

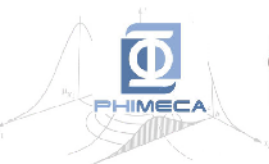
Covariance-based sensitivity indices based on polynomial chaos functional decomposition

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July 3 2013



Robust engineering

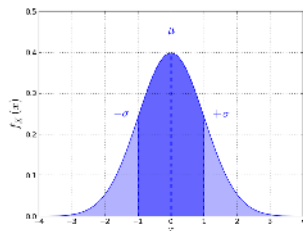
Sources of uncertainty

Uncertainties (environment, mechanical properties of materials, manufacturing tolerances, etc.) that may affect the nominal performance of the system are taken into account.

Uncertainty quantification

Design parameters are modelled by a *random vector* $X \sim F_X(x)$.

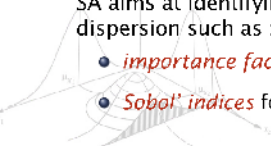
The random response of the system $Y = \mathcal{M}(X)$ is studied.



Sensitivity analysis

SA aims at identifying and prioritize the contributors to the system response dispersion such as :

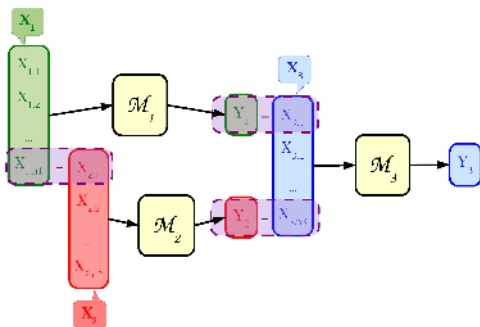
- *importance factors* in reliability analysis (FORM/SORM),
- *Sobol' indices* for the variance decomposition of the system response (ANOVA).



The concern of correlated input parameters

Uncertainty propagation

- The sensitivity of the *final performance* of the system to intermediate parameters is studied.
- Outputs of models with mutual inputs are mathematically *correlated*.
- The *joint distribution* of the intermediate parameters is implicitly defined by the uncertainty propagation in the workflow.

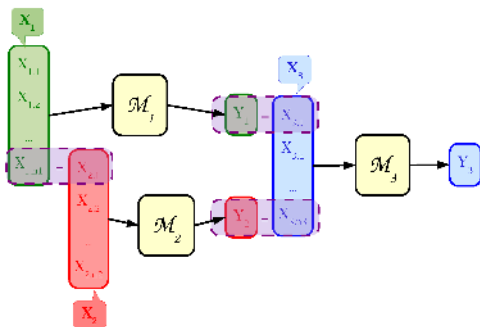


Tools for uncertainty propagation in nested models and associated sensitivity indices must be developed.

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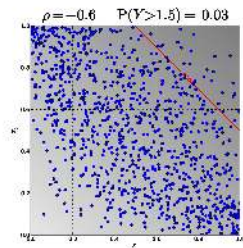
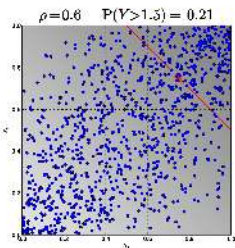
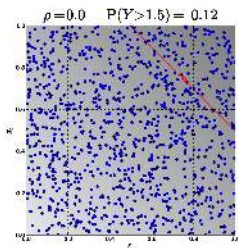
Tools for uncertainty propagation in nested models and associated sensitivity indices must be developed.

Can the correlation be ignored?

When considering the extra work induced by carrying out the copula theory (simulation, estimation), the correlation is often neglected.

Example

The probability that the sum of two random variables $X_i \sim \mathcal{U}[0, 1]$, $i = 1, 2$ exceeds a threshold $t = 1.5$ is studied.

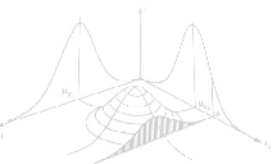


→ The correlation may either represents an *advantage* or a *drawback* for the probability of failure.

