Sensitivity analysis with generalized chaos expansion

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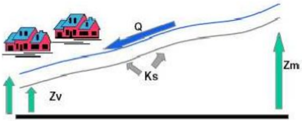
Updated slide show, following talks at SAMO 2019 conference, and at INRAE seminars. Thanks to all the participants for their feedback!

An illustrative case study



A simplified flood model [Iooss, 2011], [Iooss and Lemaitre, 2015].

- Output: cost (in million euros) of the damage on the dyke

$$Y = \mathbb{1}_{S>0} + \left[0.2 + 0.8\left(1 - \exp^{-\frac{1000}{S^4}}\right)\right]\mathbb{1}_{S\leq 0} + \frac{1}{20}\left(H_d \mathbb{1}_{H_d>8} + 8\mathbb{1}_{H_d\leq 8}\right)$$

where H is the maximal annual height of the river (in meters), and S is the maximal annual overflow (in meters)

$$S = Z_v + H - H_d - C_b \quad \text{with} \quad H = \left(\frac{Q}{BK_s\sqrt{\frac{Z_m - Z_v}{L}}}\right)^{0.6}$$

An illustrative case study

- 8 inputs variables assumed to be independent r.v., with distributions:

Input	Description	Unit	Probability distribution
$X_1 = Q$	Maximal annual flowrate	m^3/s	Gumbel $\mathcal{G}(1013, 558)$, truncated on $[500, 3000]$
$X_2 = K_s$	Strickler coefficient	-	Normal $\mathcal{N}(30, 8^2)$, truncated on $[15, +\infty[$
$X_3 = Z_v$	River downstream level	m	Triangular $\mathcal{T}(49, 50, 51)$
$X_4 = Z_m$	River upstream level	m	Triangular $\mathcal{T}(54, 55, 56)$
$X_5 = H_d$	Dyke height	m	Uniform $\mathcal{U}[7, 9]$
$X_6 = C_b$	Bank level	m	Triangular $\mathcal{T}(55, 55.5, 56)$
$X_7 = L$	River stretch	m	Triangular $\mathcal{T}(4990, 5000, 5010)$
$X_8 = B$	River width	m	Triangular $\mathcal{T}(295, 300, 305)$

The aim

The aim is to quantify the influence of the 8 inputs $X = (X_1, \ldots, X_8)$ on the output $Y = h(X) \Rightarrow$ **Global sensitivity analysis**

Specificities:

- h is costly-to-evaluate
- The gradient of h is provided (or easy-to-compute)

Summary

1. With polynomial chaos, i.e. tensor of orthonormal polynomials, (total) Sobol indices are infinite sums of squares of coefficients
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Summary

1. With polynomial chaos, i.e. tensor of orthonormal polynomials, (total) Sobol indices are infinite sums of squares of coefficients
   - *Sharp lower bounds are obtained by truncation* (with equality cases)
2. The same is true for general tensors of orthonormal functions
   - *Generalized chaos expansion*
3. When derivatives are available, we choose the orthonormal basis as the eigenfunctions of the Poincaré differential operator (PDO)
   - *PDO expansion*
   - *Sobol indices lower bounds are immediately rewritten with derivatives*

Part I

Context and notations

Sobol-Hoeffding decomposition

Framework. $X = (X_1, \ldots, X_d)$ is a vector of independent input variables with distribution $\mu_1 \otimes \cdots \otimes \mu_d$, and $h : \Delta \subseteq \mathbb{R}^d \to \mathbb{R}$ is such that $h(X) \in L^2(\mu)$.

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Theorem [Hoeffding, 1948, Efron and Stein, 1981, Sobol', 1993]

There exists a unique expansion of h of the form

$$h(X) = h_0 + \sum_{i=1}^{d} h_i(X_i) + \sum_{1 \leq i < j \leq d} h_{i,j}(X_i, X_j) + \cdots + h_{1,\dots,d}(X_1, \dots, X_d)$$

such that $E[h_I(X_I)|X_J] = 0$ for all $I \subseteq \{1, \dots, d\}$ and all $J \subsetneq I$.

