Polynomial Chaos Expansion for Uncertainties Quantification and Sensitivity Analysis

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Introduction

Uncertainties quantification in numerical simulation by Polynomial Chaos expension is a technic which has been used recently for numerous problems.
This method can also be used in global sensitivity analysis by the approximation of sensitivity indices.

Plan

1. Polynomial Chaos expansion
   - Polynomial Chaos
   - Intrusive method : Galerkin projection
   - Non-intrusive methods
     - Least square approximation
     - Non Intrusive Spectral Projection
2. Uncertainty and sensitivity analysis by PC
   - Uncertainty analysis
   - Sensitivity Analysis
     - Sobol decomposition of the PC surrogate model
     - Sensitivity indices
     - Examples
3. Application : Advection-dispersion

Polynomial Chaos expansion

Polynomial Chaos

Polynomial Chaos (PC) expansions of (2nd order) stochastic processes :

$$y(x,t,\theta) = \sum_{k=0}^{\infty} \beta_k(x,t)\Psi_k(\xi(\theta)) \quad \text{(Wiener 1938)}.$$

Application to uncertainty quantification by Ghanem and Spanos.

- $\xi = (\xi_1, \xi_2, \ldots, \xi_d)$ a set of d independent second order random variables with given joint density $p(\xi) = \prod p_i(\xi_i)$.
- $(\Psi_k(\xi))_{k\in\mathbb{N}}$ multidimensional orthogonal polynomials with regard to the inner product (mathematical expectation) $< \Psi_k, \Psi_l > \equiv \int \Psi_k(\xi)\Psi_l(\xi)p(\xi)d\xi = \delta_{kl}||\Psi_k||^2$.

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Polynomial Chaos

$$y(x,t,\xi) = \sum_{k=0}^{\infty} \beta_k(x,t)\Psi_k(\xi),$$

where $\beta_k(x,t)$ are the PC coefficients or stochastic modes of y.

Knowledge of the β_k fully characterizes the process y.

For practical use, truncature at polynomial order no :

$$P+1 = \frac{(d+no)!}{d!no!} \quad \Rightarrow y(x,t,\xi) \approx \sum_{k=0}^{P} \beta_k(x,t)\Psi_k(\xi).$$

- Fast increase of the basis dimension P according to no.
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Intrusive method : Galerkin projection

Galerkin projection

A two steps procedure to solve spectral problems :

- The introduction of the truncated spectral expansions into model equations.
- Determination of the PC coefficients such that the residual is orthogonal to the basis.

$$\mathcal{M}(y; D(\theta)) = 0 \Rightarrow \left\langle \mathcal{M}(\sum_i \beta_i \Psi_i(\xi(\theta)); D(\theta)), \Psi_k(\xi(\theta)) \right\rangle = 0 \quad \forall k.$$

Comments :

$\star$ A set of $P+1$ coupled spectral problems.

$\star$ Require rewriting / adaptation of existing codes.

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Non-intrusive methods

- Construction of a sample set $\{\xi^{(i)}\}$ of ξ and corresponding set of deterministic solutions $\{y^{(i)} = y(x, t, \xi^{(i)})\}$.
- Use the solution set to estimate/compute the PC coefficients β_k.

Comments :

$\oplus$ Solve a (large) number of **deterministic** problems.
$\oplus$ Transparent to non linearities.
$\ominus$ Convergence with the sample set dimension and error estimation.

Currently we use two different non-intrusive methods :

- Least square approximation of the β_k.
- Non Intrusive Spectral Projection (NISP).

