Propgation of uncertainties through numerical models

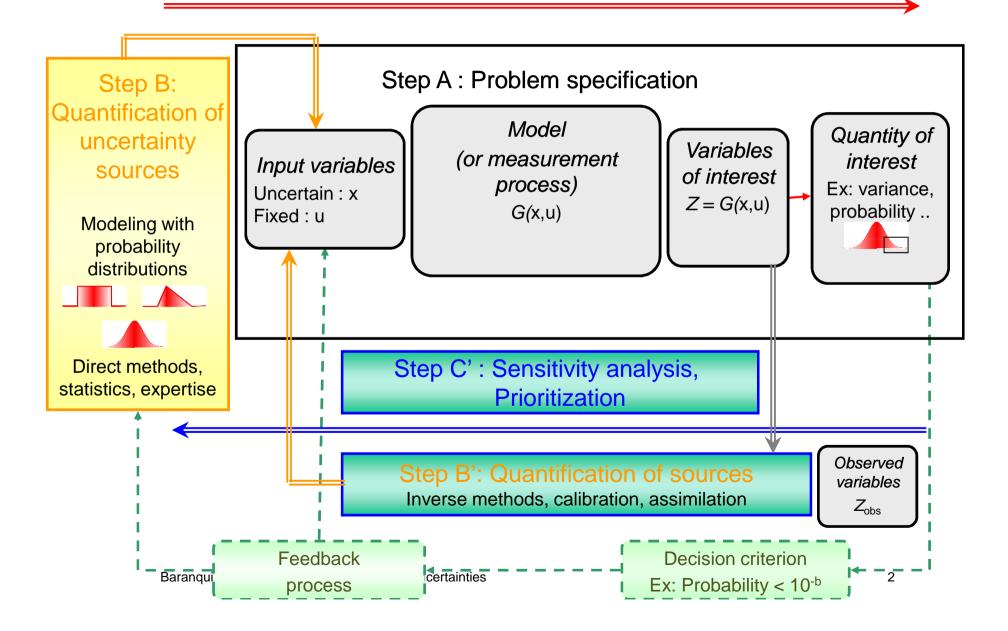
Fabrice Gamboa Bertrand looss

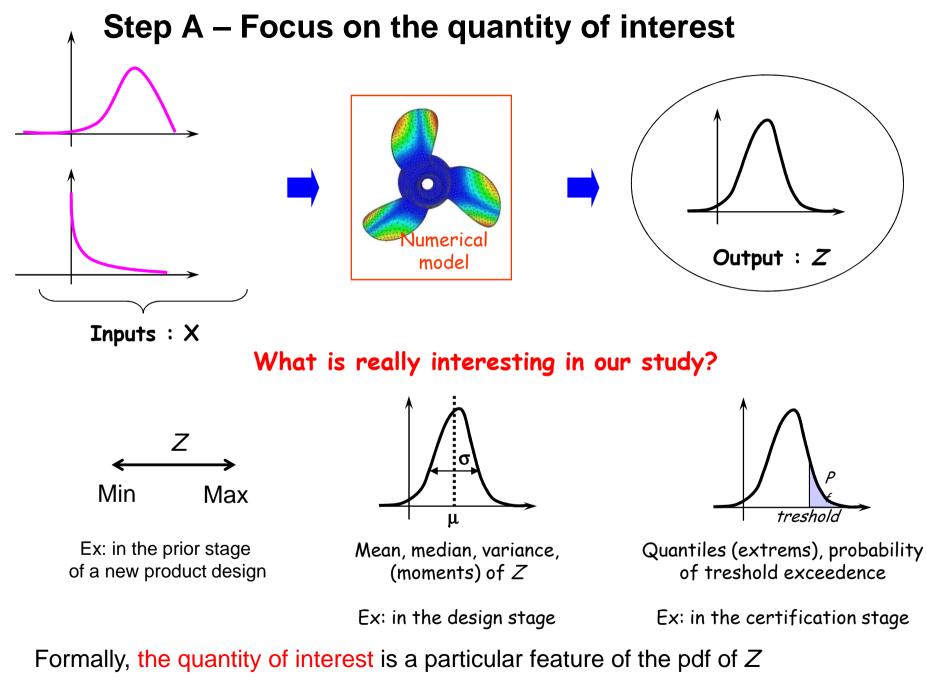
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Uncertainty management - The generic methodology

Step C : Propagation of

uncertainty sources



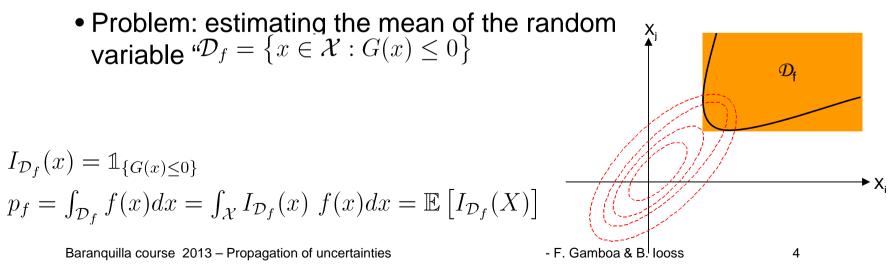


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- F. Gamboa & B. looss

A particular quantity of interest: the "probability of failure"

