

OpenTURNS Developer Training

Probabilistic uncertainty propagation

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Developers training



Probabilistic uncertainty propagation

- 1 What is uncertainty propagation?
- 2 Numerical models: the differential calculus potion
- 3 A cloud of probabilities in my code, please

Main objective

Probabilistic uncertainty propagation

OpenTURNS = Open Source Treatment of Uncertainty, Risk'N Statistics

- **Uncertainty** = unknown quantities, lack of exact knowledge, non predictable fluctuations
- **Risk** = dangerous state, critical conditions and their impact (cost, consequences)
- **Statistics** = observation and modelling of random quantities, partial knowledge
- **Treatment** = algorithmic tools to analyse, model and quantify the previous points

Main objective

UQ in a nutshell

Given:

- a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^p$ called a **model**
- a random vector X of known joint distribution \mathcal{L} of dimension n called the **sources of uncertainties**

Uncertainty quantification is focused on getting information about the **push-forward** distribution of the random vector $Y = f(X)$:

- Moments $E[h(Y)]$ where $h : \mathbb{R}^p \rightarrow \mathbb{R}^q$
- Probability of events $\mathbb{P}(Y \in B)$ as a special case ($h(y) = 1_{y \in B}$)
- Sensitivity of Y to part of X

Numerical models

Function, gradient, hessian

- **Function:** the notion of **numerical model** is a function f maps \mathbb{R}^n to \mathbb{R}^p . A shortcut is to say that:

$$f \in \mathcal{F}(\mathbb{R}^n, \mathbb{R}^p) \quad (1)$$

The integers $n \in \mathbb{N}$, $p \in \mathbb{N}^*$ are the **input** and **output** dimensions. The set $\{\underline{x} \in \mathbb{R}^n | f(\underline{x}) \text{ is well defined}\}$ is the **domain of definition** of f . For all $i \in \{1, \dots, p\}$, the function $f_i \in \mathcal{F}(\mathbb{R}^n, \mathbb{R})$ defined by $f_i(\underline{x}) = \pi_i(f(\underline{x}))$, where π_i is the projection on the i^{th} coordinate in \mathbb{R}^p , is called the **i^{th} component** of f .

- **Gradient:** a function $f \in \mathcal{F}(\mathbb{R}^n, \mathbb{R}^p)$ is said to be **differentiable** at $\underline{x} \in \mathbb{R}^n$ if one has:

$$\forall \underline{h} \in \mathbb{R}^n, f(\underline{x} + \underline{h}) = f(\underline{x}) + D(f)(\underline{x})(\underline{h}) + o(\|\underline{h}\|) \quad (2)$$

where $D(f)(\underline{x})$ is a (continuous) linear application from \mathbb{R}^n to \mathbb{R}^p :

$D(f)(\underline{x}) \in L_c(\mathbb{R}^n, \mathbb{R}^p)$. The application $D(f)$ that maps $\underline{x} \in \mathbb{R}^n$ into $L_c(\mathbb{R}^n, \mathbb{R}^p)$ is the **differential** of f . The linear application $D(f)(\underline{x})$ is always continuous in the setting of \mathbb{R}^n and has an associated matrix $\underline{\underline{M}}(\underline{x}) \in \mathcal{M}_{n,p}(\mathbb{R})$ with $M_{ij} = \frac{\partial f_i}{\partial x_j}$: it is the **jacobian matrix** of f at \underline{x} . The application that maps \underline{x} into $\underline{\underline{M}}^t(\underline{x}) \in \mathcal{M}_{p,n}(\mathbb{R})$ is the **gradient** of f at \underline{x} .

Numerical models

Function, gradient, hessian

- **Hessian**: a function $f \in \mathcal{F}(\mathbb{R}^n, \mathbb{R}^p)$ is said to be **twice differentiable** at $\underline{x} \in \mathbb{R}^n$ if the application $D(f)$ that maps \mathbb{R}^n into $L_c(\mathbb{R}^n, \mathbb{R}^p)$ is differentiable at \underline{x} . It means that:

$$\forall \underline{h} \in \mathbb{R}^n, D(f)(\underline{x} + \underline{h}) = D(f)(\underline{x}) + D^2(f)(\underline{x})(\underline{h}) + o(\|\underline{h}\|) \quad (3)$$

where $D^2(f)(\underline{x})$ is a (continuous) linear application from \mathbb{R}^n to $L_c(\mathbb{R}^n, \mathbb{R}^p)$: $D^2(f)(\underline{x}) \in L_c(\mathbb{R}^n, L_c(\mathbb{R}^n, \mathbb{R}^p))$. The application $D^2(f)$ that maps $\underline{x} \in \mathbb{R}^n$ into $L_c(\mathbb{R}^n, L_c(\mathbb{R}^n, \mathbb{R}^p))$ is the **second differential** of f . The linear application $D^2(f)(\underline{x})$ is always continuous in the setting of \mathbb{R}^n and has a tensor representation

