_k} \left[ \prod_{j=1}^{i-1} P_{f_j}(z) \right] \prod_{j=1}^{i} P_{f_j}(z) f_X(x) \, dx \]  

Noting the three following relations:

\[ \int_{\Omega} \mathbb{I}_{g_i(x,z) \leq 0} f_X(x) \, dx = \prod_{j=1}^{i} P_{f_j}(z) \]  

\[ \frac{\partial}{\partial z_k} \left[ \prod_{j=1}^{i} P_{f_j}(z) \right] = \prod_{j=1}^{i} P_{f_j}(z) \sum_{j=1}^{i-1} \frac{1}{P_{f_j}(z)} \frac{\partial P_{f_j}}{\partial z_k} \bigg|_z \]  

\[ f_X(x) = \frac{\prod_{j=1}^{i-1} P_{f_j}(z)}{\mathbb{I}_{g_{i-1}(x,z) \leq 0}} q_{i-1}(x|\Omega_{f_{i-1}}(z)) \, \forall x \in \Omega_{f_{i-1}}(z) \]  

and that the support of \( q_{i-1}(x|\Omega_{f_{i-1}}(z)) \) is \( \Omega_{f_{i-1}}(z) \), the \( i \)th intermediate sensitivity is:

\[ \frac{\partial P_{f_i}}{\partial z_k} \bigg|_z = -\int_{\Omega} \frac{\partial g_i}{\partial z_k} \delta_{g_i(x,z)} q_{i-1}(x|\Omega_{f_{i-1}}(z)) \, dx \]  

\[ - P_{f_i}(z) \sum_{j=1}^{i-1} \frac{1}{P_{f_j}(z)} \frac{\partial P_{f_j}}{\partial z_k} \bigg|_z \]  

Each of these derivatives can be estimated using the result of a SubSim. Given \( X \) a SubSim sample defined as \( X = \{ X_1, \ldots, X_m \} \) such that:

\[ X_i \sim q_0 \left( \cdot | \Omega_{f_0}(z) \right) \equiv f_X \]  

\[ X_i \sim q_{i-1} \left( \cdot | \Omega_{f_{i-1}}(z) \right) \forall i = 1, \ldots, m \]  

the estimators of the sensitivities (16) and (21) are:

\[ \frac{\partial P_{f_i}}{\partial z_k} \bigg|_z \approx -\frac{1}{N_i} \sum_{l=1}^{N_i} \frac{\partial g_l}{\partial z_k} \bigg|_{X_i^{(l)}}, \delta_{g_i(X_i^{(l)})} \]  

\[ \frac{\partial P_{f_i}}{\partial z_k} \bigg|_z \approx -\frac{1}{N_i} \sum_{l=1}^{N_i} \frac{\partial g_l}{\partial z_k} \bigg|_{X_i^{(l)}}, \delta_{g_i(X_i^{(l)})} \]  

Combining all the intermediate sensitivities, we finally get:

\[ \frac{\partial P_f}{\partial z_k} \bigg|_z = P_f(z) \sum_{i=1}^{m} \left\{ \frac{1}{P_{f_i}(z)} \cdot \left[ -\frac{1}{N_i} \sum_{l=1}^{N_i} \frac{\partial g_l}{\partial z_k} \bigg|_{X_i^{(l)}}, \delta_{g_i(X_i^{(l)})} \right. \right. \]  

\[ \left. - P_{f_i}(z) \sum_{j=1}^{i-1} \frac{1}{P_{f_j}(z)} \frac{\partial P_{f_j}}{\partial z_k} \bigg|_z \right\} \]  

4 Dirac distribution approximation

The presence of a Dirac distribution in the equations makes the numerical computation of the sensitivities intractable. To
overcome this hurdle, the Dirac distribution is approximated using a smooth function \( \hat{\delta} \) such that \( \lim_{\sigma \to 0} \hat{\delta}(\sigma) = \delta_\gamma \). This approach has been widely used in the past, (e.g., Yoo and Lee 2014, for Gaussian approximation). Five candidates are considered in this work:

