

Poincaré inequalities revisited for dimension reduction

Olivier Roustant*, Franck Barthe** and Bertrand Iooss**,***

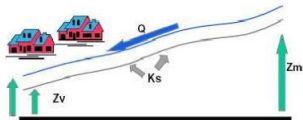
* Mines Saint-Étienne – ** Institut de Mathématiques de Toulouse – *** EDF, Chatou

ISFA – 10 March 2017, Lyon

Part I

Background and motivation

A case study for global sensitivity analysis



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

- 1 output: maximal annual overflow (in meters), denoted by S :

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

where H is the maximal annual height of the river (in meters).

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

- Aim: To detect unessential X_i 's, to quantify the influence of X_i 's on S , ...*

A case study for global sensitivity analysis

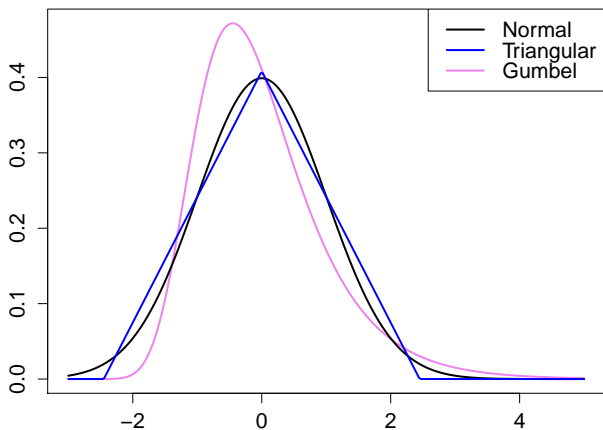


Figure: The 3 distributions types of the case study, here with mean 0 and variance 1

Towards variance-based sensitivity measures

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

Sobol-Hoeffding decomposition [Sobol, 1993, Efron and Stein, 1981]

$$g(\mathbf{X}) = g_0 + \sum_{i=1}^d g_i(X_i) + \sum_{1 \leq i < j \leq d} g_{i,j}(X_i, X_j) + \dots + g_{1,\dots,d}(X_1, \dots, X_d)$$

The g_I 's satisfy $E[g_I(X_I)|X_J] = 0$ if $J \subsetneq I$, implying orthogonality. They are obtained sequentially via

$$\mathbb{E}(g(\mathbf{X})|\mathbf{X}_I) = \int_{\mathbb{R}^{d-|I|}} g(\mathbf{x}) d\mu_{-I}(\mathbf{x}_{-I})$$

Variance-based and derivative-based measures

Variance decomposition and Sobol indices

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

$$D := \text{Var}(g(\mathbf{X})) = \sum_I D_I, \quad 1 = \sum_I S_I$$

- Total index:** $D_i^T = \sum_{J \supseteq \{i\}} D_J$, $S_i^T = \frac{D_i^T}{D}$.

Variance-based and derivative-based measures

Variance decomposition and Sobol indices

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

$$D := \text{Var}(g(\mathbf{X})) = \sum_I D_I, \quad 1 = \sum_I S_I$$

- Total index:** $D_i^T = \sum_{J \supseteq \{i\}} D_J$, $S_i^T = \frac{D_i^T}{D}$.

Derivative Global Sensitivity Measure (DGSM), [Sobol and Gershman, 1995], [Kucherenko et al., 2009]

$$v_i = \int \left(\frac{\partial g(\mathbf{x})}{\partial x_i} \right)^2 d\mu(\mathbf{x})$$

Variance-based and derivative-based measures

- **Usage for screening.**

If either $D_j^T = 0$ or $\nu_j = 0$, then X_j is non influential

- **Advantages / Drawbacks**

	Computational cost	Interpretability
Sobol indices	-	+
DGSM	+	-

Variance-based and derivative-based measures

- **Usage for screening.**

If either $D_i^T = 0$ or $\nu_i = 0$, then X_i is non influential

- **Advantages / Drawbacks**

	Computational cost	Interpretability
Sobol indices	-	+
DGSM	+	-



Can we use DGSM to do screening based on Sobol indices?

Poincaré inequality

Poincaré inequality (1-dimensional case)

A distribution μ satisfies a Poincaré inequality if the energy in $L^2(\mu)$ sense of any centered function is controlled by the energy of its derivative:

For all h in $L^2(\mu)$ such that $\int h(x)d\mu(x) = 0$, and $h'(x) \in L^2(\mu)$:

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

The best constant is denoted $C_P(\mu)$.

Link between total Sobol indices and DGSM

Theorem [Lamboni et al., 2013], extended in [Roustant et al., 2014]

If μ_i admits a Poincaré inequality, then there is a Poincaré-type inequality between total indices and DGSMs

$$D_i \leq D_i^T \leq C(\mu_i)\nu_i$$

Link between total Sobol indices and DGSM

Theorem [Lamboni et al., 2013], extended in [Roustant et al., 2014]

If μ_i admits a Poincaré inequality, then there is a Poincaré-type inequality between total indices and DGSMs

$$D_i \leq D_i^T \leq C(\mu_i)\nu_i$$

Proof. Denote $g_i^T(\mathbf{x}) := \sum_{J \ni \{i\}} g_J(\mathbf{x}_J)$. Then:

$$\frac{\partial g(\mathbf{x})}{\partial x_i} = \frac{\partial g_i^T(\mathbf{x})}{\partial x_i}$$

Link between total Sobol indices and DGSM

Theorem [Lamboni et al., 2013], extended in [Roustant et al., 2014]

If μ_i admits a Poincaré inequality, then there is a Poincaré-type inequality between total indices and DGSMs

$$D_i \leq D_i^T \leq C(\mu_i)\nu_i$$

Proof. Denote $g_i^T(\mathbf{x}) := \sum_{J \supseteq \{i\}} g_J(\mathbf{x}_J)$. Then:

$$\frac{\partial g(\mathbf{x})}{\partial x_i} = \frac{\partial g_i^T(\mathbf{x})}{\partial x_i}$$

$$\begin{aligned} D_i^T = \text{Var}(g_i^T(\mathbf{x})) &= \int (g_i^T(\mathbf{x}))^2 d\mu(\mathbf{x}) \\ &\leq C(\mu_i) \int \left(\frac{\partial g_i^T(\mathbf{x})}{\partial x_i} \right)^2 d\mu(\mathbf{x}) = C(\mu_i)\nu_i \end{aligned}$$