- G models a system (or a part of it) in operating conditions
 - Variable of interest Z→ a given state variable of the system (e.g. a temperature, a deformation, a water level etc.)
- Following an « operator » point of view
 - The system is in safe operating condition if Z is above (or below) a given "safety" threshold
- System "failure" event: $Z \leq 0$
 - Classical formulation (no loss of generality) in which the threshold is 0 and the system fails when Z is negative
 - Structural Reliability Analysis (SRA) "vision": Failure if $C-L \leq 0$ (Capacity Load)
- Failure domain:



Step B - Quantification of uncertainty sources

Different cases with respect to available information

- 1. A lot of data
 - Fitting of probability distributions
 - Statistical hypothesis test (often parametric tests)
- 2. Few data (n < 10)
 - Hypothesis on parametric probability distribution
 - Non-parametric tests : less powerfull, wide bounds
 - Expert judgement, then Bayesian inference

3. No data

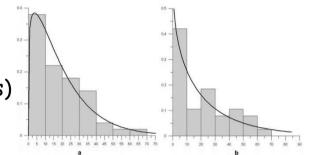
- Expert judgment techniques
- Maximum entropy principle

$$H(X) = -\int_{\mathcal{X}} f(x) \log (f(x)) \, dx$$

Measure of the "vagueness" of the information on X provided by f(x)

Information	Maximum Entropy pdf		
$X \in [a, b]$	Uniform $X \sim \mathcal{U}(a, b)$		
$\mathbb{E}(X) = \mu$ $X \in [0, \infty[$	Exponential $X \sim \mathcal{E}(1/\mu)$		
$\mathbb{E}(X) = \mu$ $\mathbb{V}(X) = \sigma^2$	Normal $X \sim \mathcal{N}(\mu, \sigma)$		



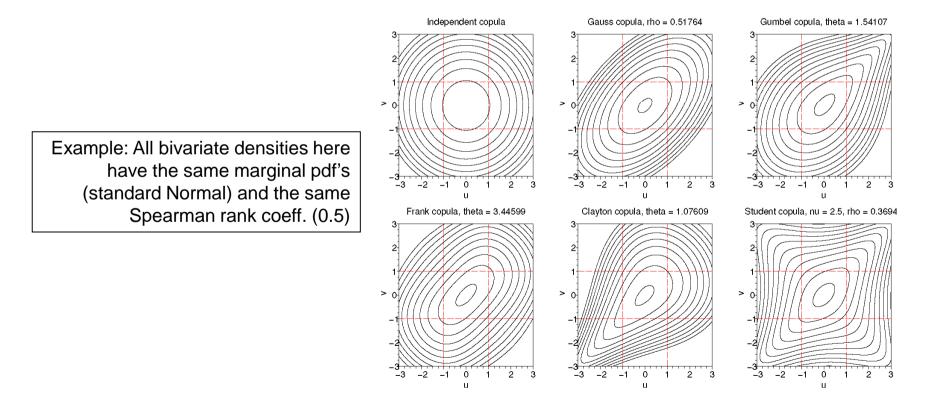


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Some comments (Step B). Dependency

- Taking into account the dependency between inputs is a crucial issue in uncertainty analysis
 - Using copulas structure \rightarrow CDF of the vector X as a function of the marginal CDF of $X_1 \dots X_n$:

 $F(x_1, x_2, \cdots, x_n) = C(F(x_1), F(x_2), \cdots, F(x_n))$



Step C - Uncertainty propagation: main principles

Propagate uncertainties from X to Z, via the deterministic function $G(\cdot)$

- Conceptually simple problem, but with sometimes a complex implementation
- Choice of method strongly depends on the quantity of interest
- => importance of step A

This quantity of interest is linked to decisional issues

Two kinds of problems :

- Central tendancy (ex. mean) or dispersion (variance)
 - Metrology
- High quantile, « probability of failure »
 - \rightarrow justification of a safety criterion



Analytical methods sometimes applicable

Numerical methods (optimization, Monte Carlo sampling)

Step C' - Sensitivity analysis: main objectives

 \cdot Reduction of the uncertainty of the model outputs by prioritization of the sources

Variables to be fixed in order to obtain the largest reduction (or a fixed reduction) of the output uncertainty

A purely mathematical variable ordering

- Most influent variables in a given output domain
 - if reducibles, then R&D prioritization
 - else, modification of the system

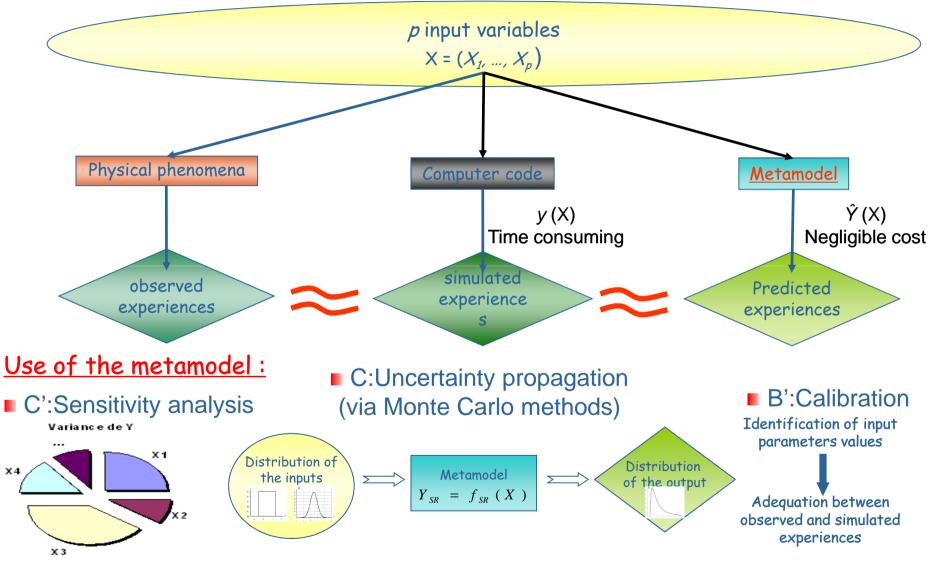
The individual cost of the reduction may change the previous variable ordering

