Uncertainty Quantification in Engineering

B. Sudret

Chair of Risk, Safety & Uncertainty Quantification



Jncertainty quantification framework Uncertainty propagation techniques Application examples

Introduction



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Introduction







Source: wikipedia/Cruas

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Computational models

Computer simulation aims at reproducing the behaviour of complex natural or man-made systems.

Computational models combine:

- A description of the physical phenomena (*e.g.* mechanics, heat transfer, fluid dynamics, etc.) by a set of equations
- Discretization procedures which transform the (partial differential) equations into linear algebra problems
- Solvers which provide an approximate solution to these equations.

From real world to computational models

Real world	Model	Underlying physics
-	R	 Aerodynamics (hyperboloïd shape) Structural mechanics (concrete shell)
		Structural mechanics (prestressed concrete)Durability (leak tightness)
	-	NeutronicsComputational fluid dynamics

• Fracture mechanics

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Inaugural lecture

Why do we use computational models in engineering?

Computational models are used as virtual prototypes which help the engineer assess and optimize the performance of the system under consideration.

Example: design of a cooling tower



From the specifications of the plant nuclear power and the existing cooling source the required cooling capacity is determined.

- Aerodynamics: size of the tower (diameter/shape/height) for optimal natural draught
- Structural mechanics: thickness of the shell, quantity of reinforcing steel bars under prescribed operating conditions and environmental loads (temperature, wind, snow, etc.)

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Incertainty quantification framework Uncertainty propagation techniques Application examples

Computational models: the abstract viewpoint

As a result of discretizing and solving the set of equations describing the physics, a computational model is a black-box program that computes quantities of interest as a function of input parameters.



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Inaugural lecture

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Where are the uncertainties?

In order to make the best use of a computational model, assumptions on the values of the input parameters shall be made in order to provide reliable predictions on the system behaviour.

Sources of uncertainty





- What is the exact thickness of the shell?
- What is the value of the concrete strength?
- What is the maximal expected wind velocity?
- Lack of knowledge (epistemic uncertainty)
- Natural variability (aleatory uncertainty)
- Model error (e.g. simplifications)

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Outline



- 2 Uncertainty quantification framework
- Oncertainty propagation techniques
 - Monte Carlo simulation
 - Surrogate models

Application examples

Global framework for uncertainty quantification



Sudret, B. Uncertainty propagation and sensitivity analysis in mechanical models, Habilitation thesis, 12007. 🖌 🗇 + 🗸 🚊 + 🧃 🛓 🔗

Global framework for uncertainty quantification



Sensitivity analysis

Sudret, B. Uncertainty propagation and sensitivity analysis in mechanical models, Habilitation thesis, (2007. 🛛 🗇 🗤 👌 🛓 🗸 🚊 🕨 🖉 🖉

Global framework for uncertainty quantification



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Global framework for uncertainty quantification



Sudret, B. Uncertainty propagation and sensitivity analysis in mechanical models, Habilitation thesis, (2007. 🛛 🗁 🔺 🚊 🕨 🖉

Step B: Quantification of the sources of uncertainty

Experimental data is available

- What does the data look like? descriptive statistics (histograms)
- What is the best probabilistic model? statistical inference

Preliminary analysis: expert judgment

- Engineering judgment (e.g. reasonable bounds)
- Best practices from the literature (i.e. lognormal distributions for material properties)

Scarce data + expert information

• Bayesian inference methods

"Available information + Data \implies Distributions"



Step C/C': Uncertainty propagation and sensitivity analysis

What is the final use of the computational model?

- Understanding a physical phenomenon
 - Parametric study: evolution of the output when one or several parameters vary in a range
 - Sensitivity analysis: detection of the important parameters
 - Calibration of the model w.r.t. available experimental data
- Robust design: variability of the system's performance in operation
- Reliability analysis: probability of non-performance / failure
- (Reliability-based) design optimization

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Monte Carlo simulatior Surrogate models

Outline

Introduction

- 2) Uncertainty quantification framework
- Oncertainty propagation techniques
 - Monte Carlo simulation
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Application examples

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Monte Carlo simulation

Some history

- The idea of random experiments using computers has been introduced by S. Ulam in 1946 to solve neutronics problem
- The name "Monte Carlo simulation" is attributed to John Von Neumann in reference to the casinos in Monaco



Source: www.monaco.mo

Principle

Reproduce numerically the variability of the model parameters using a random number generator



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Monte Carlo simulatior Surrogate models

Monte Carlo simulation for uncertainty propagation

The "Virtual Factory"

Monte Carlo simulation allows the engineer to assess the performance of a large number of virtual systems featuring different realizations of the input parameters.