'Low-cost' screening based on Sobol indices via DGSM

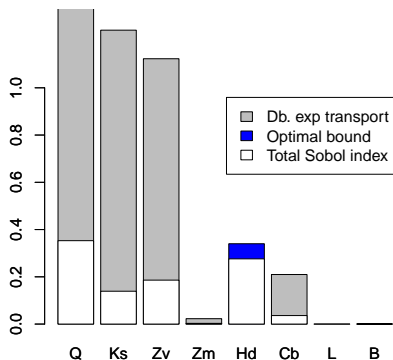


Figure: Total Sobol index S_i^T & Upper bound $C(\mu_i)\nu_i/D$

'Low-cost' screening based on Sobol indices via DGSM

- **Even if the Poincaré inequality is not accurate,**
it may be enough to screen out the less influential variables
→ Z_m, L, B in the case-study

'Low-cost' screening based on Sobol indices via DGSM

- Even if the Poincaré inequality is not accurate,
it may be enough to screen out the less influential variables
→ Z_m, L, B in the case-study
- When is the upper bound $C(\mu_i)\nu_i$ large (compared to D_i^T)?

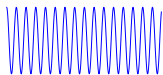
'Low-cost' screening based on Sobol indices via DGSM

- Even if the Poincaré inequality is not accurate, *it may be enough to screen out the less influential variables*
 → Z_m, L, B in the case-study
- When is the upper bound $C(\mu_i)\nu_i$ large (compared to D_i^T)?

ν_i is large



Ex: high frequency in g w.r.t. x_i
...we cannot do anything!



$C(\mu_i)$ is large

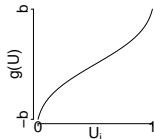
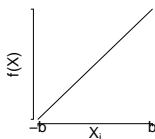


We can look for smallest $C(\mu_i)$

Why not transforming the problem to get uniform distributions?

Example with X_1, X_2 i.i.d. $\mathcal{N}(0, 1)$ truncated on $I = [-b, b]$

$$f(X_1, X_2) = X_1 + X_2 \quad \Bigg| \quad g(U_1, U_2) = F_X^{-1}(U_1) + F_X^{-1}(U_2)$$

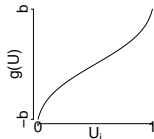
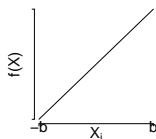


The Sobol indices of f and g are the same

Why not transforming the problem to get uniform distributions?

Example with X_1, X_2 i.i.d. $\mathcal{N}(0, 1)$ truncated on $I = [-b, b]$

$$f(X_1, X_2) = X_1 + X_2 \quad \Bigg| \quad g(U_1, U_2) = F_X^{-1}(U_1) + F_X^{-1}(U_2)$$



The Sobol indices of f and g are the same

Difference on *optimal* upper bounds computed with DGSM

$\mu(I)$	S^T	Upper bound with DGSM Original problem (with f)	Upper bound with DGSM Transformed problem (with g)
1	0.5	0.5	$+\infty$
0.95	0.5	0.52	1.48
0.75	0.5	0.56	1.00

The derivatives are larger on the transformed problem \Rightarrow larger bounds

1D Poincaré constants: Known results

pdf	Support	$C_P(\mu)$	$f_{\text{opt}}(\mathbf{x})$
Uniform	$[a, b]$	$(b - a)^2 / \pi^2$	$\cos\left(\frac{\pi(x-a)}{b-a}\right)$
$\mathcal{N}(m, s^2)$	\mathbb{R}	s^2	$x - m$
	$[r_{n,i}, r_{n,i+1}]$ (*)	$1/(n+1)$	$H_{n+1}(x)$
Double exp. $e^{- x } dx/2$	\mathbb{R}	4	×
Logistic $\frac{e^x}{(1+e^x)^2} dx$	\mathbb{R}	4	×

(*) H_n is the Hermite polynomial of degree n , and $r_{n,1}, \dots, r_{n,n}$ its zeros.

Summary and aim

- 1 *Sobol indices and DGSM are linked by Poincaré-type inequalities*

$$D_i^T \leq C(\mu_i)\nu_i \quad D_{i,j}^{\text{super}} \leq C(\mu_i)C(\mu_j)\nu_{i,j}$$

- 2 DGSM are easier to compute but Sobol indices are more interpretable
 ⇒ *DGSM may allow doing low-cost screening based on Sobol indices*

- 3 The aim: *To look for the exact Poincaré constants for distributions met in practice:*

- ▶ Frequently: Uniform – (truncated) Gaussian – Triangular – (truncated) lognormal – Exponential – (truncated) Weibull – (truncated) Gumbel
- ▶ Less frequently: (Inverse) Gamma – Beta – Trapezoidal – Generalized Extreme Value

Outline

- 1 Theory for optimal inequalities
- 2 Semi-analytical results
- 3 A numerical method
- 4 Applications

Part II

Theory for optimal inequalities

Mathematical setting

Definitions and assumptions

- Ω : an open interval (a, b) of \mathbb{R} (possibly unbounded)
- $\mu(dt) = \rho(t)dt$: A continuous measure supported by Ω .
 $\rho > 0$ on Ω , continuous on $\bar{\Omega}$ and piecewise C^1 on Ω .
- f' : *weak derivative of f* , i.e. s.t. for all ϕ of class C^∞ with compact support

$$\int_{\Omega} f(t)\phi'(t)dt = - \int_{\Omega} f'(t)\phi(t)dt.$$

- *Sobolev spaces*
 - ▶ $\mathcal{H}_{\mu}^1(\Omega) = \{f \in L^2(\mu) \text{ such that } f' \in L^2(\mu)\}$
 - ▶ $\mathcal{H}_{\mu}^{\ell}(\Omega) = \{f \in L^2(\mu) \text{ such that for all } k \leq \ell, f^{(k)} \in L^2(\mu)\}$

Mathematical setting

When weighted Sobolev spaces collapse to usual Sobolev spaces

Assume that μ is a bounded perturbation of $\mathcal{U}(\Omega)$, i.e. $0 < m < \rho(t) < M$.
Then:

$$L^2(\mu) = L^2(\mathcal{U}(\Omega)) \quad \mathcal{H}_\mu^\ell(\Omega) = \mathcal{H}_{\mathcal{U}(\Omega)}^\ell(\Omega)$$

with equivalent norms.