• Simplification of a model

- determination of the non-influent variables, that can be fixed without consequences on the output uncertainty
- building a simplified model, a metamodel

Uncertainties management for cpu time consuming models





V&V process: Verification and Validation

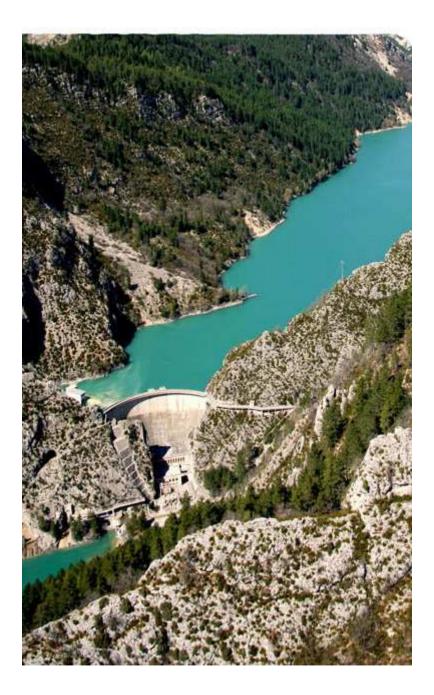
To sum up :

Verification : do I solve the equations right ?
Validation : do I solve the right equations ?
 (at least for the intended application)

Two levels for Verification :

- Code Verification : some kind of "*internal*" correctness of the code may be assessed by formal methods from Software Engineering
- Calculation Verification : concerns the calculations themselves Convergence, grid adaptation, solution algorithms, ...
 Is the solution closed to the exact one ?





Some mathematical methods for uncertainty propagation

Quadratic combination method

Data : mean values of X_i : $\mu_i = \mathbb{E}[X_i]$ variance-covariance matrix of X_i :

$$Cov [X_i, X_j] = \mathbb{E} \left[(X_i - \mu_i) (X_j - \mu_j) \right]$$
$$\rho_{ij} = \mathbb{E} \left[\frac{X_i - \mu_i}{\sigma_i} \frac{X_i - \mu_i}{\sigma_j} \right]$$

Taylor expansion of $G(\bullet)$ around E(X) :

$$G(X) = G(\mu) + \sum_{i=1}^{N} \frac{\partial G}{\partial X_i} \Big|_{X=\mu} (X_i - \mu_i)$$

+
$$\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial^2 G}{\partial X_i \partial X_j} \Big|_{X=\mu} (X_i - \mu_i) (X_j - \mu_j) + o\left(||X - \mu||^2 \right)$$

En général, dans les applications le développement est d'ordre 1

Quadratic combination method – First order

Mean of Z

 $\mathbb{E}\left[Z\right] = G(\mu)$

Variance of Z

$$\mathbb{V}[Z] = \mathbb{E}\left[\left(Z - \mathbb{E}[Z]\right)^{2}\right] = \mathbb{E}\left[\left(G(\mu) + \sum_{i=1}^{N} \frac{\partial G}{\partial X_{i}}\Big|_{X=\mu} \left(X_{i} - \mu_{i}\right) - G(\mu)\right)^{2}\right] = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial G}{\partial X_{i}}\Big|_{X=\mu} \frac{\partial G}{\partial X_{j}}\Big|_{X=\mu} \mathbb{E}\left[\left(X_{i} - \mu_{i}\right) \left(X_{j} - \mu_{j}\right)\right]$$

$$\mathbb{V}[Z] = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial G}{\partial X_{i}} \Big|_{X=\mu} \frac{\partial G}{\partial X_{j}} \Big|_{X=\mu} \rho_{ij} \sigma_{i} \sigma_{j}$$

<u>Remarks :</u>

++ Needs only mean and covariance of X

-- Do not use if G(.) is strongly non linear

-- Provides only mean and variance of Z => no extrapolation fo the distrib. law of Z ++ if X is gaussian and G(.) is linear, then Z is gaussian

Quadratic combination method – Independent case

If the X_i s are independent :

$$\mathbb{V}[Z] = \sum_{i=1}^{N} \left(\frac{\partial G}{\partial X_i} \Big|_{X=\mu} \right)^2 \sigma_i^2$$

Contribution of each input variable to the uncertainty of the output variable

Quadratic summation formula

$$\eta_i^2 = \frac{1}{\mathbb{V}\left[Z\right]} \left(\frac{\partial G}{\partial X_i}\Big|_{X=\mu}\right)^2 \sigma_i^2$$