Bridge Truss structure









Questions

- What is the range of the maximal deflection at midspan?
- How safe is the bridge w.r.t. the admissible deflection?

Sources of uncertainty

- Geometry
- Steel quality
- Applied loads

Monte Carlo simulation Surrogate models

Sample set of the quantity of interest



Monte Carlo simulation Surrogate models

Sample set of the quantity of interest



Monte Carlo simulation Surrogate models

Sample set of the quantity of interest



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Monte Carlo simulation Surrogate models

Sample set of the quantity of interest



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Scattering of the quantity of interest Statistical moments

Monte Carlo simulation provides a sample set of response quantities, say $\mathcal{Y} = \{\mathcal{M}(\boldsymbol{x}_i), i = 1, ..., N_{MCS}\}$ whose statistics may be studied:

• Mean value

$$\hat{\mu} = rac{1}{N_{MCS}}\sum_{i=1}^{N_{MCS}}\mathcal{M}(oldsymbol{x}_i)$$

• Standard deviation

$$\hat{\sigma} = \left[rac{1}{N_{MCS}-1}\sum_{i=1}^{N_{MCS}}\left(\mathcal{M}(oldsymbol{x}_i)-\hat{\mu}
ight)^2
ight]^{1/2}$$

Central trend	1
	$-\mu$

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Scattering of the quantity of interest Distribution analysis



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Monte Carlo simulation Surrogate models

Scattering of the quantity of interest Distribution analysis



Monte Carlo simulatior Surrogate models

Reliability analysis

Computational models can be used to assess the performance of a system w.r.t. some prescribed criterion. (SIA / Eurocodes in civil engineering, FAA regulations in aeronautics, etc.)

A performance function g corresponding to the margin between some quantity of interest and the associated admissible threshold t_{adm} is defined:

$$g(\boldsymbol{x}, \mathcal{M}(\boldsymbol{x})) = t_{adm} - \mathcal{M}(\boldsymbol{x})$$

• In a deterministic design paradigm, the criterion should be fulfilled when using some design value of the input vector, say x_d :

$$oldsymbol{x}_d \longrightarrow g(oldsymbol{x}_d, \, \mathcal{M}(oldsymbol{x}_d)) \longrightarrow \left\{ egin{array}{ccc} > 0 & : & {
m design} \, {
m OK} \ \leq 0 & : & {
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m not} \, {
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ight.$$

• In the world of uncertainty quantification, some realizations of the system may pass the criterion, some other may fail

"Probability of failure"

Monte Carlo simulation Surrogate models

Monte Carlo simulation for reliability analysis

Computational assessment of virtual structures



Monte Carlo simulation Surrogate models

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Monte Carlo simulation for reliability analysis

Computational assessment of virtual structures



Probability of failure

$$\hat{P}_f = \frac{N_{fail}}{N_{MCS}} = \frac{\# \text{ failed systems}}{\# \text{ virtual systems}}$$

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Monte Carlo simulatior Surrogate models

Some features of Monte Carlo simulation

Advantages

- Universal method: only rely upon simulating random numbers ("sampling") and running repeatedly the computational model
- Suited to High Performance Computing: "embarrassingly parallel"
- ullet Sound statistical foundations: convergence when $N_{MCS} \rightarrow \infty$

Drawbacks

- Statistical uncertainty: results are not exactly reproducible when a new analysis is carried out (handled through confidence intervals)
- Low efficiency

Example: suppose $P_f = 0.001$ is to be computed

- At least 1,000 samples are needed in order to observe one single failure (in the mean!)
- $\bullet\,$ About 100 times more ($\it i.e.\,$ 100,000 samples) are required to have a $\pm 10\%$ accuracy

Monte Carlo simulatior Surrogate models

Outline

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Application examples

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Monte Carlo simulation Surrogate models

Surrogate models for uncertainty quantification

A surrogate model $\tilde{\mathcal{M}}$ is an approximation of the original computational model with the following features:

- It is built from a limited set of runs of the original model \mathcal{M} called the experimental design $\mathcal{X} = \{x_i, i = 1, ..., m\}$
- $\bullet\,$ It assumes some regularity of the model ${\cal M}$ and some general functional shape

