Polynomial Chaos Expansion for Uncertainties Quantification and Sensitivity Analysis

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Introduction

A mathematical model,

$$\mathcal{M}(y; D) = 0$$

Objective : propagate uncertainty input $D(\theta)$ in the model,

$$\mathcal{M}(y(\theta); D(\theta)) = 0$$

$\longrightarrow$ characterize $y(\theta)$.

Uncertainties quantification in numerical simulation by Polynomial Chaos expansion is a technic which has been used recently for numerous physical models(elasticity, thermic, fluid mechanics,...).

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Polynomial Chaos expansion

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

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

- $\xi = (\xi_1, \xi_2, \ldots)$ a set of 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 $< \Psi_k, \Psi_l > \equiv \int \Psi_k(\xi)\Psi_l(\xi)p(\xi)d\xi = \delta_{kl}||\Psi_k||^2$.

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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 DETERMINISTIC 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 and number of random variables d :

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

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

Galerkin projection

A three steps procedure to solve spectral problems :

- Parametrization of the input data $D(\theta) \rightarrow D(\boldsymbol{\xi}(\theta))$.
- The introduction of the truncated spectral expansions into model equations.
- Determination of the PC coefficients such that the residual is orthogonal to the basis.

$$\mathcal{M}(y(\theta); D(\theta)) = 0 \Rightarrow \left\langle \mathcal{M}\left(\sum_{i=0}^{P} \beta_i \Psi_i(\boldsymbol{\xi}(\theta)); D(\boldsymbol{\xi}(\theta))\right), \Psi_k(\boldsymbol{\xi}(\theta)) \right\rangle = 0 \quad \forall k \in [0, p].$$

Comments :

⋆ A set of $P+1$ coupled spectral problems.

⋆ Require rewriting / adaptation of existing codes.

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II Non-intrusive methods

Principle

- Parametrization of the input data $D(\theta) \rightarrow D(\xi(\theta))$.
- Construction of a sample set $\{\xi^{(i)}\}$ of ξ and corresponding set of $\{y^{(i)}\}$ deterministic solutions of $\mathcal{M}(y^{(i)}; D(\xi^{(i)})) = 0$.
- Use the solution set to estimate/compute the PC coefficients β_k.

Comments :

$\oplus$ Solve a (large) number of independent **deterministic** problems.

$\oplus$ Transparent to non linearities.

$\ominus$ Slow convergence with the sample set dimension .

Currently we use two different non-intrusive methods to estimate the PC coefficients :

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

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Least square approximation

$$Z = \begin{pmatrix} \Psi_0(\xi^{(1)}) & \Psi_1(\xi^{(1)}) & \dots & \Psi_P(\xi^{(1)}) \\ \Psi_0(\xi^{(2)}) & \Psi_1(\xi^{(2)}) & \dots & \Psi_P(\xi^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_0(\xi^{(n)}) & \Psi_1(\xi^{(n)}) & \dots & \Psi_P(\xi^{(n)}) \end{pmatrix}, \quad \hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_P \end{pmatrix}$$

Least square problem for a sample set $(\xi^{(i)})$ and $\mathbf{y} = (y^{(i)})$

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

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

Sample set is constructed by SRS, LHS, ...

Non Intrusive Spectral Projection : NISP

- Exploit orthogonality of the PC basis :

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

- d-dimensional numerical integration :

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

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

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$\ominus$ Curse of dimension $\longrightarrow$ sparse grid, adaptive construction, ...

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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 $E\{(y(x,t) - E\{y(x,t)\})^2\} \approx \sum_{k=1}^{P} \beta_k^2(x,t)||\Psi_k||^2$.
- Fractiles and density estimation can be calculated by Monte-Carlo simulations of the PC model

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

(PC expansion use as a surrogate model).

Sensitivity indices

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 $f_\emptyset = f_0$.
Sensitivity indices are calculated with the formula

$$S_u = \frac{\sigma_u^2}{\sigma_f^2}$$

Where σ_f^2 is

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

and σ_u^2 are

$$\sigma_u^2 = \int f_u^2(\xi) p(\xi) d\xi$$

Computation of Sobol indices by PC expansion

Thanks to **orthogonality** of the basis and **linearity** of the PC expansion, there is a simple relation between Sobol indices and PC coefficients.

Moreover we know exactly the Sobol decomposition of the PCs.

Computation of Sobol indices by PC expansion

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

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

- 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 $\hat{y}_\emptyset = \hat{\beta}_0 \Psi_0$

- 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 : Ishigami

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

- Sensitivity indices computed from PC expansion by NISP using Smolyak cubature(Petras's library).
- Sensitivity indices estimated by Monte-Carlo simulations (LHS).

