Gradient-enhanced surrogate modeling and global sensitivity analysis with Poincaré chaos expansions

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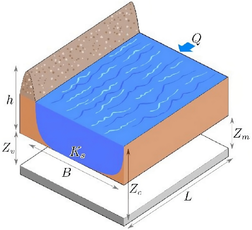
Outline

1. Introduction
2. Poincaré basis
3. Gradient-enhanced surrogate modeling and GSA
4. Numerical results
5. Conclusions

A black-box model

$$\boldsymbol{X} = \underbrace{(X_1, \dots, X_d)}_{\substack{\text{Independent}\\ \text{random variables}\\ \text{(Input)}}} \mapsto f(\boldsymbol{X}) = \underbrace{Y}_{\substack{\text{Model}\\ \text{output}}} \in \mathbb{R}$$



- Maximal overflow in one year

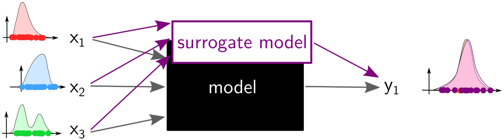
$$S = Z_v + \left(\frac{Q}{BK_s \sqrt{\frac{Z_m - Z_v}{L}}} \right)^{\frac{3}{5}} - H_d - C_b .$$

- Annual maintenance cost

$$C = \mathbb{1}_{S>0} + \left(0.2 + 0.8\left(1 - e^{-\frac{1000}{S^2}}\right)\right)\mathbb{1}_{S\leq 0} + \frac{1}{20}\max\left(H_d, 8\right).$$

Two key tasks

- Construct a surrogate model $\hat{f}(\boldsymbol{X}) \approx f(\boldsymbol{X})$, much cheaper to evaluate.



(Figure shamelessly stolen from Nora Lüthen)

- Perform Global Sensitivity Analysis to measure the influence of the input variables.

Total Sobol indices

- Hoeffding-Sobol decomposition:

$$Y = \sum_{I \subset \{1,\dots,d\}} f_I(X_I),$$

(Ex: $X_{\{1,3,5\}} = (X_1, X_3, X_5)$).

- Total Sobol index of X_k:

$$D_k^{\text{tot}} = \sum_{I \ni k} Var(f_I(X_I)),$$

$$S_k^{\text{tot}} = \frac{1}{Var(Y)} D_k^{\text{tot}} \in [0,1].$$

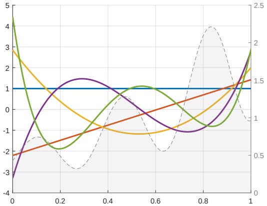
Using Polynomial Chaos Expansions (PCE)

- The model can be written as

$$f(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} c_{\boldsymbol{\alpha}}\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} c_{\boldsymbol{\alpha}}\, \psi^{(1)}_{\alpha_1}(X_1)\dots\psi^{(d)}_{\alpha_d}(X_d),$$

where each $(\psi^{(k)}_n)$ is a family of 1D orthogonal polynomials w.r.t. $X_k \sim \mu_k$.

1D orthogonal polynomials:



- Classical ones:

Hermite polynomials $\sim \mathcal{N}(0,1)$

Laguerre polynomials $\sim \Gamma(\alpha,\beta)$

Jacobi polynomials $\sim \mathcal{B}(a,b)$.

Surrogate model and total Sobol indices estimators

- One estimates the coefficients $c_{\boldsymbol{\alpha}}$ using model evaluations $f(\boldsymbol{X}^1),\dots,f(\boldsymbol{X}^N)$.

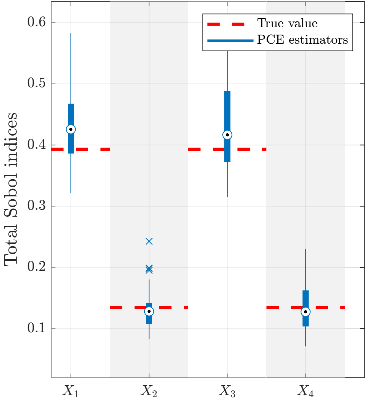
$$\tilde{f}(\boldsymbol{X}) = \sum_{\alpha\in\tilde{\mathcal{A}}} \hat{c}_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{X}), \qquad \tilde{S}^{\mathrm{tot}}_k = \frac{\sum_{\alpha\in\tilde{\mathcal{A}},\alpha_k>0}\hat{c}^2_{\alpha}}{\sum_{\alpha\in\tilde{\mathcal{A}},\alpha\neq 0}\hat{c}^2_{\alpha}}.$$

