Poincaré inequalities in dimension 1.
Applications to sensitivity analysis.

Summer school “Global sensitivity analysis and Poincaré inequalities”
6-8 July 2022

Olivier Roustant
INSA Toulouse & IMT

This talk is based on various works, including collaborations with
F. Barthe, F. Gamboa (IMT), B. Iooss (EDF & IMT),
N. Lüthen, S. Marelli and B. Sudret (ETH).

Part I

Poincaré inequalities in dimension 1.

Here we present the paper written with F. Barthe and B. Iooss [Roustant et al., 2017], in a specific slide show [download].

Part II

Complements: Poincaré basis, Poincaré chaos

Poincaré basis

Consider the spectral decomposition associated to the Poincaré inequalities. The eigenfunctions (e_n) define a Hilbert basis of $L^2(\mu_1)$, called *Poincaré basis.*

Caracterization of Poincaré basis [Lüthen et al., 2021]

Under our assumption on μ_1, the Poincaré basis is the only orthonormal basis of $L^2(\mu_1)$ in $H^1(\mu_1)$ *such that its derivative (e'_n) also form an orthogonal basis*.

In particular, the derivative of the Poincaré basis is an orthogonal system:

$$\langle e'_m, e'_n \rangle = \lambda_n \langle e_m, e_n \rangle = \lambda_n \delta_{n,m}$$

The proposition above states that it remains dense in $L^2(\mu_1)$, and that the Poincaré basis is the only one to do this.

Caracterization of the Poincaré basis: sketch of proof

Direct sense.

- We already mentionned that (e'_n) remains an orthogonal *system*.
- Let us check that (e'_n) is *dense* in $L^2(\mu)$, by showing that its orthogonal space is null.

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As $f \in L^2(\mu) = L^2(a,b)$, $\exists g \in H^1(a,b) = H^1(\mu)$ such that $f = g'$, with:

$$g(x) = g(a) + \int_a^x f(t)dt.$$

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This implies that g is proportional to $e_0 = 1$, thus $f = 0$.

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Reverse sense, unicity of the basis.

- Let (φ_n) a system of $H^1(\mu)$ with $\varphi_0 = 1$. Assume that (φ_n) is an orthonormal basis of $L^2(\mu)$ and $(\varphi'_n)_{n\geq 1}$ is an orthogonal basis of $L^2(\mu)$.

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- Notice that (φ_n) is an orthogonal basis of $H^1(\mu)$.
  - Orthogonal by assumption: $\langle \varphi_n, \varphi_m \rangle_{H^1(\mu)} = \langle \varphi_n, \varphi_m \rangle + \langle \varphi_n', \varphi_m' \rangle \propto \delta_{n,m}$.

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$$f \in H^1(\mu) \to \langle f', \varphi_n' \rangle.$$

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By Riesz theorem, there exists a unique $\zeta_n \in H^1(\mu)$ such that

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With $f = \varphi_m, (m \neq n)$, by density of $(\varphi_n) \in H^1(\mu)$, we get $\zeta_n \propto \varphi_n$.
With $f = \varphi_n$, we get $\langle f', \varphi'_n \rangle = \lambda_n \langle f, \varphi_n \rangle$, and $(\varphi_n)_n$ is the Poincaré basis.

Computation of Poincaré constant and basis

- By finite elements (FE) in 1D (or 2D). [Roustant et al., 2017]
  If V is of class C^k (with $d\mu_1(x) = e^{-V(x)}dx$), then with n knots for FE:
  - Convergence of estimated eigenvalues at the speed $1/n^{2(k+1)}$
  - Convergence of estimated eigenfunctions at the speed $1/n^{k+1}$

- For any dimension, it is possible to estimate the Poincaré constant from a sample of μ (any dim.), by using a RKHS dense in $H^1(\mu)$. [Pillaud-Vivien et al., 2019]
  - Convergence at the speed $1/\sqrt{n}$, where n is the sample size

Remark. Both methods involve a eigen decomposition of a matrix of size n $\Rightarrow n \leq 10\,000$