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such that $E[h_I(X_I)|X_J] = 0$ for all $I \subseteq \{1, \ldots, d\}$ and all $J \subsetneq I$. Moreover:

$$\begin{aligned} h_0 &= \mathbb{E}[h(X)] \\ h_i(X_i) &= \mathbb{E}[h(X)|X_i] - h_0 \\ h_I(X_I) &= \mathbb{E}[h(X)|X_I] - \sum_{J \subsetneq I} h_J(X_J) \qquad \text{(recursion)} \\ &= \sum_{J \subseteq I} (-1)^{|I|-|J|} \mathbb{E}[h(X)|X_J] \qquad \text{(inclusion-exclusion)} \end{aligned}$$

Variance decomposition

- The non-overlapping condition

$$\mathbb{E}[h_I(X_I)|X_J] = 0 \quad \text{for all} \quad J \subsetneq I$$

avoids one term to be considered as a more complex one.

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- It implies that *$h_I(X_I)$ is orthogonal to $L^2(X_J)$ such that $J \cap I \subsetneq I$*:

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In particular *the decomposition is orthogonal (ANOVA)*:

$$D := \mathrm{Var}(h(X)) = \sum_{I \subseteq \{1,\dots,d\}} \mathrm{Var}(h_I(X_I))$$

Sensitivity indices

Sobol indices

- Partial variances: $D_I = \mathrm{Var}(h_I(X_I))$, and *Sobol indices* $S_I = D_I/D$

$$D = \sum_I D_I, \qquad 1 = \sum_I S_I$$

- $D_i^{\text{tot}} = \sum_{J \supseteq \{i\}} D_J$, $\quad S_i^{\text{tot}} = \frac{D_i^{\text{tot}}}{D}$ *Total index*
- $D_I^{\text{tot}} = \sum_{J \supseteq \{I\}} D_J$, $\quad S_I^{\text{tot}} = \frac{D_I^{\text{tot}}}{D}$ *Total interaction, superset importance*

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Derivative Global Sensitivity Measure (DGSM)

$$\nu_i = \int \left(\frac{\partial h(x)}{\partial x_i} \right)^2 d\mu(x), \qquad \nu_I = \int \left(\frac{\partial^{|I|} h(x)}{\partial x_I} \right)^2 d\mu(x)$$

Usage for screening

Assume that:

- h is continuous on $\Delta = [0, 1]^d$
- for all i, the support of μ_i contains $[0, 1]$

- **Variable screening**
  If either $D_i^{tot} = 0$ or $\nu_i = 0$, then X_i is non influential

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- **Interaction screening**
  If either $D_{i,j}^{tot} = 0$ or $\nu_{i,j} = 0$, then $(x_i, x_j) \mapsto h(x)$ is additive

  Total interactions can be visualized on the *FANOVA graph*, where the edge size is proportionnal to the index value.

Illustration on a toy example

8D g-Sobol function, with uniform inputs on $[0, 1]$:

$$h(x) = \prod_{j=1}^{8} \frac{|4x_j - 2| + a_j}{1 + a_j}$$

with $a = c(0, 1, 4.5, 9, 99, 99, 99, 99)$.

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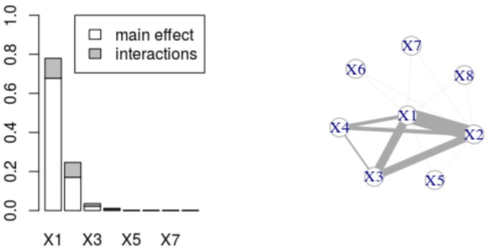

Figure: 1st order analysis (left) and 2nd order analysis (right) with 10^5 simulated data

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A 6D block-additive function, with uniform inputs on $[-1, 1]$:

$$h(x) = \cos([1, x_1, x_2, x_3]^\top \beta) + \sin([1, x_4, x_5, x_6]^\top \gamma))$$

with $\beta = (-0.8, -1.1, 1.1, 1)^\top$ and $\gamma = (-0.5, 0.9, 1, -1.1)^\top$.

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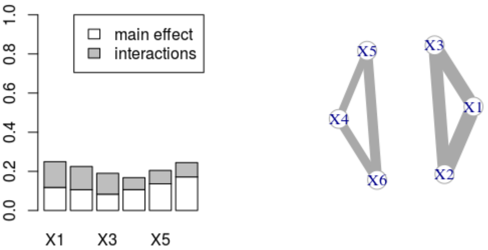

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Derivative-based upper bounds of Sobol indices with Poincaré inequalities

Reminder: μ *satisfies a Poincaré inequality if for all h in* $L^2(\mu)$ *such that* $\int h(x)d\mu(x) = 0$*, and* $h'(x) \in L^2(\mu)$*:*

$$\int h(x)^2 d\mu(x) \leq C(\mu) \int h'(x)^2 d\mu(x)$$

$\rightarrow$ *Optimal values of* $C(\mu)$ *have been investigated in [Roustant et al., 2017]*

