Statistical learning for computer experiment

Atelier GDR MASCOT NUM 2011

14:00 – 14:07 : F. Mangeant : Introduction

14:07 – 14:59 : G. Obozinski : Survey of statistical learning trends

15:00 – 15:45 : N. Rachdi : Application of statistical learning techniques

15:46 – 16:01 : Break

16:01 – 16:58 : Open discussion

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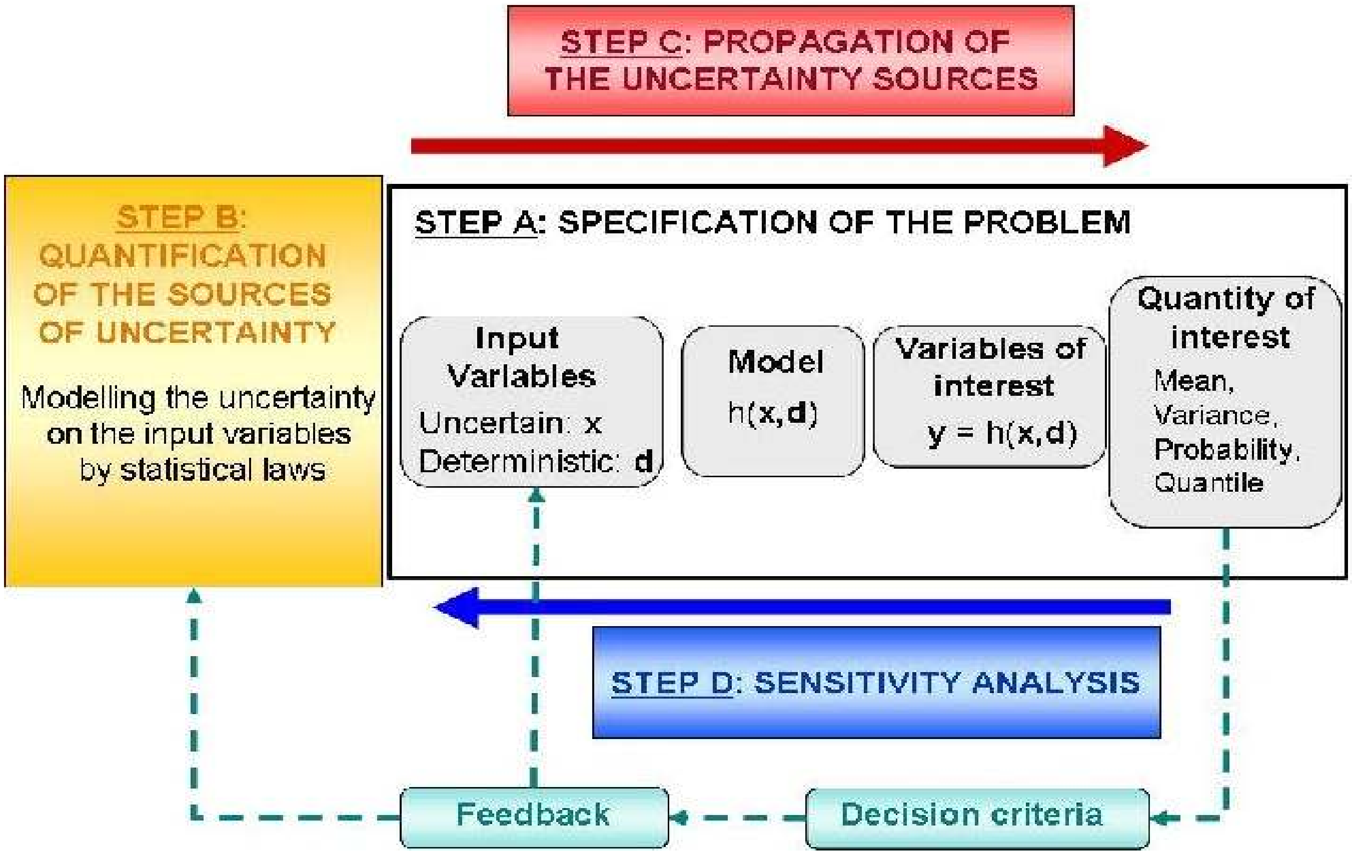
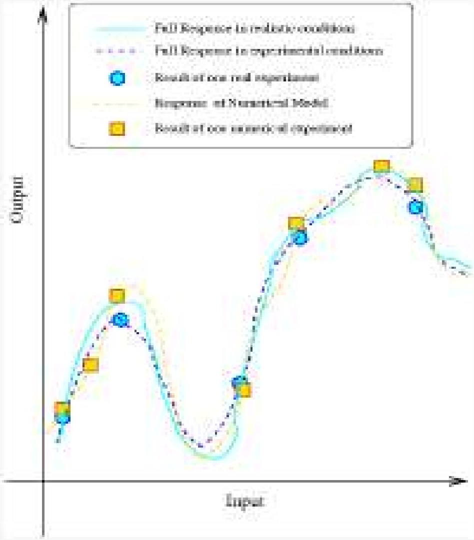
Once again, the engineer's point of view !