Illustrations

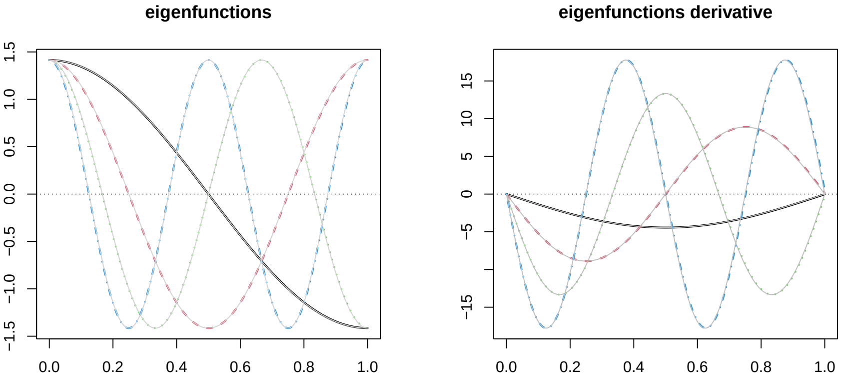

Figure: Estimated first eigenfunctions and their derivatives for the *uniform* pdf on [0, 1]. The superimposed grey solid lines are the true curves, cor. to $e_n(x) = \sqrt{2}\cos\left(\frac{2\pi nx}{2}\right)$.

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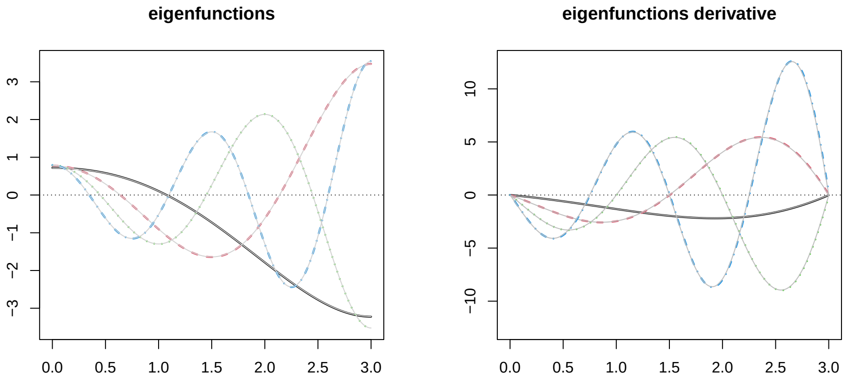

Figure: Estimated first eigenfunctions and their derivatives for the *exp.* pdf $\mathcal{E}(1)$, truncated on $[0, 3]$. The superimposed grey solid lines are the true curves.

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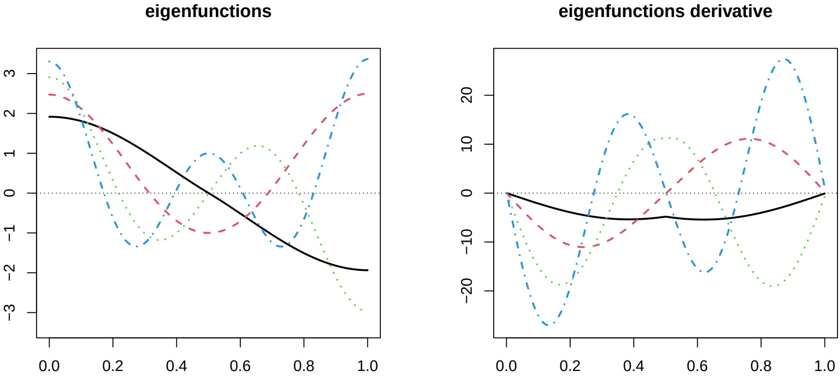

Figure: Estimated first eigenfunctions and their derivatives for the *triangle* pdf on [0, 1]. Software used: sensitivity R package [Iooss et al., 2021].

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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For any centered function h, denote $c_{\underline{\ell}} = \langle h, e_{\underline{\ell}} \rangle$. Then $h = \sum_{\underline{\ell}} c_{\underline{\ell}} e_{\underline{\ell}}$, and:

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$$h_1^{\text{tot}} = \sum_{\ell_1 \geq 1, \ell_2,\dots,\ell_d} c_{\underline{\ell}}\, e_{\underline{\ell}}, \qquad D_1^{\text{tot}}(h) = \sum_{\ell_1 \geq 1, \ell_2,\dots,\ell_d} c_{\underline{\ell}}^2$$

Poincaré chaos expansions, application to sensitivity analysis

Define the Poincaré expansion (PoinCE) as the chaos expansion obtained with *the Poincaré basis*.

Properties (variance-based indices with Poincaré chaos)

For all h in $H^1(\mu)$, we can rewrite (total) Sobol indices with derivatives:

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

When using derivatives?

Consider a squared integral $\theta = (\int g(x) d\mu(x))^2$, 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 $\phi_i, \phi_j, \psi_1, \ldots$.

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 $X^1, \ldots, X^n$ 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}.