• The more the absolute correlation, the less it should be neglected.

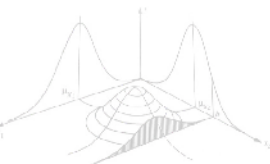
Plan de la présentation

- 1 Global sensitivity analysis
- 2 Applications



Plan de la présentation

- 1 Global sensitivity analysis
 - ANOVA Decomposition
 - ANCOVA Decomposition
 - Estimation of the sensitivity indices
- 2 Applications



Functional decomposition

[Hoeffding (1948)]

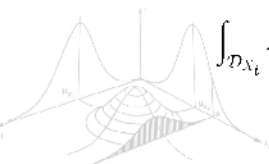
Separation of the effects

Let X be a n -dimensional random vector. The model \mathcal{M} may be uniquely decomposed by a *sum of function of increasing dimension* :

$$\begin{aligned}\mathcal{M}(X) &= \mathcal{M}_0 + \sum_{i=1}^n \mathcal{M}_i(X_i) + \sum_{1 \leq i < j \leq n} \mathcal{M}_{i,j}(X_i, X_j) + \dots + \mathcal{M}_{1,\dots,n}(X_1, \dots, X_n) \\ &= \mathcal{M}_0 + \sum_{\mathbf{u} \subset \{1, \dots, n\}} \mathcal{M}_{\mathbf{u}}(X_{\mathbf{u}})\end{aligned}$$

where \mathcal{M}_0 is a constant and the multi index notation \mathbf{u} stands for a subset of $\{1, \dots, n\}$.

The terms of the decomposition have *zero mean* and *pairwise orthogonal* :



$$\int_{\mathcal{D}_{X_i}} \mathcal{M}_i(x_i) dx_i = 0 \quad \text{et} \quad \int_{\mathcal{D}_X} \mathcal{M}_i(x_i) \mathcal{M}_j(x_j) dx = 0$$

Decomposition of the model output variance [Sobol' (1993)]

ANOVA decomposition

The ANOVA (*ANalysis Of VAriance*) decomposition consists in identifying the *shares of variance* of $Y = \mathcal{M}(X)$ associated to one or more variables.

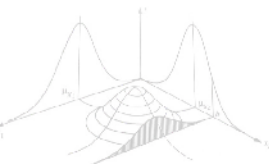
It can be decomposed in the form :

$$\mathbb{V}[Y] = \sum_{\mathbf{u} \subseteq \{1, \dots, n\}} \mathbb{V}[\mathcal{M}_{\mathbf{u}}(X_{\mathbf{u}})]$$

First order sensitivity indices

The *contribution* of a variable X_i to the variance of the model response Y is defined by the first order Sobol' index :

$$S_i = \frac{\mathbb{V}[\mathbb{E}[Y|X_i]]}{\mathbb{V}[Y]} = \frac{\mathbb{V}[\mathcal{M}_i(X_i)]}{\mathbb{V}[Y]}$$



Decomposition of the model output variance [Sobol' (1993)]

2^{nd} order sensitivity indices

The *interaction* between two variables X_i and X_j is described by the 2^{nd} order Sobol' index :

$$S_{i,j} = \frac{\mathbb{V}[\mathbb{E}[Y|X_i, X_j]]}{\mathbb{V}[Y]} - S_i - S_j$$

Total order indices

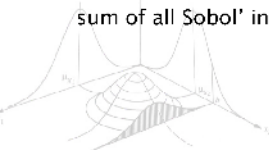
The total order index takes both the *intrinsic contribution* of the variable X_i and its interaction with the other variables $X_{j \neq i}$ into account :

$$S_i^T = S_i + \sum_{j \neq i} S_{i,j} + \sum_{k \neq i,j} S_{i,j,k} + \dots + S_{1\dots n}$$

Unitary sum

When all the interaction orders of the decomposition are taken into account, the sum of all Sobol' indices equals 1, *i.e.* the total variance is completely explicated :

$$\sum_{i=1}^n S_i + \sum_{j \neq i} S_{i,j} + \dots + S_{1\dots n} = 1$$

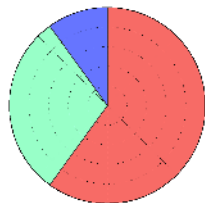


The issue of correlated variables

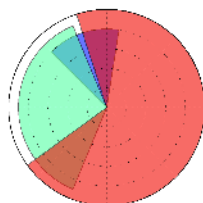
The ANOVA decomposition allows one to explain the total variance of the model response provided the variables are independent.