Sensitivity indices (normed)

Methods of Monte Carlo simulation

- General mthods to evaluate a numerical quantity, using some random simulations
- In uncertainty propagation : use a random sample of G(X) to evaluate the quantity of interest
- We suppose that we know how to simulate an i.i.d (independent and identically distributed) sample of X_i following its probability distribution f_i

Monte Carlo in general (1/3)

• Computation of the integral :

Monte Carlo estimator

Monte Carlo (2/3)

• Variance of the Monte Carlo estimator

$$\mathbb{V}\left[\frac{1}{n}\sum_{i=1}^{n}h(X^{(i)})\right] = \frac{1}{n^2} \ n\mathbb{V}\left[h(X)\right] = \frac{1}{n}\mathbb{V}\left[h(X)\right] \qquad \begin{array}{c} \text{Variance of the sum} \\ \text{of n r.v. i.i.d.} \end{array}$$

- Variance of h(X) is given via its estimator :

$$\mathbb{V}[h(X)] \approx \frac{1}{n} \sum_{i=1}^{n} \left(h(x^{(i)}) - \hat{I} \right)^2$$

- General expression for the variance of the MC estimator

$$\mathbb{V}\left[\hat{I}\right] \approx \frac{1}{n^2} \sum_{i=1}^n \left(h(x^{(i)}) - \hat{I}\right)^2$$

- We note :

$$\sigma_{\hat{I}}^2 = \mathbb{V}\left[\hat{I}\right]$$

Monte Carlo (3/3)

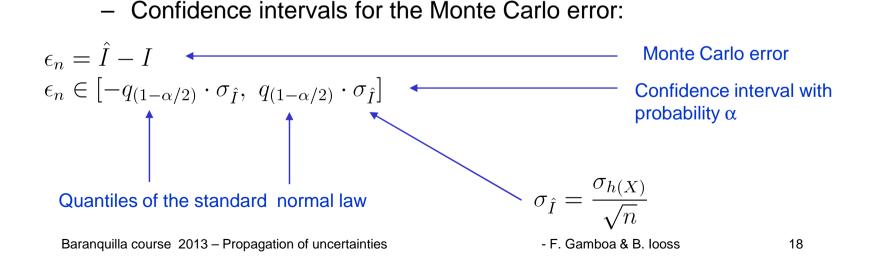
• Asymptotic law of the estimator from Central Limit Theorem:

$$\frac{\sqrt{n}}{\sigma_{h(X)}} \left(\hat{I} - I \right) \sim \mathcal{N}(0, 1) \quad \text{with} \quad \sigma_{h(X)} = \sqrt{\mathbb{V}[h(X)]}$$

Low convergence speed (in $1/\sqrt{n}$) but:

Independence with respect to the dimension of X and to the form of h(•) Unbiased estimator

Precision only depends on n (then on the cpu time of h(.))



Monte Carlo and uncertainty propagation

• Propagation of the uncertainties of X to Z=G(X)

 $x^{(1)}, x^{(2)}, \dots, x^{(n)}$

n-sample of X

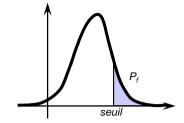
• Monte Carlo estimator of mean and variance of Z :

$$\mathbb{E}[G(X)] \approx \frac{1}{n} \sum_{i=1}^{n} G(x^{(i)})$$
$$\mathbb{V}[G(X)] \approx \frac{1}{n} \sum_{i=1}^{n} \left[G(x^{(i)}) - \frac{1}{n} \sum_{i=1}^{n} G(x^{(i)}) \right]^2$$

• Moments of Z are estimated by the empirical moments

Estimation of a probability of failure

• System failure : event $Z \le 0$

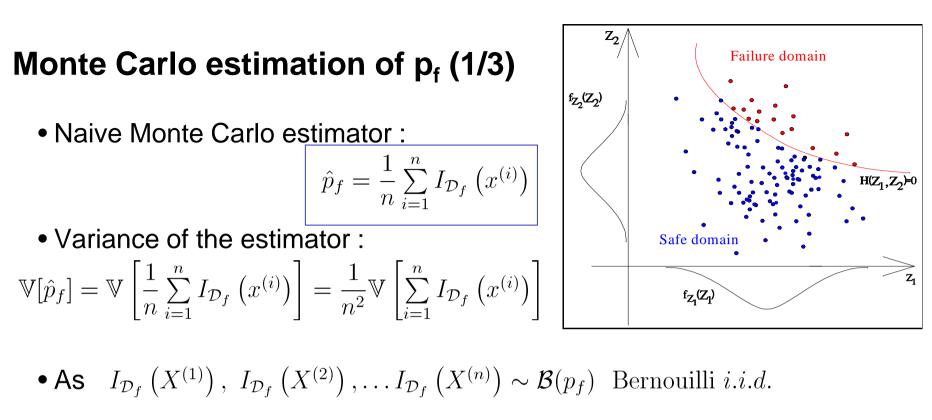


- Failure domain: $\mathcal{D}_f = \{x \in \mathcal{X} : G(x) = z \le 0\}$
- Failure probability: $p_f = \int_{\mathcal{D}_f} f(x) dx = \int_{\mathcal{X}} I_{\mathcal{D}_f}(x) f(x) dx = \mathbb{E} \left[I_{\mathcal{D}_f}(X) \right]$

