OpenTURNS Developer Training
Probabilistic uncertainty propagation

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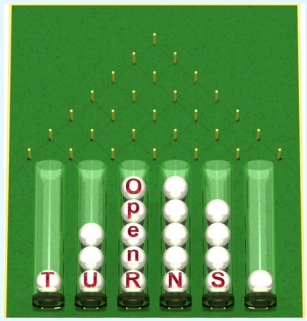
Developers training



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 predictible 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

The main objective of OpenTURNS is to quantify and analyse a critical *event* E built upon a *quantity of interest* Y that is linked to *sources of uncertainty* $\underline{X}$ through a *numerical model* f:

$$E = \mathbf{1}_{Y>s} \quad , Y = f(\underline{X}) \tag{1}$$

where $s \in \mathbb{R}$ is a given threshold, $\underline{X}$ is a random vector, E is the critical event. The quantification of this event is typically the evaluation of its *probability of occurence* $\mathbb{P}(E)$.

Numerical models

Function, gradient, hessian

- Function: the notion of numerical model is identified with the notion of numerical function, it means a function f maps $\mathbb{R}^n$ to $\mathbb{R}^p$. A shortcut is to say that:

$$f \in \mathcal{F}(\mathbb{R}^n, \mathbb{R}^p) \tag{2}$$

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 $i \in \{1, \ldots, p\}$, 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:

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

where $D(f)(\underline{x})$ is a (continuous) linear application from $\mathbb{R}^n$ to $\mathbb{R}^p$: $D(f)(\underline{x}) \in L_c(\mathbb{R}^n, R^p)$. The application $D(f)$ that maps $\underline{x} \in \mathbb{R}^n$ into $L_c(\mathbb{R}^n, R^p)$ 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 $\underline{\underline{M}}(\underline{x}) \in \mathcal{M}_{n,p}(\mathbb{R})$ whith $M_{ij} = \frac{\partial f_i}{\partial x_j}$: it is the jacobian matrix of f at $\underline{x}$. The application that maps $\underline{x}$ into $M^t(\underline{x}) \in \mathcal{M}_{p,n}(\mathbb{R})$ 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 $L_c(\mathbb{R}^n, R^p)$ is differentiable at $\underline{x}$. It means that:

$$\forall \underline{h} \in \mathbb{R}^n, D(f)(\underline{x} + \underline{h}) = D(f)(\underline{x}) + D^2(f)(\underline{x})(\underline{h}) + o(||\underline{h}||) \tag{4}$$

where $D^2(f)(\underline{x})$ is a (continuous) linear application from $\mathbb{R}^n$ to $L_c(\mathbb{R}^n, \mathbb{R}^p)$: $D^2(f)(\underline{x}) \in L_c(\mathbb{R}^n, L_c(R^n, R^p))$. The application $D^2(f)$ that maps $\underline{x} \in \mathbb{R}^n$ into $L_c(\mathbb{R}^n, L_c(\mathbb{R}^n, R^p))$ 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 $\underline{\underline{T}}(\underline{x}) \in \mathcal{T}_{n,n,p}(\mathbb{R})$ whith $M_{ijk} = \frac{\partial^2 f_i}{\partial x_j \partial x_k}$: it is the second jacobian tensor of f at $\underline{x}$. The application that maps $\underline{x}$ into $T^t(\underline{x}) \in \mathcal{T}_{p,n,n}(\mathbb{R})$ 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:

$$\forall B \in \mathcal{B}(\mathbb{R}), \mu_{\underline{X}}(B) = \mathbb{P}(\underline{X}^{-1}(B)) \tag{5}$$

- 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:

$$F_{\underline{X}}(\underline{x}) = \mathbb{P}(X_1 \leq x_1, \ldots, X_n \leq x_n) \tag{6}$$

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:

$$p_{\underline{X}}(\underline{x}) = \mathbb{P}(\underline{X} = \underline{x}) \tag{7}$$

  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:

$$F_{\underline{X}}(\underline{x}) = \int_{\mathbb{R}^n} p_{\underline{X}}(\underline{x})\, d\underline{x} \tag{8}$$

