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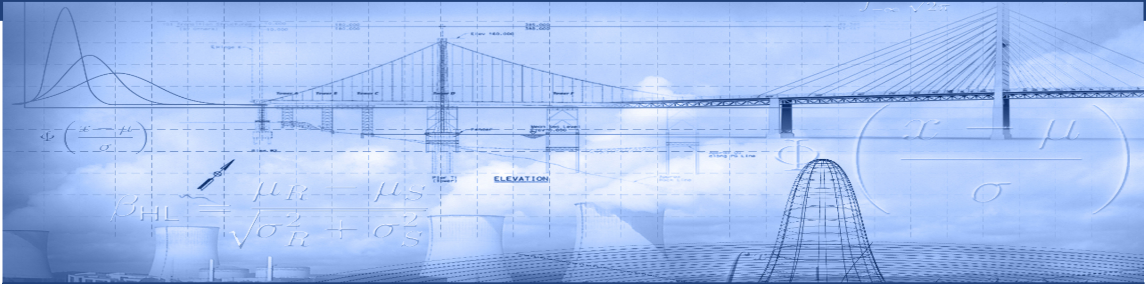

Poincaré chaos expansions for derivative-enhanced surrogate modelling and sensitivity analysis

UQSay #41

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- Poincaré inequalities
- Sensitivity analysis
- ...

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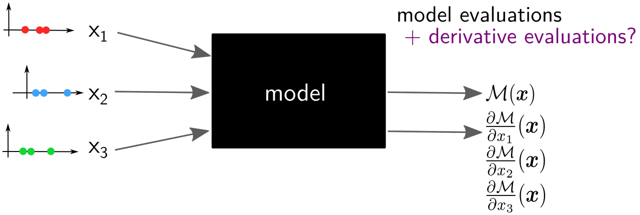
- UQ for engineering models
- Surrogate modelling
  in particular, sparse polynomial chaos expansions
- ...

Global sensitivity analysis using derivative-based sparse Poincaré chaos expansions, `https://arxiv.org/abs/2107.00394`

Poincaré chaos expansions: Topics

Black-box model
Surrogate modelling
Sensitivity analysis
Using derivative information



Outline

Spectral expansions as surrogate models

Variance-based and derivative-based sensitivity analysis

Poincaré constants and the associated differential operator

Computing Poincaré chaos expansions

Numerical example

Conclusion & Outlook

Chaos expansions as surrogate models

Setting:

- Input random vector $\boldsymbol{X}$ with d independent components and joint distribution $f_{\boldsymbol{X}}$
- Model $\mathcal{M} \in L^2_{f_{\boldsymbol{X}}}$ (square-integrable)
- Output random variable $Y = \mathcal{M}(\boldsymbol{X})$

We want to model random variable Y

Let $(\psi_k)_{k\in\mathbb{N}}$ be a basis of $L^2_{f_{\boldsymbol{X}}}$. Then:

$$Y = \mathcal{M}(\boldsymbol{X}) = \underbrace{\sum_{k\in\mathbb{N}} c_k \psi_k(\boldsymbol{X})}_{\text{surrogate model}}$$

For example:

- (Fourier expansion)
- Polynomial chaos expansion
- Poincaré chaos expansion

Approximation of Y by orthogonal polynomials in X ($d = 1$)

Theorem: Density of polynomials in $L^2_{f_X}(\mathcal{D})$ — Ernst et al (2012)

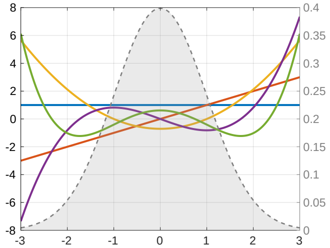
Assume that X possesses finite moments of all orders, and that F_X is continuous.
If the distribution function is uniquely defined by the sequence of its moments, then the polynomials are dense in $L^2_{f_X}(\mathcal{D})$.

Hermite chaos

Wiener (1938); Ghanem, Spanos (1991)

- X Gaussian $\to$ Hermite polynomials:

$$\psi_0(x) = 1,\ \psi_1(x) = x,\ \psi_2(x) = \frac{x^2 - 1}{2}, \ldots$$



Hermite polynomials

Generalized chaos

Xiu, Karniadakis (2002)

- X uniform $\to$ Legendre polynomials
- X Beta $\to$ Jacobi polynomials
- X Gamma $\to$ Laguerre polynomials

Approximation of Y by orthogonal polynomials in X ($d = 1$)

Ernst et al (2012)

Theorem: Density of polynomials in $L^2_{f_X}(\mathcal{D})$

Assume that X possesses finite moments of all orders, and that F_X is continuous.
If the distribution function is uniquely defined by the sequence of its moments, then the polynomials are dense in $L^2_{f_X}(\mathcal{D})$.