Problematic

In the presence of correlation between the variables, does the sensitivity of output Y to an input X_i results from its intrinsic contribution in \mathcal{M} or its correlation with another influential variable X_j ?



Independent variables



Correlated variables

Should the two types of contribution be separated?

ANCOVA decomposition

[Li and Rabitz (2010)]

Objectif

Extension of the ANOVA decomposition to the case of correlated variables.

The variance of the model output can be expressed as the *covariance* between Y and its functional decomposition of $\mathcal{M}(X)$:

$$\begin{aligned}
 \mathbb{V}[Y] &= \text{Cov}[Y, Y] \\
 &= \text{Cov} \left[Y, \sum_{i=1}^n \mathcal{M}_i(X_i) + \sum_{1 \leq i < j \leq n} \mathcal{M}_{i,j}(X_i, X_j) + \dots + \mathcal{M}_{1,\dots,n}(X) \right] \\
 &= \text{Cov} \left[Y, \sum_{\mathbf{u} \subseteq \{1,\dots,n\}} \mathcal{M}_{\mathbf{u}}(X_{\mathbf{u}}) \right] \\
 &= \sum_{\mathbf{u} \subseteq \{1,\dots,n\}} \left[\underbrace{\mathbb{V}[\mathcal{M}_{\mathbf{u}}(X_{\mathbf{u}})]}_{\text{ANOVA structural part}} + \underbrace{\text{Cov}[\mathcal{M}_{\mathbf{u}}(X_{\mathbf{u}}), \mathcal{M}_{\bar{\mathbf{u}}}(X_{\bar{\mathbf{u}}})]}_{\text{correlative part, 0 if } R=I} \right]
 \end{aligned}$$

The variability of the model response is decomposed in a first part related to the *model structure* and a second part related to the *dependence structure* of the variables.

ANCOVA sensitivity indices

[Li and Rabitz (2010)]

Separation of the contributions

A triplet of sensitivity indices $\{S_i, S_i^S, S_i^C\}$ is proposed for each variable X_i :

- *Total contribution* index of X_u :


$$S_u = \frac{\text{Cov}[Y, \mathcal{M}_u(X_u)]}{\mathbb{V}[Y]}$$

- *Structural contribution* index of X_u :

$$S_u^S = \frac{\mathbb{V}[\mathcal{M}_u(X_u)]}{\mathbb{V}[Y]}$$

- *Correlative contribution* index of X_u :

$$S_u^C = \frac{\text{Cov}[\mathcal{M}_u(X_u), \mathcal{M}_{\bar{u}}(X_{\bar{u}})]}{\mathbb{V}[Y]}$$



Properties

The ANCOVA indices verify

$$S_u = S_u^S + S_u^C$$

Identification of the components

[Li and Rabitz (2010)]

Challenge

Identifying all the components of the functional decomposition.

Possibilities

1 - Identification using a *projection method* (Monte Carlo estimation of integrals) :

$$\mathcal{M}_0 = \int_{\mathbb{D}_X} \mathcal{M}(\mathbf{x}) d\mathbf{x}, \quad \mathcal{M}_i(x_i) = \int_{\mathbb{D}_{X_{\sim i}}} \mathcal{M}(\mathbf{x}_{\sim i}) d\mathbf{x}_{\sim i} - \mathcal{M}_0, \quad \dots$$

2 - HDMR approach : model decomposition on a *basis of functions* :

- simple polynomials,
- B-splines,
- orthonormal polynomials :

$$\varphi_1(x) = \sqrt{3}(2x - 1), \quad \varphi_2(x) = 6\sqrt{5}(x^2 - x + \frac{1}{6}), \quad \dots$$



Didactic example

Polynomial model

$$Y = \mathcal{M}(X) = X_1 + X_2 + X_2^2 + X_1X_2 + 3$$

with $X_i \sim \mathcal{N}(0, 1)$, $i = 1, 2$ et $R_{12} = \rho_S$.