$\underline{\underline{T}}(\underline{x}) \in \mathcal{T}_{n,n,p}(\mathbb{R})$ with $M_{ijk} = \frac{\partial^2 f_i}{\partial x_j \partial x_k}$: it is the **second jacobian tensor** of f at \underline{x} . The application that maps \underline{x} into $\underline{\underline{T}}(\underline{x}) \in \mathcal{T}_{p,n,n}(\mathbb{R})$ is the **hessian tensor** of f at \underline{x} . This tensor is made of sheets $T_{k,..} \in \mathcal{M}_{n,n}(\mathbb{R})$ that are **symmetric**.

Random vector, distribution

Definition

- A **random vector** \underline{X} is a measurable function from a probability space $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$ into the probability space $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \mu_{\underline{X}})$.
- The associated **distribution** is the probability measure $\mu_{\underline{X}}$ defined by:

$$\forall B \in \mathcal{B}(\mathbb{R}), \mu_{\underline{X}}(B) = \mathbb{P}(\underline{X}^{-1}(B)) \quad (4)$$

- The **main advantage** of a random vector is that we are now working on a **numeric space** \mathbb{R}^n instead of a general set Ω .
- The different values $\forall \omega \in \Omega, \underline{X}(\omega)$ taken by a random vector \underline{X} are called the **realizations** of the random vector.
- A distribution is completely defined by its **cumulative distribution function or CDF** $F_{\underline{X}}$ which maps \mathbb{R}^n into $[0, 1]$ and is defined by:

$$F_{\underline{X}}(\underline{x}) = \mathbb{P}(X_1 \leq x_1, \dots, X_n \leq x_n) \quad (5)$$

Random vector, distribution

Discrete random vectors, continuous random vectors

There are two distinguished classes of random vectors:

- Those that take their values in \mathbb{N}^n and are called **discrete integral** random vectors. The distribution of this kind of random vectors is equivalently described by the function $p_{\underline{X}}$ that maps \mathbb{N}^n into $[0, 1]$ such that:

$$p_{\underline{X}}(\underline{x}) = \mathbb{P}(\underline{X} = \underline{x}) \quad (6)$$

The function $p_{\underline{X}}$ is called its **probability distribution function or PDF**.

- Those such that there exist a function $p_{\underline{X}}$ that maps \mathbb{R}^n into R^+ such that:

$$F_{\underline{X}}(\underline{x}) = \int_{\mathbb{R}^n} p_{\underline{X}}(\underline{x}) d\underline{x} \quad (7)$$

These random vectors are called **absolutely continuous** random vectors with respect to the Lebesgue measure $d\underline{x}$. The function $p_{\underline{X}}$ is called its **probability density function or PDF**.

WARNING 1: The PDF acronym is used for two distinct functions, but the context makes it clear which kind of PDF is relevant in practical applications.

WARNING 2: A random vector can be neither discrete nor continuous!

PDF and CDF, 1D case

Continuous



Discrete

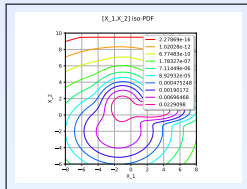


General

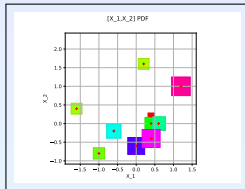


PDF and CDF, 2D case

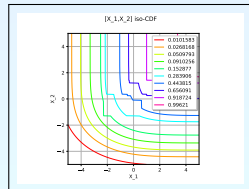
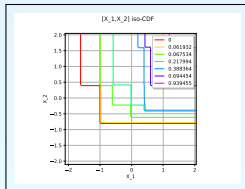
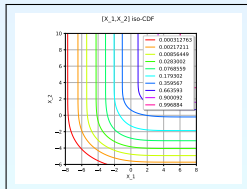
Continuous



Discrete



General



Expectation, mean, covariance

Definition

- The **expectation** $\mathbb{E}[\underline{X}]$ of a real random vector \underline{X} of dimension n is the deterministic vector of \mathbb{R}^n defined by:

$$\mathbb{E}[\underline{X}]_i = \int_{\mathbb{R}} x_i d\mu_{X_i}(x_i) \quad (8)$$

where μ_{X_i} is the distribution of the 1D random vector corresponding to the projection of \underline{X} on its i^{th} coordinate. It is thus a quantity that is defined component by component. For bell shaped distributions, it is an indication of the location of most of the realizations of \underline{X} .

