(Non)linear dimension reduction of input parameter space using gradient information

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Journée Réduction de dimension
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This work was supported by the Inria associate team UNQUESTIONABLE (UNcertainty QUantification is ESenTIal for OceaNic & Atmospheric flow proBLEms).

⋆ Our framework is the following:

$$\mathcal{M} : \left\{ \begin{array}{rcl} \mathcal{X} = \prod_{i=1}^{d} \mathcal{X}_i & \rightarrow & \mathcal{Y} \\ \mathbf{x} & \mapsto & y = \mathcal{M}(x_1, \ldots, x_d) \end{array} \right. \quad \text{with}$$

- $\mathcal{M}$ expensive to evaluate,
- high dimension $d \gg 1$.

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  - exploit gradient information when available (e.g., automatic differentiation, adjoint method).

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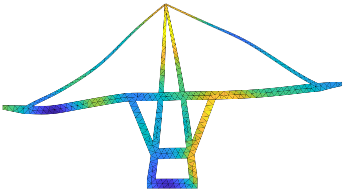
- More precisely, we seek for a decomposition of the form:

$$\mathcal{M}(x_1, \ldots, x_d) \approx f \circ g(\mathbf{x}) = f\left(g_1(x_1, \ldots, x_d), \ldots, g_r(x_1, \ldots, x_d)\right)$$

with $r \leq d$.

Illustration: resonance frequency of a bridge



Parametrized eigenvalue problem

$$\mathcal{M}(\mathbf{x}) = \min_{v \in \mathbb{R}^{\mathcal{N}}} \frac{v^T K(\mathbf{x}) v}{v^T M v}$$

- $K(\mathbf{x})$: stiffness matrix, M: mass matrix
- $v \in \mathbb{R}^{\mathcal{N}}$, $\mathcal{N} = 960$ nodes in the finite element mesh
- the Young modulus field, $E(\mathbf{x}) = \exp\left(\sum_{i=1}^{d} x_i \sqrt{\sigma_i} \psi_i\right)$, with $\psi_i : \Omega \to \mathbb{R}$ and σ_i the i-th leading eigenfunctions and eigenvalues of kernel $c(s,t) = \sqrt{5}\exp(-\|s-t\|_2^2/20)$, is parametrized by $\mathbf{x} \sim \mathcal{N}_d(0, Id)$, $d = 32$.

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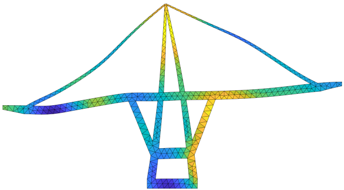

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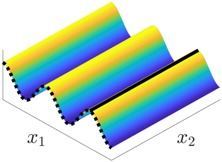
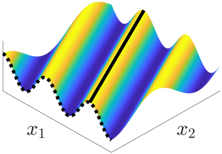
For this example, it is easy to compute model gradient $\nabla \mathcal{M}(\mathbf{x}) = (\partial_{x_1} \mathcal{M}(\mathbf{x}), \cdots, \partial_{x_d} \mathcal{M}(\mathbf{x}))$:

$$\partial_{x_i} \mathcal{M}(\mathbf{x}) = \frac{v(\mathbf{x})^T (\partial_{x_i} K(\mathbf{x})) v(\mathbf{x})}{v(\mathbf{x})^T M v(\mathbf{x})}, \text{ with } v(\mathbf{x}) = \operatorname*{argmin}_{v \in \mathbb{R}^{\mathcal{N}}} \frac{v^T K(\mathbf{x}) v}{v^T M v}.$$



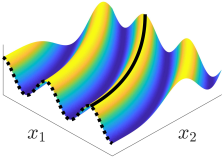
$\sin(x_1)$

$\underbrace{g(\mathbf{x}) = x_1}_{\text{linear in first canonical coordinate}}$



$\sin(x_1 + x_2)$

$\underbrace{g(\mathbf{x}) = x_1 + x_2}_{\text{linear}}$



$\sin(x_1 + x_2^2)$

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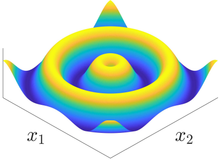

$\sin(x_1^2 + x_2^2)$

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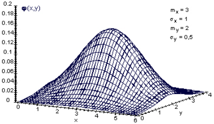
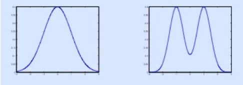
Uncertainty quantification framework

Uncertain input parameters are modeled by a probability distribution μ on $\mathcal{X}$, from experts' knowledge or from observations.



E.g., if the inputs are independent, this probability distribution is characterized by its marginals: $\mu(d\mathbf{x}) = \prod_{i=1}^{d} \mu_i(dx_i)$.



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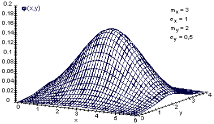

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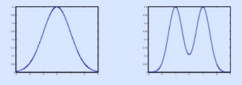
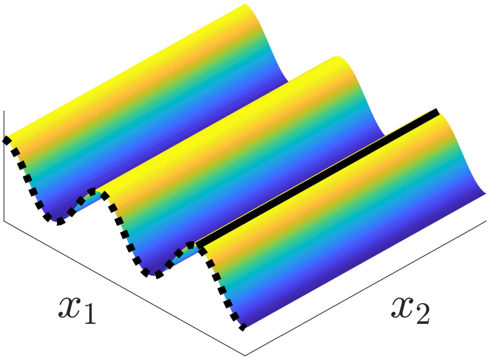


Approximation error is measured as

$$\mathbb{E}\left(\|\mathcal{M}(\mathbf{X}) - f \circ g(\mathbf{X})\|_{\mathcal{Y}}^{2}\right),$$

with some specific norm on $\mathcal{Y}$.


x_1
x_2

In the following,

$$\mathcal{M} : \begin{cases} \mathcal{X} = \mathbb{R}^d & \to & \mathcal{Y} = \mathbb{R}^p \\ \mathbf{x} & \mapsto & y = \mathcal{M}(x_1, \ldots, x_d) \end{cases}$$

For $p = 1$ (scalar output) and $\mathbf{u} \subset \{1, \ldots, d\}$, one defines the total Sobol' index for $\mathcal{M}$ associated to $\mathbf{u}$ as:

$$S_{\mathbf{u}}^{\text{tot}} = 1 - \frac{\mathrm{Var}\left[\mathbb{E}\left(Y|X_{-\mathbf{u}}\right)\right]}{\mathrm{Var}[Y]} = \frac{\mathbb{E}\left[\mathrm{Var}\left(Y|X_{-\mathbf{u}}\right)\right]}{\mathrm{Var}[Y]}$$

with $X_{-\mathbf{u}} = (X_i\ ,\ i \notin \mathbf{u})$ (see, e.g., Da Veiga et al. [2021]).