- **Gaussian** \( \hat{\delta}_\gamma(\sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) = \frac{1}{\sigma} \phi\left(\frac{x}{\sigma}\right) \)
- **Truncated Gaussian** \( \hat{\delta}_\gamma(\sigma) = \frac{\frac{1}{\sigma} \phi\left(\frac{x}{\sigma}\right)}{\Phi_1(\frac{\sigma}{\sqrt{2}})} \) \( \mathbb{I}_{-\sigma \leq y \leq \sigma} \)
- **Sinc** \( \hat{\delta}_\gamma(\sigma) = \frac{\sin(\frac{x}{\sigma})}{\pi x} \)
- **Bump** \( \hat{\delta}_\gamma(\sigma) = \frac{1}{\sigma \pi} \exp\left(-\frac{1}{\sigma^2}x^2\right) \) \( \mathbb{I}_{-\sigma \leq y \leq \sigma} \)
- **Poisson** \( \hat{\delta}_\gamma(\sigma) = \frac{1}{\pi (\sigma^2+y^2)} \)

All these functions include a scalar parameter \( \sigma \) which dictates the “width” of the Dirac approximation. The choice of the approximation as well as \( \sigma \) is of prime importance. Ideally, one would like \( \sigma \) to tend to zero. However, because we are using sampling-based methods, only a finite amount of information is available. For this reason, an “optimal” value of \( \sigma \) needs to be chosen.

### 5 Numerical experiments. Selection of \( \sigma \)

The optimal value of \( \sigma \) and the choice of Dirac approximation might be problem dependent. Statistically, the optimal choice is the one that minimizes the error between the actual and the estimated sensitivity. Knowing the true sensitivity, traditional performance metrics of an estimator can be computed, such as normalized bias (Bias), standard deviation (Std) and root mean square error (RMSE):

\[
\text{Bias (\%)} = 100 \times \frac{|E[\tilde{\psi}] - \psi|}{\psi} \quad (27)
\]

\[
\text{Std (\%)} = 100 \times \sqrt{\frac{E[\tilde{\psi}^2] - E[\tilde{\psi}]^2}{\psi}} \quad (28)
\]

\[
\text{RMSE (\%)} = 100 \times \sqrt{\frac{E[(\tilde{\psi} - \psi)^2]}{\psi}} \quad (29)
\]

where \( \psi \) is the actual sensitivity as defined in (34) and \( \tilde{\psi} \) is an estimator of \( \psi \), as defined in (8). At this point, it is important to recall that the estimator of the sensitivity encompasses two levels of approximation:

\[
\frac{\partial P_f}{\partial z_k} \bigg|_z = -\int_{\Omega} \frac{\partial g}{\partial x_k} \bigg|_{x,z} \delta_g(x,z) f_X(x) dx = -\int_{\Omega} \frac{\partial g}{\partial x_k} \bigg|_{x,z} \delta_g(x,z) f_X(x) dx \quad (30)
\]

\[
\approx -\int_{\Omega} \frac{\partial g}{\partial x_k} \bigg|_{x,z} \delta_g(x,z) f_X(x) dx \approx -\frac{1}{N} \sum_{i=1}^{N} \frac{\partial g}{\partial x_k} \bigg|_{x,y(x^{(i)},z)} \delta_{y(x^{(i)},z)} \quad (31)
\]

Because Monte Carlo estimators are unbiased, (31) only introduces variance in the estimator. On the other hand, (30) is an analytical approximation, and only introduces bias on the estimator. Although the variance could be estimated using the standard error, the bias is not strictly speaking statistical. Therefore it cannot be quantified statistically, such as with leave one out approaches.