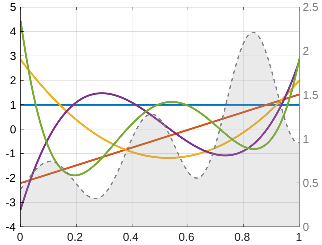
- Notable exception: lognormal distribution!

Arbitrary chaos

Wan and Karniadakis (2006); Oladyshkin and Nowak (2012)

- One can compute an orthogonal polynomial basis for any distribution that fulfills the assumptions (e.g., with compact support)

By the way: the term *polynomial chaos* goes back to Wiener (1938)
$\rightarrow$ Use of the word "chaos" older than Chaos theory in mathematics! (1938 vs 1977)



Orth. polynomials for arbitrary distribution

Polynomial chaos expansion ($d \geq 1$)

Model

Surrogate model

Output

Input

Coefficients

$$Y = \mathcal{M}(\boldsymbol{X}) \approx \mathcal{M}^{\text{PCE}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

Multivariate polynomial

with tensor product basis functions

1D polynomial in x_i of degree α_i

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \prod_{i=1}^{d} \psi^{(i)}_{\alpha_i}(x_i),$$

where the multi-index $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$ defines the degree

and set of multi-indices $\mathcal{A}$, e.g., total-degree basis of degree p:

$$\mathcal{A} = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \sum_{i=1}^{d} \alpha_i \leq p\}$$

- If for each X_i the moment problem is uniquely solvable, then the multivariate polynomials are dense in $L^2_{f_{\boldsymbol{X}}}(\mathcal{D})$ and this approximation converges in mean-square to Y Ernst et al (2012)

How to compute a PCE?

$$Y = \mathcal{M}(\boldsymbol{X}) \approx \mathcal{M}^{\text{PCE}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

Ingredients of a PCE:

- (Basis functions $\{\psi_{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \mathbb{N}^d\}$ defined by input distribution.)
- Need to decide subset of multi-indices $\mathcal{A} \subset \mathbb{N}^d$
- Need to choose points $\boldsymbol{x} \in \mathcal{X} \subset \mathcal{D}$ (experimental design) and collect the corresponding model evaluations $y = \mathcal{M}(\boldsymbol{x})$
- Need to compute the coefficients $\boldsymbol{c}$
  - Projection:

$$c_{\boldsymbol{\alpha}} = \langle \mathcal{M}, \psi_{\boldsymbol{\alpha}} \rangle$$

integration in d dimensions

  - Regression:

$$\boldsymbol{c} = \min_{\boldsymbol{c}'} \left\| \boldsymbol{y} - \boldsymbol{\Psi} \boldsymbol{c}' \right\|_2 \text{ (+ regularization)}$$

properties of $\boldsymbol{\Psi}$ are crucial

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Sobol'-Hoeffding / ANOVA decomposition

Hoeffding (1948); Sobol (1993)

Any $\mathcal{M} \in L^2_{f_{\boldsymbol{X}}}$ can be decomposed uniquely as a sum of terms of increasing complexity

$$\mathcal{M}(\boldsymbol{X}) = m_0 + \sum_{1 \leq i \leq d} m_i(X_i) + \sum_{1 \leq i < j \leq d} m_{i,j}(X_i, X_j) + \cdots + m_{1,\dots,d}(X_1, \dots, X_d)$$

where the terms satisfy $\int m_I(\boldsymbol{X}_I) f_{X_k}(x_k) \mathrm{d}x_k = 0$ for all $k \in I \subset \{1, \dots, d\}$.