– Problem : computation of the mean of the random variable $I_{\mathcal{D}_f}(x)$

• Failure indicator : $I_{\mathcal{D}_f}(x) = \mathbb{1}_{\{G(x) \le 0\}}$

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• We have:
$$\mathbb{V}[\hat{p}_f] = \frac{1}{n^2} \sum_{i=1}^n \mathbb{V}\left[I_{\mathcal{D}_f}(x)\right] = \frac{1}{n^2} n p_f(1-p_f)$$

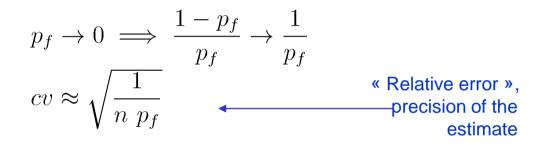
 $\mathbb{V}[\hat{p}_f] = \frac{1}{n} p_f(1-p_f)$ Estimated by: $\mathbb{V}[\hat{p}_f] \approx \frac{1}{n} \hat{p}_f(1-\hat{p}_f)$

 Asymptotical convergence to a normal law and other MC estimator properties

- Monte Carlo estimation of p_f (2/3) Decrease in square root of n : $\sigma_{\hat{p}_f} = \frac{1}{\sqrt{p_f}} \sqrt{p_f(1-p_f)}$
- Variation coefficient :

$$cv = \frac{\sigma_{\hat{p}_f}}{\mathbb{E}[\hat{p}_f]} = \sqrt{\frac{p_f(1-p_f)}{n}\frac{1}{p_f^2}} = \sqrt{\frac{1-p_f}{n p_f}}$$

• For small values of p_f :



• For example, if we estimate a proba $p_f = 10^{-r}$ with cv = 10%,

 \Rightarrow prohibitive required cpu times

 \Rightarrow Use of improved methods: approximate methodes (FORM/SORM), accelerated Monte Carlo methods, metamodel-based methods, ...

Importance sampling (1/3)

 <u>Idée</u> : modifying the sampling prob. distribution of X in order to concentrate the samples in most interesting regions (in terms of contribution to computation of expectation of h(X))

$$I = \int_{\mathcal{X}} h(x)f(x)dx = \int_{\mathcal{X}} h(x)\frac{f(x)}{\varphi(x)}\varphi(x)dx = \int_{\mathcal{X}} h(x)w(x)\varphi(x)dx$$

• It's the expectation of the function h(x)w(x), $X \sim \varphi(x)dx$

1) Produce a sample (x⁽ⁱ⁾) from density
$$\varphi(x)dx$$

2) Then, compute : $\hat{I}^{is} = \frac{1}{n} \sum_{i=1}^{n} h(x^{(i)}) w(x^{(i)})$
 $\mathbb{V}\left[\hat{I}^{is}\right] = \frac{1}{n} \mathbb{V}\left[h(X) \frac{f(x)}{\varphi(x)}\right]$

- Unbiased estimator of I, in condition that the support of $\phi(x)$ contains the one of f(x)

Importance sampling (2/3)

- This method does not guarantee any variance reduction $\forall \phi(x)$
- The choice of the « instrumental law » $\phi(x)$ is crucial
 - theoretically: optimal density :

$$\varphi^*(x) = \frac{\mid h(x) \mid f(x)}{\int_{\mathcal{X}} \mid h(x) \mid f(x) dx}$$

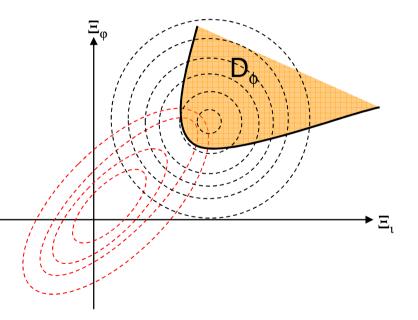
- The normalization constant is as difficult to evaluate as evaluating I !
- However, practical result ...
- Estimation of a failure probability p_f by importance sampling

- Here:
$$h(x) = I_{\mathcal{D}_f}(x) = \mathbb{1}_{\{G(x) \le 0\}}$$

- Optimal density : $\varphi^*(x) = \frac{I_{\mathcal{D}_f}(x)f(x)}{\int_{\mathcal{X}} I_{\mathcal{D}_f}(x)f(x)dx} = \frac{I_{\mathcal{D}_f}(x)f(x)}{p_f}$