Example using PCE

- Toy model with interactions ($N = 40$)

$$f(X) = \prod_{k=1}^{4} \frac{1}{1 + (X_k - a_k)^2}, \quad a_i = \frac{(-1)^k}{k+1}, \quad X_k \sim \mathcal{U}(-1, 1).$$

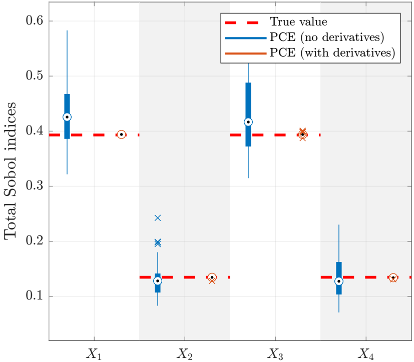
- $(\psi_n^{(k)})_{n \geq 0}$ are Legendre polynomials (Jacobi polynomials).



Gradient-enhanced PCE

Q: What if we also have derivative information $\partial_k f(\boldsymbol{X}^1), \ldots, \partial_k f(\boldsymbol{X}^N)$?

- For Legendre (Jacobi) polynomials Adcock & Sui (2019):



- Peng (2016), Guo (2018). Similar results can be obtained using

  Hermite $\sim \mathcal{N}(0,1)$, Laguerre $\sim \mathrm{Gamma}(\alpha, \beta)$, Jacobi $\sim \mathrm{Beta}(a, b)$.
- What about **other** probability distributions?
- **Key property:** those three polynomial families, are **Poincaré bases**.

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1D Weighted Poincaré Inequality

- Let $\mu(dx) = \rho(x)\mathbb{1}_{(a,b)}(x)\,dx$ be a probability measure and $w\colon (a,b) \to \mathbb{R}^+$ a weight.
- μ satisfies a weighted Poincaré inequality with weight w if:

$$\int_a^b g^2\, d\mu \leq C_P(\mu, w) \int_a^b w\,(g')^2\, d\mu, \quad \forall g \ \text{ centered} \quad (\int_a^b g\, d\mu = 0).$$

- $C_P(\mu, w)$ is the smallest (optimal) constant.

Connection with Derivative Global Sensitivity Measures (DGSM):

- If $X_k \sim \mu_k$ satisfies a weighted Poincaré inequality with $w_k \geq 0$, then

$$S_k^{\mathrm{tot}} \leq \frac{C_P(\mu_k, w_k)}{\mathrm{Var}(f(\boldsymbol{X}))}\, \mathbb{E}\underbrace{\left[w_k(X_k)\left(\frac{\partial f}{\partial x_k}(\boldsymbol{X})\right)^2\right]}_{\text{Weighted DGSM}}.$$

- Classical case ($w_k \equiv 1$)
  - Kucherenko et al. (2009).
  - Lamboni et al. (2013).
  - Roustant et al. (2017).
- Weighted case ($w_k \not\equiv 1$)
  - Song et al. (2018).
  - Heredia et al. (2026).

Two eigenvalue problems

$$C_P(\mu, w) = \underbrace{\sup_{g \text{ centered}} \frac{\int_a^b g^2 \, d\mu}{\int_a^b w\,(g')^2 d\mu}}_{\text{Optimisation problem}}, \qquad \left(\int_a^b g^2 \, d\mu \leq C_P(\mu, w) \int_a^b w\,(g')^2 \, d\mu \right).$$

Characterization:

The optimal constant satisfies

$$C_P(\mu, w) = 1/\lambda_1,$$

where λ_1 is the smallest positive eigenvalue in the equivalent problems:

(P1) Find (λ, g), solutions of

$$\lambda \int_a^b g\,h\,d\mu = \int_a^b w\,g'\,h'\,d\mu, \qquad \text{for all } h.$$

(P2) Find (λ, g), solutions of

$$-L_w g := -\frac{1}{\rho}(w\,g'\,\rho)' = \lambda\,g, \qquad (+\text{ boundary conditions})$$

Poincaré basis

- Under some conditions on ρ and w, (P1) and (P2) admit a countable family of solutions $(\lambda_n, \psi_n)_{n\geq 0}$:

(P1) $$\lambda_n \int_a^b \psi_n \, h \, d\mu = \int_a^b w \, {\psi_n}' \, h' \, d\mu, \qquad \text{for all } h,$$

Numerical computation: finite elements

- $(\psi_n)_{n\geq 0}$ constitute an orthogonal basis of $L^2(\mu)$ — we call it **Poincaré basis**

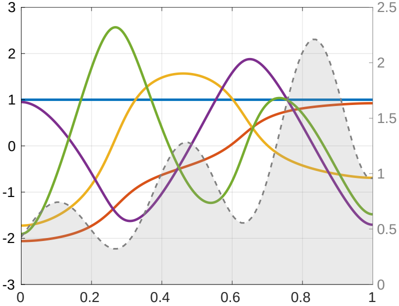
The key property: The family of derivatives $(\psi_n')_{n\geq 1}$ is orthogonal in $L^2(\mu, w)$:

$$\int_a^b w \, \psi_n' \, \psi_m' \, d\mu = \lambda_n \int_a^b \psi_n \, \psi_m \, d\mu = 0, \qquad \text{for all } n \neq m.$$

One can show that it is an orthogonal **basis**.

The Poincaré basis depends on the weight

- Given μ, the choice of w determines the Poincaré basis.
  - $w \equiv 1$ — classical Poincaré basis [Roustant et al. (2020)].



- ψ_1 is always monotonic and centered.

The power to fix a basis function

Idea: Given μ, can we fix the eigenfunction ψ_1?

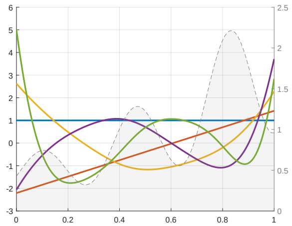
Weight construction [Germain and Swan (2022)] [Heredia et al. (2026)]:

Take your favorite centered monotonic function g. Can we have $g = \psi_1$? **R:** Yes.

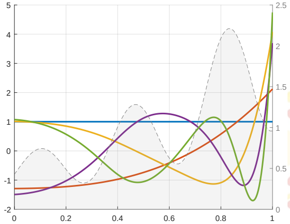
$w_g($ $w_g =$ "weight for which $g = \psi_1$" $g\Big)$

Examples:

Poincaré basis when g is linear

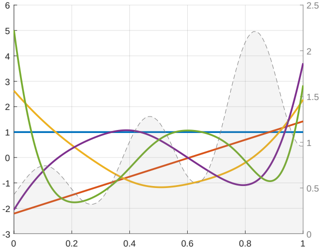


Poincaré basis when $g(x) \approx x^3$



Poincaré basis using the linear standard weight

- Consider $w_{lin} := w_g$, with g linear.



Examples:

μ	w_{lin}	Operator $L_{w_{lin}}$	$(\psi_n)_{n\geq 0}$
$\mathcal{N}(0,1)$	1	Hermite	Hermite polynomials
$\mathrm{Gamma}(\alpha,\beta)$	x/β	Laguerre	Laguerre polynomials
$\mathrm{Beta}(a,b)$	$x(1-x)/(a+b)$	Jacobi	Jacobi polynomials

Note: Poincaré bases coincide with polynomials in these three cases ***only****.*

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Poincaré chaos expansion

- Consider tensor products of 1D Poincaré bases $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \psi^{(1)}_{\alpha_1}(x_1)\dots\psi^{(d)}_{\alpha_d}(x_d)$.

Surrogate models: Regression problem:

$$f(\boldsymbol{x}) \approx \sum_{\alpha\in\tilde{\mathcal{A}}} \hat{c}_\alpha\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \qquad\qquad \Psi\hat{c} \approx y$$

$$\xrightarrow{\boldsymbol{x}^1,\dots,\boldsymbol{x}^d}$$

$$\sqrt{w_k(x_k^i)}\,\partial_k f(\boldsymbol{x}) \approx \sum_{\alpha\in\mathcal{A}} \hat{c}_\alpha \sqrt{w_k(x_k^i)}\,\partial_k\psi_{\boldsymbol{\alpha}}(x) \qquad\qquad \Psi_{\partial_k}\hat{c} \approx y_{\partial_k}$$

where

$$\Psi_{i\,\alpha} = \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}^i), \quad (\Psi_{\partial_k})_{i\,\alpha} = \sqrt{w_k(x_k^i)}\,\partial_k\psi_{\boldsymbol{\alpha}}(x^i)$$

$$y_i = f(\boldsymbol{x}^i), \qquad (y_{\partial_k})_i = \sqrt{w_k(x_k^i)}\,\partial_k f(x^i)$$

- Combined system:

$$\begin{bmatrix} \Psi \\ \Psi_{\partial_1} \\ \vdots \\ \Psi_{\partial_d} \end{bmatrix} \hat{c} \approx \begin{bmatrix} y \\ y_{\partial_1} \\ \vdots \\ y_{\partial_d} \end{bmatrix}$$

Note: It is simple because the Poincaré derivatives form an orthogonal basis!