In this article, the “optimal” \( \sigma \) is obtained through experiments. Although it is not the optimal value for any problem, this educated guess would lead to better results than an arbitrary one. As a demonstrative case, consider the following linear analytical limit state, for which analytical sensitivities can be derived:

\[
g(x,z) = -x - z + d \leq 0 \quad (32)
\]

where \( X \sim \mathcal{N}(0, 1) \). Because the limit state function is linear, the probability of failure and its derivative can be obtained exactly:

\[
P_f(z) = 1 - \Phi(d - z) \quad (33)
\]

\[
\frac{dP_f}{dz} \bigg|_z = \phi(d - z) \quad (34)
\]

where \( \phi \) (resp. \( \Phi \)) is the standard normal probability density (resp. cumulative distribution) function. The number of CMC samples \( N \) is defined to ensure a 5% coefficient of variation on the probability of failure:

\[
N(z) = \left[ \left( \frac{\sqrt{1 - P_f(z)} + 0.05}{P_f(z) \times 0.05} \right) \right]^2 \quad (35)
\]

where \( P_f \) is defined by (33).

\( \sigma \) is a function of the number of points (i.e. the amount of information) available, which is in turn influenced by the value of \( P_f \). For this reason, a parameter \( \alpha \) is introduced to define a fraction \( N_r \) of the available samples so that \( N_r = \left[ P_f \times N \times \alpha \right] \), where \( P_f \) is estimated using (7).

Because the optimal value of \( \sigma \) is also dependent on the order of magnitude of \( g \), the following quantities are
Fig. 1 Normalized bias ($\text{Bias}$), standard error ($\text{Std}$) and root mean square error ($\text{RMSE}$) for four levels of probability of failure.
defined. Let $y$ be the vector of responses such that $y_i = g(X_i^j, z)$, $|y|$ the vector of absolute values of $y$ and the rank operator such that $y_{(1)} = \min(y)$ and $y_{(N)} = \max(y)$. $\sigma$ is therefore defined as $|y|_{(N_i)}$ so that only the $N_i$ closest points from the limit state have function value within $\pm \sigma$. These points are the most relevant to the calculation of the sensitivity of $P_f$ because they will potentially lead to a variation of $f_{g(x,z)}$.

The experiment is repeated for four values of $d$ such that $P_f$ equals $10^{-1}$, $10^{-2}$, $10^{-3}$, and $10^{-4}$. For SubSim, each probability step (here, $10^{-1}$) is estimated using CMC (w.r.t a conditional distribution). Figure 1 shows the plots of normalized bias (27), standard error (28) and root mean square error (29) for the example introduced in (32). Expectations of $P_f$ are calculated out of 300 repetitions. The experiment is repeated for 4 levels of probability. Two immediate conclusions arise:

– The Poisson approximation shows a poor performance compared to the other approximations,
– The Sinc approximation provides inconsistent results.

Out of the three remaining approximations, the Gaussian one has the lowest variance across the experiments. Note that this is a very favorable feature for optimization. In gradient-based optimization, the variance of the sensitivities will impair the convergence properties more than the bias. For these reasons, the Gaussian approximation is elected.

From the results in Fig. 1, in the case of a Gaussian approximation, a graphical inspection shows that a value of $\alpha = 0.5$ is a satisfactory choice for the minimization of RMSE. This value can be compared the solution of the following optimization problem:

$$\alpha_{opt} = \arg \min_{\alpha} RMSE(\alpha)$$

(36)

Table 1 shows normalized bias (27), standard error (28) and root mean square error (29) for $\alpha = \alpha_{opt}$ and $\alpha = 0.5$. Except for the case $P_f = 10^{-1}$, $\alpha = 0.5$ yields similar results to $\alpha = \alpha_{opt}$. For $P_f = 10^{-1}$ it yields an increase in the RMSE of about 1%.

### 6 Conclusion

In this note, an expression of the sensitivity of probability of failure with respect to decision variables is derived. Estimators are proposed based on Crude Monte Carlo and Subset Simulation. Numerical concerns regarding the approximation of the Dirac distribution are addressed. Experiments seem to show that Gaussian approximation should be favored with a value of $\alpha = 0.5$. However, this result might not always be true and an automatic tuning algorithm to find the optimal $\alpha$ (i.e., $\sigma$) as in (Morio et al. 2013) will be investigated.

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