Variance decomposition

$$\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right] = \sum_{1 \leq i \leq d} \mathrm{Var}\left[m_i(X_i)\right] + \sum_{1 \leq i < j \leq d} \mathrm{Var}\left[m_{i,j}(X_i, X_j)\right] + \cdots + \mathrm{Var}\left[m_{1,\dots,d}(X_1, \dots, X_d)\right]$$

$\rightarrow$ ANalysis Of VAriance decomposition

Sobol' indices

Variance decomposition

$$\underbrace{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right]}_{:=D} = \sum_{1 \leq i \leq d} \mathrm{Var}\left[m_i(X_i)\right] + \sum_{1 \leq i < j \leq d} \mathrm{Var}\left[m_{i,j}(X_i, X_j)\right] + \cdots + \mathrm{Var}\left[m_{1,\ldots,d}(X_1, \ldots, X_d)\right]$$

total variance

First-order Sobol' index:

$$S_i^1 = \frac{\mathrm{Var}\left[m_i(X_i)\right]}{D},$$

Total Sobol' index:

$$S_i^{\text{tot}} = \frac{1}{D} \sum_{J : i \in J} \mathrm{Var}\left[m_J(X_J)\right]$$

PCE ♡ Sobol' indices

Sudret (2008)

The ANOVA decomposition of a PCE $\mathcal{M}^{\text{PCE}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d} c_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$ is given by

$$m_I(\boldsymbol{X}) := \sum_{\substack{\boldsymbol{\alpha}:\alpha_i>0, i\in I,\\ \alpha_j=0, j\notin I}} c_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

$\psi_{\boldsymbol{\alpha}}$ constant in $j \notin I$

From orthonormality in $L^2_{f_{\boldsymbol{X}}}$ it follows that

$$\mathrm{Var}\left[m_I(\boldsymbol{X})\right] = \sum_{\substack{\boldsymbol{\alpha}:\alpha_i>0, i\in I\\ \alpha_j=0, j\notin I}} c_{\boldsymbol{\alpha}}^2$$

and the total variance and the Sobol' indices are given by

$$D = \sum_{\boldsymbol{\alpha}\neq\boldsymbol{0}} c_{\boldsymbol{\alpha}}^2, \qquad S_i^1 = \frac{1}{D}\sum_{\substack{\boldsymbol{\alpha}:\alpha_i>0,\\ \alpha_j=0, j\neq i}} c_{\boldsymbol{\alpha}}^2, \qquad S_i^{\text{tot}} = \frac{1}{D}\sum_{\boldsymbol{\alpha}:\alpha_i>0} c_{\boldsymbol{\alpha}}^2$$

Any tensor-product orthonormal basis, made from 1D bases that each contain the constant function, allows the same construction

Derivative-based global sensitivity measure (DGSM)

Kucherenko et al. (2009)

Another sensitivity measure: DGSM

$$\nu_i = \mathbb{E}\left[\left(\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{X})\right)^2\right] = \int_{\mathcal{D}} \left(\frac{\partial \mathcal{M}}{\partial x_i}(\boldsymbol{x})\right)^2 f_{\boldsymbol{X}}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \left\| \frac{\partial \mathcal{M}}{\partial x_i} \right\|^2.$$

Relation to Sobol' indices:

Sobol and Kucherenko (2009); Lamboni et al. (2013)

$$S_i^{\text{tot}}\, D \leq C_P\, \nu_i$$

with Poincaré constant C_P of measure $f_{X_i}\mathrm{d}x_i$
$\rightarrow$ low-cost variable screening

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The Poincaré constant in 1D

Definition: The Poincaré constant C_P associated to a measure μ is the best possible constant C with

$$\int g^2 d\mu \leq C \int (g')^2 d\mu \tag{1}$$

for all $g \in H^1_\mu$ with $\int g d\mu = 0$.

"A function with a small (weak) derivative (in the sense of μ)
is close to a constant function (in the sense of μ)."

Useful for:

- Bounding total Sobol' indices — Lamboni et al (2013)
- Convergence rate of Markov chains — Pillaud-Vivien et al (2020)
  Quantifying multimodality of μ
- . . .

In 1D, $C_P(\mu)$ can be computed accurately for a large class of measures μ! — Roustant, Barthe, Iooss (2017)

Eigenproblem for Poincaré differential operator

Roustant, Barthe, Iooss (2017)

Assumption

Assume that f_X is supported on a bounded interval (a,b) and that $f_X(x) = e^{-V(x)}$ with V continuous and piecewise C^1 on $[a,b]$.

