Treatment of uncertainties in numerical simulation

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07/03/2013



Introduction

Starting point: uncertainties everywhere in a modeling chain !

Main problem: credibility of predictions



Similar safety and uncertainty issues in CS&E and Nature sciences CS&E : Computational Science & Engineering



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Exemple 1: particle dispersion in atmosphere (1/3)

Accidental scenario of pollutant release

Domain of study: 10 km around an industrial site

2 arbitrary sources (at ground level) : * source 1 : tracer (gas) * source 2 : iodine (particles)

Projection for 4 days

Meteorological data: wind, temperature, humidity, rain

Rugosity of the ground (vegetation)

Topography and location of sources



[Source : CEA]

Exemple 1: particle dispersion in atmosphere (2/3)

Computation of wind field (direction and amplitude)

Visualization of the wind with flux lines



Exemple 1: particle dispersion in atmosphere (3/3)

Use of a <u>computer code</u> of lagrangian particle dispersion (solving the Euler equations of fluid mechanics)

Visualisztion of gas concentrations en gaz after a 5 hours' release



Plume under the particular form

Concentration plume (at 10 m level)

Results are strongly sensitive to meteorological data

Exemple 2: Models in hydrology



Uncertainties in model parameters that govern surface and ground water transport, ...

Exemple 3: Uncertainties in oil reservoir characterization

- Scalar uncertain parameters :
 - Reservoir Geometry : limits, thickness, faults, etc...
 - Petrophysical properties : porosity, permeability,...
 - Fluid properties water/Oil/Gaz : contacts between fluids, viscosity,...
 - Rock/Fluid interactions, Well Data, etc...
- Spatial uncertain parameters :
 - several realizations of a unique geological structure
 - geostatistical parameter \Rightarrow represented as a "seed variable"
 - Exemples:
 - · geostatistical seed
 - Structure maps
 - Stochastic fracture networks



[Source : IFP EN]



Effect of geostatistical uncertainties ?



Main stakes of uncertainty management

- Modeling phase:
 - <u>Improve</u> the model
 - <u>Explore</u> the best as possible different input combinations
 - Identify the predominant inputs and phenomena in order to priorize R&D
- Validation phase:
 - <u>Reduce</u> prediction uncertainties
 - <u>Calibrate</u> the model parameters
- Practical use of a model:
 - Safety studies: <u>assess</u> a risk of failure (rare events)
 - Conception studies: <u>optimize</u> system performances and robustness





Which (parametric) uncertainty sources?

• Epistemic uncertainty

- It is related to the lack of knowledge or precision about a parameter which is deterministic in itself (or can be considered deterministic under some accepted hypotheses). E.g. a characteristic of a material.
- Stochastic (or aleatory) uncertainty
 - It is related to the real variability of a parameter, which cannot be reduced (e.g. the discharge of a river in flood risk assessment of a riverside area). The parameter is stochastic in itself.
- Reducible vs non-reducible uncertainties
 - Epistemic uncertainties are (at least theoretically) reducible
 - Instead, stochastic uncertainties are (in general) irreducible (the discharge of a river will never be predicted with certainty)

A (very) simplified example: flood water level calculation





- \triangleright Z_c: Flood level (variable of interest)
- Z_m et Z_v : level of the riverbed, upstream and downstream (random)
- Q : river discharge (random)
- K_s : Strickler's roughness coefficient (random)
- B, L: Width and length of the river cross section (deterministic)



Which output variable of interest?

• Formally, we can link the output variable of interest Z to a number of continuous or discrete uncertain inputs X through the function G: Z = C(X, d)

Z = G(X, d)

 d denotes the "fixed" variables of the study, representing, for instance a given scenario. In the following we will simply note:

$$Z = G(X)$$

- The output variable of interest can be of dimension 1 or >1
- The function G can present itself as:
 - an analytical formula or a complex finite element code,
 - with high / low computational costs (measured by its CPU time),
- The uncertain inputs are modeled thanks to a random vector X, composed of p univariate random variables $(X_1, X_2, ..., X_p)$ linked by a dependence structure.



