# OpenTURNS Developer Training Probabilistic uncertainty propagation

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#### Developers training



# Probabilistic uncertainty propagation

What is uncertainty propagation?

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

# Main objective

## UQ in a nutshell

#### Given:

- a function  $f: \mathbb{R}^n \to \mathbb{R}^p$  called a model
- ullet 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  $\mathrm{E}\left[h(Y)\right]$  where  $h:\mathbb{R}^p \to \mathbb{R}^q$
- 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:

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

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  $\pi_i$  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:

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

where  $D(f)(\underline{x})$  is a (continuous) linear application from  $\mathbb{R}^n$  to  $\mathbb{R}^p$ :  $D(f)(\underline{x}) \in L_c(\mathbb{R}^n, R^p)$ . 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  $\underline{M}(\underline{x}) \in \mathcal{M}_{n,p}(\mathbb{R})$  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:

where  $D^2(f)(x)$  is a (continuous) linear application from  $\mathbb{R}^n$  to  $L_c(\mathbb{R}^n, \mathbb{R}^p)$ :

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

 $D^2(f)(\underline{x}) \in L_c(\mathbb{R}^n, L_c(R^n, R^p))$ . 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  $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \mu_X)$ .
- The associated distribution is the probability measure  $\mu_X$  defined by:

$$\forall B \in \mathcal{B}(\mathbb{R}), \mu_{\underline{X}}(B) = \mathbb{P}(\underline{X}^{-1}(B))$$
(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  $\Omega$ .
- 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<sub>X</sub> which maps R<sup>n</sup> into [0, 1] and is defined by:

$$F_{\underline{X}}(\underline{x}) = \mathbb{P}(X_1 \le x_1, \dots, X_n \le x_n)$$
 (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  $p_X$  that maps  $\mathbb{N}^n$  into [0,1] such that:

$$\rho_{\underline{X}}(\underline{x}) = \mathbb{P}(\underline{X} = \underline{x}) \tag{6}$$

The function  $p_X$  is called its probability distribution function or PDF.

• Those such that there exist a function  $p_X$  that maps  $\mathbb{R}^n$  into  $R^+$  such that:

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

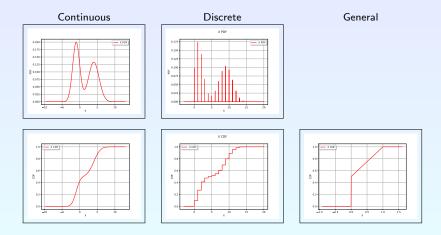
These random vectors are called absolutely continuous random vectors with respect to the Lebesgue measure  $d\underline{x}$ . The function  $p\underline{x}$  is called its probability density function or PDF.

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.

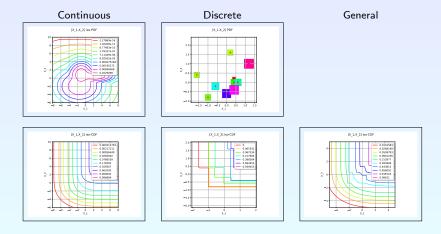
WARNING 2: A random vector can be neither discrete nor continuous!



# PDF and CDF, 1D case



# PDF and CDF, 2D case



## Expectation, mean, covariance

#### Definition

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

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

where  $\mu_{X_i}$  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  $\operatorname{Cov}[X]$  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:

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

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

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

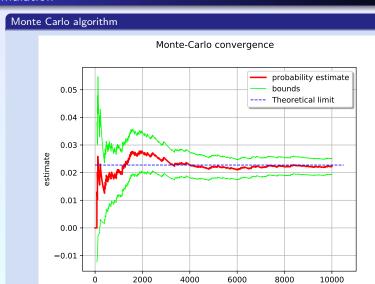
## Simulation

#### 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  $f\in\{(\mathbb{R}^n,\mathbb{R}^p)\text{ such that }\mathbb{E}[f(\underline{X}_1)]$  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  $\operatorname{Cov}[\underline{X}_1]$  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  $\operatorname{Cov}[\underline{X}_1]$

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  $\phi(\underline{y}) = \mathbf{1}_{\{\underline{\tilde{y}} \in \mathbb{R}^p \mid \underline{\tilde{y}}_i \leq y_i}$  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



outer iteration

## 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!