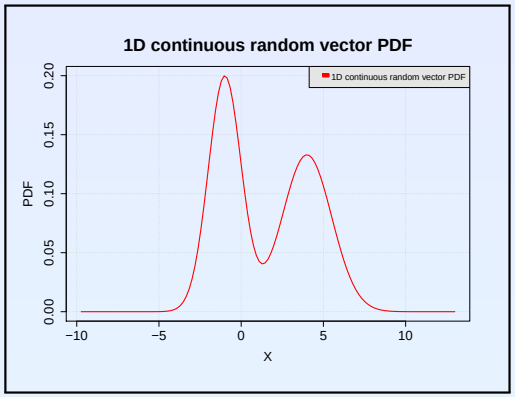
  These random vectors are called absolutely continuous random vectors with respect to the Lebesgue measure $d\underline{x}$. The function $p_{\underline{X}}$ is called its probability density function or PDF.

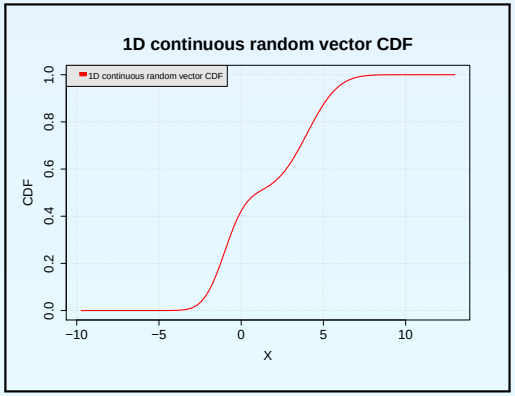
WARNING 1: The PDF acronym is used for two distinct functions, but the context makes it clear which kind of PDF is relevant in practical applications.