Name	Shape	Parameters
Polynomial chaos expansions	$ ilde{\mathcal{M}}(oldsymbol{x}) = \sum a_{oldsymbol{lpha}} \Psi_{oldsymbol{lpha}}(oldsymbol{x})$	a_{lpha}
Kriging	$\tilde{\mathcal{M}}(\boldsymbol{x}) = \boldsymbol{\beta}_{m}^{T} \cdot \boldsymbol{f}(\boldsymbol{x}) + Z(\boldsymbol{x}, \omega)$	$oldsymbol{eta},\sigma_Z^2,oldsymbol{ heta}$
Support vector machines	$ ilde{\mathcal{M}}(oldsymbol{x}) = \sum_{i=1} a_i K(oldsymbol{x}_i, oldsymbol{x}) + b$	$oldsymbol{a},b$

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Monte Carlo simulation Surrogate models

Ingredients for building a surrogate model

- Select an experimental design \mathcal{X} that covers at best the domain of input parameters: Latin Hypercube Sampling, low-discrepancy sequences
- \bullet Run the computational model ${\cal M}$ onto ${\cal X}$ exactly as in Monte Carlo simulation
- \bullet Smartly post-process the data $\{\mathcal{X}\,,\,\mathcal{M}(\mathcal{X})\}$ through a learning algorithm

Name	Learning method
Polynomial chaos expansions	sparse grids, regression, LAR
Kriging	maximum likelihood, Bayesian inference
Support vector machines	quadratic programming

• Validate the surrogate model

Monte Carlo simulation Surrogate models

Validation of a surrogate model

• An error estimate allows one to assess the accuracy of a surrogate model built from a given experimental design, *e.g.* the mean-square error:

$$egin{split} arepsilon &= \mathbb{E}\left[\left(\mathcal{M}(oldsymbol{X}) - ilde{\mathcal{M}}(oldsymbol{X})
ight)^2
ight] \ &pprox rac{1}{N_{val}}\sum_{k=1}^{N_{val}}\left[\mathcal{M}(oldsymbol{x}_k) - ilde{\mathcal{M}}(oldsymbol{x}_k)
ight]^2 \end{split}$$

- \bullet For the sake of robustness a validation set that is different from the learning set ${\mathcal X}$ should be used
- Techniques such as the leave-one-out cross-validation or bootstrap may be used to decrease the computational burden

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Monte Carlo simulation Surrogate models

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Uncertainty propagation techniques

Surrogate models

Truss structure

Problem statement



Input: 10 independent random variables

- Bars properties (2 cross-sections, 2 Young's moduli)
- Loads (6 parameters)

Output: maximal deflection

Uncertainty guantification

- Distribution of the maximal deflection?
- Mean value and standard deviation?
- Reliability analysis: $\operatorname{Prob}\left[v \geq \frac{L}{200} = 12 \text{ cm}\right]$?

Blatman, G. Adaptive sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis. Université Blaise Pascal Clermont-Ferrand 2009.

Monte Carlo simulation Surrogate models

Truss structure

	Reference	Monte Carlo	Polynomial chaos
	100,000 runs	3	0 runs
Mean (cm)	7.94	8.02 ± 0.49	7.98
Std. dev. (cm)	1.11	1.36 ± 0.10	1.10



Reliability analysis

	Reference	Polynomial chaos
	100,000 runs	500 runs
10 cm	4.39e-02 \pm 3.0%	$4.30\text{e-}02\pm0.9\%$
11 cm	$8.61\text{e-}03\pm6.7\%$	8.71e-03 \pm 2.1%
12 cm	$1.62\text{e-}03\pm15.4\%$	1.51e-03 \pm 5.1%
13 cm	$2.20\text{e-}04\pm41.8\%$	$2.03\text{e-}04\pm13.8\%$

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Risk analysis for a pressure vessel



Question

What is the probability of crack propagation in a pressure vessel in case of a severe pressurized thermal shock?

Uncertainties

- Size and position of metallurgical defects
- Steel toughness (which depends on the alloy composition)
- Ageing due to irradiation

Conditional probability of crack propagation for different incident scenarios (transients) combined into a global probabilistic safety assessment

Dubourg, V. et al. Échantillonnage préférentiel quasi-optimal par krigeage pour l'évaluation de la fiabilité des cuves de réacteurs, Proc. 7th JN'Eiab Conf., Chambéry (2012) 🚊 🔊 🔍

Natural hazards: performance-based design w.r.t earthquakes





Question

What is the probability of collapse of a building as a function of the "intensity" of a potentiel earthquake?

Uncertainties

- Properties of the structure (material strength, stiffness of the connections, etc.)
- Earthquake magnitude, duration, peak ground acceleration

Non linear transient finite element analysis of the structure for different synthetic earthquakes

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Natural hazards: performance-based design w.r.t earthquakes



- The vulnerability is represented by a fragility curve (probability of attaining some state of damage conditionally on the PGA)
- Seismologists provide models for the PGA w.r.t. the local seismicity (occurrence / magnitude)
- Damage-related costs may be incorporated towards a global risk assessment

Performance-based earthquake engineering

Yang, T., Moehle, J., Stojadinovic, B. & Der Kiureghian, A. Seismic performance evaluation of facilities: methodology and implementation J. Struct. Eng. (ASCE), 2009, 135, 1146-1154.