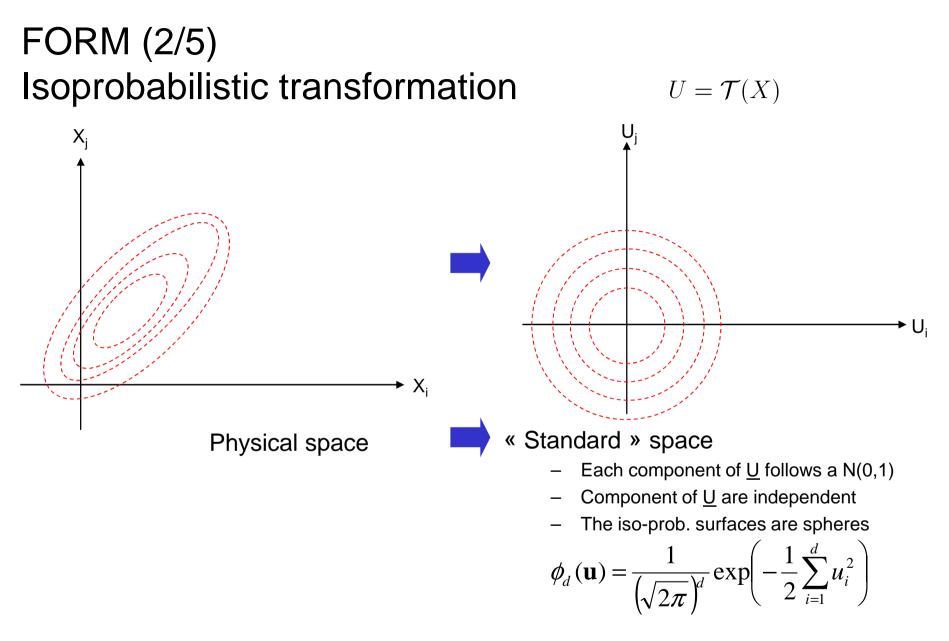
Importance sampling (3/3)

- The optimal density id the conditional law of de X knowing that $X \in D_f$
- Intuitive result→ the method is mostly efficient if it produces samples in the failure domain
- Some practical algorithms:
 - Obtain a first idea of the configuration of D_f (first Monte Carlo runs)
 - Center the instrumental law on a point of D_f (for example on the design point P* obtained with the FORM method)



FORM method (1/5)

- FORM: First Order Reliability Method
- From structural safety domain
- 3 steps :
- Transformation of inputs X_i to other inputs whose probability distributions have « good properties »
 Isoprobabilistic transformation → standard Gaussian space
- 2. Search of the most probable failure conditions
- 3. Estimation of the failure probability



Points which mostly contribute to p_f are the nearest to the origin in the standard space

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FORM : isoprobabilistic transformation

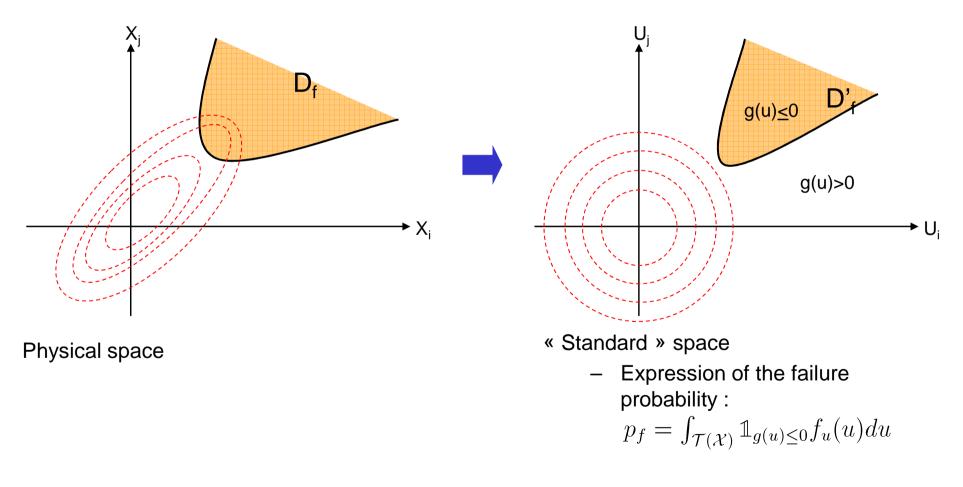
Rosenblatt transformation

T :
$$u_1 = \Phi^{-1}(F_1(z_1))$$

 $u_2 = \Phi^{-1}(F_2(z_2|z_1))$
:
 $u_N = \Phi^{-1}(F_N(z_N|z_{N-1}, \dots, z_2, z_1))$

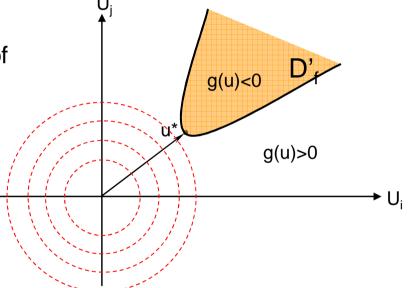
FORM (3/5) – Isoprobabilistic transformation

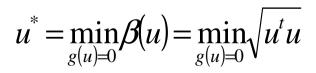
• New expression of the failure probability $\mathbb{P}(G(X) \le 0) = \mathbb{P}(G(\mathcal{T}^{-1}(U) \le 0) = \mathbb{P}(g(U) \le 0)$



FORM (4/5) – Search of the most probable failure conditions

- To each point of the standard space, some operating or failure conditions are associated
 - The most probable failure point is the nearest from the origin (where the desnity is max because the mean of of U is the null vector)
 - Reminder : the value of density f_U(u) depends only on ||u|| (distance of u from origin)
 - Call it P* : designpoint
 - Call u* the vector OP*
 - The search of u*, (with an uniqueness hyp.), is an optimization problem under constraints





FORM (5/5) – Evaluation of p_f

• Hypothesis :

=> N(0,1)