The "model" uncertainty

What are the components of model uncertainty?

- **Reference model h^***: Usually not accessible, expression of a natural or a complex technical object.
- **Theoretical model $\tilde{h}$**: Scientific expert activity (theoretical solution of a PDE system, ...), corresponding to the level of understanding and simplification of the problem.
- **Numerical model $\hat{h}$**: Numerical solution of the theoretical model (effects of meshing, choice of a numerical scheme)
- **Implementation model h**: Software implementation of the model on a given hardware architecture (computer accuracy, choice of coding rules, ..).



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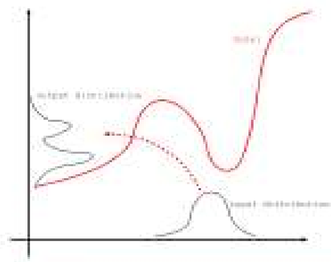
Other components of uncertainty

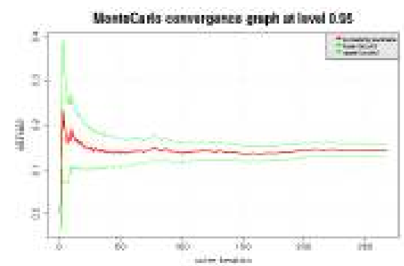
Uncertainty on the input parameters

Uncertainty due to the choice of probability measure $\mathbb{P}^{\mathbf{X}}$ on the input parameters $\mathbf{X}$ compared to $\mathbb{P}^{\mathbf{X}}_{*}$

Uncertainty on the stochastic convergence

Approximation of the criterion of interest $\rho(Y)$ by a stochastic computation $\hat{\rho}_N(Y)$





Is it possible to define a sort of contribution's metrics?

$$\Delta \leq \underbrace{\mathcal{N}_{\mathcal{S}}(h^*, \tilde{h})}_{\text{Scientific Validation}} + \underbrace{\mathcal{N}_{\mathcal{N}}(\tilde{h}, \hat{h})}_{\text{Numerical Validation}} + \underbrace{\mathcal{N}_{\mathcal{I}}(\hat{h}, h)}_{\text{Hardware / Software Validation}} + \underbrace{\mathcal{N}_{\mathcal{Q}}(\mathbb{P}^{\mathbf{X}}_{*}, \mathbb{P}^{\mathbf{X}})}_{\text{Statistical Validation}} + \underbrace{\mathcal{N}_{\mathcal{P}}(\rho(Y), \hat{\rho}_N(Y))}_{\text{Propagation Validation}}$$

Engineering basic metrics!

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Specification of the model, input/output/criteria

- **To characterize the properties of the model**
  - **Dimension**: h is classically a real function belonging to $\mathcal{F}(\mathbb{R}^P \times \mathbb{R}^T, \mathbb{R}^Q)$. Even if the dimension of $\mathbf{x}$ can be large, most of the engineering problems we are focused on only contain $P \leq 50$ and $Q \leq 5$.
  - **Computational budget**: A single computation of h can be very expensive. The computational budget will represent the number of runs N affordable to solve the problem.
  - **Black box/white box**: h is either a black box (*the inner operations of the model are not accessible*), a grey box (*part of the inner operations is accessible*) or a white box (*all the operations of the model are accessible*).
  - **Mathematical properties**: the basic mathematical properties (regularity, monotony, linearity or non linearity towards certain parameters) may be unknown to the engineer.
  - **Domain of validity**: h should be delivered with its domain of validity $\mathcal{V}^{[\epsilon]} \subseteq \mathbb{R}^P \times \mathbb{R}^T$.

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What kind of information is available in many of our computer experiment ?

- Couples (Xi, Yi)
- Database of {Xi} and database of {Yj} not obtained simultaneously
- Panoply of numerical models {h1, h2, h3}

  → ***Considered deterministic this afternoon***
- Different quantities of interest
  - Probability, quantile, moments
  - Probability density function, cumulative density function, …

Example :
h1: Interpolation in database Lookup table,
h2: Analytical model,
h3: 2D PDE model,
h4: 3D PDE solved by a numerical method

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Requirements of the algorithms to be developed

- Best use of the information for a given objective (*ie* quantity of interest)

- Non asymptotic approaches (linked to the size of the database and the CPU budget)

- Adaptative building of surrogate models for a given objective

- Measure of accuracy of the estimator/algorithm

- Validation/Verification strategies

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Challenge 1 – Metrics to selec the right level of fidelity for a given goal

In many applications, several numerical codes are available
for the same type of application *(Example : Rule of the thumb, excell sheet, 2D model, 3D FE model, …)*

A compromise has to be found between the « complexity » of the model and the « objective » of the simulation.

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Challenge 2 – How to develop new surrogate models adapted to specific purpose ?

Kriging, polynomial chaos as they are built today for a L2 norm and may be not well fitted for some specific objectives

Challenge 3 – How to develop validation and verification strategies ?

To be able to evaluate the different types components of validation