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

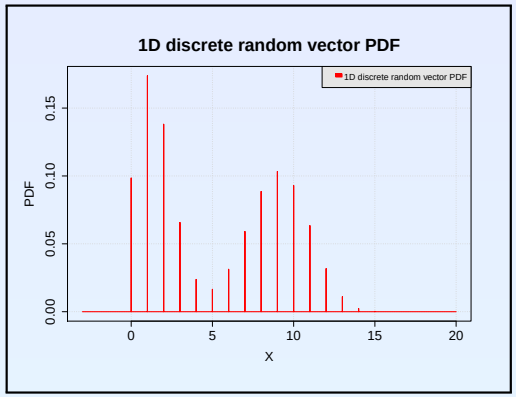
PDF and CDF, 1D case

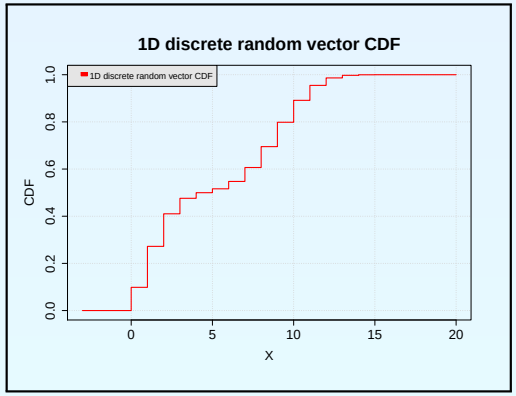
Continuous



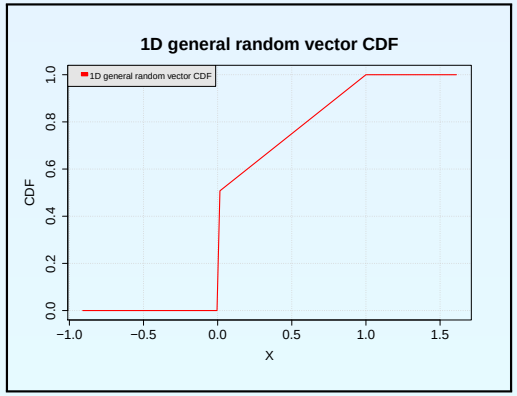


Discrete



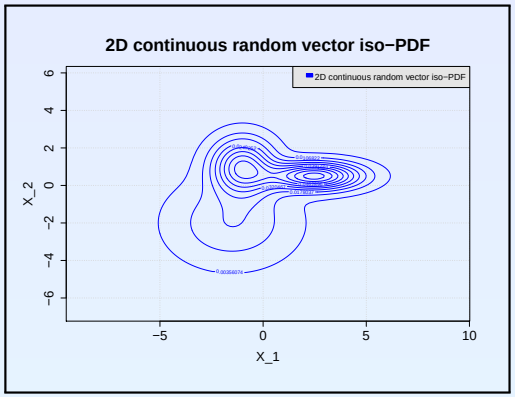


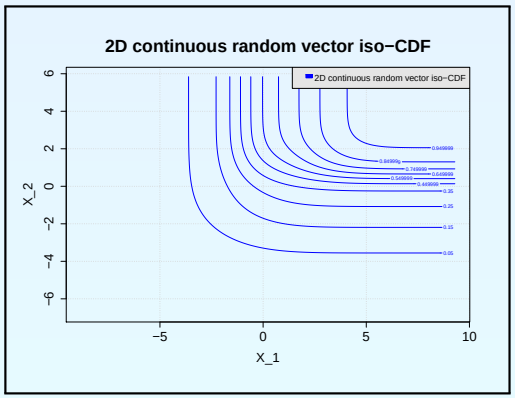
General



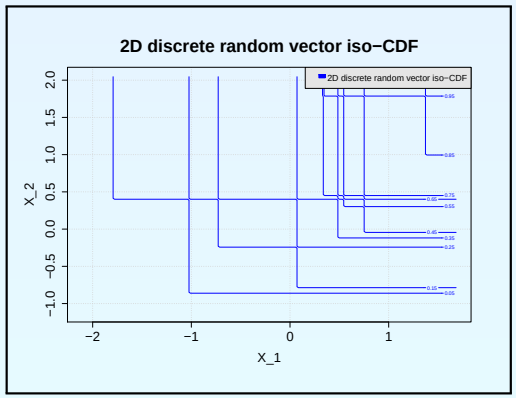
PDF and CDF, 2D case

Continuous

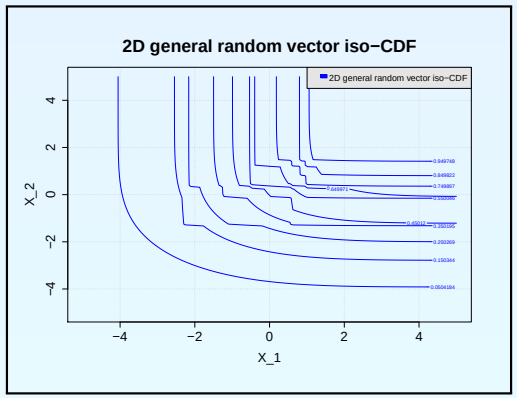




Discrete



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:

$$\mathbb{E}[\underline{X}]_i = \int_{\mathbb{R}} x_i \, d\mu_{X_i}(x_i) \tag{9}$$

  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 $\mathrm{Cov}\,[\underline{X}]$ 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:

$$\mathrm{Cov}\,[\underline{X}]_{ij} = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])] \tag{10}$$

  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:

$$\mathbb{P}[\{\omega \in \Omega \,|\, \underline{X}_n(\omega) \not\to \underline{X}(\omega) \text{ as } n \to \infty\}] = 0 \tag{11}$$

- 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:

$$\forall \phi \in \mathcal{C}^b(\mathbb{R}^n, \mathbb{R}), \lim_{n\to\infty} \mathbb{E}[\phi(\underline{X}_n)] = \mathbb{E}[\phi(\underline{X})] \tag{12}$$