Coefficient computation

- Coefficients $\hat{c}$ computed by ℓ^1-minimization:

$$\hat{c} = \arg\min_{c} \left(\|\Psi c - y\|_2^2 + \sum_{k=1}^{d} \|\Psi_{\partial_k} c - y_{\partial_k}\|_2^2 + \gamma \|c\|_1 \right).$$

- Algorithm: Least-Angle Regression (LARS) with γ chosen by leave-one-out error, using UQLab – ETH Zurich (check their website).

Sobol' indices

Computed from coefficients:

$$\widehat{S}_k^{\mathrm{tot}} = \frac{\sum_{\alpha\in\mathcal{A},\alpha_i>0} \hat{c}_\alpha^2}{\sum_{\alpha\in\mathcal{A},\alpha\neq 0} \hat{c}_\alpha^2}$$

Global error (H^1 on validation set X_{val}):

$$\begin{aligned} E_{H^1} = {} & \hat{\mathbb{E}}[(f(X_{\mathrm{val}}) - \widehat{f}(X_{\mathrm{val}}))^2] \\ & + \sum_{k=1}^{d} \hat{\mathbb{E}}\left[w_k(X_{k,\mathrm{val}}) \left(\partial_k f(X_{\mathrm{val}}) - \partial_k \widehat{f}(X_{\mathrm{val}})\right)^2 \right] \end{aligned}$$

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Flood model

- Maximal annual overflow:

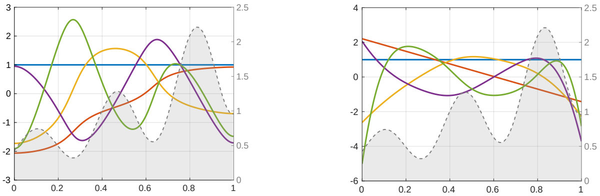
$$S = Z_v + \left(\frac{Q}{BK_s\sqrt{\frac{Z_m - Z_v}{L}}} \right)^{\frac{3}{5}} - H_d - C_b.$$

- Annual maintenance cost

$$C = \mathbb{1}_{S>0} + \left(0.2 + 0.8\left(1 - e^{-\frac{1000}{S^2}}\right)\right)\mathbb{1}_{S\leq 0} + \frac{1}{20}\max\left(H_d, 8\right).$$

- Input variables: The inputs are Q (Truncated Gumbel), K_s (Truncated Normal), H_d (Uniform), and Z_v, Z_m, C_b, L, B (Triangular).

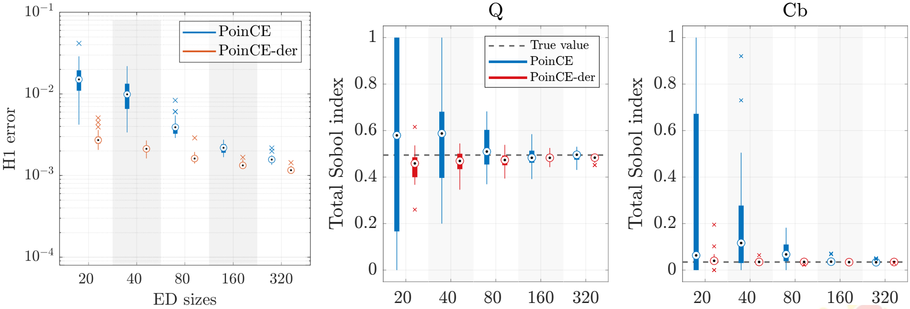
Two Poincaré bases:



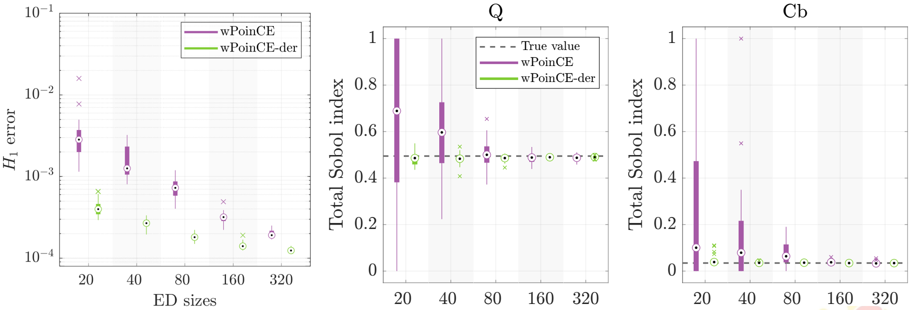
Using $w \equiv 1$

Using w_{lin}

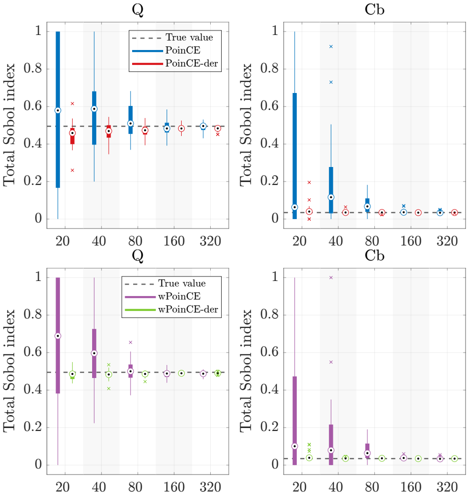
Flood cost model ($w \equiv 1$)



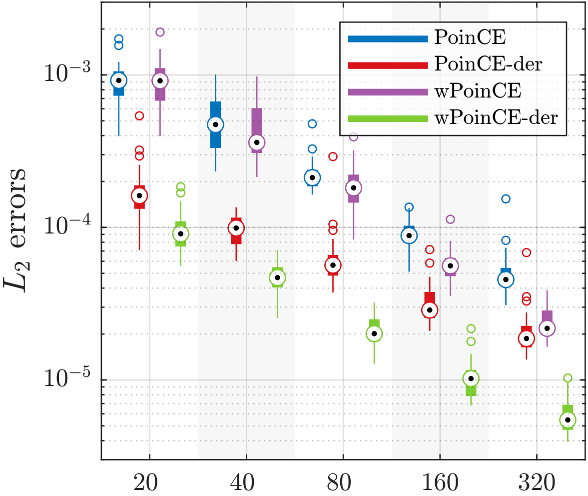
Flood cost model (w_{lin})



Flood cost model ($w \equiv 1$ vs $w = w_{lin}$)



Flood cost model ($w \equiv 1$ vs $w = w_{lin}$)



Conclusions

Poincaré bases offer multiple advantages:

- Well suited when working with derivatives.
- Control on the basis functions.
- Being able to deal with general distributions.

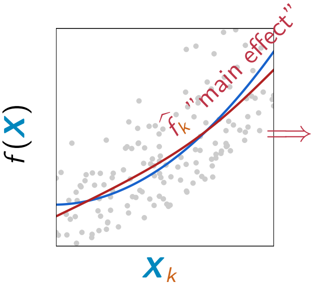
This work generalizes:

- The classical framework when $w \equiv 1$.
- Gradient-enhanced PCE with Hermite, Laguerre and Jacobi polynomials.

Next steps:

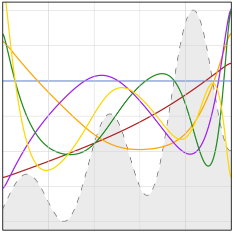
- Make it available in UQlab (ETH Zurich).
- Use other Poincaré bases for models whose behavior is not linear.
  - Data-driven weights.

Data-driven weight



$\Longrightarrow$ $\widehat{w}_k$: "weight for which $\widehat{f}_k = \psi_1$" $\Longrightarrow$

$\Downarrow$

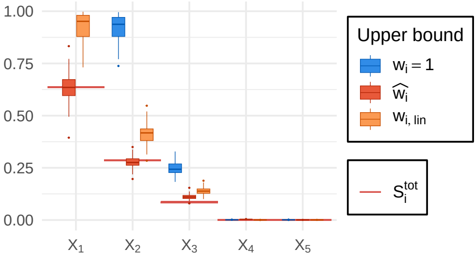


Upper bounds

Heredia et al. (2026)

$$S_k^{\text{tot}} \lesssim \mathbb{E}\left[w_k(X_k)\left(\frac{\partial f}{\partial x_k}(\boldsymbol{X})\right)^2\right]$$

$$f(\boldsymbol{X}) = \prod_{k=1}^{5}\left(a_k\left(\underbrace{X_k^4}_{\mathcal{U}(0,1)} - \frac{1}{5}\right)+1\right).$$