Methodology

The "global methodology" of uncertainty management



Let us focus on "step B"

- We stay in the case where uncertainty sources are modeled by random variable
 - Probabilistic setting
 - X is a multi-dimensional random variable
 - Its uncertainty is described by a joint distribution
 - A key question: the dependence between the components of X
- Situations encountered in common industrial practice:
 - No data \rightarrow Expertise for assessing the distribution of X
 - Data available \rightarrow Fitting parametric or non-parametric distributions
 - Indirectly observed data \rightarrow inverse modeling
 - Bayesian approach \rightarrow Combining expertise and data

No data

- In industrial practice, it may happen the only available information is an expert's advice
- Elicitation methods
 - Formal translation of the expertise into a probability distribution
 - Particularly interesting problem in Bayesian statistics
- Open question, object of several research works
- A way to build probability distributions from minimalist information: the Maximum Entropy Method

Statistical Entropy (1/3)

- Definition given by Shannon (1948), then formalized by Jaynes (1957)
- Discrete case: X is a discrete r.v. the distribution of which is $P_X = \{p_1, p_2, ..., p_k\}$ $H(X) = -\sum_{i=1}^k p_i \log(p_i)$ Statistical Entropy
- Properties :

 $\begin{array}{l} H(X) \geq 0 \\ H(X) = 0 \Leftrightarrow \exists ! p_i : p_i = 1, \quad \forall i \neq j \quad p_j = 0 \end{array} \begin{array}{l} \text{Always positive, except for a} \\ \text{particular case (minimum = 0)} \end{array}$

- The maximum, equal to log(k), is reached in case of uniform distribution

$$p_i = \frac{1}{k} \forall i \Rightarrow H(X) = -\sum_{i=1}^k \frac{1}{k} \log\left(\frac{1}{k}\right) = -\frac{1}{k} \ k \ \log(\frac{1}{k}) = \log(k)$$

Statistical Entropy (2/3)

- Intuitive interpretation of entropy
 - Minimum in case of "perfect" information → no doubt on the value of de X between the k possible values
 - Maximum in the case when the information given by the prob. is the most "vague" possible → each possible value of X is equiprobable
 - Entropy: (inverse) measure of the information on X brought by its prob. distribution



Statistical Entropy (3/3)

• Extension to a continuous r.v. : $H(X) = -\int_{\mathcal{X}} f(x) \log (f(x)) dx$

- Maximum Entropy Principle
 - Among all possible distributions, one chooses the one that brings the minimum information \rightarrow i.e. the one maximizing the entropy
 - Justification : Research of "objectivity"
 - Do not add any information, except the one given by the expert

Maximum Entropy application

- Trivial Application: an expert tells that X is a discrete r.v that can take k values → choice of the discrete uniform distribution
 :
- More generally, let us imagine an expert gives in pieces of information concerning X under the form:

 $\int_{\mathcal{X}} g_j(x) f(x) dx = c_j$

The maximum entropy problem consists in finding a function f(x) maximizing H(X) et respecting the N +1 conditions:

$$\begin{cases} \int_{\mathcal{X}} f(x) dx = 1\\ \int_{\mathcal{X}} g_j(x) f(x) dx = c_j \quad j = 1...N \end{cases}$$

Constrained Optimization

 Justification : Among all possible distributions, one chooses the one that brings the minimum information compatible with available information

Maximum Entropy application - examples (1/2)

Given information	Distribution maximizing entropy		
$X \in [a, b]$	Uniform	$X \sim \mathcal{U}(a, b)$	
$\mathbb{E}(X) = \mu$ $X \in [0, \infty[$	Exponential	$X \sim \mathcal{E}(1/\mu)$	
$ \begin{split} \mathbb{E}(X) &= \mu \\ \mathbb{V}(X) &= \sigma^2 \end{split} $	Normal	$X \sim \mathcal{N}(\mu, \sigma)$	