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Least square approximation

Least square problem for a sample sets $\mathcal{B} = (\xi^{(i)})$ and $\mathbf{y} = (y^{(i)})$.

$$\hat{\beta}^R(\mathcal{B}) = (Z^T Z)^{-1} Z^T \mathbf{y}$$

where $Z^T Z$ is the Fisher matrix :

$$Z = \begin{pmatrix} 1 & \Psi_1(\xi^{(1)}) & \dots & \Psi_P(\xi^{(1)}) \\ 1 & \Psi_1(\xi^{(2)}) & \dots & \Psi_P(\xi^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \Psi_1(\xi^{(n)}) & \dots & \Psi_P(\xi^{(n)}) \end{pmatrix}$$

Open questions :

- Selection of the sample set ?
- Design Optimal Experiment, active learning ?
- Error estimation ?
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Non Intrusive Spectral Projection : NISP

- Exploit orthogonality of the PC basis :

$$\beta_k = \frac{\langle y(\xi), \Psi_k(\xi) \rangle}{\langle \Psi_k^2 \rangle}, \quad \langle y(\xi), \Psi_k \rangle = \int_\Omega y(\xi)\Psi_k(\xi)pdf(\xi)d\xi.$$

- Numerical integration :

$$\int_\Omega y(\xi)\Psi_k(\xi)pdf(\xi)d\xi \approx \sum_{i=1}^{N} y(\xi^{(i)})\Psi_k(\xi^{(i)})w^{(i)} = \hat{\beta}_k \langle \Psi_k^2 \rangle,$$

with $\xi^{(i)}$ and $w^{(i)}$ are integration quadrature points / weights.

⊕ Independent computation of the PC coefficients.
⊖ Curse of dimension (cubature formula, adpative construction, Monte-Carlo, . . .)

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Uncertainty and sensitivity analysis by PC

Uncertainty analysis

Uncertainty analysis from PC coefficients is immediate :

- The expectation and the variance of the process are given by $E\{y(x,t)\} = \beta_0(x,t)$ and $E\{(y(x,t) - E\{y(x,t)\})^2\} = \sum_{k=1}^{\infty} \beta_k^2(x,t)||\Psi_k||^2$.
- Higher moments too.
- Fractiles and density estimation can be calculated by Monte-Carlo simulations of the PC surrogate model

$$y(x,t,\xi) \approx \sum_{k=0}^{P} \beta_k(x,t)\Psi_k(\xi)$$

(only polynomials to be computed : not the full model).

Global Sensitivity Analysis

The computation of sensitivity indices from PC coefficients is also immediate.

Indeed we know exactly the Sobol decomposition of the PCs.

So thanks to **orthogonality** of the basis and **linearity** of the PC expansion one can immediately deduce the Sobol decomposition of the PC expansion.

Sobol decomposition of the PC surrogate model

- For each integrable function f, there is a unique decomposition :

$$f(\xi) = \sum_{u \subseteq \{1,2,\ldots,d\}} f_u(\xi_u), \quad (Sobol 1993)$$

with $f_\emptyset = f_0$.

- The Sobol decomposition of a troncated PC expansion $\hat{y}$ is,

$$\hat{y}(\xi) = \sum_{u \subseteq \{1,2,\ldots,d\}} \hat{y}_u(\xi_u) = \sum_{k=0}^{P} \hat{\beta}_k \Psi_k(\xi)$$

- The terms of the decomposition are

$$\hat{y}_u(\xi_u) = \sum_{k \in K_u} \hat{\beta}_k \Psi_k(\xi)$$

with $K = \{0, 1, ..., P\}$, $K_u := \{k \in K | \Psi_k(\xi) = \Psi_k(\xi = \xi_u)\}$
and $\hat{y}_\emptyset = \hat{\beta}_0 \Psi_0$

Sensitivity indices

Sensitivity indices are calculated with the formula

$$S_u = \frac{\sigma_u^2}{\sigma_{\hat{y}}^2}$$

Where $\sigma_{\hat{y}}^2$ is

$$\sigma_{\hat{y}}^2 = \sum_{u \subseteq \{1,2,\ldots,d\} \setminus \emptyset} \sigma_u^2$$

and σ_u^2 are explicits for PC expansions

$$\sigma_u^2 = \int \hat{y}_u^2(\xi) p(\xi) d\xi = \sum_{k \in K_u} \hat{\beta}_k^2 ||\Psi_k||^2$$