Theorem: 1D Poincaré basis

Under this assumption, for the solutions of the eigenproblem

$$\begin{aligned} L\psi := \psi'' - V'\psi' &= -\lambda\psi, \\ \psi'(a) = \psi'(b) &= 0 \end{aligned}$$

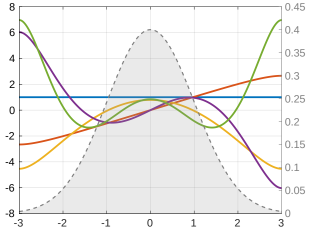
it holds that

- The eigenfunctions $(\psi_k)_{k\geq 0}$ form an orthonormal basis of $L^2_{f_X}$
- Eigenvalues: $0 = \lambda_0 < \lambda_1 < \ldots \to \infty$
- $\lambda_0 = 0$ and $\psi_0(x) = 1$
- $C_P(f_X) = \frac{1}{\lambda_1}$, and ψ_1 attains equality in Eq. (1)

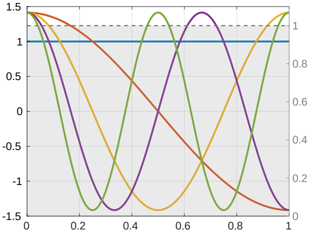
Poincaré basis (1D)

Roustant, Gamboa, Iooss (2020)

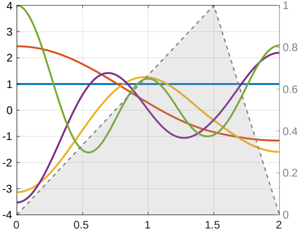
- In general not polynomial
  - Exception: f_X Gaussian $\rightarrow$ Hermite polynomials
  - f_X uniform leads to cosine basis functions (Fourier basis)
- Behavior similar to polynomials:
  - ψ_k has k zeros, i.e., higher-order functions oscillate more
- If $f_X \in C^m$, $\psi_k \in C^{m+1}$ ($f_X \in C^0$ by assumption)



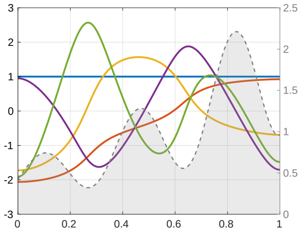
Gaussian



Uniform



Triangular



Custom

Poincaré basis (1D)

Special property

$$\left\langle g', \psi_k' \right\rangle_{f_X} = \lambda_k \left\langle g, \psi_k \right\rangle_{f_X} \text{ for all } g \in H^1_{f_X}$$

- Consequence: the derivatives of the Poincaré basis form again an orthogonal basis of $L^2_{f_X}$, i.e., an orthogonal system that is dense in $L^2_{f_{\boldsymbol{X}}}$:

$$\left\langle \psi_j', \psi_k' \right\rangle_{f_X} = \lambda_k \left\langle \psi_j, \psi_k \right\rangle_{f_X} = \begin{cases} \lambda_k, & \text{if } j = k \\ 0 & \text{else} \end{cases}$$

$\rightarrow$ Well suited for dealing with derivatives.

- The Poincaré basis is the only basis with this property!

Lüthen et al (2021, preprint)

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Poincaré chaos expansion ($\geq$ 1D)

Roustant, Gamboa, Iooss (2020)

Define the Poincaré chaos expansion (PoinCE) by

$$\mathcal{M}(\boldsymbol{X}) \;\approx\; \mathcal{M}^{\text{PoinCE}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

with $(\psi_{\boldsymbol{\alpha}})_{\boldsymbol{\alpha} \in \mathcal{A}}$ tensorized Poincaré basis associated to $f_{\boldsymbol{X}} = \prod_{i=1}^{d} f_{X_i}$

- Basis for $L^2_{f_{\boldsymbol{X}}}(\mathcal{D}) \rightarrow$ chaos expansion just like PCE
- In particular, coefficients of PoinCE yield moments and Sobol' sensitivity indices
- Partial derivatives of multivariate basis functions are orthogonal: for all $g \in H^1_{f_{\boldsymbol{X}}}$,

$$\left\langle \frac{\partial}{\partial x_i} \psi_{\boldsymbol{\alpha}}, \frac{\partial}{\partial x_i} g \right\rangle_{f_{\boldsymbol{X}}} \;=\; \lambda_{i,\alpha_i} \left\langle \psi_{\boldsymbol{\alpha}}, g \right\rangle_{f_{\boldsymbol{X}}}$$

Computation of DGSM from Poincaré coefficients

Lüthen et al (2021, preprint)