- In spite of the justification, several objections can be made (e.g. on the choice of an uniform distribution...)
- Nevertheless, these choices are common in practice

Maximum Entropy application - examples (2/2)







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Other common distributions – no data (1/2)

- Triangular distribution $\mathcal{T}(a, b, m)$
 - When the expert gives an interval and a mode m (most probable value)



Other common distributions – no data (2/2)

- Beta distribution $\mathcal{B}(\alpha,\beta)$
 - If the r.v. is the probability for a single event to occurr
 - The expert gives a number of "successes" N' over N virtual expériments $\alpha = N'$

$$\beta = N - N'$$

- Gamma distribution $\mathcal{G}(\alpha,\beta)$
 - If the r.v. is a failure rate
 - The expert gives a number of "failures" N' observed over a "virtual" observation period T

$$\alpha = N' \quad \beta = T$$





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Data available

• Problem:

- From an i.i.d. sample of the r.v. X:
- Building the probability distribution of X, for:
 - ➡ Predicting its moments, quantiles etc.
 - Random sampling the r.v. X (e.g. Monte Carlo)

Independent and identically distributed

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

- We will focus here on uni-dimensional variables
- Non-parametric fitting
- Parametric fitting

• ...

• Verifying the quality of the fitting

Non-parametric fitting

- Empirical cumulated distribution function
- Empirical Histogram
 - "Basic" and well-known tools for the engineer

• Kernel smoothing techniques

Empirical cumulated distribution function

• i.i.d. sample of X, of size n:

 $x^{(1)}, x^{(2)}, ..., x^{(n)}$

• Empirical cumulated distribution function:

- Proportion of observations <a> a fixed value x of la v.a. X
- "Inversion" of the empirical cumulated distribution function
 - Empirical quantile:

$$\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\left\{x^{(i)} \le x\right\}}$$
$$\hat{F}_n(x) \to F(x) \quad \text{a.s.}$$







Histogram approximation of the density

• Divide the domain of X in m intervals, of equal length h

• Approximate the density of X by the step function: $]x^* + jh, x^* + (j+1)h] \ j \in \mathbb{N}$

$$\hat{f}_n(x) = \frac{1}{nh} \sum_{i=1}^n \mathbb{1}_{\left\{x^{(i)} \in \mathcal{I}(x)\right\}} \longrightarrow \mathcal{I}(x) \text{ interval containing } x$$
Number of elements of the same interval as x

• Kernel approximation of the density is inspired by histogram approximation



Х

Kernel approximation (1/4)

• Estimation of the density of X:
$$\hat{f}_{n,h}(x) = \frac{1}{nh} \sum_{i=1}^{N} K\left(\frac{x - x^{(i)}}{h}\right)$$

- h is called "bandwidth"
 - Smoothing parameter, the higher h, the "smoother" the density
- K is a function, called "kernel", positive and such as: $\int_{\mathcal{X}} K(x) dx = 1$
- K is, in general, a symmetric density, e.g. a normal distribution $\mathcal{N}(0,1)$ In this case:

$$K\left(\frac{x-x^{(i)}}{h}\right) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_i)^2}{2h^2}}$$

• Other kernels: triangular, uniform, Epanechnikov ...



Kernel approximation (2/4)

- Idea underlying this method
 - Histogram estimation: for x fixed, each point x⁽ⁱ⁾ of the sample contributes to the value of f(x) in a "binary" way (yes/no)
 - Kernel estimation: the contribution is continuous and depends on the distance between x et x⁽ⁱ⁾.