Sudret, B., Mai, C.V, Computing seismic fragility curves using polynomial chaos expansions, ICOSSAR'2013, New York.

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Durability of concrete structures



(Source: http://www.cement.org)

Questions

- What is the probability of corrosion-induced damage after 20 years of service?
- What is the expected (resp. 95%- quantile) concrete surface that is affected by concrete rebars corrosion due to concrete carbonation (resp. chloride ingress)?



(Source: http://www.structuremag.org)

Uncertainties

- CO₂ (resp. chlorides) diffusion parameters
- Rebars position (concrete cover)
- Corrosion kinetics
- Spatial variability

Sudret, B. Probabilistic models for the extent of damage in degrading reinforced concrete structures Reliab. Eng. Sys. Safety, 2008, 93, 410-422

Indicators for long-term infrastructure management

Durability of concrete structures



(Source: http://www.cement.org)

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- What is the probability of corrosion-induced damage after 20 years of service?
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- Corrosion kinetics
- Spatial variability

Sudret, B. Probabilistic models for the extent of damage in degrading reinforced concrete structures Reliab. Eng. Sys. Safety, 2008, 93, 410-422

Indicators for long-term infrastructure management

Robust design of submarine hulls



Question

How to minimize the volume of a single bay reference structure while ensuring a high reliability level w.r.t buckling failure?

 $\min \mathcal{V}(\boldsymbol{d})$ such that $\mathbb{P}\left(p_{coll}(\boldsymbol{X}, \boldsymbol{d}) < p_{serv}\right) \leq 10^{-k}$



Dubourg, V. Adaptive surrogate models for reliability analysis and reliability-based design optimization, Université Blaise Pascal, Clermont-Ferrand, France, 2011

Robust design of submarine hulls

Uncertainties

- Tolerances in the dimensions / straightness of the stiffeners
- Geometrical imperfections of the shell
- Variability of the material properties (elasto-plastic constitutive laws)

Optimal robust design ensuring a high level of structural reliability





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Dubourg, V. et al. Modélisation probabiliste de champs d'imperfections géométriques de coques résistantes de sous-marins, Proc. 10^e Coll. Nat.Calcul des Structures, Giens, 2011.

Effect of electromagnetic waves onto human bodies

Courtesy J. Wiart (Orange Labs) / PhD A. Ghanmi





- The specific absorption rate (*SAR*) characterizes the energy absorbed by the human body exposed to waves (*e.g.* cellular phones, wifi, etc.)
- Computational dosimetry allows one to estimate the *SAR* for a given "phantom", *i.e.* a computational model of the human body (Maxwell equations solved by FDTD (finite difference in time domain))

$$SAR = \sigma \frac{E^2}{\rho}$$

- E : electric field
- σ : tissues conductivity

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 ρ : mass density

Question

How to assess the variability of the SAR over a population wit different morphology, different phones, different use, etc.?

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Question

How to assess the variability of the $S\!AR$ over a population with different morphology, different phones, different use, etc.?



Effect of electromagnetic waves onto human bodies

Uncertainties

- Morphology of the body (e.g. children vs. adults)
- Posture
- Type of cellular phone / Position of the phone



After Findlay & Dimbylow (2007)

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Estimation of the distribution of SAR within a given population to provide regulating authorities with detailed information

A.Ghanmi et al., Analysis of the influence of the position of the mobile on SAR induced using polynomial chaos decomposition, Proc. XXXth URSI Scientific symposium, 2011.

Conclusion

- Uncertainty quantification has become a hot topic in many (if not all) domains of applied science and engineering
- It is a transdisciplinary field which takes advantage from research progress in the mathematical- (statistics, PDEs), engineering- (civil, mechanical, chemical, etc.) and computer science communities
- Generic analysis tools may be developed and disseminated towards the community "The UQLab platform"
- Good UQ studies rely upon fruitful discussions between the field- and UQ- specialists: scientists and engineers should have a significant education in statistics and probability theory

Future research trends

- More accurate modelling of the input uncertainty in case of statistical dependence (copula theory)
- Progress in surrogate models: parsimonious *vs.* robust models in order to tackle large-scale simulation problems
- Dissemination of good practices towards the engineering community (reduce the mathematical abstraction to the minimum)

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