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We then have the following equality Hart and Gremaud [2018]:

$$S_{\mathbf{u}}^{\text{tot}} = \frac{\|Y - \mathbb{E}\left(Y|X_{-\mathbf{u}}\right)\|^2}{\|Y - \mathbb{E}\left(Y\right)\|^2},$$

with $\|Y - \mathbb{E}\left(Y|X_{-\mathbf{u}}\right)\|^2 = \mathbb{E}\left(|\mathcal{M}(\mathbf{X}) - \mathbb{E}\left(Y|X_{-\mathbf{u}}\right)|^2\right)$.

From

$$S_{\mathbf{u}}^{\text{tot}} = \frac{\| Y - \mathbb{E}(Y|X_{-\mathbf{u}}) \|^2}{\| Y - \mathbb{E}(Y) \|^2},$$

with $\| Y - \mathbb{E}(Y|X_{-\mathbf{u}}) \|^2 = \mathbb{E}\left(|\mathcal{M}(\mathbf{X}) - \mathbb{E}(Y|X_{-\mathbf{u}})|^2\right)$, we deduce:

$$\begin{aligned} S_{\mathbf{u}}^{\text{tot}} \approx 0 \quad &\Leftrightarrow \quad \mathcal{M}(\mathbf{X}) \approx f(\mathbf{X}_{-\mathbf{u}}) \\ &\Leftrightarrow \quad \mathbf{X}_{\mathbf{u}} \text{ is useless to "explain" } Y = \mathcal{M}(\mathbf{X}) \end{aligned}$$

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Note that if $\mu(d\mathbf{x}) = \prod_{i=1}^{d} \mu_i(dx_i)$ then

$$S_{\mathbf{u}}^{\text{tot}} = \sum_{\mathbf{v} \subseteq \{1,\dots,d\}\,,\ \mathbf{u} \cap \mathbf{v} \neq \emptyset} S_{\mathbf{v}} \text{ and}$$

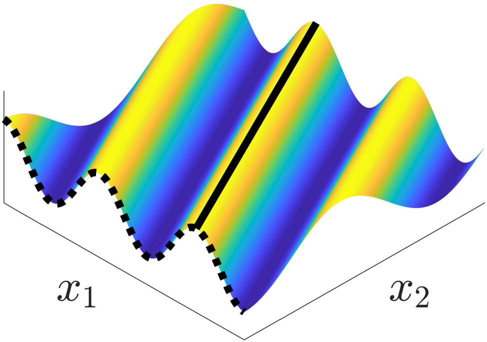
$$\begin{aligned} S_{\mathbf{u}}^{\text{tot}} \approx 0 \quad &\Leftrightarrow \quad \mathcal{M}(\mathbf{X}) \approx \mathcal{M}(\mathbf{x}_{\mathbf{u}}, \mathbf{X}_{-\mathbf{u}}) \text{ for } \textstyle\prod_{i \in \mathbf{u}} \mu_i\text{-almost all } \mathbf{x}_{\mathbf{u}} \\ &\Leftrightarrow \quad \mathbf{X}_{\mathbf{u}} \text{ is useless to "explain" } Y = \mathcal{M}(\mathbf{X}) \\ &\Leftrightarrow \quad \mathbf{X}_{\mathbf{u}} \text{ "can be fixed" to any value in the model} \end{aligned}$$

A natural extension to the vector-valued case:

$$S_{\mathbf{u}}^{\text{tot}} = \frac{\mathbb{E}(\|\mathcal{M}(\mathbf{X}) - \mathbb{E}(\mathcal{M}(\mathbf{X})|\mathbf{X}_{-\mathbf{u}})\|_{\mathcal{Y}}^2)}{\mathbb{E}(\|\mathcal{M}(\mathbf{X}) - \mathbb{E}(\mathcal{M}(\mathbf{X}))\|_{\mathcal{Y}}^2)},$$

with $\mathcal{Y} = \mathbb{R}^p$ endowed with a hilbertian norm $\|\cdot\|_{\mathcal{Y}}$ (see Lamboni et al. [2011], Gamboa et al. [2013], Zahm et al. [2020]).

Gradient based linear dimension reduction Constantine and Diaz [2017], Zahm et al. [2020]



Framework:

$$\mathbf{x} \in \mathbb{R}^d \mapsto \mathcal{M}(x_1, \ldots, x_d) \ \in \mathcal{Y}$$

with $\mathcal{Y} = \mathbb{R}^p$ endowed with a Hilbertian norm $\|\cdot\|_\mathcal{Y}$.

One aims at approximating $\mathcal{M}$ by a ridge function (a function which is constant along a subspace). More specifically, one seeks for $r \leq d$ and $A \in \mathbb{R}^{r\times d}$ such that:

$$\mathcal{M}(\mathbf{x}) \approx f(A\,\mathbf{x}) \text{ with } f : \mathbb{R}^r \to \mathcal{Y}\,,$$

or equivalently for $r \leq d$ and a rank-r projector $P_r \in \mathbb{R}^{d\times d}$ such that:

$$\mathcal{M}(\mathbf{x}) \approx h(P_r\,\mathbf{x}) \text{ with } h : \mathbb{R}^d \to \mathcal{Y}\,.$$

We assume $\mathbf{X} \sim \mu = \mathcal{N}(m, \Sigma)$.