Proposition: DGSM formula for Poincaré chaos

Let $\mathcal{M} = \sum_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}$ be the expansion of $\mathcal{M} \in H^1_{f_{\boldsymbol{X}}}$ in the Poincaré basis. Then the DGSM index of $\mathcal{M}$ with respect to X_i is

$$\nu_i = \sum_{\boldsymbol{\alpha}:\alpha_i>0} \lambda_{i,\alpha_i} (c_{\boldsymbol{\alpha}})^2$$

This is an extension of a previous result for Hermite PCE. Sudret and Mai (2015)

We obtain lower and upper bounds to total partial variances:

$$\sum_{\boldsymbol{\alpha}\in\mathcal{A}:\alpha_i>0} (c_{\boldsymbol{\alpha}})^2 \;\leq\; S_i^{\text{tot}} D \;\leq\; C_P(f_{X_i})\,\nu_i \;=\; \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d:\alpha_i>0} \frac{\lambda_{i,\alpha_i}}{\lambda_{i,1}} (c_{\boldsymbol{\alpha}})^2 \,.$$

Poincaré derivative expansion

Roustant, Gamboa, Iooss (2020)

PoinCE

$$\mathcal{M}(\boldsymbol{x}) \approx \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

An alternative way to compute the coefficients $(c_{\boldsymbol{\alpha}})_{\boldsymbol{\alpha} \in \mathcal{A}}$: Make use of model partial derivatives

PoinCE-der

$$\frac{\partial}{\partial x_i} \mathcal{M}(\boldsymbol{x}) \approx \sum_{\boldsymbol{\alpha} \in \mathcal{A}, \alpha_i > 0} \tilde{c}_{\boldsymbol{\alpha}} \frac{\partial}{\partial x_i} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

- Theoretically $c_{\boldsymbol{\alpha}} = \tilde{c}_{\boldsymbol{\alpha}}$ for $\boldsymbol{\alpha} \in \mathcal{A}$ with $\alpha_i > 0$
- In practice (when computed from data) they are not equal!
- Terms with $\alpha_i = 0$ vanish when differentiated w.r.t. x_i
  - $+$ Fewer coefficients to estimate from same number of data points!
  - $-$ Some coefficients cannot be estimated from a single partial derivative expansion: unnormalized Sobol indices can be computed, but not e.g. variance
- Aggregate the coefficients from the partial derivative expansions to get the full picture

Poincaré derivative expansion: Aggregation of coefficients

Lüthen et al (2021, preprint)

PoinCE-der-i

$$\frac{\partial}{\partial x_i}\mathcal{M}(\boldsymbol{x}) \approx \sum_{\boldsymbol{\alpha}\in\mathcal{A},\alpha_i>0} \tilde{c}_{\boldsymbol{\alpha}}^{\partial,i} \frac{\partial}{\partial x_i}\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

- PoinCE-der-i computes the coefficients corresponding to the multi-indices $\{\boldsymbol{\alpha} \in \mathcal{A}, \alpha_i > 0\}$
- For each multi-index $\boldsymbol{\alpha} \neq \mathbf{0}$, average over all active variables:

$$\tilde{c}_{\boldsymbol{\alpha}}^{\partial,\text{avg}} = \frac{1}{\#\{\underbrace{i : 1 \leq i \leq d, \alpha_i > 0}_{\psi_{\boldsymbol{\alpha}} \text{ is not constant in } x_i}\}} \sum_{\substack{i:1\leq i\leq d,\\ \alpha_i>0}} \tilde{c}_{\boldsymbol{\alpha}}^{\partial,i}$$

$\rightarrow$ The coefficients $(\tilde{c}_{\boldsymbol{\alpha}}^{\partial,\text{avg}})_{\boldsymbol{\alpha}\in\mathcal{A}\setminus\mathbf{0}}$ can be used for computing total variance and sensitivity indices

- For surrogate modelling: Compute the remaining coefficient $\tilde{c}_{\mathbf{0}}^{\partial,\text{avg}}$ of the constant term by OLS on the residual

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Application to dyke cost toy model

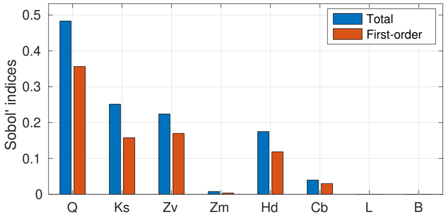
The model describes the cost in million euros given by