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Perspective: multi-dimensional case

- **Multi-dimensional** setting:

$$X = (\underbrace{(X_{I_1}), \dots, (X_{I_d})}_{\substack{\text{Independent} \\ \text{random } \textbf{vectors} \\ \text{(Input)}}}) \mapsto f(X) = \underbrace{Y}_{\substack{\text{Model} \\ \text{output}}}$$

Multi-dim weighted Poincaré inequality

$$\int g^2 \, d\mu \leq C_P(\mu, W) \int \langle W \nabla g, \nabla g \rangle \, d\mu$$

Upper bound

$$S^{\text{tot}}_{I_k} \lesssim \mathbb{E}\left[\langle W_{I_k} \nabla_{I_k} f(\boldsymbol{X}), \nabla_{I_k} f(\boldsymbol{X}) \rangle \right]$$

Multi-dim Poincaré basis

$$\lambda_n \int \psi_n \, h \, d\mu = \int \langle W \nabla \psi_n, \nabla h \rangle \, d\mu$$

$$-L_W \psi_n = -\frac{1}{\rho} \operatorname{div}(W \, \nabla \psi_n \, \rho) = \lambda_n \psi_n$$

Chaos expansion

$$\tilde{f}(\boldsymbol{X}) = \sum_{\alpha \in \tilde{\mathcal{A}}} \hat{c}_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

$$\tilde{S}^{\text{tot}}_{I_k} = \frac{\sum_{\alpha \in \tilde{\mathcal{A}}, \alpha_{I_k} > 0} \hat{c}_{\alpha}^2}{\sum_{\alpha \in \tilde{\mathcal{A}}, \alpha \neq 0} \hat{c}_{\alpha}^2}$$

Perspective: multi-dimensional case

- We establish Weighted Poincaré inequalities for:
  - Elliptical distributions:

    $$\rho(\boldsymbol{x}) \approx h\left(\langle \Sigma(\boldsymbol{x}-m), \boldsymbol{x}-m\rangle\right).$$

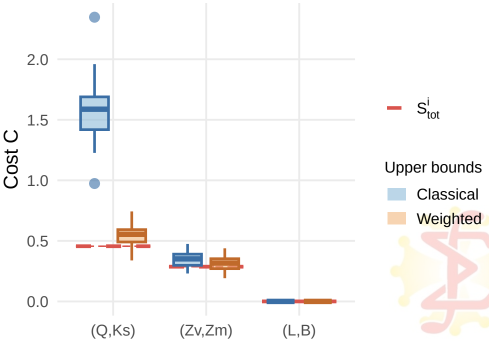
    Ex: Multivariate Normal.
  - Multivariate Liouville distributions:

    $$\rho(\boldsymbol{x}) \approx h\left(\sum_{k=1}^{n} x_k\right), \qquad x_k > 0.$$

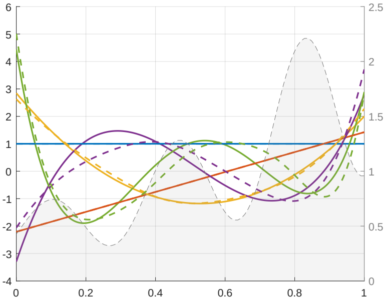
    Ex: Multivariate Pareto.
  - Copulas + transport $\Longrightarrow$ more general distributions.

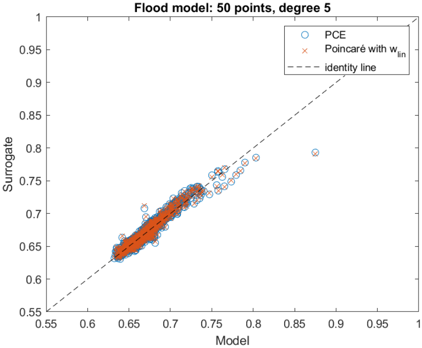
Application:

- Flood cost model.
  (Q, K_s), (Z_v, Z_m) (L, B) $\sim$ Gaussian copula.