Controlled approximation problem Given $\varepsilon \geq 0$, find r, h and a rank-r projector P_r such that

$$\mathbb{E}(\|\mathcal{M}(\mathbf{X}) - h(P_r \mathbf{X})\|_{\mathcal{Y}}^2) \leq \varepsilon.$$

Procedure:

1. derive an upper bound for the error
$$\|\mathcal{M} - h \circ P_r\| \leq \mathcal{R}(h, P_r)$$
2. fix r and solve
$$\min_{h, P_r} \mathcal{R}(h, P_r)$$
3. increase r until
$$\min_{h, P_r} \mathcal{R}(h, P_r) \leq \varepsilon$$

Note that P_r is not restricted to be a projector onto the canonical coordinates.

Derivation of the upper bound

For any projector P_r,

$$\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M}|\sigma(P_r))\| = \min_h \|\mathcal{M} - h \circ P_r\|.$$

From Poincaré type inequalities, we can deduce that for $\mathcal{M} : \mathbb{R}^d \to \mathcal{Y}$ smooth vector-valued and for any projector P_r,

$$\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M}|\sigma(P_r))\| \leq \sqrt{\mathrm{trace}\big(H(I_d - P_r)\Sigma(I_d - P_r)^T\big)}$$

with matrix $H \in \mathbb{R}^{d\times d}$ defined by

$$\boxed{H = \int (\nabla\mathcal{M})^*(\nabla\mathcal{M})\mathrm{d}\mu}$$

where

$$\begin{cases} \nabla\mathcal{M}(x) : \mathbb{R}^d \to \mathbb{R}^p \text{ Jacobian of } \mathcal{M} \text{ at } x \\ \nabla\mathcal{M}(x)^* \text{ is the adjoint of } \nabla\mathcal{M}(x) \end{cases}$$

What is the matrix H ?

$$H = \int (\nabla \mathcal{M})^* (\nabla \mathcal{M}) \mathrm{d}\mu \quad \in \mathbb{R}^{d \times d}$$

- Vector-valued case: $\mathcal{Y} = \mathbb{R}^p$ with $\|\cdot\|_{\mathcal{Y}}$ such that $\|v\|_{\mathcal{Y}}^2 = v^T R_{\mathcal{Y}} v$ for some SPD matrix $R_{\mathcal{Y}} \in \mathbb{R}^{p \times p}$. Then

$$H = \int (\nabla \mathcal{M})^T R_{\mathcal{Y}} (\nabla \mathcal{M}) \, \mathrm{d}\mu$$

with

$$\nabla \mathcal{M} = \begin{pmatrix} \frac{\partial \mathcal{M}_1}{\partial x_1} & \cdots & \frac{\partial \mathcal{M}_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathcal{M}_p}{\partial x_1} & \cdots & \frac{\partial \mathcal{M}_p}{\partial x_d} \end{pmatrix}$$

- Scalar-valued case: $\mathcal{Y} = \mathbb{R}$ with $\|\cdot\|_{\mathcal{Y}} = |\cdot|$, then

$$H = \int (\nabla \mathcal{M})(\nabla \mathcal{M})^T \, \mathrm{d}\mu$$

with

$$\nabla \mathcal{M} = \begin{pmatrix} \frac{\partial \mathcal{M}}{\partial x_1} \\ \vdots \\ \frac{\partial \mathcal{M}}{\partial x_d} \end{pmatrix}$$

$\rightsquigarrow\rightsquigarrow$ Active-Subspace method Constantine and Diaz [2017]

Minimizing the upper bound

Let (v_i, λ_i) be the i-th generalized eigenpair of (H, Σ^{-1}):

$$H v_i = \lambda_i \Sigma^{-1} v_i.$$

One has $\lambda_1 \geq \cdot \geq \lambda_i \geq \cdot \geq \lambda_d$ and

$$\min_{P_r} \sqrt{\text{trace}(H(I_d - P_r)\Sigma(I_d - P_r)^T)} = \sqrt{\sum_{i=r+1}^{d} \lambda_i}$$

A solution is the Σ^{-1}-orthogonal proj. P_r onto $\text{span}\{v_1, \ldots, v_r\}$, $P_r = \left(\sum_{i=1}^r v_i v_i^T\right) \Sigma^{-1}$, and

- a fast decay in λ_i ensures $\sqrt{\sum_{i=r+1}^d \lambda_i} \leq \varepsilon$ for $r = r(\varepsilon) \ll d$,
- H provides a test that reveals the low-effective dimension.

Let's come back to the upper bound, namely,

$$\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M}|\sigma(P_r))\| \leq \sqrt{\text{trace}(H(I_d - P_r)\Sigma(I_d - P_r)^T)}.$$

Choosing $\mathcal{Y} = \mathbb{R}^p$ and P_r as the projector that extracts the coordinates of $\mathbf{X}$ indexed by $\mathbf{u}$, we get:

$$S_{\mathbf{u}}^{\text{tot}} = \frac{\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M}|\sigma(I_d - P_r))\|^2}{\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M})\|^2}$$

thus

$$\begin{aligned} S_{\mathbf{u}}^{\text{tot}} &\leq \frac{\text{trace}\left(\Sigma P_r^T H P_r\right)}{\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M})\|^2} \\ &= \frac{\sum_{i\in\mathbf{u}} \mathrm{Var}(X_i) H_{i,i}}{\|\mathcal{M} - \mathbb{E}_\mu(\mathcal{M})\|^2}. \end{aligned}$$

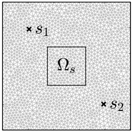
See, e.g., Sobol' & Kucherenko, 2009 and Lamboni *et al.*, 2013 for similar results in the case $p = 1$ (scalar output).