Poincaré inequality and Rayleigh ratio

Rayleigh ratio

For $f \in \mathcal{H}_\mu^1(\Omega)$:

$$J(f) = \frac{\int_\Omega f'^2 d\mu}{\int_\Omega f^2 d\mu} = \frac{\|f'\|^2}{\|f\|^2}$$

Finding the Poincaré constant is equivalent to:

$$\min_{f \in \mathcal{H}_\mu^1(\Omega)} J(f) \quad \text{s.t.} \quad \int_\Omega f d\mu = 0$$

and $C_P(\mu)$ denotes the *inverse* of the minimum.

Optimizing a Rayleigh ratio in finite dimensions

Exercise!

Let A a positive definite matrix on \mathbb{R}^n . Find:

$$\min_{x \in \mathbb{R}^n} \frac{\|x\|_A^2}{\|x\|^2}$$

with $\|x\|_A^2 = x^T A x$

Optimizing a Rayleigh ratio in finite dimensions

Exercice!

Let A a positive definite matrix on \mathbb{R}^n . Find:

$$\min_{x \in \mathbb{R}^n} \frac{\|x\|_A^2}{\|x\|^2}$$

with $\|x\|_A^2 = x^T A x$

Solution. A is diagonalisable in an orthonormal basis u_k :

$$A u_k = \lambda_k u_k$$

with $\lambda_1 \geq \dots \geq \lambda_n > 0$.

Expand x in the basis: $x = \sum x_k u_k$, then $Ax = \sum \lambda_k x_k u_k$:

$$\frac{\|x\|_A^2}{\|x\|^2} = \frac{\sum \lambda_k x_k^2}{\sum x_k^2} \geq \lambda_1$$

with equality if $x = u_1$.

Spectral interpretation and link to a 2nd-order differential equation

Theorem (Synthesis from [Bobkov and Götze, 2009] and [Dautray and Lions, 1990])

Assume that $\Omega = (a, b)$ is bounded, and that $\rho(t) = e^{-V(t)} > 0$ on $\bar{\Omega} = [a, b]$. A minimizer f of the Rayleigh ratio is obtained by solving

$$Lf := f'' - V'f' = -\lambda f \quad \text{with} \quad f'(a) = f'(b) = 0$$

when $\lambda =: \lambda(\mu)$ is the smallest possible value, called spectral gap. Furthermore, $\lambda(\mu)$ is a simple eigenvalue and f is strictly monotone.

Spectral interpretation and link to a 2nd-order differential equation

Theorem (Synthesis from [Bobkov and Götze, 2009] and [Dautray and Lions, 1990])

Assume that $\Omega = (a, b)$ is bounded, and that $\rho(t) = e^{-V(t)} > 0$ on $\bar{\Omega} = [a, b]$. A minimizer f of the Rayleigh ratio is obtained by solving

$$Lf := f'' - V'f' = -\lambda f \quad \text{with} \quad f'(a) = f'(b) = 0$$

when $\lambda =: \lambda(\mu)$ is the smallest possible value, called spectral gap. Furthermore, $\lambda(\mu)$ is a simple eigenvalue and f is strictly monotone.

Ideas for the proof. Show the connections between the three problems

P1 Find $f \in \mathcal{H}_\mu^1(\Omega)$ s.t. $J(f) = \frac{\|f'\|^2}{\|f\|^2}$ is minimum under $\int f d\mu = 0$

P2 Find $f \in \mathcal{H}_\mu^1(\Omega)$ s.t. $\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$

P3 Find $f \in \mathcal{H}_\mu^2(\Omega)$ s.t. $f'' - V'f' = -\lambda f$ and $f'(a) = f'(b) = 0$

Spectral interpretation and link to a 2nd-order differential equation

(P1) \iff (P2) (for the smallest positive λ). Start from (P2):

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Spectral interpretation and link to a 2nd-order differential equation

(P1) \iff (P2) (for the smallest positive λ). Start from (P2):

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Up to a switch in order to make coercive the left side, we can 'diagonalize': there exists a Hilbert basis $(u_k)_{k \geq 0}$ and an increasing sequence $(\lambda_k)_{k \geq 0}$ of positive numbers that tends to infinity such that:

$$\langle u'_k, g' \rangle = \lambda_k \langle u_k, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Spectral interpretation and link to a 2nd-order differential equation

(P1) \iff (P2) (for the smallest positive λ). Start from (P2):

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Up to a switch in order to make coercive the left side, we can 'diagonalize': there exists a Hilbert basis $(u_k)_{k \geq 0}$ and an increasing sequence $(\lambda_k)_{k \geq 0}$ of positive numbers that tends to infinity such that:

$$\langle u'_k, g' \rangle = \lambda_k \langle u_k, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Remark that:

- $\lambda_k = 0 \iff k = 0$, and $u_0 = 1$
- $\int f d\mu = 0 \iff \langle f, 1 \rangle = 0$

Thus f is written: $f = \sum_{k \geq 1} f_k u_k$.

Spectral interpretation and link to a 2nd-order differential equation

(P1) \iff (P2) (for the smallest positive λ). Start from (P2):

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Up to a switch in order to make coercive the left side, we can 'diagonalize': there exists a Hilbert basis $(u_k)_{k \geq 0}$ and an increasing sequence $(\lambda_k)_{k \geq 0}$ of positive numbers that tends to infinity such that:

$$\langle u'_k, g' \rangle = \lambda_k \langle u_k, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Remark that:

- $\lambda_k = 0 \iff k = 0$, and $u_0 = 1$
- $\int f d\mu = 0 \iff \langle f, 1 \rangle = 0$

Thus f is written: $f = \sum_{k \geq 1} f_k u_k$. Finally,

$$J(f) = \frac{\|f'\|^2}{\|f\|^2} = \frac{\sum_{k=1}^{+\infty} \lambda_k f_k^2}{\sum_{k=1}^{+\infty} f_k^2} \geq \lambda_1 > 0$$

with equality iff $f \in \mathbb{R} u_1$.