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

where H_d is the dyke height and S is the maximal annual overflow given by

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

Q	Maximal annual flowrate	truncated Gumbel
K_s	Strickler coefficient	truncated Gaussian
Z_v	River downstream level	Triangular
Z_m	River upstream level	Triangular
H_d	Dyke height	Uniform
C_b	Bank level	Triangular
L	Length of river stretch	Triangular
B	River width	Triangular



Methods for estimating sensitivity indices

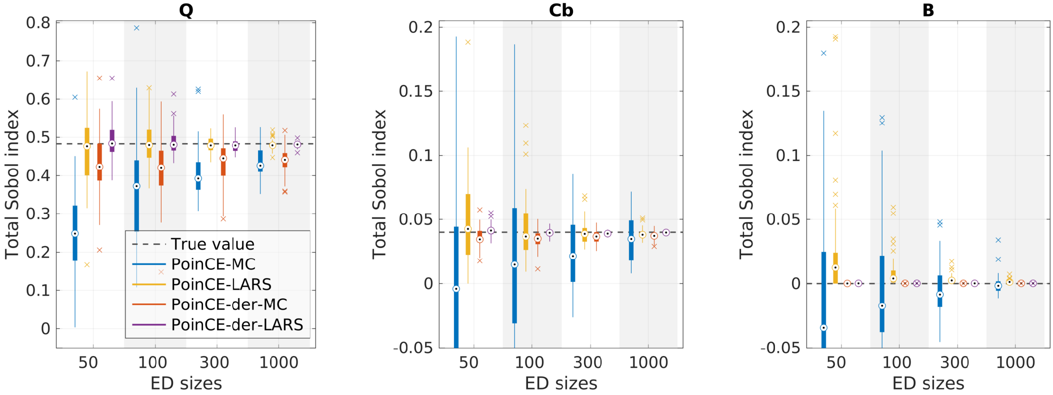
Sobol' indices

- Sample-based estimation — Janon et al (2014)
- Through ANOVA decomposition
  - Poincaré basis, coefficients computed through MC-projection — Roustant, Gamboa, Iooss (2020)
  - ——————— sparse regression — Lüthen et al (2021, preprint)
  - Poincaré derivative basis, coefficients computed through MC-projection — Roustant, Gamboa, Iooss (2020)
  - ——————— sparse regression, aggregated — Lüthen et al (2021, preprint)
  - PCE basis, coefficients computed through sparse regression

DGSM indices

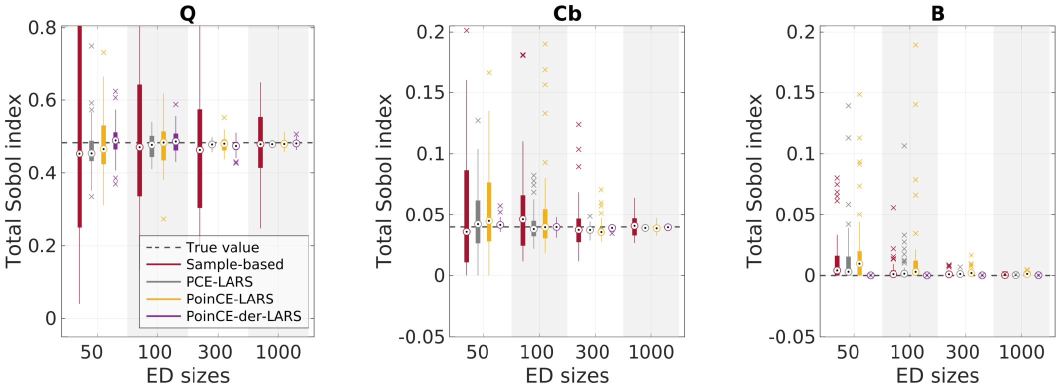
- Sample-based estimation — Kucherenko et al (2009)
- Analytical computation from Poincaré derivative basis, coefficients computed through sparse regression — Lüthen et al (2021, preprint)