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Theorem [Lamboni et al., 2013]

The total Sobol index is bounded with DGSM, thanks to a Poincaré inequality:

$$\underbrace{D_i^{\text{tot}}}_{\text{interpretable but costly}} \leq \underbrace{C(\mu_i)}_{\text{Poincaré constant}} \times \underbrace{\int_{\mathbb{R}^d} \left(\frac{\partial h}{\partial x_i}(x)\right)^2 \mu(dx)}_{\text{economical but less interpretable}}$$

Derivative-based upper bounds of Sobol indices with Poincaré inequalities

Actually, *the same tool can be used to obtain lower bounds* on Sobol indices!
As for matricial problems, the minimum of the Rayleigh ratio (s.t. $\int h d\mu = 0$)

$$\frac{\int h'(x)^2 d\mu(x)}{\int h(x)^2 d\mu(x)} = \frac{\|h'\|^2}{\|h\|^2}$$

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$$\langle h', e_n' \rangle = \lambda_n \langle h, e_n \rangle \qquad (\star)$$

with $0 < \lambda_1 = \frac{1}{C(\mu_1)} < \lambda_2 < \cdots < \lambda_n \to +\infty$.

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Poincaré differential operator (PDO)

The underlying operator is $Lh = h'' - V'h'$, and solving $(\star)$ is equivalent to

$$Lh = -\lambda h, \qquad \text{with} \quad h'(a) = h'(b) = 0.$$

This can be solved numerically (fastly!) with 1-dimensional finite elements.

Part II

Generalized chaos expansion

Generalized chaos expansion

For all j, let $e_{j,0} = 1, e_{j,1}, \dots, e_{j,n_j-1}$ *be orthonormal functions in* $L^2(\mu_j)$.
We call *generalized chaos* a tensor of the form:

$$e_{\underline{\ell}}(x) = \prod_{j=1}^{d} e_{j,\ell_j}(x_j)$$

where $\underline{\ell} = (\ell_1, \dots, \ell_d)$ is a multi-index.
When the $e_{.,.}$ are (orthonormal) polynomials, we recover *polynomial chaos*.

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Property

The subset of tensors that involve *exactly (resp. at least)* x_1 is an Hilbert basis of the corresponding space. Thus, for any centered function h:

$$h_1 = \sum_{\ell_1 \geq 1} \langle h, e_{1,\ell_1} \rangle e_{1,\ell_1}, \qquad h_1^{\text{tot}} = \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \langle h, e_{\underline{\ell}} \rangle e_{\underline{\ell}}$$

$$D_1(h) = \sum_{\ell_1 \geq 1} \langle h, e_{1,\ell_1} \rangle^2, \qquad D_1^{\text{tot}}(h) = \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \langle h, e_{\underline{\ell}} \rangle^2$$

N.B. This material is inspired from [Antoniadis, 1984, Tissot, 2012].

PDO expansions

Define PDO expansion as the generalized chaos expansion obtained with *the eigenfunctions of the Poincaré differential operator*.

Property

$$
\begin{aligned}
D_1(h) &= \sum_{\ell_1 \geq 1} \langle h, e_{1,\ell_1} \rangle^2 = \sum_{\ell_1 \geq 1} \frac{1}{\lambda_{1,\ell_1}^2} \langle \frac{\partial h}{\partial x_1}, e'_{1,\ell_1} \rangle^2. \\
D_1^{\text{tot}}(h) &= \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \langle h, e_{1,\ell_1} \dots e_{d,\ell_d} \rangle^2 \\
&= \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \frac{1}{\lambda_{1,\ell_1}^2} \langle \frac{\partial h}{\partial x_1}, e'_{1,\ell_1} e_{2,\ell_2} \dots e_{d,\ell_d} \rangle^2.
\end{aligned}
$$

PDO expansions

Example of lower bound. Limiting ourselves to the first eigenfunction in all dimensions, and to first and second order tensors involving x_1, we obtain:

- A derivative-free PDO lower bound:

$$D_1^{\text{tot}}(h) \geq \underbrace{\langle h, e_{1,1} \rangle^2}_{\text{lower bound for } D_1} + \sum_{i=2}^{d} \langle h, e_{1,1} e_{i,1} \rangle^2$$

- A derivative-based PDO lower bound:

$$D_1^{\text{tot}}(h) \geq \underbrace{C(\mu_1)^2 \langle \frac{\partial h}{\partial x_1}, e'_{1,1} \rangle^2}_{\text{lower bound for } D_1} + C(\mu_1)^2 \sum_{i=2}^{d} \langle \frac{\partial h}{\partial x_1}, e'_{1,1} e_{i,1} \rangle^2$$

Equality case: when h has the form

$$h(x) = \alpha_1 e_{1,1}(x_1) + \sum_{i=2}^{d} \alpha_i e_{1,1}(x_1) e_{i,1}(x_i) + g(x_2, \ldots, x_d)$$

When using derivatives?