Spectral interpretation and link to a 2nd-order differential equation

(P2) \iff (P3) Formally the link comes from an **integration by part (IPP)**:

$$\langle f', g' \rangle = \int_a^b f' g' \rho = [(f' \rho) g]_a^b - \int_a^b (f' \rho)' g$$

Spectral interpretation and link to a 2nd-order differential equation

(P2) \iff (P3) Formally the link comes from an **integration by part (IPP)**:

$$\langle f', g' \rangle = \int_a^b f' g' \rho = [(f' \rho) g]_a^b - \int_a^b (f' \rho)' g$$

$$\lambda \langle f, g \rangle = \lambda \int_a^b f g \rho = - \int_a^b (\lambda f \rho) g$$

Spectral interpretation and link to a 2nd-order differential equation

(P2) \iff (P3) Formally the link comes from an **integration by part (IPP)**:

$$\langle f', g' \rangle = \int_a^b f' g' \rho = [(f' \rho) g]_a^b - \int_a^b (f' \rho)' g$$

$$\lambda \langle f, g \rangle = \lambda \int_a^b f g \rho = - \int_a^b (\lambda f \rho) g$$

Thus the two are equal for all $g \in \mathcal{H}_\mu^1(\Omega)$ iff:

- $f'(a) = f'(b) = 0$ (since $\rho > 0$)
- $(f' \rho)' = -\lambda f \rho$, i.e. $(f'' - V' f') \rho = -\lambda f \rho$

Spectral interpretation and link to a 2nd-order differential equation

(P2) \iff (P3) Formally the link comes from an **integration by part (IPP)**:

$$\langle f', g' \rangle = \int_a^b f' g' \rho = [(f' \rho) g]_a^b - \int_a^b (f' \rho)' g$$

$$\lambda \langle f, g \rangle = \lambda \int_a^b f g \rho = - \int_a^b (\lambda f \rho) g$$

Thus the two are equal for all $g \in \mathcal{H}_\mu^1(\Omega)$ iff:

- $f'(a) = f'(b) = 0$ (since $\rho > 0$)
- $(f' \rho)' = -\lambda f \rho$, i.e. $(f'' - V' f') \rho = -\lambda f \rho$

This proves (P2) \Leftarrow (P3), since f is regular enough (IPP is valid).

Conversely, an **argument of regularity** is necessary. One can show that **if f is solution of (P2), then $(f' \rho)$ is of class C^1** , and more precisely:

$$f'(x) = \frac{\lambda}{\rho(x)} \int_x^b f(t) \rho(t) dt.$$

Spectral interpretation and link to a 2nd-order differential equation

Neumann and Dirichlet spectral gaps

If f is enough derivable, finding $f \uparrow$ of the Neumann spectral problem

$$Lf := f'' - V'f' = -\lambda f, \quad f'(a) = f'(b) = 0$$

is equivalent to finding $g > 0$ of the *Dirichlet* spectral problem

$$Kg := g'' - V'g' - V''g = -\lambda g, \quad g(a) = g(b) = 0$$

Spectral interpretation and link to a 2nd-order differential equation

Neumann and Dirichlet spectral gaps

If f is enough derivable, finding $f \uparrow$ of the Neumann spectral problem

$$Lf := f'' - V'f' = -\lambda f, \quad f'(a) = f'(b) = 0$$

is equivalent to finding $g > 0$ of the *Dirichlet* spectral problem

$$Kg := g'' - V'g' - V''g = -\lambda g, \quad g(a) = g(b) = 0$$

Main idea. Consider $g = f'$

$$\begin{array}{ll} (Lf)' = f''' - V'f'' - V''f' = -\lambda f' & f'(a) = f'(b) = 0 \\ \updownarrow & \updownarrow \\ Kg = g'' - V'g' - V''g = -\lambda g & g(a) = g(b) = 0 \end{array}$$

Other useful properties: Optimal constants on intervals

1 *Monotonicity with respect to the interval*

$$I \subseteq J \quad \Rightarrow \quad C_P(\mu|_I) \leq C_P(\mu|_J)$$

Other useful properties: Optimal constants on intervals

1 *Monotonicity with respect to the interval*

$$I \subseteq J \quad \Rightarrow \quad C_P(\mu|_I) \leq C_P(\mu|_J)$$

2 *Continuity with respect to the support*

$$I_\epsilon \uparrow I \quad \Rightarrow \quad C_P(\mu|_{I_\epsilon}) \rightarrow C_P(\mu|_I)$$

Other useful properties: Optimal constants on intervals

1 *Monotonicity with respect to the interval*

$$I \subseteq J \quad \Rightarrow \quad C_P(\mu|_I) \leq C_P(\mu|_J)$$

2 *Continuity with respect to the support*

$$I_\epsilon \uparrow I \quad \Rightarrow \quad C_P(\mu|_{I_\epsilon}) \rightarrow C_P(\mu|_I)$$

Consequence.

We can assume that $\Omega = (a, b)$ is bounded and that ρ does not vanish on $\bar{\Omega}$.

Other useful properties: Optimal constants on intervals

Sketch of proof for monotonicity.

For $f \in \mathcal{H}^1(\mu|_I)$, extend it on J with a constant outside I . This is \tilde{f} .

Other useful properties: Optimal constants on intervals

Sketch of proof for monotonicity.

For $f \in \mathcal{H}^1(\mu|_I)$, extend it on J with a constant outside I . This is \tilde{f} .

$$\text{Var}_{\mu|_I}(f) = \inf_a \int_I (f - a)^2 \frac{d\mu}{\mu(I)}$$

Other useful properties: Optimal constants on intervals

Sketch of proof for monotonicity.

For $f \in \mathcal{H}^1(\mu|_I)$, extend it on J with a constant outside I . This is \tilde{f} .

$$\begin{aligned}\text{Var}_{\mu|_I}(f) &= \inf_a \int_I (f - a)^2 \frac{d\mu}{\mu(I)} \\ &\leq \inf_a \int_J (\tilde{f} - a)^2 \frac{d\mu}{\mu(I)}\end{aligned}$$

Other useful properties: Optimal constants on intervals

Sketch of proof for monotonicity.

For $f \in \mathcal{H}^1(\mu|_I)$, extend it on J with a constant outside I . This is \tilde{f} .

$$\begin{aligned} \text{Var}_{\mu|_I}(f) &= \inf_a \int_I (f - a)^2 \frac{d\mu}{\mu(I)} \\ &\leq \inf_a \int_J (\tilde{f} - a)^2 \frac{d\mu}{\mu(I)} \leq C_P(\mu) \int_J (\tilde{f}')^2 \frac{d\mu}{\mu(I)} \end{aligned}$$

Other useful properties: Optimal constants on intervals

Sketch of proof for monotonicity.

For $f \in \mathcal{H}^1(\mu|_I)$, extend it on J with a constant outside I . This is \tilde{f} .

$$\begin{aligned} \text{Var}_{\mu|_I}(f) &= \inf_a \int_I (f - a)^2 \frac{d\mu}{\mu(I)} \\ &\leq \inf_a \int_J (\tilde{f} - a)^2 \frac{d\mu}{\mu(I)} \leq C_P(\mu) \int_J (\tilde{f}')^2 \frac{d\mu}{\mu(I)} = C_P(\mu) \int_I (f')^2 d\mu|_I. \end{aligned}$$

Other useful properties: Optimal constants on intervals

Sketch of proof for monotonicity.