- The obtained function is continuous
 - The algorithm setting is made by:
 - The type of kernel
 - The value of h (smoothing parameter)

Kernel approximation (3/4)

• Quality of the approximation measured by:

- Mean squared error : $MSE[\hat{f}_{n,h}(x)] = \mathbb{E}\left[\left(\hat{f}_{n,h}(x) f(x)\right)^2\right]$
- Mean squared error integrated over the values de X: $\text{MISE}[\hat{f}_{n,h}(x)] = \int_{\mathcal{X}} \text{MSE}[\hat{f}_{n,h}(x)]dx$
- Asymptotical value of MISE:

 $\operatorname{AMISE}[\hat{f}_{n,h}(x)]$

 By the expression of the limited development of the AMISE, it is possible, in dimension 1, to obtain a value of h minimizing it:

$$h_{\text{AMISE}} = \left[\frac{R(K)}{n\mu_2^2(K)R(f'')}\right]^{1/5} \quad \text{where} \quad \begin{array}{l} R(K) = \int_{\mathcal{X}} (K(x))^2 \, dx \\ \mu_2^2(K) = \int_{\mathcal{X}} x^2 K(x) \, dx \end{array}$$

Kernel approximation (4/4)

• The most important parameter is the bandwidth h

- Examples obtained with the R function density()
- 500 i.i.d. values of $\mathcal{N}(\mu = 500, \sigma = 100)$
- **O** Default algorithm in R (h*=24.9)
- **2** H=h*3 \rightarrow Oversmoothing (too smooth!)
- Θ H=h/3 \rightarrow Undersmoothing





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Parametric fitting

- Fundamental hypothesis: the distribution of X belongs to a given family of parametric distributions
 - $f(\cdot) \in \mathcal{D}_{\theta}$ We use the notation: $\begin{array}{c} X \sim f_{\theta}(x) & \text{continuous case} \\ X \sim P_{\theta}(x) & \text{discrete case} \end{array}$
- The distribution is completely determined by the value of its parameter θ (generally of dimension 1, 2 or 3 for the usual distributions)
- Parametric fitting consists in estimating, under the base of the available information on X, the value of the parameter θ of its under-lying distribution

Maximum Likelihood Estimation (1/4)

• Likelihood function:

$$\mathcal{L}(x^{(1)}, \dots, x^{(n)} | \theta) = \prod_{i=1}^{n} f_{\theta}(x^{(i)}) \quad \text{continuous case}$$
$$\mathcal{L}(x^{(1)}, \dots, x^{(n)} | \theta) = \prod_{i=1}^{n} P_{\theta}(x^{(i)}) \quad \text{discrete case}$$

• Maximum Likelihood Estimator (ML) :

$$\hat{\theta}_{\mathrm{ML}} = \operatorname*{ArgMax}_{\theta} \left[\mathcal{L}(x^{(1)}, \dots, x^{(n)} | \theta) \right] = \operatorname*{ArgMax}_{\theta} \left[\log \left(\mathcal{L}(x^{(1)}, \dots, x^{(n)} | \theta) \right) \right]$$

- Value of θ that maximizes the likelihood (or the log-likelihood)
- Intuitively, we look for the value which maximizes the "probability" to observe the given sample
- It is an optimization problem

Maximum Likelihood Estimation (2/4)

- If the likelihood id differentiable (twice)
 - The two conditions below ensure $\hat{\theta}_{\rm ML}$ is a local maximizing point for the likelihood:

$$\frac{\partial \mathcal{L}}{\partial \theta}\Big|_{\theta=\hat{\theta}_{\mathrm{ML}}} = 0 \qquad \qquad \frac{\partial^2 \mathcal{L}}{\partial \theta^2}\Big|_{\theta=\hat{\theta}_{\mathrm{ML}}} \le 0$$

• Some "classical" examples :