We must compute squared integrals $\theta = (\int g(x) d\mu(x))^2$, when g is equal to:

$$g_{\text{dir}} = h\phi_1, h\phi_1\phi_j, \dots \qquad \text{or} \qquad g_{\text{der}} = \frac{\partial h}{\partial x_1}\psi_1, \frac{\partial h}{\partial x_1}\psi_1\phi_j, \dots$$

for some functions $\phi_i, \phi_j, \psi_1, \dots$.

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for some functions $\phi_i, \phi_j, \psi_1, \dots$.

The reason why we should compute θ with / without derivatives is numerical.
The sample estimate $\hat{\theta} = \left(\frac{1}{n}\sum_{i=1}^{n} g(X^i)\right)^2$, with $X^1, \dots, X^n$ i.i.d. $\sim \mu$, verifies:

$$\hat{\theta} \approx \mathcal{N}\left(\theta, \frac{4\theta}{n}\mathrm{Var}_{\mu}(g)\right)$$

Hence, for one squared integral, using the derivative form can reduce estimation error when g_{der} is less variable than g_{dir}.

Particular cases

- *For uniform distributions, PDO expansion = Fourier expansion*
  - Indeed, the PDO is the Laplacian, whose eigenfunctions are trigo. functions
- *For normal distributions, PDO expansion = PC expansion*
  - This is the only case where PDO expansion = PC expansion

Weight-free derivative-based lower bounds

All the integrals above can involve derivatives by integrating by part.
But this often induce weights; Here is an alternative to PDO, avoiding weights.

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But this often induce weights; Here is an alternative to PDO, avoiding weights.

Assume that μ_j *is continuous with pdf* $p_j \in \mathcal{H}^1(\mu_j)$ vanishing at the boundaries but not inside, and such that $p_j' \not\equiv 0$ and $p_j'/p_j \in L^2(\mu_j)$. Denote:

$$Z_j(x_j) = (\ln p_j)'(x_j), \qquad I_j = \mathrm{Var}(Z_j(X_j)).$$

Then, by choosing $e_{j,1}(x_j) = I_j^{-1/2} Z_j(x_j)$, we have:

$$D_1^{\mathrm{tot}} \geq \underbrace{I_1^{-1} c_1^2}_{\text{lower bound for } D_1} + I_1^{-1} \sum_{j=2}^{d} I_j^{-1} c_{1,j}^2$$

with

$$c_1 = \int h(x) Z_1(x_1) d\mu(x) = -\int \frac{\partial h(x)}{\partial x_1} d\mu(x)$$

$$c_{1,j} = \int h(x) Z_1(x_1) Z_j(x_j) d\mu(x) = -\int \frac{\partial h(x)}{\partial x_1} Z_j(x_j) d\mu(x) = \int \frac{\partial^2 h(x)}{\partial x_1 \partial x_j} d\mu(x)$$

Weight-free derivative-based lower bounds

For normal variables $N(m_j, s_j^2)$:

$$D_1^{\text{tot}} \geq \underbrace{s_1^2 \left(\int \frac{\partial h(x)}{\partial x_1} d\mu(x) \right)^2}_{\text{lower bound for } D_1} + s_1^2 \sum_{j=2}^{d} s_j^2 \left(\int \frac{\partial^2 h(x)}{\partial x_1 \partial x_j} d\mu(x) \right)^2$$

Dist. name	Support	p	Z	I
Normal	$\mathbb{R}$	$\frac{1}{s\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(x-m)^2}{s^2}\right)$	$-(X-m)/s^2$	$1/s^2$
Laplace	$\mathbb{R}$	$\frac{1}{2s} \exp\left(\frac{\lvert x-m\rvert}{s}\right)$	$-\mathrm{sgn}(X-m)/s$	$1/s^2$
Cauchy	$\mathbb{R}$	$\frac{1}{\pi}\frac{s}{(x-x_0)^2+s^2}$	$\frac{-2(x-x_0)}{(x-x_0)^2+s^2}$	$1/(2s^2)$