Replacement of the limit surface g(u)=0by the hyperplan intersecting P* and orthogonal to u*, with equation : β : norme de u* $\sum_{i=1}^{n} \alpha_i u_i + \beta = 0$ α_i cos. direct de u* Approximation based on the hyp. that points far away from P* have small contributions to $p_f \rightarrow$ their proba is very small ► U: $p_f \approx \mathbb{P}\left(\sum_{i=1}^N \alpha_i u_i + \beta \le 0\right) =$ $\mathbb{P}\left(\sum_{i=1}^{N} \alpha_{i} u_{i} \leq -\beta\right) = \Phi(-\beta)$ β : « Reliability index » α_i : « Importance factors» FORM \rightarrow sensitivity indices of variables Ui to Linear combination of r.v. **Distribution function** pf N(0,1) with normed coeff. αi of N(0,1)

FORM/SORM : Pros and cons

Pros:

reduced computing times with respect to other methods
No dependancy between computing times and value of pf
Getting the importance factors and a design point

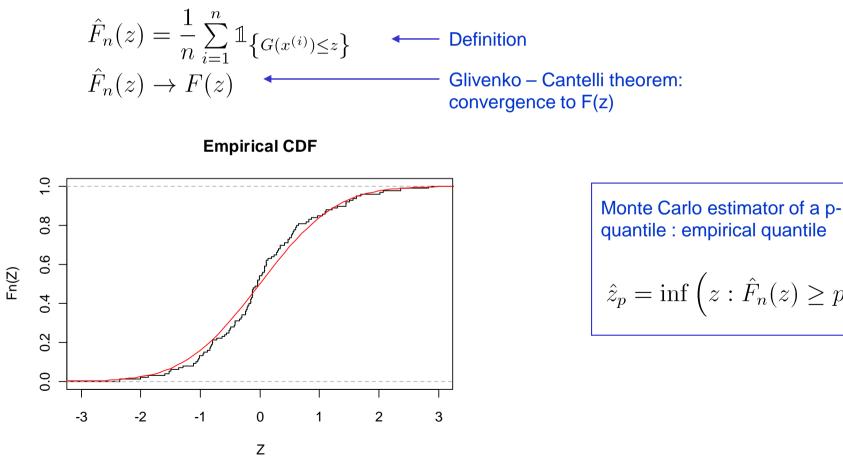


Cons:

- Approximation not always valid
- No measure of the error which is made:
- G has to be differentiable
- Hypothesis of a unique design point

Quantile estimation (1/2)

Probability distribution function and quantile estimator



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quantile : empirical quantile
$$\hat{z}_p = \inf\left(z:\hat{F}_n(z) \ge p\right)$$

Quantile estimation (2/2)

- In practice:
 - Build an <u>ordered</u> sample from $G(x^{(1)}), G(x^{(2)}), ..., G(x^{(n)})$

- Call it:
$$z^{(1)}, z^{(2)}, ..., z^{(n)}$$
 $z^{(1)} \le z^{(2)} \le ... \le z^{(n)}$

 $- \hat{z}_p = z^{(\lceil np \rceil)}$

• For example, if n=100 and p=0.95, then we have to take 96th value in the ordered sample

• Of course, we need
$$\frac{1}{N}$$

• Asymptotic law of the estimator:

$$\frac{\sqrt{n}}{\tau} \left(\hat{z}_p - z_p \right) \sim \mathcal{N}(0, 1) \qquad \tau^2 = \frac{p(1-p)}{\left(f(z_p) \right)^2}$$

Quantile estimation – Wilks formula

•We can show that:

 $\mathbb{P}\left(z^{(np+r)} > z_p\right) = \sum_{j=n(1-p)-r+1}^{n} \mathbb{P}\left(j \text{ parmi les } z^{(i)} \text{ sont } > z_p\right) = 1 - C_p(n,r)$ $C_p(n,r) = \sum_{j=0}^{n(1-p)-r} \binom{n}{j} (1-p)^j p^{n-j}$

- Then, if r is the smallest integer such that $C_p(n,r) \le 1-\beta \implies 1-C_p(n,r) \ge \beta$

- then,
$$\mathbb{P}\left(z^{(np+r)} > z_p\right) \geq \beta$$

- We obtain the Wilks method
 - Conservative estimator of quantiles :
 - With a fixed n, find β (the confidence level of the quantile)
 - With a fixed β fixé, find n (required number of code runs)

Sampling via Wilks formula

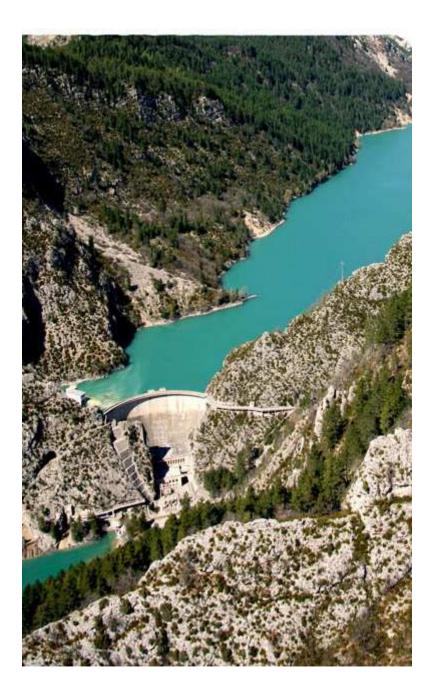
Comments:
Robust method
No hypothesis on the distribution function
Constraint :
Can only be applied to pure random sample (i.i.d.)