A numerical example

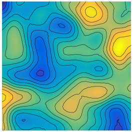
Diffusion problem on $\Omega = [0,1]^2$: $\begin{cases} \nabla \cdot \kappa \nabla u &= 0 & \text{in } \Omega \\ u &= x + y & \text{on } \partial\Omega \end{cases}$

- Random diffusion field κ, log-normal distribution.
- After finite element discretization:

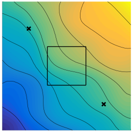
$$x = \log(\kappa) \in \mathbb{R}^{3252} \sim \mu = \mathcal{N}(0, \Sigma)$$



(a) mesh, 3252 elements



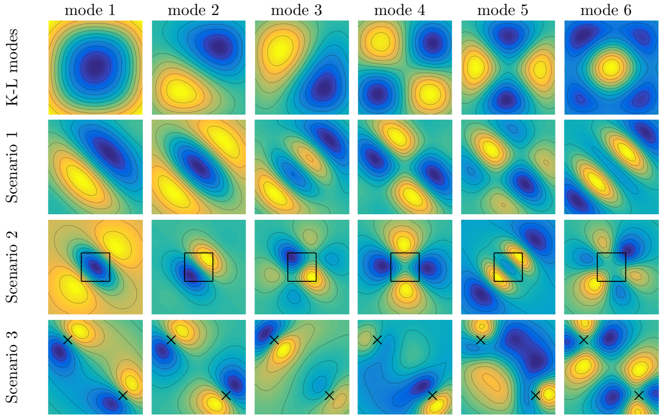
(b) log. diffusion field



(c) solution

1. Scenario 1 $\mathcal{M} : x \mapsto u \in \mathcal{Y} \subset H^1(\Omega)$, $p = 1691$ (number of nodes in the mesh for FEM);
2. Scenario 2 $\mathcal{M} : x \mapsto u_{|\Omega_s} \in \mathcal{Y} \subset H^1(\Omega_s)$, $p = 168$;
3. Scenario 3 $\mathcal{M} : x \mapsto (u_{|s_1}, u_{|s_2}) \in \mathcal{Y} = \mathbb{R}^2$ (canonical norm).

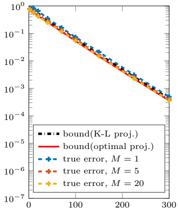
Modes $v_1, v_2, \ldots$



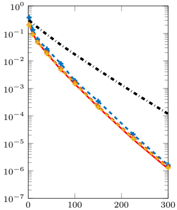
$$\text{Im}(P_r) = \text{span}\{v_1, v_2, \ldots, v_r\}$$

Approximation of the conditional expectation assuming H is known

$$\mathbb{E}_\mu(\mathcal{M}|\sigma(P_r)) \;\approx\; \hat{F}_r : x \mapsto \frac{1}{M}\sum_{k=1}^{M} \mathcal{M}(P_r x + (I_d - P_r)\mathbf{Z}^{(k)}), \quad \mathbf{Z}^{(k)} \overset{iid}{\sim} \mu$$



$\mathcal{M} : x \mapsto u$



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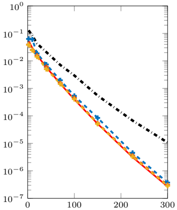


$\mathcal{M} : x \mapsto (u_{|s_1}, u_{|s_2})$

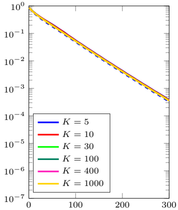
$$\|\mathcal{M} - \hat{F}_r\| = function(r)$$

We can show that

$$\mathbb{E}\left(\|\mathcal{M} - \hat{F}_r\|^2\right) \leq (1 + M^{-1})\ \mathrm{trace}(\Sigma(I_d - P_r^T)H(I_d - P_r))$$

Approximation of H to get the projector

$$H \approx \widehat{H} = \frac{1}{K}\sum_{k=1}^{K} (\nabla \mathcal{M}(\mathbf{X}^{(k)}))^* (\nabla \mathcal{M}(\mathbf{X}^{(k)})), \quad \mathbf{X}^{(k)} \overset{iid}{\sim} \mu$$



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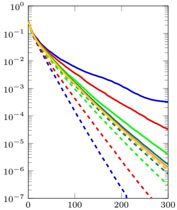

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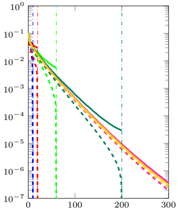

$\mathcal{M} : x \mapsto \left(u_{|s_1}, u_{|s_2}\right)$

$\sqrt{\mathrm{trace}(\Sigma(I_d - \hat{P}_r^T)\widehat{H}(I_d - \hat{P}_r))} = \mathit{function}(r)$ (dashed curves)

$\sqrt{\mathrm{trace}(\Sigma(I_d - \hat{P}_r^T)H(I_d - \hat{P}_r))} = \mathit{function}(r)$ (solid curves)

Notice that $\mathrm{rank}(\widehat{H}) \leq K \ \max_{1\leq k\leq K} \mathrm{rank}\left(\nabla\mathcal{M}(\mathbf{X}^{(k)})\right) \leq K \dim(\mathcal{Y})$ (see also Zahm et al. [2022])

Beyond Gaussian uncertainty

Let $d\mu(x) \sim \exp\Big(- V(x) - \Psi(x) \Big) dx$. Assume

1. $\mathrm{supp}(\mu)$ **convex**,
2. (**Bakry–Émery** theorem) V a **convex** potential with
$$\nabla^2 V(x) \succeq \Gamma, \text{ with } \Gamma \text{ SPD matrix,}$$
3. (**Holley–Stroock** perturbation lemma) Ψ **bounded** with
$$\exp(\sup \Psi - \inf \Psi) \leq \kappa\,.$$

Then μ satisfies the subspace Poincaré inequality (Zahm et al. [2022]):

$$\|\mathcal{M} - \mathbf{E}[\mathcal{M}(\mathbf{X})|{P_r}^T \mathbf{X}]\|^2 \leq \kappa\, \mathrm{trace}[\Sigma(I_d - {P_r}^T) H (I_d - P_r))]$$

for any smooth function $\mathcal{M}$ and any projector P_r.