Improvements on existing works (in [Kucherenko and Iooss, 2017])

- *For uniforms on* $[0, 1]$ using the orthonormal function obtained from x_1^m, and an integration by part, we obtain:

$$D_1^{\text{tot}} \geq D_1 \geq \frac{2m+1}{m^2} \left(\int (h(1, x_{-1}) - h(x))dx - w_1^{(m+1)} \right)^2$$

where $w_1^{(m+1)} = \int \frac{\partial h(x)}{\partial x_1} x_1^{m+1} dx$. This improves on the known lower bound which has the same form, with the smaller multiplicative constant $\frac{2m+1}{(m+1)^2}$.

- *For normal distributions*, we improve on:

$$D_1^{\text{tot}} \geq D_1 \geq s_1^2 \left(\int \frac{\partial h(x)}{\partial x_1} d\mu(x) \right)^2.$$

N.B. Better bounds are obtained by adding orth. funct. of the form $\psi_1 \psi_j$.

Weights and connexion with PC expansions

1. PDO expansion can be extended to weighted Poincaré inequalities,

$$\mathrm{Var}_{\mu_1}(h) \leq C \int_{\mathbb{R}} h'(x)^2 w(x) \mu_1(dx)$$

by solving $\langle h', e_n' \rangle_w = \lambda_n \langle h, e_n \rangle$ with $\langle h, g \rangle_w := \int h(x) g(x) w(x) \mu_1(dx)$.

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2. Using weighted Poincaré inequalities has already been proposed in SA: [Song et al., 2019] choose w such that e_1 is a 1st order polynomial.
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2. Using weighted Poincaré inequalities has already been proposed in SA: [Song et al., 2019] choose w such that e_1 is a 1st order polynomial.
$\rightarrow$ *Except from 3 cases, the other eigenfunctions e_n are not all polynomials.*

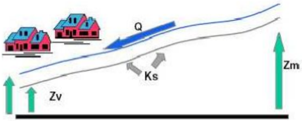
3. There are exactly 3 cases where PDO expansions = PC expansions, i.e. where all eigenfunctions are polynomials [Bakry et al., 2014]:

Law	Interval	Polynomials	Weight
Normal	$\mathbb{R}$	Hermite	$w(x) = 1$
Gamma	$\mathbb{R}_+$	Laguerre	$w(x) \propto x^{\alpha-1} e^{-\alpha x}$
Beta	$[-1, 1]$	Jacobi	$w(x) \propto (1-x)^{\alpha-1}(1+x)^{\beta-1}$

Part III

An application

A case study for global sensitivity analysis



A simplified flood model [Iooss, 2011], [Iooss and Lemaitre, 2015].

- Output: cost (in million euros) of the damage on the dyke

$$Y = \mathbb{1}_{S>0} + \left[0.2 + 0.8\left(1 - \exp^{-\frac{1000}{S^4}}\right)\right]\mathbb{1}_{S\leq 0} + \frac{1}{20}\left(H_d \mathbb{1}_{H_d>8} + 8\mathbb{1}_{H_d\leq 8}\right)$$

where H is the maximal annual height of the river (in meters), and S is the maximal annual overflow (in meters)

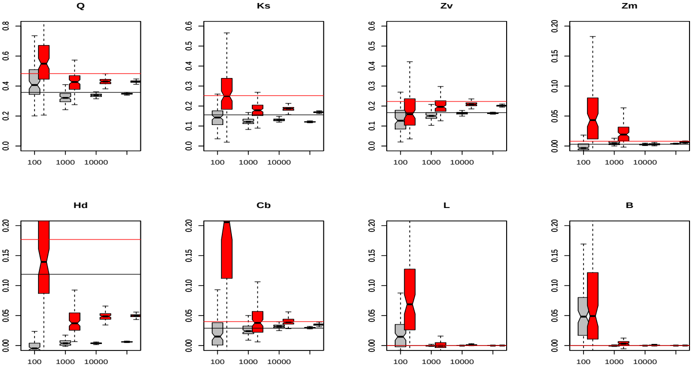
$$S = Z_v + H - H_d - C_b \quad \text{with} \quad H = \left(\frac{Q}{BK_s\sqrt{\frac{Z_m - Z_v}{L}}}\right)^{0.6}$$