Property (derivative-based sensitivity measure with DGSM)

For all h in $H^1(\mu)$, DGSM can be computed with the Poincaré basis coef.:

$$\nu_1(h) = \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \lambda_{1,\ell_1} \langle h, e_{\underline{\ell}} \rangle^2 = \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \frac{1}{\lambda_{1,\ell_1}} \langle \frac{\partial h}{\partial x_1}, e'_{1,\ell_1} e_{2,\ell_2} \dots e_{d,\ell_d} \rangle^2.$$

Proof:

$$\nu_1(h) = \left\| \frac{\partial h}{\partial x_1} \right\|^2 = \left\| \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \langle h, e_{\underline{\ell}} \rangle \frac{\partial e_{\underline{\ell}}}{\partial x_1} \right\|^2 = \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \langle h, e_{\underline{\ell}} \rangle^2 \left\| \frac{\partial e_{\underline{\ell}}}{\partial x_1} \right\|^2$$

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Remark: $$\nu_1(h) \geq \lambda_{1,1} \sum_{\ell_1 \geq 1, \ell_2, \dots, \ell_d} \langle h, e_{\underline{\ell}} \rangle^2 = \frac{1}{C(\mu_1)} D_1^{\text{tot}}(h)$$

Hence we retrieve the upper bound: $D_1^{\text{tot}}(h) \leq C(\mu_1) \nu_1(h)$

Poincaré chaos expansion (PoinCE) vs polynomial chaos exp. (PCE)

On the flood model, using derivatives with PoinCE gives more accurate results especially for small indices, and outperforms PCE [Lüthen et al., 2021]

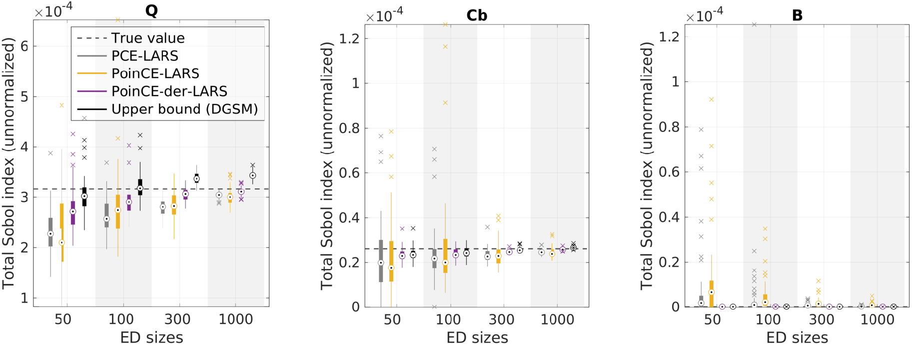

Figure: Estimates of unnormalized total Sobol' indices for the flood cost model, via sparse regression. Software used: UQLab [Marelli and Sudret, 2014].

Part III

Conclusion and perspectives

Some conclusions

- Poincaré inequalities give an *upper bound of Sobol indices with DGSM*
- A *Poincaré basis remains an orthogonal basis by derivation* (and is the only one to do so).
  - Particular cases: Hermite polynomials for the Normal distribution, a kind of Fourier basis for the uniform distribution.
  - Efficient numerical method based on finite elements
- *Poincaré chaos give simple expressions for Sobol indices and DGSM*, as a sum of (weighted) squared, *involving (or not) derivatives*
- *Using derivatives* for sensitivity analysis *is very efficient for screening, provided the function is smooth*. Couterexample: oscillations!

Perspectives

- Use the derivative information to build the chaos expansion
- Extension to 2D problems, assuming independence of pairs of variables
  $\rightarrow$ *Attend the PhD defense of Clément Steiner to learn more!*
- Active subspaces
  $\rightarrow$ *See the course of Clémentine Prieur in this summer school*

Iooss, B., Veiga, S. D., Janon, A., and Pujol, G. (2021).
sensitivity: Global Sensitivity Analysis of Model Outputs.
R package version 1.25.0.

Lüthen, N., Roustant, O., Gamboa, F., Iooss, B., Marelli, S., and Sudret, B. (2021).
Global sensitivity analysis using derivative-based sparse Poincaré chaos expansions.

Marelli, S. and Sudret, B. (2014).
UQLab: A framework for uncertainty quantification in Matlab.
In *Vulnerability, Uncertainty, and Risk (Proc. 2nd Int. Conf. on Vulnerability, Risk Analysis and Management (ICVRAM2014), Liverpool, United Kingdom)*, pages 2554–2563.

Pillaud-Vivien, L., Bach, F., Lelièvre, T., Rudi, A., and Stoltz, G. (2019).
Statistical estimation of the poincaré constant and application to sampling multimodal distributions.

Roustant, O., Barthe, F., and Iooss, B. (2017).
Poincaré inequalities on intervals - application to sensitivity analysis.
Electron. J. Statist., 11(2):3081–3119.