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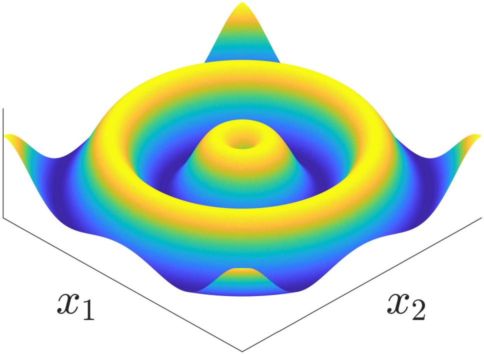
for any smooth function $\mathcal{M}$ and any projector P_r.

- Gaussian mixtures,
- uniform measures on compact & convex sets
- any measure such that $d\mu(\mathbf{x}) \geq \alpha > 0$ on compact & convex sets.

Extension to nonlinear dimension reduction Bigoni et al. [2022]



$$\mathcal{M} : \begin{cases} \mathcal{X} \subset \mathbb{R}^d & \rightarrow & \mathbb{R} \\ \mathbf{x} & \mapsto & y = \mathcal{M}(x_1, \ldots, x_d) \end{cases}$$

$$\mathcal{M}(x_1, \ldots, x_d) \approx f \circ g(\mathbf{x}) = f\left(g_1(x_1, \ldots, x_d), \ldots, g_r(x_1, \ldots, x_d)\right),$$

with the feature map g is not necessarily linear.

We propose, for any $r \leq d$, a two-step procedure.

- Step 1, construction of the feature map g:
  solve $\min_{g \in \mathcal{G}_r} J(g_1, \ldots, g_r)$ with J a gradient-based cost function.

- Step 2, construction of the profile fucntion f:

$$\text{solve} \quad \min_{f \in \mathcal{F}_r} \mathbb{E}\left[\left(\mathcal{M}(\mathbf{X}) - f \circ g(\mathbf{X})\right)^2\right].$$

Choice of the cost function J

Note that, if $\mathcal{M}(x_1, \ldots, x_d) = f \circ g(\mathbf{x})$, then

$$\nabla\mathcal{M}(\mathbf{x}) = \underbrace{\nabla g(\mathbf{x})^T}_{\in\mathbb{R}^{d\times r}} \underbrace{\nabla f(g(\mathbf{x}))}_{\in\mathbb{R}^{r}} \Rightarrow \nabla\mathcal{M}(\mathbf{x}) \in \mathrm{range}(\nabla g(x)^T).$$

A natural choice for J is then

$$J(g) := \mathbb{E}\left[\left\|\nabla\mathcal{M}(\mathbf{X}) - \Pi_{\mathrm{range}(\nabla g(\mathbf{X})^T)}\nabla\mathcal{M}(\mathbf{X})\right\|^2\right].$$

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We have proven $\mathcal{M} = f\circ g \Rightarrow J(g) = 0$. Question a) Is the reciprocal true?

Question a): is the reciprocal $\Uparrow$ true? yes!

Proposition:

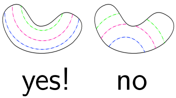
Assume $\mathcal{M} \in \mathcal{C}^1(\mathcal{X};\mathbb{R})$ and $g \in \mathcal{G}_r \subset \mathcal{C}^1(\mathcal{X};\mathbb{R}^r)$.
Assume that the level-sets of g are such that

$$g^{-1}(\{\mathbf{z}\}) = \{\mathbf{x} \in \mathcal{X} : g(\mathbf{x}) = \mathbf{z}\},$$

are **pathwise-connected** for any $z \in \mathbb{R}^r$. Then

$$J(g) = 0 \Rightarrow \exists\, f \text{ such that } \mathcal{M} = f \circ g$$

Are g's level sets pathwise-connected?



Examples of feature maps $g : \mathcal{X} \to \mathbb{R}$ with $\mathcal{X}$ convex and with smoothly pathwise connected level-sets:

Affine feature map Any function $g(\mathbf{x}) = A\mathbf{x} + b$ with $A \in \mathbb{R}^{m \times d}$ and $b \in \mathbb{R}^m$;

Feature map following from a C^1-diffeomorphism Any function $g(\mathbf{x}) = (\phi_1(\mathbf{x}), \dots, \phi_m(\mathbf{x}))$ where $\phi_i(\mathbf{x})$ is the i-th component of $\phi(\mathbf{x})$, with $\phi : \mathcal{X} \to \mathcal{X}$ a C^1-diffeomorphism;

Polynomial feature map Any polynomial function on $\mathcal{X} = \mathbb{R}^d$ such that for all $\mathbf{z} \in g(\mathcal{X})$, the zeros of the polynomial $\mathbf{x} \mapsto g(\mathbf{x}) - \mathbf{z}$ are pathwise-connected.

Examples of feature maps $g : \mathcal{X} \to \mathbb{R}$ with $\mathcal{X}$ convex and with smoothly pathwise connected level-sets:

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Question b): does $J(g) \approx 0$ implies $\mathcal{M} \approx f \circ g$? yes!

Denote by $\mathbb{C}(Z)$ the **Poincaré constant** of a random vector Z, that is, the smallest constant such that

$$\mathrm{Var}(h(Z)) \leq \mathbb{C}(Z)\,\mathbb{E}\left[\left\|\nabla h(Z)\right\|^2\right]$$

holds for any smooth function $h : \mathrm{supp}(Z) \to \mathbb{R}$.