For $f \in \mathcal{H}^1(\mu|_I)$, extend it on J with a constant outside I . This is \tilde{f} .

$$\begin{aligned} \text{Var}_{\mu|_I}(f) &= \inf_a \int_I (f - a)^2 \frac{d\mu}{\mu(I)} \\ &\leq \inf_a \int_J (\tilde{f} - a)^2 \frac{d\mu}{\mu(I)} \leq C_P(\mu) \int_J (\tilde{f}')^2 \frac{d\mu}{\mu(I)} = C_P(\mu) \int_I (f')^2 d\mu|_I. \end{aligned}$$

Sketch of proof for continuity.

- From monotonicity, $C_P(\mu|_{I_\epsilon}) \leq C_P(\mu|_I)$
- Then, choose $f \in \mathcal{H}^1(\mu|_I)$, and check with Lebesgue theorem that:

$$\frac{\text{Var}_{\mu|_I}(f)}{\int_\Omega f'^2 d\mu|_I} = \lim_{\epsilon \rightarrow 0} \frac{\text{Var}_{\mu|_{I_\epsilon}}(f)}{\int_{I_\epsilon} f'^2 d\mu|_{I_\epsilon}} \leq \lim_{\epsilon \rightarrow 0} C_P(\mu|_{I_\epsilon})$$

Properties for symmetric measures on symmetric intervals

Let $I = (-a, a)$ be a symmetric interval, and μ an even measure on \mathbb{R} .

1 *Improved result for monotonicity*

$$C_P(\mu|_I) \leq \mu(I)^2 C_P(\mu)$$

Properties for symmetric measures on symmetric intervals

Let $I = (-a, a)$ be a symmetric interval, and μ an even measure on \mathbb{R} .

1 *Improved result for monotonicity*

$$C_P(\mu|_I) \leq \mu(I)^2 C_P(\mu)$$

2 *Symmetry and odd functions*

The infimum of the Rayleigh ratio on I can be found among odd functions

Part III

Semi-analytical results

An example: The truncated normal distribution

Poincaré constant of the truncated Normal distribution

Define:

$$h_0(\lambda, t) = M_{\frac{1-\lambda}{2}, \frac{1}{2}} \left(\frac{t^2}{2} \right) \quad h_1(\lambda, t) = M_{\frac{2-\lambda}{2}, \frac{3}{2}} \left(\frac{t^2}{2} \right)$$

where the so-called *Kummer's function* $M_{a_1, b_1}(z) = {}_1F_1(a_1; b_1; z)$ is an example of *hypergeometric series* $\sum_{p \geq 0} x_p$ satisfying

$$\frac{x_{p+1}}{x_p} = \frac{(p + a_1)z}{(p + b_1)(p + 1)}, \quad x_0 = 1$$

Notice that h_0 and h_1 generalize *Hermite polynomials*: When λ is an odd (resp. even) positive integer, then $t \mapsto h_0(\lambda, t)$ (resp. $t \mapsto t \cdot h_1(\lambda, t)$) is proportional to the Hermite polynomial of degree $\lambda - 1$.

Then the spectral gap of $\mathcal{N}(0, 1)_{|[a, b]}$ is the first zero of the function

$$d(\cdot) = bh_0(\cdot, a)h_1(\cdot, b) - ah_0(\cdot, b)h_1(\cdot, a)$$

Sketch of proof. Consider the Dirichlet problem

$$g'' - t g' = -(\lambda - 1)g, \quad g(a) = g(b) = 0$$

Sketch of proof. Consider the Dirichlet problem

$$g'' - t g' = -(\lambda - 1)g, \quad g(a) = g(b) = 0$$

- *Look for a series expansion $g(t) = \sum_{n \geq 0} c_n t^n \Rightarrow c_{n+2} = \frac{n - (\lambda - 1)}{(n+1)(n+2)} c_n$.*

Sketch of proof. Consider the Dirichlet problem

$$g'' - t g' = -(\lambda - 1)g, \quad g(a) = g(b) = 0$$

- *Look for a series expansion $g(t) = \sum_{n \geq 0} c_n t^n \Rightarrow c_{n+2} = \frac{n - (\lambda - 1)}{(n+1)(n+2)} c_n$.*
Split g into even an odd part, $g(t) = g_0(t) + t.g_1(t)$. Then:

$$g(t) = c_0 h_0(\lambda, t) + c_1 t.h_1(\lambda, t)$$

Sketch of proof. Consider the Dirichlet problem

$$g'' - t g' = -(\lambda - 1)g, \quad g(a) = g(b) = 0$$

- *Look for a series expansion $g(t) = \sum_{n \geq 0} c_n t^n \Rightarrow c_{n+2} = \frac{n - (\lambda - 1)}{(n+1)(n+2)} c_n$.*
Split g into even an odd part, $g(t) = g_0(t) + t.g_1(t)$. Then:

$$g(t) = c_0 h_0(\lambda, t) + c_1 t.h_1(\lambda, t)$$

- Now, $g(a) = g(b) = 0$ lead to the linear system $Xc = 0$, with:

$$X = \begin{pmatrix} h_0(\lambda, a) & a h_1(\lambda, a) \\ h_0(\lambda, b) & b h_1(\lambda, b) \end{pmatrix} \quad c = \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}$$

Sketch of proof. Consider the Dirichlet problem

$$g'' - t g' = -(\lambda - 1)g, \quad g(a) = g(b) = 0$$

- *Look for a series expansion $g(t) = \sum_{n \geq 0} c_n t^n \Rightarrow c_{n+2} = \frac{n - (\lambda - 1)}{(n+1)(n+2)} c_n$. Split g into even an odd part, $g(t) = g_0(t) + t.g_1(t)$. Then:*

$$g(t) = c_0 h_0(\lambda, t) + c_1 t.h_1(\lambda, t)$$

- Now, $g(a) = g(b) = 0$ lead to the linear system $Xc = 0$, with:

$$X = \begin{pmatrix} h_0(\lambda, a) & ah_1(\lambda, a) \\ h_0(\lambda, b) & bh_1(\lambda, b) \end{pmatrix} \quad c = \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}$$

This system must be singular, otherwise g would be identically zero. Thus $\det(X) = 0$, leading to $d(\lambda) = 0$.