Results: Sobol' indices – MC-projection vs sparse regression



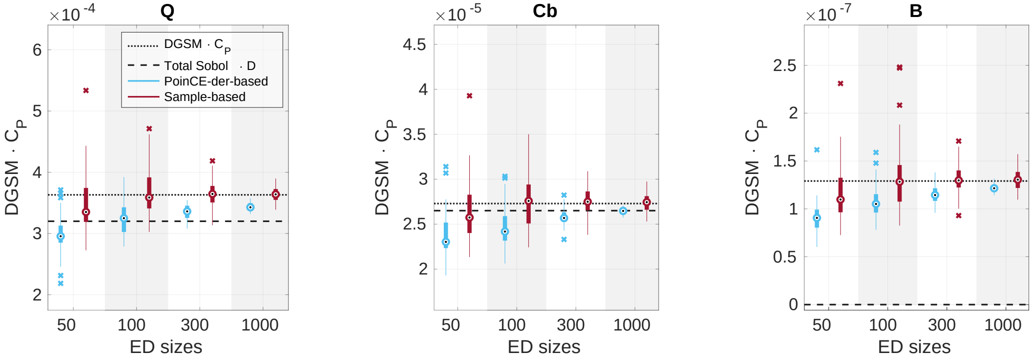
- Projection underestimates the Sobol' index, sparse regression gives more accurate estimates
- PoinCE-der estimates have a smaller variance than PoinCE estimates

Results: Sobol' indices – PoinCE vs PCE and sample-based



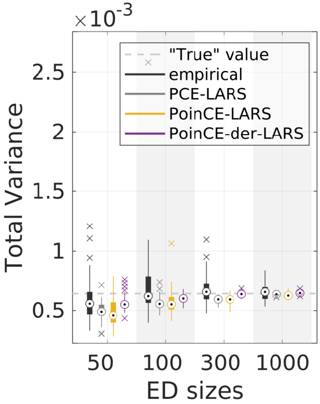
- PoinCE-der outperforms PCE especially for low-importance variables ($\rightarrow$ screening)
- Sample-based estimation shows large variability for important variables

Results: DGSM indices



- Poincaré-based estimate for DGSM underestimates the true value ($C_P \nu_i = \sum_{\boldsymbol{\alpha}:\alpha_i>0} \frac{\lambda_{i,\alpha_i}}{\lambda_{i,1}} (c_{\boldsymbol{\alpha}})^2$)
- Sample-based DGSM more accurate

Results: Total variance



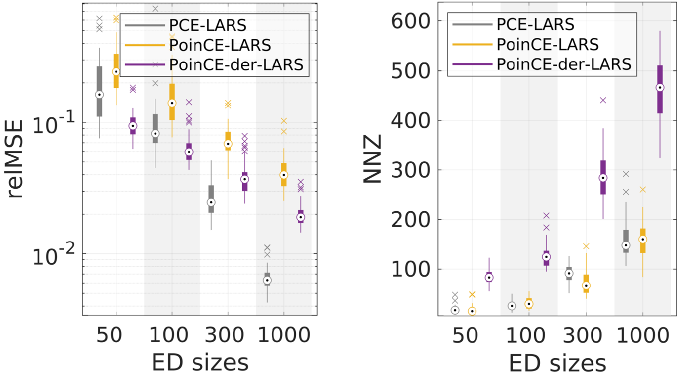
Variance

- PoinCE-der (aggregated coefficients) estimates the variance well

Results: Performance as global surrogate model

Relative mean squared error

$$= \frac{\mathbb{E}_{\boldsymbol{X}}\left[\left(\mathcal{M}(\boldsymbol{X}) - \hat{\mathcal{M}}(\boldsymbol{X})\right)^2\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right]}$$



Relative mean-squared error

Number of nonzeros in expansion

- PoinCE-der estimates the variance well, but PCE gives a better approximation in terms of $L^2_{f_{\boldsymbol{X}}}$-error

Conclusion

- Poincaré chaos expansions (PoinCE) are like PCE, but with a different basis consisting of the eigenfunctions of the Poincaré differential operator
- Sobol' indices and DGSM can be computed analytically from the PoinCE coefficients
- The Poincaré basis is the only orthogonal basis for $L^2_{f_{\boldsymbol{X}}}(\mathcal{D})$ for which the partial derivatives form again an orthogonal basis for the same space
- PoinCE is well suited to sensitivity analysis and to utilizing derivatives

Outlook:

- Work in progress: Use model evaluations and derivatives at once for computing the coefficients (in the spirit of gradient-enhanced PCE)
- Non-polynomial basis with special derivative property – usefulness for UQ in practice?

Thank you for your attention!

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