Normal $\mathcal{N}(\mu, \sigma)$	$\hat{\mu}_{\mathrm{ML}} = \overline{x}, \hat{\sigma}_{\mathrm{ML}} = (1/n) \sum_{i} (x^{(i)} - \overline{x})^2$ avec $\overline{x} = (1/n) \sum_{i} x^{(i)}$		
Exponential $\mathcal{E}(\lambda)$	$\hat{\lambda}_{\rm ML} = 1/\overline{x}$		
Uniform $\mathcal{U}(a,b)$	$\hat{a}_{\mathrm{ML}} = \min(x^{(i)}), \hat{b}_{\mathrm{ML}} = \max(x^{(i)})$ Case where de derivative is never null		

Maximum Likelihood Estimation (3/4)

- Properties of the ML estimator
 - Convergent (consistent): $n \to \infty$, $\hat{\theta}_{ML} \to \theta$ a.s.
 - Asymptotically normally distributed:

 $n \to \infty, \quad \sqrt{n} \left(\hat{\theta}_{\mathrm{ML}} - \theta \right) \sim \mathcal{N}(0, \sigma) \qquad \qquad \text{Fisher information Matrix} \\ \sigma^2 = \left(\mathcal{I}(\theta) \right)^{-1} \qquad \qquad \qquad \mathcal{I}(\theta) = \mathbb{E} \left[\left(\frac{\partial}{\partial \theta} \log \left(\mathcal{L}(X|\theta) \right) \right)^2 \right]$

- Asymptotically unbiased $n \to \infty$, $\mathbb{E}\left[\hat{\theta}_{\mathrm{ML}} \theta\right] \to 0$
 - ... but not necessarily unbiased for finite n
 - Example : estimator of the variance of a normal distribution

Maximum Likelihood Estimation (4/4)

- Properties of the ML estimator (more)
 - Asymptotically effective: among all unbiased estimators of θ , the ML estimator has a minimal variance
 - Invariant with respect to re-parameterization. Let us suppose to differently re-parameterize the distribution of X:

 $\xi = g(\theta)$ $\hat{\xi}_{\rm ML} = g(\hat{\theta}_{\rm ML})$

- Some good properties, but the ML estimator is not always calculable
 - Another usual estimation technique: the method of moments

Method of moments

• Under existence condition, let us consider the first r moments of the probability distribution of X:

$$m_j = \int_{\mathcal{X}} x^j f_{\theta}(x) dx, \qquad j = 1 \dots r$$

– Estimated by the empirical moments : \hat{m}_{i} =

$$b_j = (1/n) \sum_{i=1}^n [x^{(i)}]^j$$

• Method of moments consists in solving in θ the system of equations:

$$\begin{cases} m_j = \hat{m}_j \qquad j = 1...r \end{cases}$$

- Properties : Convergence, asymptotic normality, but not efficiency → "less precise" estimator than the ML
- Used when maximizing the likelihood is particularly tricky (e.g. Weibull)

Verifying the quality of the fitting

- Graphical verification
 - superimposition of theoretical and empirical cumulative distribution functions
 - QQ plot
- Goodness-of-fit tests
 - Kolmogorov Smirnov
 - Cramer Von Mises
 - Anderson Darling
 - ... many others
- Example: fitting a probability distribution on 149 data of maxima annual discharges of a river

Parametric or non-parametric?

- No "unique" answer to the question!
- Generally, if possible, parametric fitting is chosen
 - Easier manipulation of the distribution
- Non-parametric fitting is interesting
 - When a great number of data is available
 - When the distribution is expected to be of "unusual" shape, e.g. multi-modal

Example of fitting (1/2)



Example of fitting (2/2) – ML estimation

- Parametric fitting (maximum of likelihood)
 - Normal distribution
 - $(\hat{\mu}, \hat{\sigma}) = (1335, 711)$
 - Log-normal distribution • $(\hat{\mu}_{log}, \hat{\sigma}_{log}) = (7.0, 0.60)$
 - Exponential distribution
 - $\hat{\lambda} = 1/1335$
 - Gumbel distribution
 - $(\hat{\mu}, \hat{\beta}) = (1013, 557)$

Visual verification of the quality of fitting



Goodness-of-fit tests (1/4)

• Goodness-of-fit test:

Hypothesis H_0 : the sample is an outcome of the given distribution Hypothesis H_1 : H_0 is not true

- These tests are based on the evaluation of a function of the data (named "test statistic") which, under the hypothesis H₀, is distributed according to a known distribution
- Significance level α : the probability to wrongly reject the null hypothesis H₀ (i.e. when H₀ is true)
- For a classical unilateral (at right) test, la decision rule is:

Accept
$$H_0$$
 if $\tau(x^{(1)}, \dots, x^{(n)}) \leq \tau_{1-\alpha}$
Value of the test statistic for the
sample under investigation
$$(1-\alpha)$$
 quantile of the test statistic, under the
hypothesis $H_0 \rightarrow$ This quantity is known
(tables, statistical software)

Goodness-of-fit tests (2/4)

Kolmogorov – Smirnov (KS)

• $\tau_{KS} = \sup \sqrt{n} \left| F_n(x) - F(x) \right|$

• Quelques tests

- Cramer – Von Mises (CM) • $\tau_{CM} = \int_{-\infty}^{+\infty} [F_n(x) - F(x)]^2 dF(x) =$ $\frac{1}{12n} \sum_{i=1}^n \left[\frac{2i-1}{2n} - F(x^{(i)}) \right]^2$ After an ordering of the sample - Anderson – Darling (AD) • $\tau_{AD^2} = n \int_{-\infty}^{+\infty} \frac{[F_n(x) - F(x)]^2}{F(x) \cdot (1 - F(x))} dF(x) =$ $- n - \frac{1}{n} \sum_i \left[\log(F(x^{(i)}) + \log(1 - F(x^{(n-i+1)})) \right]$

Goodness-of-fit tests (3/4)

- The KS test takes into account the maximum deviation between empirical CDF and theoretical
- The CM test takes more into account the "global" fitting
- The AD test particularly consider the fitting on the tails of the distributions, by weighting the deviations with the factor:



Goodness-of-fit tests (4/4)

	Normal distrib.	Log-normal distrib.	Gumbel distrib.
Kolmogorov – Smirnov	τ _{KS} = 0.091	τ _{KS} = 0.087	τ _{KS} = 0.043
$\tau_{95\%} = 0.11$	p-val = 0.17	p-val = 0.20	p-val = 0.94
Cramer – Von Mises	τ _{CM} = 0.29	τ _{CM} = 0.23	τ _{CM} = 0.038
$\tau_{95\%} = 0.46$	p-val = 0.17	p-val = 0.21	p-val = 0.94
Anderson Darling	$\tau_{AD} = 2.08$	$\tau_{AD} = 1.44$	τ _{AD} = 0.25
	p-val = 0	p-val = 0.02	p-val = 1

- Preference for the Gumbel distribution
- But other distribution could not be rejected. How to choose?
- Other selection tools (based on likelihoods ratio) :

 $AIC = 2k - 2\log(\mathcal{L})$ $BIC = k\log(n) - 2\log(\mathcal{L})$

Just a word on Bayesian approach (1/2)

• That topic deserves an entire training course!

• Idea : updating, by data observation, a preliminary knowledge on the parameters of the statistical model, described by a *prior distribution*

- Appealing approach in industrial practice, for incorporating expertise in statistical analysis
- Allows to explicitly account for uncertainty tainting the parameter θ , which is described here as a random variable...

Just a word on Bayesian approach (2/2)

- An unique probability distribution for describing the so-called "aleatory" (per se, irreducible) and "epistemic" (lack of knowledge, reducible) uncertainties
- A important point: the choice of the prior distribution
 - Non-informative distrib. \rightarrow minimizing the information brought by the prior
 - Informative distrib. \rightarrow properly modeling the expertise
- Bayesian computing
 - No analytical solution for the integral at denominator in Bayes formula
 - Use of simulation methods for getting a sample of the posterior distribution (the expression of which is always known up to a multiplicative constant)