Example with Wilks at first order and unilateral quantile Z_{max} is the maximal value of the N-sample (i.i.d) of Z

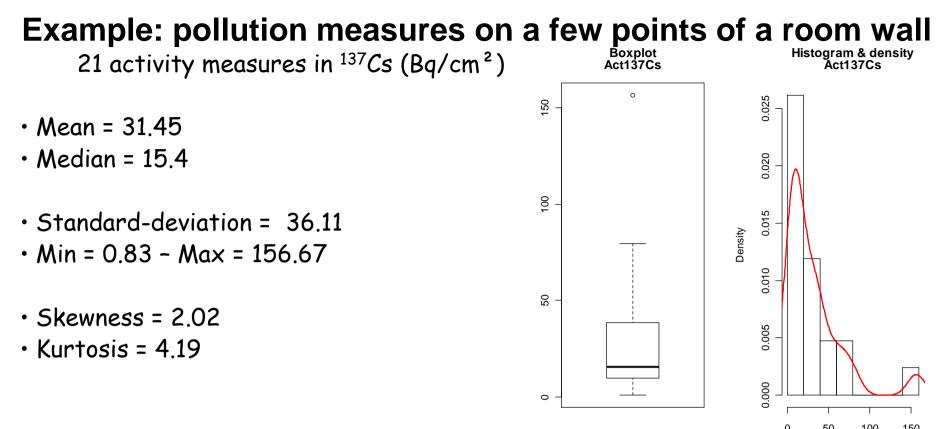
$$P[P(Z \le Z_{\max}) \ge \alpha] \ge \beta, \quad N \text{ solution of } 1 - \alpha^N \ge \beta$$

α	0.50	0.90	0.90	0.95
β	0.95	0.90	0.95	0.90
n	5	22	29	45

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Application example



Safety issue: guarantee (with a certain confidence level) that the contamination does not exceed a treshold over all the room wall

<u>Examples</u> : prediction of the amount of different category of wastes (proportion of activities < 50 Bq / cm² , > 100 Bq / cm² , ...) waste quantities in different types of storage (deep geologic, subsurface, no storage)

different costs

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Useful probabilistic tools: universal inequalities

For a random variable X with mean μ and variance σ^2 , we can use for X > μ :

• the Bienaymé-Tchebytcheff inequality:
$$P(X \le \mu + k\sigma) > \frac{k^2}{1+k^2}$$

More than 72% of the surface < 100 Bq/cm² Pessimistic bound μ and σ^2 are replaced by their empirical estimates

• the Guttman inequality:

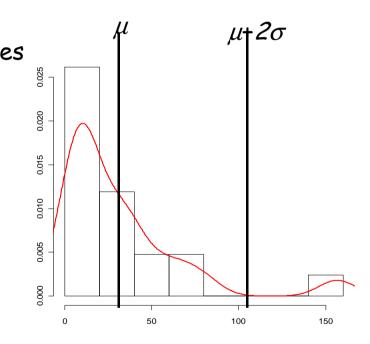
$$P(X \le \mu + k\sigma) > \frac{q^2}{1+q^2}$$
 with $q^2 = \frac{(k^2-1)^2}{\gamma_2 - 1}$

More than 82% of the surface < 100 Bq/cm² Needs the knowledge of the kurtosis

• the Meidell inequality (<u>unimodality hypothesis</u>):

$$P(X \le \mu + k\sigma) > \frac{(3k/2)^2}{1 + (3k/2)^2}$$

More than 89% of the surface < 100 Bq/cm²



All these tools give unsafe estimates

Using the Wilks formula

For an i.i.d. sample $\{X_1, ..., X_n\}$ of a random variable X, if n is solution of $1 - \alpha^n \ge \beta$ and $X_{\max} = \max\{X_1, ..., X_n\}$ we have $P[P(X \le X_{\max} | (X_1, ..., X_n)) \ge \alpha] \ge \beta$

It gives:

1. the minimal sample size n for α and β 2. for a given sample, the α -quantile value,

with a β confidence degree

Ĩ	α	0.50	0.90	0.95	0.95
Î	β	0.95	0.95	0.90	0.95
	n	5	29	45	59

No hypothesis on distribution function and no needs of parameter estimates

More general result linking *n* and order *r* (rank in the ordered sample $\{X_{(1)}, \dots, X_{(n)}\}$)

Application (measures in ^{137}Cs):

• Wilks (n=21, r=2, $\beta=0.9$) -> more than 83% of the surface < 80 Bq/cm² (with a 90% degree of confidence)

• Meidell (unimod., σ estimate) -> more than 80% of the surface < 80 Bq/cm²

Conclusions on step C (uncertainty propagation)

- Challenge: balance between precision of the estimate and cpu time cost
- Use **Monte Carlo** if possible: independent of input dimension, unbiased estimation, gives a confidence interval

BUT : needs large number of model runs to obtain convergence

- If this cost is unreachable, alternative methods exist:
 - Accelerated Monte Carlo method (importance sampling, etc.)
 - Méthodes quasi-Monte Carlo (cf. cours 2) <u>But:</u> curse of dimensionality
 - <u>Approximate methids</u>:
 - Quadratique summation <u>But:</u> linear hypothesis
 - FORM/SORM : fast estimation of p_f. Can be used to initialize another method (importance sampling)
 - Using a surrogate model of the computer code (metamodel)

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