A case study for global sensitivity analysis

- 8 inputs variables assumed to be independent r.v., with distributions:

Input	Description	Unit	Probability distribution
$X_1 = Q$	Maximal annual flowrate	m^3/s	Gumbel $\mathcal{G}(1013, 558)$, truncated on $[500, 3000]$
$X_2 = K_s$	Strickler coefficient	-	Normal $\mathcal{N}(30, 8^2)$, truncated on $[15, +\infty[$
$X_3 = Z_v$	River downstream level	m	Triangular $\mathcal{T}(49, 50, 51)$
$X_4 = Z_m$	River upstream level	m	Triangular $\mathcal{T}(54, 55, 56)$
$X_5 = H_d$	Dyke height	m	Uniform $\mathcal{U}[7, 9]$
$X_6 = C_b$	Bank level	m	Triangular $\mathcal{T}(55, 55.5, 56)$
$X_7 = L$	River stretch	m	Triangular $\mathcal{T}(4990, 5000, 5010)$
$X_8 = B$	River width	m	Triangular $\mathcal{T}(295, 300, 305)$

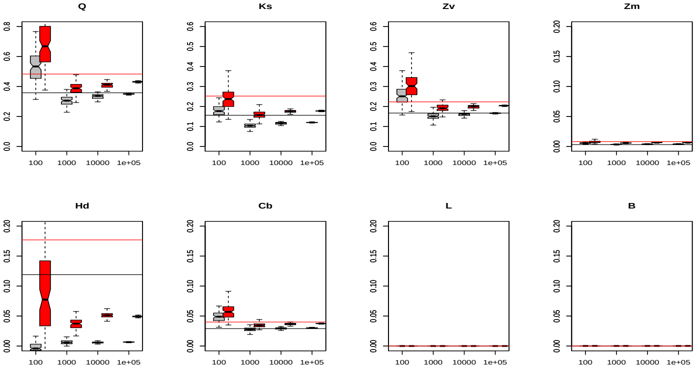
Illustration on the flood problem: PDO lower bounds without derivatives



MC estimate of PDO lower bound of (total) Sobol indices, for various sample sizes:

$$D_1^{\text{tot}} \geq \underbrace{\langle h, e_{1,1} \rangle^2}_{\text{lower bound for } D_1} + \sum_{i=2}^{d} \langle h, e_{1,1} e_{i,1} \rangle^2$$

Illustration on the flood problem: PDO lower bounds using derivatives



MC estimate of PDO lower bound of (total) Sobol indices, for various sample sizes:

$$D_1^{\text{tot}} \geq \underbrace{C(\mu_1)^2 \left\langle \frac{\partial h}{\partial x_1}, e'_{1,1} \right\rangle^2}_{\text{lower bound for } D_1} + C(\mu_1)^2 \sum_{i=2}^{d} \left\langle \frac{\partial h}{\partial x_1}, e'_{1,1} e_{i,1} \right\rangle^2$$

Conclusions on the application

1. Lower bounds are easily computed, even for exotic input distributions
2. The estimation error can be large for small sample sizes
   - Bootstrap confidence intervals are required
3. The (estimated) lower bounds of the total Sobol' indices are often informative, i.e. larger than the (estimated) first order Sobol' indices
4. Using derivatives (then DGSM) gives excellent results, even for small sample size cases

Part IV

Conclusions and perspectives

Take-home messages

1. Polynomial chaos (PC) expansion is *extended to tensor Hilbert bases*
   - Gives lower bound for Sobol indices, with equality cases
2. *When derivatives are available, a good Hilbert basis is given by the eigenfunctions of the Poincaré Differential Operator* (PDO expansion)
   - Suitable lower bounds for Sobol indices are obtained with first eigenvalues
   - Improves on existing results on derivative-based sensitivity measures
3. PDO expansion can be computed fastly for various prob. distributions
   - 1-dimensional finite element methods
4. PDO expansion $\neq$ PC expansion, except for the Normal distribution
   - Only two other exceptions, when using weights: Gamma & Beta.
   - For the uniform distribution, PDO expansion = Fourier expansion.

Perspectives

1. To investigate finite sample properties of estimators
   - Reduce bias for small sample size in both PDO and PC expansions
2. To adapt L^1 techniques for PDO expansions
   - In order to choose relevant terms (not only the first eigenvalues)
3. To compare PDO and PC expansions in engineering problems

To go further into details, discover the related publication
in *Electronic Journal of Statistics*.

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