Functional decomposition $\mathcal{M}(X) = \underbrace{\mathcal{M}_0}_{3} + \underbrace{\mathcal{M}_1(X_1)}_{X_1} + \underbrace{\mathcal{M}_2(X_2)}_{X_2 + X_2^2} + \underbrace{\mathcal{M}_{1,2}(X_1, X_2)}_{X_1X_2}$

ρ_S	0.0	S_i	S_i^S	S_i^C	
		X_1	0.20	0.20	0.00
		X_2	0.60	0.60	0.00
		$X_{1,2}$	0.20	0.20	0.00
		Σ	1.00	1.00	0.00

ρ_S	0.8	S_i	S_i^S	S_i^C	
		X_1	0.19	0.10	0.09
		X_2	0.52	0.29	0.23
		$X_{1,2}$	0.29	0.14	0.15
		Σ	1.00	0.53	0.47

The independent case corresponds to the ANOVA (Sobol' indices).
The correlated case exhibits the sensitivities of Y to the correlations.

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Metamodelling

Objectif

Substitute the physical model numerically expensive to evaluate with a mathematical representation referred to as *metamodel* (or response surface).

Design of experiments

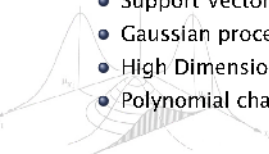
The metamodel $\widehat{\mathcal{M}}$ is built from a *finite number* of calls to the physical model \mathcal{M} that constitute the DOE \mathcal{D} .

It is evaluated on N -sample of randomly generated points (MCS, LHS, LCVT).

$$\mathcal{D} = \{ \mathbf{x}^{(k)}, y^{(k)} = \mathcal{M}(\mathbf{x}^{(k)}), k = 1, \dots, N \}$$

Types of metamodels

- Support Vector Regression,
- Gaussian process metamodels (*Kriging*),
- High Dimensional Model Representation,
- Polynomial chaos expansions.



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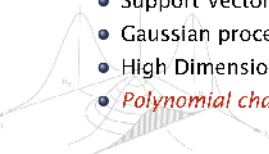
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- Gaussian process metamodels (*Kriging*),
- High Dimensional Model Representation,
- *Polynomial chaos expansions*.

Motivations :

- numerical efficiency
- separation of the effects



Polynomial chaos expansions

[Ghanem and Spanos (2003)]

Principle

Expansion of the random response Y of the model on a *orthonormal polynomial basis* selected according to the distribution of the input variables.

$$Y = \sum_{j=0}^{-\infty} a_j \Psi_j(\mathbf{X})$$

with :

Ψ_j base des polynômes de chaos, e.g. $\Psi_j(\boldsymbol{\xi}) = \prod_{i=1}^n He_i^j(\xi_i)$

(multivariate Hermite polynomials for Gaussian variables)

a_j Coefficients of the expansion to be determined

Truncature of the basis

The expansion converges to the response when the size of the basis tends to ∞ .

In practice, it is usually truncated to a *degree p* so that :

$$Y \approx \sum_{|\alpha| \leq p} a_\alpha \Psi_\alpha(\mathbf{X}), \quad \alpha \in \mathbb{N}^n$$



Estimation of the ANCOVA indices

Proposed methodology

- Functional decomposition :
Analytical expression of the components by *identification* of linear combinations of multivariate polynomials :

$$\mathcal{M}_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) \equiv \sum_{\{\alpha_i > 0\} \subset \mathbf{u}} a_{\alpha} \Psi_{\alpha}(\mathbf{X})$$

Example with $n = 5$:

$\mathbf{u} = \{1, 2, 4\}$ corresponds to $\alpha = \{\alpha_1, \alpha_2, 0, \alpha_4, 0\}$ with $\alpha_{1,2,4} \in \mathbb{N}^*$

- Evaluation of the variances and covariances :
Evaluation of the basis multivariate polynomials on a sample \mathbf{X} from the joint distribution of the inputs.

$$\mathbf{y} = \{\mathbf{y}_j = \Psi_j(\mathbf{X}), j = 0, \dots, P - 1\}$$

Estimation of the variances and covariances of *linear combinations* of the columns of \mathbf{y} ($N \times P$).