- The **covariance** $\text{Cov}[\underline{X}]$ of a real random vector \underline{X} of dimension n is the deterministic symmetric square matrix of $\mathcal{M}_{n,n}(\mathbb{R})$ defined by:

$$\text{Cov}[\underline{X}]_{ij} = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])] \quad (9)$$

where X_i and X_j are the i^{th} and j^{th} components of \underline{X} . This matrix is semidefinite positive. For bell shaped distributions, this quantity express the dispersion of the distribution around its mean value.

Convergence

Definition

- A sequence of random vectors $(\underline{X})_{n \in \mathbb{N}}$ defined over the **same** probability space $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$ is said to **converge almost surely** to the random vector \underline{X} if and only if:

$$\mathbb{P}[\{\omega \in \Omega \mid \underline{X}_n(\omega) \not\rightarrow \underline{X}(\omega) \text{ as } n \rightarrow \infty\}] = 0 \quad (10)$$

- A sequence of random vectors $(\underline{X})_{n \in \mathbb{N}}$ defined over the probability spaces $(\Omega_n, \mathcal{B}(\Omega_n), \mathbb{P}_n)$ is said to **converge in law** to the random vector \underline{X} defined over the probability space $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$ if and only if:

$$\forall \phi \in \mathcal{C}^b(\mathbb{R}^n, \mathbb{R}), \lim_{n \rightarrow \infty} \mathbb{E}[\phi(\underline{X}_n)] = \mathbb{E}[\phi(\underline{X})] \quad (11)$$

where $\mathcal{C}^b(\mathbb{R}^n, \mathbb{R})$ is the set of bounded continuous functions defined on \mathbb{R}^n and taking value into \mathbb{R} .

Simulation

Strong number law and Central Limit Theorem

- **(Strong law of large numbers)** For all sequence of random vectors $(\underline{X})_{n \in \mathbb{N}}$ defined over the **same** probability space $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$, **independent** and **sharing the same distribution** $\mu_{\underline{X}}$, for all measurable function $f \in \{(\mathbb{R}^n, \mathbb{R}^p)$ such that $\mathbb{E}[f(\underline{X}_1)]$ exists, **the sequence of random vectors** $(\frac{1}{n} \sum_{k=1}^n f(\underline{X}))_{n \in \mathbb{N}}$ **converges almost surely to the constant random vector** $\mathbb{E}[f(\underline{X}_1)]$
- **(Central Limit Theorem)** Moreover, if $\text{Cov}[\underline{X}_1]$ is well-defined and finite, the sequence of random vectors defined by $(\sqrt{n} (\frac{1}{n} \sum_{k=1}^n f(\underline{X}) - \mathbb{E}[f(\underline{X}_1)]))_{n \in \mathbb{N}}$ **converges in law to a multivariate Normal distribution with covariance** $\text{Cov}[\underline{X}_1]$

The first theorem gives a mean to compute any quantity related to a random vector \underline{Y} defined as the image of a random vector \underline{X} through a numerical model f , for exemple its CDF: generate many independent realizations of \underline{Y} , take $\phi(\underline{y}) = 1_{\{\tilde{\underline{y}} \in \mathbb{R}^p \mid \tilde{y}_i \leq y_i\}}$ and the quantity $\frac{1}{n} \sum_{k=1}^n \phi(\underline{Y})$ will almost surely converge towards $\mathbb{E}[\phi(\underline{Y})] = \mathbb{P}[Y_1 \leq y_1, \dots, Y_n \leq y_n] = F_{\underline{Y}}(\underline{y})$. It is the so-called **Monte Carlo method**. The second theorem gives a mean to quantify the ecision of a Monte Carlo approximation for large but finite values of n . As we know the asymptotic behaviour of the fluctuations of $(\frac{1}{n} \sum_{k=1}^n f(\underline{X}))_{n \in \mathbb{N}}$ we can determine a region R for which the needed quantity has a large probability to be, and we see that this region shrinks with a speed proportional to $\frac{1}{\sqrt{n}}$.

Simulation

Monte Carlo algorithm



The end

No more maths!

- The probabilistic approach to uncertainty propagation involves some high level maths,
- The following presentations will show that an OpenTURNS developer must have a basic knowledge of these maths (at least the basic vocabulary) in order to be comfortable with the platform and its objects...
- ... but he/she has not to be an expert in order to be efficient!