Proposition:

Assume $\mathcal{G}_r \subset \mathcal{C}^1(\mathbf{X}; \mathbb{R}^r)$ and $\mathrm{rank}\left(\nabla g(\mathbf{x})^T\right) = r\ \forall\, g \in \mathcal{G}_r$, $\forall\, \mathbf{x} \in \mathcal{X}$. Assume

$$\mathbb{C}(\mathbf{X}|\mathcal{G}_r) := \sup_{g\in\mathcal{G}_r} \sup_{\mathbf{z}\in g(\mathcal{X})} \mathbb{C}(\mathbf{X}|g(\mathbf{X}) = \mathbf{z}) < \infty.$$

Then for any $g \in \mathcal{G}_r$, there exists a profile $f : \mathbb{R}^r \to \mathbb{R}$ such that

$$\mathbb{E}\left[\left(\mathcal{M}(\mathbf{X}) - f \circ g(\mathbf{X})\right)^2\right] \leq \mathbb{C}(\mathbf{X}|\mathcal{G}_r)\, J(g).$$

Example: if $\mathcal{G}_r = \{\mathbf{x} \mapsto U^T\mathbf{x} : U \in \mathbb{R}^{d\times r} \text{ orth. columns}\}$ and if $\mathbf{X} \sim \mathcal{N}(0, I_d)$, then

$$\mathbb{C}(\mathbf{X}|\mathcal{G}_r) = 1$$

Although assuming $\mathbb{C}(\mathbf{X}|\mathcal{G}_r) < \infty$ is usual, e.g., in the analysis of Markov semigroups or in molecular dynamics, proving it remains an open challenge in more general settings.

Question c): how to minimize $g \mapsto J(g)$? We seek for g solving

$$\min_{g=(g_1,\dots,g_r)\in\mathcal{G}_r} J(g) = \mathbb{E}\left[\left\|\nabla\mathcal{M}(\mathbf{X}) - \Pi_{\mathrm{range}(\nabla g(\mathbf{X})^T)}\nabla\mathcal{M}(\mathbf{X})\right\|^2\right]$$

with $\mathcal{G}_r = \mathcal{G}^r = \mathrm{span}\{\Phi_1,\dots,\Phi_K\}^r$.

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It is equivalent to seek for g solving

$$\max_{G\in\mathbb{R}^{\#\mathcal{G}\times r}} \mathcal{R}(G) = \mathbb{E}\left[\mathrm{trace}(G^T H(\mathbf{X})G)(G^T\Sigma(\mathbf{X})G)^{-1}\right] \text{ where}$$

$$H(\mathbf{x}) = \nabla\Phi(\mathbf{x})(\nabla\mathcal{M}(\mathbf{x})\nabla\mathcal{M}(\mathbf{x})^T)\nabla\Phi(\mathbf{x})^T,$$
$$\Sigma(\mathbf{x}) = \nabla\Phi(\mathbf{x})\nabla\Phi(\mathbf{x})^T, \text{ with } \Phi(\mathbf{x}) = (\Phi_1(\mathbf{x}),\dots,\Phi_K(\mathbf{x})).$$

Maximization is solved with a quasi-Newton algorithm.

For linear feature maps, $g(\mathbf{x}) = A\,\mathbf{x}$, our procedure coincides with active subspace method.

Adaptive construction of g from $\{\mathbf{X}^{(i)}, \mathcal{M}(\mathbf{X}^{(i)}), \nabla\mathcal{M}(\mathbf{X}^{(i)})\}_{i=1}^{N}$

Empirical cost

We first replace $\mathcal{R}(G)$ by its empirical counterpart:

$$\hat{\mathcal{R}}^N(G) = \frac{1}{N}\sum_{i=1}^{N} \mathrm{trace}(G^T H(\mathbf{X}^{(i)}) G)(G^T \Sigma(\mathbf{X}^{(i)}) G)^{-1}.$$

For any $1 \leq r \leq d$, we adapt the complexity of $\mathcal{G}_r = \mathcal{G}^r$ to the sample size N.

Matching Pursuit

We use a state-of-the-art Migliorati [2015, 2019] reduced-set matching pursuit algorithm on downward-closed polynomial spaces to build g.

Cross Validation

is used to know when to stop the iterations (before it overfits).

More precisely, to adapt the complexity of $\mathcal{G}$ with respect to the sample size N, one uses the following tools:

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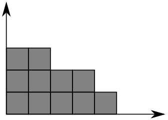
Downward closed polynomial spaces

$$\mathcal{G} = \mathbb{P}_\Lambda[\mathbb{R}^d] = \text{span}\{x_1^{\nu_1} \dots x_d^{\nu_d}, \nu \in \Lambda\}$$

where $\Lambda \subset \mathbb{N}^d$ is a downward closed set, that is:

$$\nu \in \Lambda \text{ and } \mu \leq \nu \quad \Rightarrow \quad \mu \in \Lambda$$



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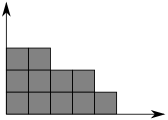
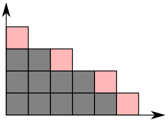


Matching Pursuit

$$\Lambda_{k+1} = \Lambda_k \cup \{\nu_{k+1}\}$$

$$\nu_{k+1} \in \underset{\nu \in \text{ReducedMargin}(\Lambda_k)}{\text{argmax}} |\partial_\nu \hat{\mathcal{R}}^N(G_k^*)|$$



where G_k^* is the minimizer of $\hat{\mathcal{R}}^N(\cdot)$ over Λ_k.

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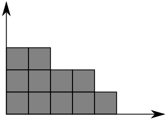

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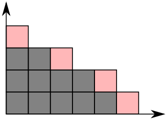

where G_k^* is the minimizer of $\hat{\mathcal{R}}^N(\cdot)$ over Λ_k.

Cross Validation

To know when to stop the iterations (before it overfits).

Once g is computed, how to construct f?

$$\min_{f\in\mathcal{F}_r} \frac{1}{N}\sum_{i=1}^{N}\left(\mathcal{M}(\mathbf{X}^{(i)}) - f\circ g(\mathbf{X}^{(i)})\right)^2 \underbrace{+\|\nabla\mathcal{M}(\mathbf{X}^{(i)}) - \nabla f\circ g(\mathbf{X}^{(i)})\|^2}_{\text{recycle the gradients}}$$