Example : Homma-Saltelli

$$f(\xi) = sin(\xi_1) + 7sin^2(\xi_2) + 0.1\xi_3^4 sin(\xi_1) \ .$$

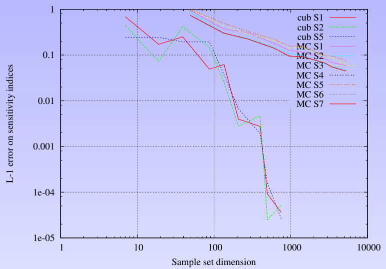
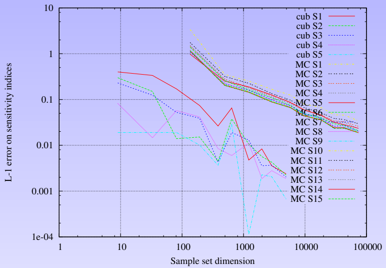


FIG.: L-1 error sensitivity indices computed by PC coefficients and Monte-Carlo simulation vs. the sample set dimension

- β_k computed by NISP using Smolyak cubature.
- The figure shows the expectation of the error on the computation by Monte-Carlo over 100 simulations.

Example : Saltelli-Sobol, non smooth function

$$g(\xi) = \prod_{i=1}^{p}(|4\xi_i - 2| + a_i)/(1 + a_i), a_i = (i-1)/2, p = 5 \ .$$



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Application : Advection-dispersion in a porous media

Equation of advection-dispersion

$$(1+R)\theta\frac{\partial C}{\partial t}(z,t) = -\frac{\partial}{\partial z}\left(qC(z,t) - \theta(D_0 + \lambda|q|)\frac{\partial C}{\partial z}(z,t)\right),$$

(+ Initial and boundary conditions).

Deterministic input

- $R \geq 0$ decay rate,
- q Darcy velocity,
- $\theta \in]0,1]$ porosity,
- D_0 mol. diffusivity.

Input uncertainties

λ hydrodynamic dispersion coefficient :

$$\lambda = a\theta^b,$$

where a and b random

$$log(a) \sim \mathcal{U}([10^{-4}, 10^{-2}]), \quad b \sim \mathcal{U}([-3.5, -1]).$$

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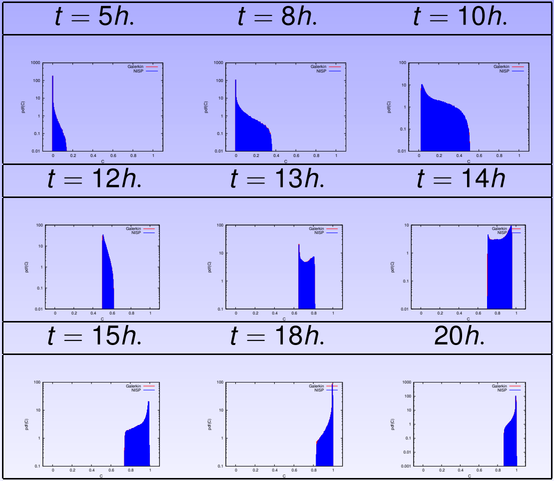

FIG.: Comparison between pdf of the concentration at $x = 0.5$ for different times obtained by Galerkin and NISP ($no = 6$).

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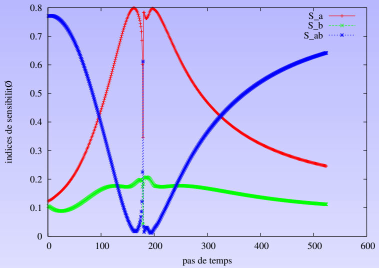

FIG.: Sensitivity indices computed thanks to the PC coefficients computed vs. time

Conclusion

Summary

- Alternative techniques (intrusive / non-intrusive) available for practicle determination of PC coefficients ;
- PC expansion contains a great deal of information in a convenient compact format ;
- Global sensitivity analysis proceeds immediately from PC expansion ;
- Limited to low-moderate dimensionality of the input uncertainty ;
- Issues in application to non-smooth processes (remedy : use non-smooth basis).

Conclusion

Perspectives

- Improvement of non-intrusive methods (development of efficient adaptive quadrature techniques, automatic enrichment of sample sets using active learning techniques) ;
- Reduced basis approximation ;
- Application to industrial problems ;
- Application to identification and optimization problems.