Polynomials vs Poincaré basis





- Solid lines: Orthogonal polynomials.
- Dashed lines: Poincaré eigenfunctions.

Enforcing other eigenfunctions ψ_n?

- The weight for which $g = \psi_n$ (centered) is always given by

$$w_g(x) = -\frac{\lambda_n}{g'\rho(x)} \int_a^x g(y)\rho(y)\,dy \quad \left(w_g\, g'(x) = -\frac{\lambda_n}{\rho(x)} \int_a^x g(y)\rho(y)\,dy \right).$$

- Two ideas, given g:
  - If g is such that

$$g(x) = 0 \Leftrightarrow \int_a^x g(y), \rho(y)\,dy = 0,$$

then (I think) $w_g \geq 0$.

  - (Olivier Zahm) Denoting $g^\uparrow(x) = \int_a^x g'(y)\,dy$ and $m = \int_a^b g^\uparrow(y)\rho(y)\,dy$, consider

$$\boxed{w_g^*(x) = -\frac{\mathrm{Var}_\rho(g)}{\mathrm{Var}_\rho(g^\uparrow)} \frac{1}{\rho(x) g^{\uparrow\prime}(x)} \int_a^x \left(g^\uparrow(t) - m\right) \rho(t)\,dt}.$$

Poincaré basis existence

- Poincaré basis functions $(\psi_n)_{n\geq 0}$ are solutions of the Sturm Liouville problem:

(P2)
$$\begin{cases} -L_w g := -\frac{1}{\rho}(w\, g'\, \rho)' = \lambda\, g, \\ (wg'\rho)(a) = (wg'\rho)(b) = 0. \end{cases}$$

- Some sufficient conditions of existence Zettl (2005)
  - $\int_a^b \frac{1}{w\rho} < \infty$ (Regular sturm Liouville problem).
  - The anti-derivatives of $\frac{1}{w\rho}$ belong to $L^2(\mu)$ (Limit circle).
- A case where the Poincaré basis does not exist:

$$\rho(x) = e^{-x}, \quad w(x) = 1, \quad x > 0.$$

Indeed, $C_P(\mu, w) = 1$, with "$\psi_1(x)$" $= \left(1 - \frac{1}{2}\gamma x\right) e^{\frac{1}{2}\gamma x} \notin L^2(\mu)$.

Data-driven weight consistency

Suppose that:

- $\widehat{f_k}$ is centered with respect to μ_k.
- $\widehat{f_k}$ satisfies $\widehat{f_k}'(a) \neq 0$ and $\widehat{f_k}'(b) \neq 0$.
- As $n \to \infty$, we have the almost sure convergence:

$$\left\|\widehat{f_k} - f_k\right\|_\infty \to 0 \quad \text{and} \quad \left\|\widehat{f_k}' - f_k'\right\|_\infty \to 0$$

Then $\widehat{w_k}$ converges almost surely:

$$\left\|\widehat{w_k} - w_{f_k}\right\|_\infty \to 0$$

Moreover

$$\frac{1}{n}\sum_{i=1}^{n} \widehat{w}_i(\boldsymbol{X}_k^i)\left(\frac{\partial f}{\partial x_k}(\boldsymbol{X}^i)\right)^2 \to \mathbb{E}\left[w_k(\boldsymbol{X}_k)\left(\frac{\partial f}{\partial x_k}(\boldsymbol{X})\right)^2\right].$$

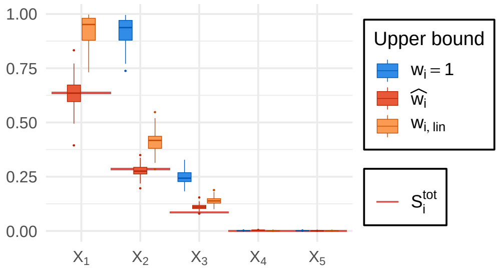
Data-driven weight application

The model

- $X_1, \dots, X_5 \sim \mathcal{U}(0,1)$.
- $f(X) = \prod_{i=1}^{5} \left(\underbrace{a_i \left(X_i^4 - \frac{1}{5} \right)}_{f_i(X_i)} + 1 \right)$,

where $a = \left(\frac{1}{2}, \frac{1}{3}, \frac{1}{5.5}, \frac{1}{91}, \frac{1}{91} \right)$.
- $N = 150$.

Indices and upper bounds



Main effects and their monotonic estimators