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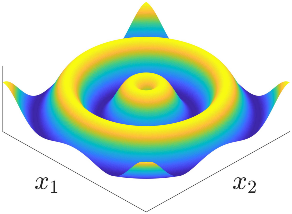
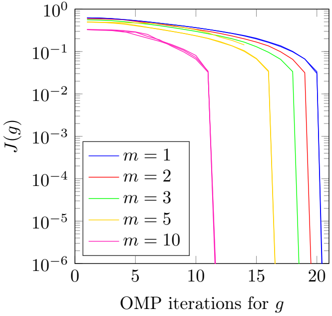
Benchmark algorithm (without dimension reduction):

$$\min_{v\in\mathcal{V}} \frac{1}{N}\sum_{i=1}^{N} \left(\mathcal{M}(\mathbf{X}^{(i)}) - v(\mathbf{X}^{(i)})\right)^2 \underbrace{+\|\nabla\mathcal{M}(\mathbf{X}^{(i)}) - \nabla v(\mathbf{X}^{(i)})\|^2}_{\text{recycle the gradients}}$$

Illustration: isotropic function

$$\mathcal{M}(\mathbf{x}) = \cos\left(\sqrt{x_1^2 + \ldots + x_d^2}\right)$$
$$\mu = \mathcal{N}(0, I_d)$$
$$\mathbf{x} \in \mathbb{R}^{20}$$
$$N = 100$$





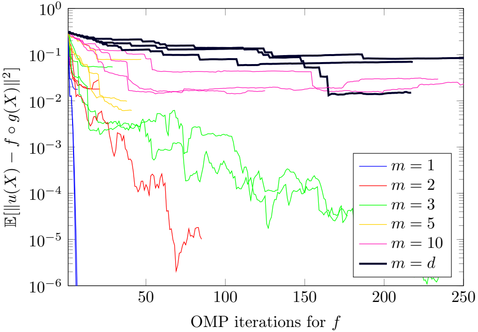
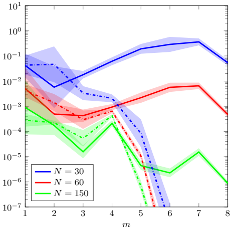
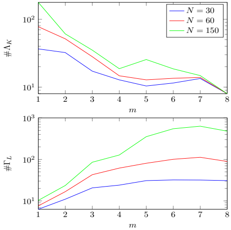


Illustration: Borehole function

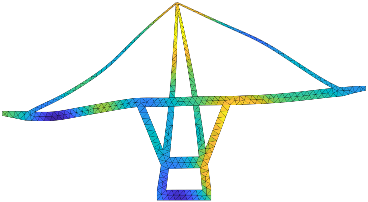
$$\mathcal{M}(\mathbf{x}) = \frac{2\pi T_{\mathcal{M}}(H_{\mathcal{M}} - H_\ell)}{\ln(r/r_\omega)\left(1 + \frac{2LT_{\mathcal{M}}}{\ln(r/r_\omega) r_\omega{}^2 K_\omega} + \frac{T_{\mathcal{M}}}{T_\ell}\right)}, \quad \begin{cases} x_1 = r_\omega & \sim \mathcal{N}(0.1, 3 \cdot 10^{-4}) \\ x_2 = r & \sim \log\mathcal{N}(7.71, 1.0112) \\ x_3 = T_{\mathcal{M}} & \sim \mathcal{U}(63\,070, 115\,600) \\ x_4 = H_{\mathcal{M}} & \sim \mathcal{U}(990, 1110) \\ x_5 = T_\ell & \sim \mathcal{U}(63.1, 116) \\ x_6 = H_\ell & \sim \mathcal{U}(700, 820) \\ x_7 = L & \sim \mathcal{U}(1120, 1\,680) \\ x_8 = K_\omega & \sim \mathcal{U}(9\,855, 12\,045) \end{cases}$$





Continuous lines: mean squared error $\mathbb{E}[(\mathcal{M}(\mathbf{X}) - f \circ g(\mathbf{X}))^2]$, Dashed lines: cost function $J(g)$. The width of the shaded region corresponds to the standard deviation over 20 experiments.

Illustration: resonance frequency of a bridge



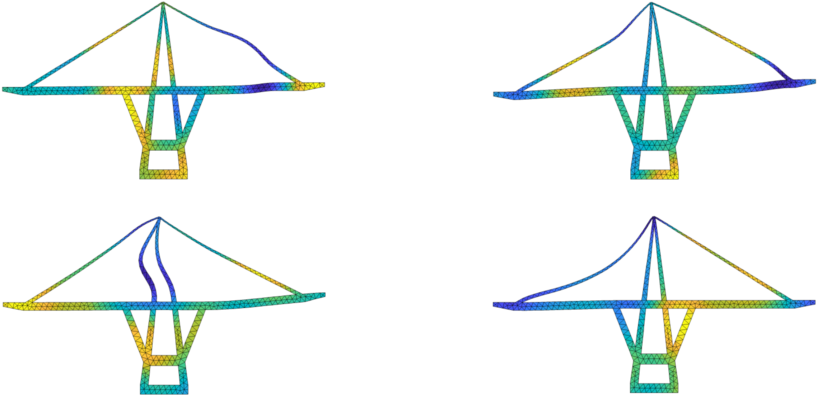
Parametrized eigenvalue problem

$$\mathcal{M}(\mathbf{x}) = \min_{v\in\mathbb{R}^{\mathcal{N}}} \frac{v^T K(\mathbf{x}) v}{v^T M v}$$

- $K(\mathbf{x})$: stiffness matrix
- M: mass matrix
- $v \in \mathbb{R}^{\mathcal{N}}$, $\mathcal{N} = 960$ nodes in the finite element mesh
- $\mathbf{x} \in \mathbb{R}^d$: Young modulus field ($d = 32$ KL modes)
- $N = 100$ (20 trials)

For this example, it is easy to compute model gradient $\nabla\mathcal{M}(\mathbf{x}) = (\partial_{x_1}\mathcal{M}(\mathbf{x}), \cdots, \partial_{x_d}\mathcal{M}(\mathbf{x}))$:

$$\partial_{x_i}\mathcal{M}(\mathbf{x}) = \frac{v(\mathbf{x})^T (\partial_{x_i} K(\mathbf{x})) v(\mathbf{x})}{v(\mathbf{x})^T M v(\mathbf{x})}, \text{ with } v(\mathbf{x}) = \operatorname*{argmin}_{v\in\mathbb{R}^{\mathcal{N}}} \frac{v^T K(\mathbf{x}) v}{v^T M v}.$$



Resonance frequency of a bridge. Four realizations of the Young modulus field **X** (color of the elements) and the associated resonance mode $v(\mathbf{X})$ (displacement of the mesh).