Estimation of the ANCOVA indices

Orthogonality of the basis

- The orthogonality of the basis is satisfied provided the variables are independent.
 - If the components are independent, then the covariances are zero.

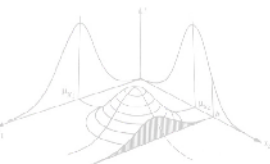
Proposition

- ① Building the expansion using the joint distribution X featuring an *independent copula* $C_{I_{n \times n}}$ in order to preserve the orthogonality of the functional decomposition.
- ② Simulating realizations of the joint distribution X featuring the *real copula* of the input random vector for the estimation of the covariances.

The polynomial chaos expansions is used here as a response surface providing the sought functional decomposition.

Plan de la présentation

- 1 Global sensitivity analysis
- 2 **Applications**

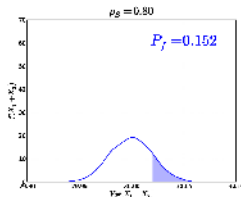
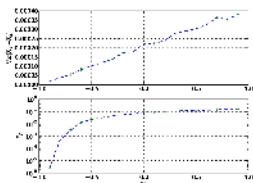


Interpretation - A tolerancing problem

Let us consider a distance Y as the sum of two distances X_1 and X_2 machined by the same CNC unit :

$$Y = X_1 + X_2 \quad X_1 \sim \mathcal{N}(10, 0.01) \quad X_2 \sim \mathcal{N}(20, 0.01) \quad \rho_S(X_1, X_2)$$

The probability that Y exceeds a threshold $t = 30.02$ is studied.



	S_i	S_i^S	S_i^C
X_1	0.50	0.27	0.23
X_2	0.50	0.27	0.23
Σ	1.00	0.54	0.46

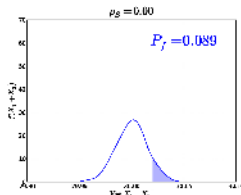
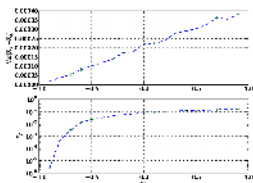
The negative correlative contribution indices mean a reduction in the variance response due to the correlation.

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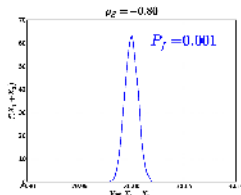
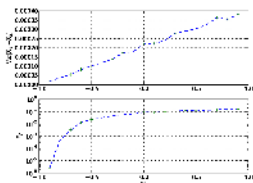
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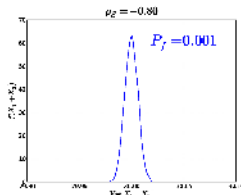
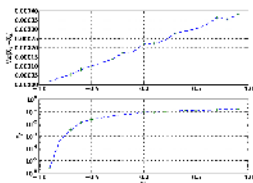
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Industrial application

Diesel engine



Spontaneous ignition due to high pressure (volume ratio 20 :1) and temperature (over 900°C).