Truncated normal distribution – Symmetric case: $I = [-b, b]$

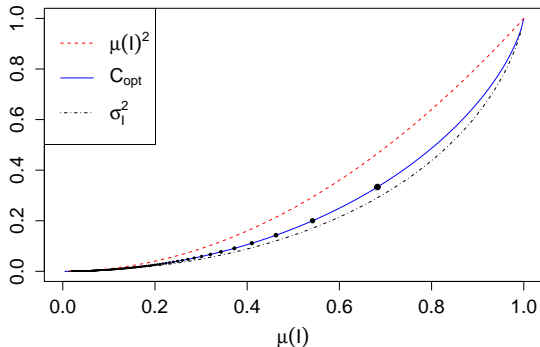


Figure: Poincaré constant of $\mu = \mathcal{N}(0, 1)$ truncated on $I = [-b, b]$, vs $\mu(I)$

σ_I^2 : variance of the truncated normal on I – Black points: Hermite polynomials of even degree.

Truncated normal distribution – General case

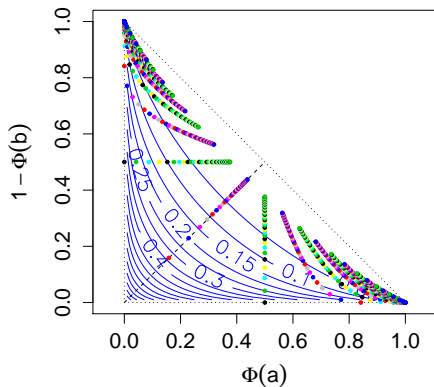


Figure: Poincaré constant of $\mathcal{N}(0, 1)$ truncated on $I = [a, b]$.

Colored points: Hermite polynomials (up to degree 100).

Summary: General methodology for finding optimal constants on $[a, b]$

- 1 Consider the spectral problem $f'' - V'f' = -\lambda f \quad f'(a) = f'(b) = 0$
- 2 Find a basis of 2 independent solutions $f_{1,\lambda}(t), f_{2,\lambda}(t)$
- 3 The Neumann conditions lead to a *singular* linear system

$$\begin{pmatrix} f'_{1,\lambda}(a) & f'_{2,\lambda}(a) \\ f'_{1,\lambda}(b) & f'_{2,\lambda}(b) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$\lambda = 1/C_{opt}$ is then the first zero of: $\lambda \mapsto f'_{1,\lambda}(a)f'_{2,\lambda}(b) - f'_{1,\lambda}(b)f'_{2,\lambda}(a)$

Summary: General methodology for finding optimal constants on $[a, b]$

- 1 Consider the spectral problem $f'' - V'f' = -\lambda f \quad f'(a) = f'(b) = 0$
- 2 Find a basis of 2 independent solutions $f_{1,\lambda}(t), f_{2,\lambda}(t)$
- 3 The Neumann conditions lead to a *singular* linear system

$$\begin{pmatrix} f'_{1,\lambda}(a) & f'_{2,\lambda}(a) \\ f'_{1,\lambda}(b) & f'_{2,\lambda}(b) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$\lambda = 1/C_{opt}$ is then the first zero of: $\lambda \mapsto f'_{1,\lambda}(a)f'_{2,\lambda}(b) - f'_{1,\lambda}(b)f'_{2,\lambda}(a)$

Variants.

- Dirichlet problem (ex: Truncated Gaussian)
- Symmetry (ex: Triangular)

1D Poincaré constants: Additional results

pdf	Support	\mathbf{C}_{opt}	Form of $\mathbf{f}_{\text{opt}}(\mathbf{x})$
Uniform	$[a, b]$	$(b - a)^2 / \pi^2$	$\cos\left(\frac{\pi(x-a)}{b-a}\right)$
$\mathcal{N}(\mu, \sigma^2)$	\mathbb{R}	σ^2	$x - \mu$
	$[r_{n,i}, r_{n,i+1}]$	$1/(n+1)$	$H_{n+1}(x)$
	$[a, b]$	<i>see before</i>	<i>related to Kummer</i>
Db. exp. $e^{- x } dx / 2$	\mathbb{R}	4	×
(*)	$[a, b], ab > 0$	$(\frac{1}{4} + \omega^2)^{-1}$	$e^{x/2} \cos(\omega x + \phi)$
(*, **)	$[a, b], ab \leq 0$	$> (\frac{1}{4} + \omega^2)^{-1}$	$e^{ x /2} \times \text{trig. spline}$
Logistic $\frac{e^x}{(1+e^x)^2} dx$	\mathbb{R}	4	×
<i>Triangular</i>	$[-1, 1]$	≈ 0.1729	<i>linked to Bessel J_0</i>

(*) For the truncated Exponential on $[a, b] \subseteq \mathbb{R}^+$, we use $\omega = \pi/(b - a)$

(**) If $a < 0 < b$, the spectral gap is the zero in $]0, \min(\pi/|a|, \pi/|b|)[$ of $x \mapsto \cotan(|a|x) + \cotan(|b|x) + 1/x$

Part IV

A numerical method

Principle: Finite elements

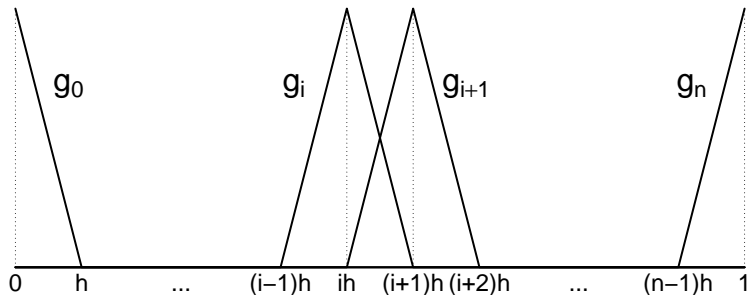


Figure: Basis of finite elements \mathbb{P}_1 on $[0, 1]$. The g_i 's are hat functions for $i = 1, \dots, n - 1$, truncated at the boundaries ($i = 0$ and $i = n$).

Principle: Finite elements

The idea is to solve numerically the spectral problem (P2)

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Solutions are obtained as the limit of solutions in the finite dim. space \mathbb{P}_1 .

Principle: Finite elements

The idea is to solve numerically the spectral problem (P2)

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Solutions are obtained as the limit of solutions in the finite dim. space \mathbb{P}_1 .