Results:

	$r=1$	$r=2$	$r=3$	$r=4$	$r=6$	$r=8$	$r=16$	$r=32$
Mean $\times 10^{12}$	1.6	1.5	1.1	1.2	1.3	1.5	1.6	1.4
Std $\times 10^{12}$	0.80	0.69	0.22	0.24	0.28	0.83	0.39	0.43
$\#\Lambda_K$	148 ($\pm$64)	129 ($\pm$45)	91 ($\pm$21)	80 ($\pm$23)	64 ($\pm$16)	57 ($\pm$9)	51 ($\pm$1)	32 ($\pm$0)
$\#\Gamma_L$	5 ($\pm$1)	8 ($\pm$1)	11 ($\pm$1)	15 ($\pm$3)	24 ($\pm$7)	44 ($\pm$24)	133 ($\pm$102)	102 ($\pm$70)

Mean and standard deviation of mean squared error $\mathbf{E}[(\mathcal{M}(\mathbf{X}) - f \circ g(\mathbf{X}))^2]$ over 20 experiments, where g and f are constructed adaptively with $N = 100$ samples. Mean squared error is computed on a (fixed) validation set of size 1000. The last two lines give mean($\pm$ std) of the cardinality of $\#\Lambda_K$ and $\#\Gamma_L$, which represent the complexity of g and f, respectively.

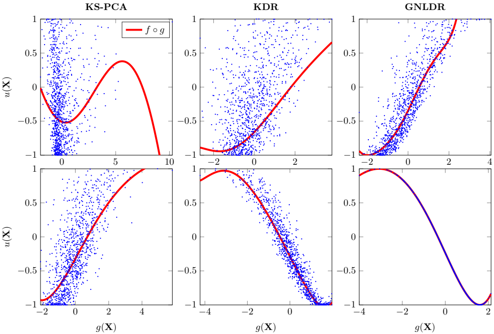
Comparison with nonlinear (NL) kernel supervised PCA and NL kernel dimension reduction.

$$\mathbf{Y} = \begin{pmatrix} \mathcal{M}(\mathbf{X}) \\ \nabla\mathcal{M}(\mathbf{X}) \end{pmatrix} \in \mathbb{R}^{1+d}.$$

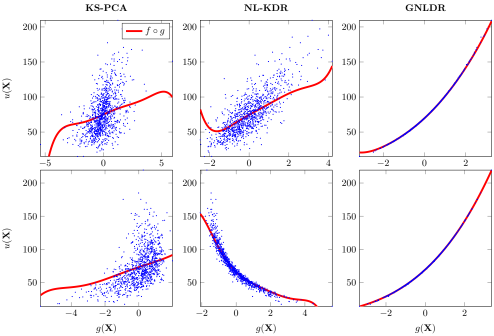
Kernel supervised PCA Barshan et al. [2011] aims to maximize the dependence between $G^T\Phi(\mathbf{X})$ and $\mathbf{Y}$ measured with the Hilbert-Schmidt norm of the cross-covariance operator restricted to an arbitrary reproducing kernel Hilbert space (RKHS).

Kernel dimension reduction Fukumizu et al. [2009] aims to minimize the dependence between $\mathbf{Y}$ and $\mathbf{Y}|G^T\Phi(\mathbf{X})$ measured with the Hilbert-Schmidt norm of the conditional covariance operator restricted to some RKHS.

In our experiments, we used squared exponential kernels for both $\kappa_{\mathbf{X}}$ and $\kappa_{\mathbf{Y}}$.



Isotropic function. Comparison of KS-PCA and NL-KDR with our method (GNLDR) for $m = 1$. Blue points: 1000 samples of $(g(\mathbf{X}), \mathcal{M}(\mathbf{X}))$. Red lines: function $g(\mathbf{x}) \mapsto f \circ g(\mathbf{x})$ with either $N = 50$ (top row) or $N = 500$ (bottom row). Here, f is a univariate polynomial of degree 6 and g a multivariate polynomial of degree 2.



Borehole function. Comparison of KS-PCA and NL-KDR with our method (GNLDR) for $m = 1$. Blue points: 1000 samples of $(g(\mathbf{X}), \mathcal{M}(\mathbf{X}))$. Red lines: function $g(\mathbf{x}) \mapsto f \circ g(\mathbf{x})$ with either $N = 30$ (top row) or $N = 300$ (bottom row). Here, f is a univariate polynomial of degree 6 and g a multivariate polynomial of degree 2.

Conclusion

- In this talk, we presented a trip around global sensitivity analysis (via total Sobol' indices) and (non)linear dimension reduction.
- We proposed a two-step algorithm to build the approximation $\mathcal{M}(\mathbf{x}) \approx f \circ g(\mathbf{x})$ adaptively with respect to the input/output sample. This algorithme takes into account gradient information.

Conclusion

- In this talk, we presented a trip around global sensitivity analysis (via total Sobol' indices) and (non)linear dimension reduction.
- We proposed a two-step algorithm to build the approximation $\mathcal{M}(\mathbf{x}) \approx f \circ g(\mathbf{x})$ adaptively with respect to the input/output sample. This algorithme takes into account gradient information.

Perspectives

- It would be interesting to propose an optimal (or at least a clever) sampling procedure.
- Beyond polynomial approximation?
- Although assuming $\mathbb{C}(\mathbf{X}|\mathcal{G}_r) < \infty$ is usual, proving it remains an open challenge. Is it possible to choose the approximation class $\mathcal{G}_r$ such that $\mathbb{P}_{\mathbf{X}|\mathcal{G}_r}$ is the push-forward measure of the standard normal distribution through a Lipschitz map.
- ...

Thanks for your attention!

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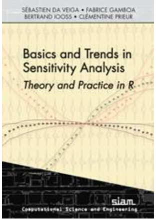
And a little bit of advertisement



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