Common rail : pressure up to 2000 bars

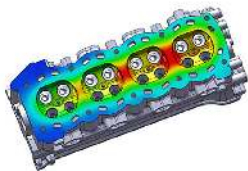
Compromise performance / reliability / pollution / noise / costs

Cylinder head

Fatigue resistance of the weak points (fireface, bridge)

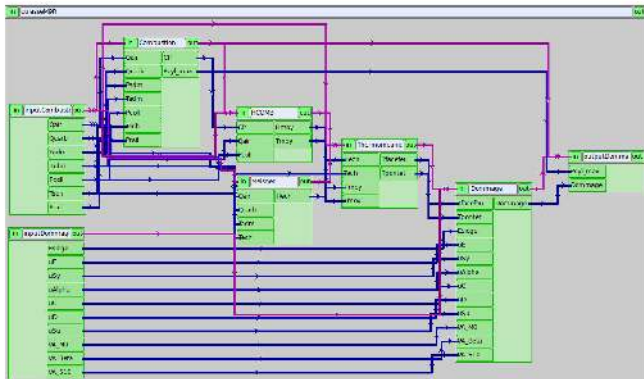
Damage explained by a *complex physics* (thermomechanical stress).

Mechanical, thermal and fatigue mechanisms modelled by *seperated softwares*.



Nested modelling of the system

Nested modelling scheme

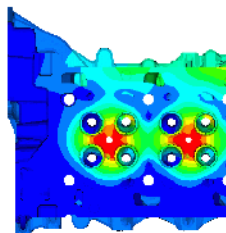


- 17 input variables, 7 output variables, 5 physical models,
- Expansion of order $p = 4$, 7×5985 coefficients to be determined, DOE of size $N = 10^4$.

Results

Sensitivity of the temperature in the cylinder head

Temperatures of the fireface and bridge



Paramètre	S	S^U	S^C
H_{ech}	1.17	1.83	-0.67
T_{ech}	0.09	0.07	0.01
H_{moy}	-0.01	0.01	-0.03
T_{moy}	-0.24	0.29	-0.53
Σ	1.00	2.21	-1.21

$$\rho_S = \begin{vmatrix} 1 & 0 & -0.54 & -0.81 \\ 0 & 1 & 0 & 0.05 \\ -0.54 & 0 & 1 & 0.92 \\ 0.81 & 0.05 & 0.92 & 1 \end{vmatrix}$$

→ The exhaust *heat transfer coefficient* H_{ech} and the mean temperature T_{moy} are the most influent contributors to the dispersion in the temperatures.

• The *negative correlation* between H_{ech} and T_{moy} tends to lower the total variance.

Results

Sensitivity of the damage of the cylinder head

Degradation of the physical properties that may lead to the cracking of the cylinder head.



Paramètre	S	S^U	S^C
T_{face}	0.02	0.01	0.01
T_{pontet}	0.02	0.01	0.01
E_{sieg}	0.00	0.00	0.00
u_E	0.00	0.00	0.00
u_{S_y}	0.00	0.00	0.00
u_α	0.00	0.00	0.00
u_C	0.00	0.00	0.00
u_D	0.00	0.00	0.00
u_{S_u}	0.02	0.02	0.00
$V_{A_{MO}}$	0.20	0.20	0.00
$V_{A_{Beta}}$	0.12	0.12	0.00
$V_{A_{S10}}$	0.00	0.00	0.00
Σ	0.38	0.36	0.02

- The main contributors to the dispersion of the damage are the *fatigue parameters* whose c.o.v. is high *because hard to determine*.
- The *low* sum of the first order indices (0.38) indicates that *strong* interactions resulting from a complex physics exist.

Conclusion & Perspectives

Conclusion

- 1 The issue of global sensitivity analysis with *correlated input variables* is addressed.
- 2 The ANalysis Of COVariance represents a *generalization of the ANOVA*.
- 3 This technique allows one to distinguish the *structural contribution* from the *correlative contribution*.
- 4 The indices can be computed using *polynomial chaos expansions*.
- 5 The *interpretation* of indices may be tricky (negative indices, indices > 1 , etc.).

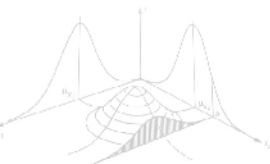
Perspectives

- 1 Define *total indices* (correlative and interactive contribution are mixed).
- 2 Find a way to *normalize* the indices when the correlated variance is less than the independent variance.



End of the presentation

Thank you for your attention.



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