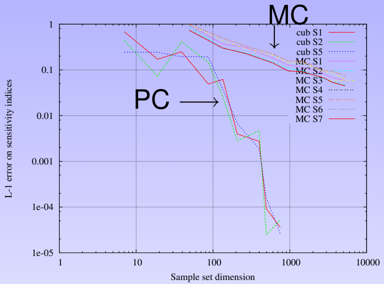

FIG.: L-1 on error sensitivity indices computed by PC coefficients and Monte-Carlo simulation (average over 100 LHS realisations) vs. the number of model evaluations

Example : g-function, 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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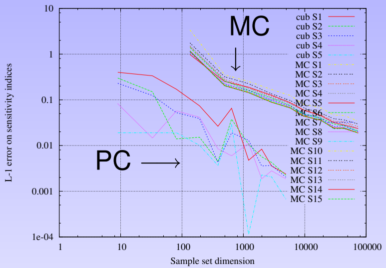

FIG.: L-1 on error sensitivity indices computed by PC coefficients and Monte-Carlo simulation (average over 100 LHS realisations) vs. the number of model evaluations

Application : Nuclear waste disposal

Mathematical Model

Modelisation of the radio-nucleides concentration $y(x,t)$ by an equation of advection-dispersion,

$$(1+R)\phi\frac{\partial y}{\partial t}(x,t) = -\frac{\partial}{\partial x}\left(qy(x,t) - \phi(D_0+\lambda|q|)\frac{\partial y}{\partial x}(x,t)\right),$$

(+ Initial and boundary conditions).

Deterministic input

- $R \geq 0$ decay rate,
- q Darcy velocity,
- $\phi \in]0,1]$ saturation in fluid,
- D_0 mol. diffusivity.

Input uncertainties

λ hydrodynamic dispersion coefficient :

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

where a and b are uncertain

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

Results from PC expansion - I

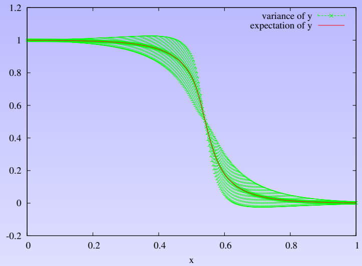

FIG.: Expectation and variance of the process concentration $y(x, t = 12h)$.

Results from PC expansion - II

Time evolution of sensitivity indices for the process concentration $y(x = 0.5, t)$

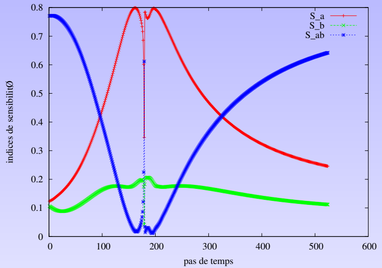

FIG.: Sensitivity indices, $S_u(x = 0.5, t)$, computed thanks to the PC coefficients.

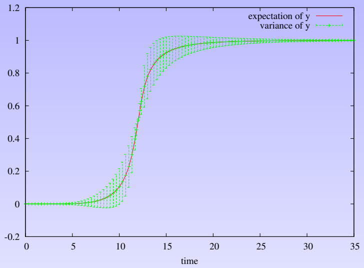

FIG.: Expectation and variance of the concentration $y(x = 0.5, t)$.

$$S_a(x = 0.5, t) + S_b(x = 0.5, t) + S_{ab}(x = 0.5, t) = 1.$$

Results from PC expansion - III

Time evolution of the pdf for the concentration $y(x = 0.5, t)$

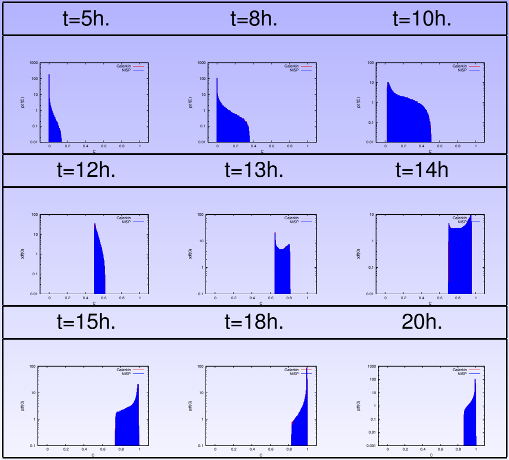

FIG.: Pdf of the concentration $y(x = 0.5, t)$ (PC degree = 6).

Conclusion

Summary

- PC expansion contains a great deal of information in a convenient compact format ;
- Global sensitivity analysis proceeds immediately from PC expansion ;
- Alternative techniques (intrusive / non-intrusive) available for practicle determination of PC coefficients ;
- 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 NISP method by the development of efficient adaptive sparse grid technics ;
- Automatic enrichment of sample sets using active learning technics ;
- Reduced basis approximation for high dimensional problems ;
- Application to industrial problems ;