In \mathbb{P}_1 , the problem is to find $\mathbf{f}_h \in \mathbb{R}^{n+1}$ such that

$$K_h \mathbf{f}_h = \lambda M_h \mathbf{f}_h$$

with: $K_h = (\langle g'_i, g'_j \rangle)_{0 \leq i, j \leq n}$ and $M_h = (\langle g_i, g_j \rangle)_{0 \leq i, j \leq n}$.

Principle: Finite elements

The idea is to solve numerically the spectral problem (P2)

$$\langle f', g' \rangle = \lambda \langle f, g \rangle \quad \forall g \in \mathcal{H}_\mu^1(\Omega)$$

Solutions are obtained as the limit of solutions in the finite dim. space \mathbb{P}_1 .

In \mathbb{P}_1 , the problem is to find $\mathbf{f}_h \in \mathbb{R}^{n+1}$ such that

$$K_h \mathbf{f}_h = \lambda M_h \mathbf{f}_h$$

with: $K_h = (\langle g'_i, g'_j \rangle)_{0 \leq i, j \leq n}$ and $M_h = (\langle g_i, g_j \rangle)_{0 \leq i, j \leq n}$.

Using the Choleski dec. of $M_h = L_h L_h^T$, we obtain an **eigenvalues problem**

$$\widetilde{K}_h \widetilde{\mathbf{f}}_h = \lambda \widetilde{\mathbf{f}}_h$$

with $\widetilde{K}_h = L_h^{-1} K_h (L_h^T)^{-1}$ and $\widetilde{\mathbf{f}}_h = L_h^T \mathbf{f}_h$.

Convergence properties

Proposition

Assume that Ω is bounded and $\rho > 0$ on $\bar{\Omega}$.

Consider the solutions of the spectral problem in \mathbb{P}_1 ,

$$0 = \lambda_{0,h} \leq \lambda_{1,h} \leq \dots \leq \lambda_{n,h}$$

and $u_{0,h}, u_{1,h}, \dots, u_{n,h}$ corr. eigenvectors. Let $\ell \geq 1$ s.t. $f_{\text{opt}} \in \mathcal{H}_\mu^{\ell+1}(\Omega)$. Then:

$$|\lambda_{1,h} - \lambda(\mu)| = O(h^{2\ell}), \quad |u_{1,h} - f_{\text{opt}}| = O(h^\ell)$$

Convergence properties

Proposition

Assume that Ω is bounded and $\rho > 0$ on $\bar{\Omega}$.

Consider the solutions of the spectral problem in \mathbb{P}_1 ,

$$0 = \lambda_{0,h} \leq \lambda_{1,h} \leq \dots \leq \lambda_{n,h}$$

and $u_{0,h}, u_{1,h}, \dots, u_{n,h}$ corr. eigenvectors. Let $\ell \geq 1$ s.t. $f_{\text{opt}} \in \mathcal{H}_{\mu}^{\ell+1}(\Omega)$. Then:

$$|\lambda_{1,h} - \lambda(\mu)| = O(h^{2\ell}), \quad |u_{1,h} - f_{\text{opt}}| = O(h^{\ell})$$

Proof. If $\mu = \mathcal{U}(\Omega)$, the result comes from theory on finite elements (see e.g. [Raviart and Thomas, 1988]), as all eigenvalues are simple.

Convergence properties

Proposition

Assume that Ω is bounded and $\rho > 0$ on $\bar{\Omega}$.

Consider the solutions of the spectral problem in \mathbb{P}_1 ,

$$0 = \lambda_{0,h} \leq \lambda_{1,h} \leq \dots \leq \lambda_{n,h}$$

and $u_{0,h}, u_{1,h}, \dots, u_{n,h}$ corr. eigenvectors. Let $\ell \geq 1$ s.t. $f_{\text{opt}} \in \mathcal{H}_{\mu}^{\ell+1}(\Omega)$. Then:

$$|\lambda_{1,h} - \lambda(\mu)| = O(h^{2\ell}), \quad |u_{1,h} - f_{\text{opt}}| = O(h^{\ell})$$

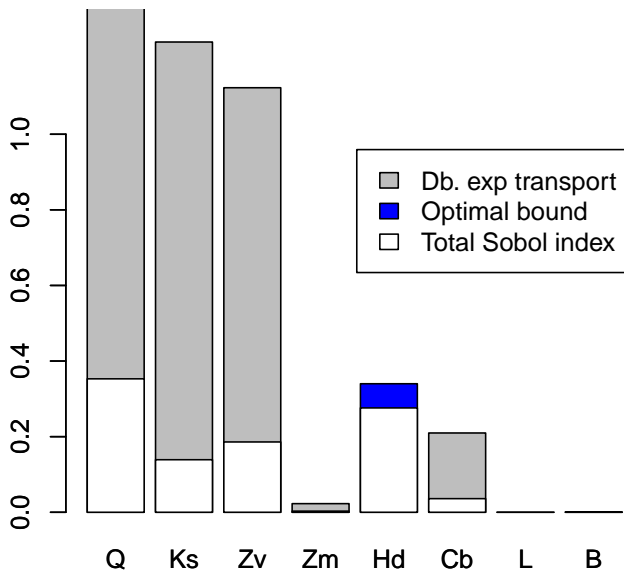
Proof. If $\mu = \mathcal{U}(\Omega)$, the result comes from theory on finite elements (see e.g. [Raviart and Thomas, 1988]), as all eigenvalues are simple.

This also applies under the assumptions above since μ is a bounded perturbation of $\mathcal{U}(\Omega)$: $0 < m < \rho(t) < M$.