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

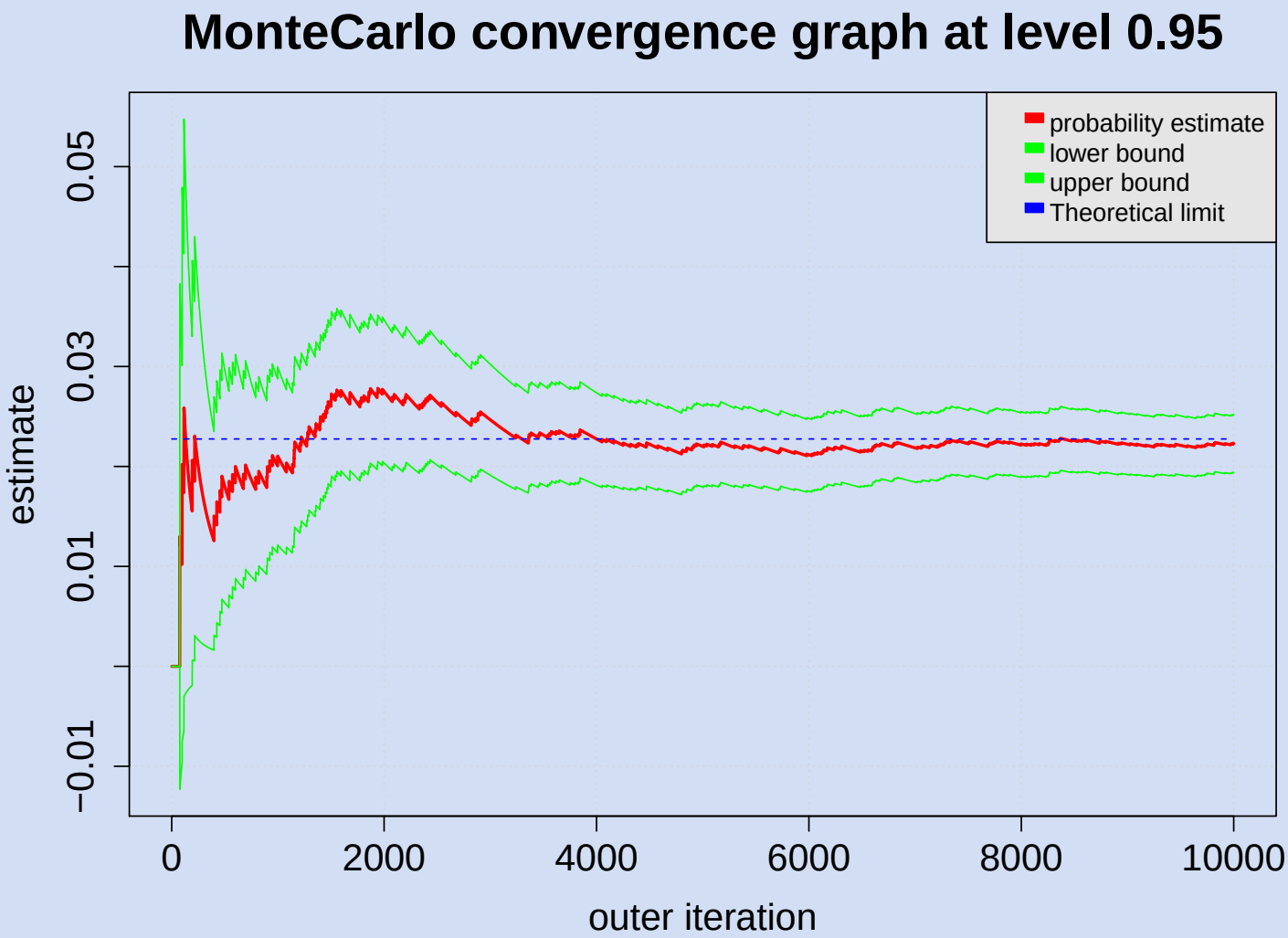
Strong number law and Central Limit Theorem

- (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 $\left(\frac{1}{n}\sum_{k=1}^{n} f(\underline{X})\right)_{n\in\mathbb{N}}$ converges almost surely to the constant random vector $\mathbb{E}[f(\underline{X}_1)]$
- (Central Limit Theorem) Moreover, if $\mathrm{Cov}\,[\underline{X}_1]$ is well-defined and finite, the sequence of random vectors defined by $\left(\sqrt{n}\left(\frac{1}{n}\sum_{k=1}^{n} f(\underline{X}) - \mathbb{E}[f(\underline{X}_1)]\right)\right)_{n\in\mathbb{N}}$ converges in law to a multivariate Normal distribution with covariance $\mathrm{Cov}\,[\underline{X}_1]$

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 $\phi(\underline{y}) = \mathbf{1}_{\{\underline{\tilde{y}}\in\mathbb{R}^p \mid \tilde{y}_i \leq y_i}$ and the quantity $\frac{1}{n}\sum_{k=1}^{n}\phi(\underline{Y})$ will almost surely converge towards $\mathbb{E}[\phi(\underline{Y})] = \mathbb{P}[Y_1 \leq y_1, \ldots, Y_n \leq y_n] = F_{\underline{Y}}(\underline{y})$. 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 $\left(\frac{1}{n}\sum_{k=1}^{n} f(\underline{X})\right)_{n\in\mathbb{N}}$ 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!