Generalized chaos expansions
Lower bounds on Sobol indices

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Summary

1. With polynomial chaos, (total) Sobol indices are infinite sums of squares
   - *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*

Part I

Context and notations

Context and notations

ANOVA decomposition

There is a unique decomposition for $h \in L^2(\mu)$, with $\mu = \mu_1 \otimes \cdots \otimes \mu_d$

$$h(x) = h_0 + \sum_{i=1}^{d} h_i(x_i) + \sum_{i<j} h_{i,j}(x_i, x_j) + \cdots + h_{1,\dots,d}(x_1, \dots, x_d)$$

s.t. $\mathbb{E}(h_I(x_I)|x_J) = 0$ if $J \subsetneq I$. All the terms are orthogonal. Hence:

$$\mathrm{Var}(h(x)) = \sum_{i=1}^{d} \mathrm{Var}(h_i(x_i)) + \sum_{i<j} \mathrm{Var}(h_{i,j}(x_i, x_j)) + \dots$$

Sobol indices

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

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

Context and notations

Total indices and derivative-based measures

$$I \subseteq \{1, \dots, d\} : \qquad D_I^{\text{tot}} = \sum_{J \supseteq I} D_J, \qquad \nu_I = \int \left(\frac{\partial^{|I|} h(x)}{\partial x_I} \right)^2 d\mu(x)$$

These indices can be used to screen out useless variables or interactions:

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

Derivative-based upper bounds of Sobol indices with Poincaré inequalities

Theorem [Lamboni et al., 2013]

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

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

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]*

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. $\int h d\mu = 0$)

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

is given by the smallest eigenvalue of a spectral problem. More precisely, if μ_1 has density $\exp(-V)$ on a bounded interval $[a, b]$, then $\exists(\lambda_n, e_n)_{n\geq 0}$ s.t. $\forall h$:

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

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

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 $e_{\cdot,\cdot}$ are (orthonormal) polynomials, we recover *polynomial chaos*.

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

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

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

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:

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

where $w_1^{(m+1)} = \int \frac{\partial g(x)}{\partial x_1} x_1^{m+1} dx$. 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:

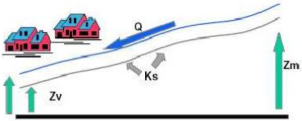
$$D_1^{\text{tot}} \geq D_1 \geq s_1^2 \left(\int \frac{\partial g(x)}{\partial x_1} d\mu(x)\right)^2.$$

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

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)

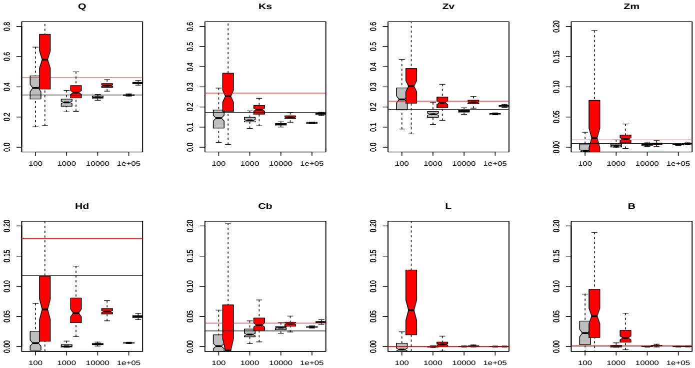
$$S = Z_v + H - H_d - C_b \quad \text{with} \quad H = \left(\frac{Q}{BK_s\sqrt{\frac{Z_m - Z_v}{L}}}\right)^{0.6}$$

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 $\mathcal{T}(295, 300, 305)$

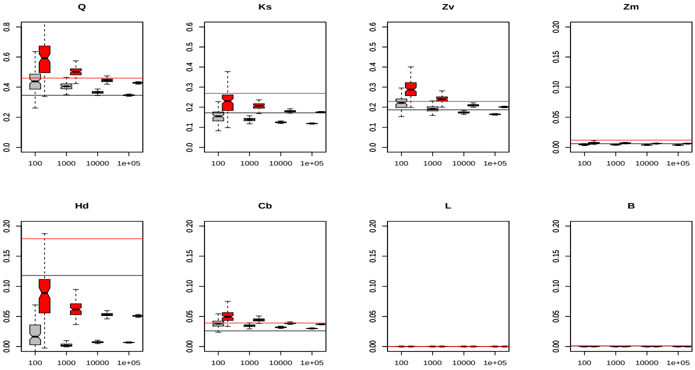
Illustration on the flood problem: PDO lower bounds without derivatives



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 preprint here

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Appendix. 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 $\langle h, g \rangle_w := \int h(x)g(x)w(x)\mu(dx)$.

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