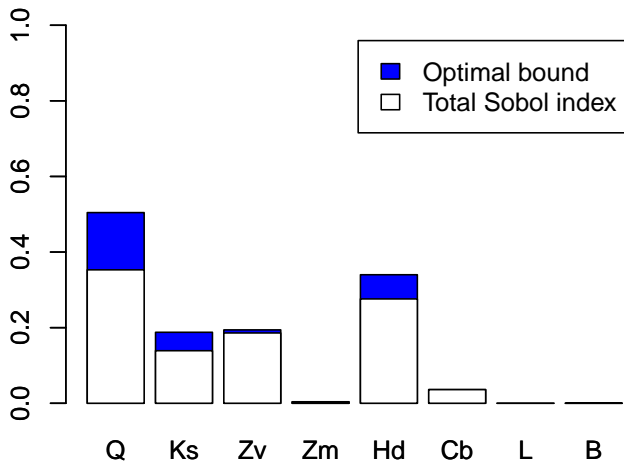
Part V

Applications

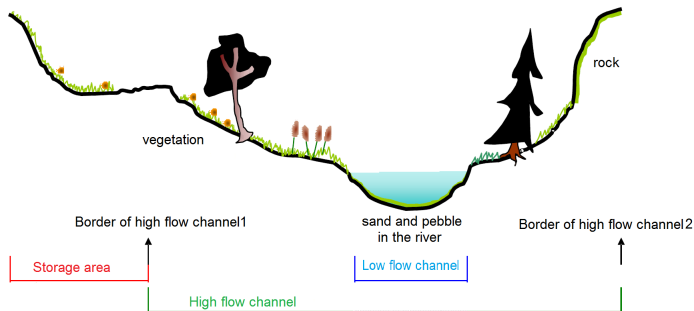
Come-back to the case study



Come-back to the case study



Application on a 1D hydraulic model



- Mascaret simulator on Vienne river (Saint Venant Lab.)
- $d = 37$ random inputs (uniform and truncated Gaussian)
- Output: The water level at a specific river location
- Adjoint model gives derivatives (cost independent of d) and DGSM [Petit et al., 2016]

Application on a 1D hydraulic model

Study with $n = 20,000$ on 5 inputs previously identified as active

Inputs	$K_{s,c}^{11}$	$K_{s,c}^{12}$	dZ^{11}	dZ^{12}	Q
μ	\mathcal{U}	\mathcal{U}	\mathcal{TN}	\mathcal{TN}	\mathcal{TN}
S^T	0.456 ($2e-3$)	0.0159 ($1e-4$)	0.293 ($1e-3$)	0.015 ($1e-4$)	0.239 ($1e-3$)
By double exponential transport					
Upper bound	-	-	1.844 ($2e-3$)	0.116 ($2e-3$)	1.504 ($1.5e-2$)
By logistic transport					
Upper bound	-	-	0.461 ($4e-3$)	0.028 ($5e-4$)	0.376 ($4e-3$)
Optimal Poincaré constant					
Optimal bound	0.625 ($2e-4$)	0.029 ($1e-5$)	0.288 ($3e-3$)	0.017 ($3e-4$)	0.235 ($2e-3$)

Part VI

Conclusion

Conclusions

Conclusions

- ① *DGSM allow doing low-cost screening based on Sobol indices*
⇒ Will work if the function is not varying too quickly

Conclusions

- 1 *DGSM allow doing low-cost screening based on Sobol indices*
⇒ Will work if the function is not varying too quickly
- 2 $C_P(\mu)$ can be computed semi-analytically for simple distributions, e.g. *in blue* in our initial list:
 - ▶ Frequently: *Uniform* – (truncated) *Gaussian* – *Triangular* – (truncated) lognormal – *truncated Exp.* – (truncated) Weibull – (truncated) Gumbel
 - ▶ Less frequently: (Inverse) Gamma – Beta – Trapezoidal – Generalized Extreme Value
- 3 $C_P(\mu)$ can be computed numerically with finite elements.

See more details on our preprint

<https://hal.archives-ouvertes.fr/hal-01388758>

Acknowledgements






Part of this research was conducted within the frame of the Chair in Applied Mathematics OQUAIDO, gathering partners in technological research (BRGM, CEA, IFPEN, IRSN, Safran, Storengy) and academia (CNRS, Ecole Centrale de Lyon, Mines Saint-Etienne, University of Grenoble, University of Nice, University of Toulouse) around advanced methods for Computer Experiments.

We are also grateful to:

- Fabrice Gamboa, who initiated this research.
- Saint Venant Lab. for providing the Mascaret test case and Sébastien Petit who has performed the computations on this model.
- Laurence Grammont and the members of the team 'Génie Mathématique & Industriel' for useful discussions.
- The participants of the previous conferences where this research was presented!

Part VII

References - Thank you for your attention!

-  Ané, C., Blachère, S., Chafaï, D., Fougères, P., Gentil, I., Malrieu, F., Roberto, C., and Scheffer, G. (2000).
Sur les inégalités de Sobolev logarithmiques, volume 10 of *Panoramas et Synthèses*.
Société Mathématique de France, Paris.
-  Bobkov, S. and Götze, F. (2009).
Hardy Type Inequalities via Riccati and Sturm-Liouville Equations, pages 69–86.
Springer New York.
-  Bobkov, S. G. and Houdré, C. (1997).
Isoperimetric constants for product probability measures.
The Annals of Probability, 25(1):184–205.
-  Dautray, R. and Lions, J. (1990).
Mathematical Analysis and Numerical Methods for Science and Technology: Volume 3 Spectral Theory and Applications.
Springer.
-  Efron, B. and Stein, C. (1981).
The jackknife estimate of variance.

The Annals of Statistics, 9(3):586–596.



Iooss, B. (2011).

Revue sur l'analyse de sensibilité globale de modèles numériques.

Journal de la Société Française de Statistique, 152:1–23.



Iooss, B. and Lemaitre, P. (2015).

A review on global sensitivity analysis methods.

In Meloni, C. and Dellino, G., editors, *Uncertainty management in Simulation-Optimization of Complex Systems: Algorithms and Applications*, pages 101–122. Springer.



Kucherenko, S., Rodriguez-Fernandez, M., Pantelides, C., and Shah, N. (2009).

Monte carlo evaluation of derivative-based global sensitivity measures.

Reliability Engineering and System Safety, 94:1135–1148.



Lamboni, M., Iooss, B., Popelin, A.-L., and Gamboa, F. (2013).

Derivative-based global sensitivity measures: General links with Sobol' indices and numerical tests.

Mathematics and Computers in Simulation, 87:45–54.



Petit, S., Zaoui, F., Popelin, A.-L., Goeury, C., and Goutal, N. (2016).

Couplage entre indices à base de dérivées et mode adjoint pour l'analyse de sensibilité globale. Application sur le code Mascaret.

Preprint, <https://hal.archives-ouvertes.fr/hal-01373535>.



Raviart, P. and Thomas, J. (1988).

Introduction à l'analyse numérique des équations aux dérivés partielles. Masson.



Roustant, O., Fruth, J., looss, B., and Kuhnt, S. (2014).

Crossed-derivative based sensitivity measures for interaction screening. *Mathematics and Computers in Simulation*, 105:105 – 118.



Sobol, I. (1993).

Sensitivity estimates for non linear mathematical models.

Mathematical Modelling and Computational Experiments, 1:407–414.



Sobol, I. and Gershman, A. (1995).

On an alternative global sensitivity estimator.

In *Proceedings of SAMO 1995*, pages 40–42, Belgirate, Italy.