

Surrogate to Poincaré inequalities on manifolds for dimension reduction in nonlinear feature spaces

Alexandre PASCO

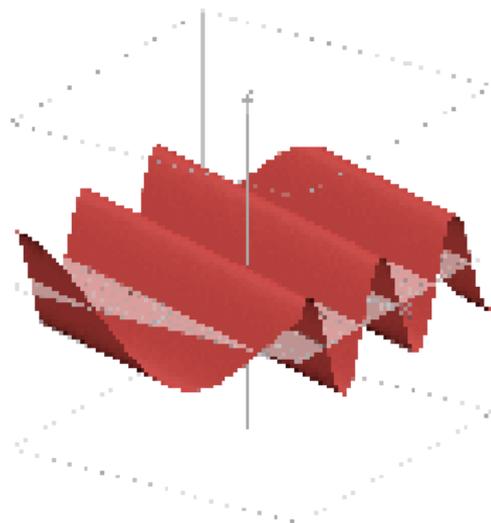
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In collaboration with Anthony NOUY.



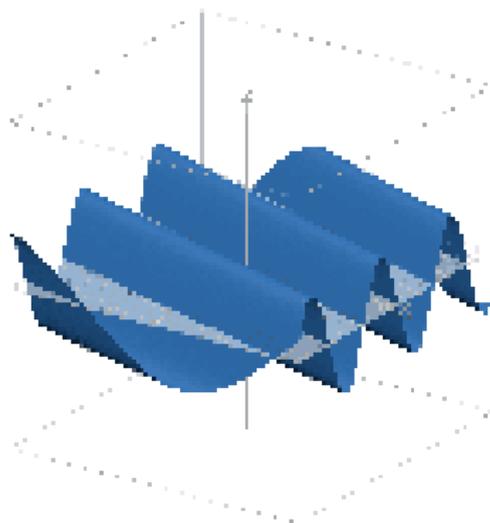
- ① Introduction
- ② Measuring the quality of g
- ③ Surrogate one feature
- ④ Surrogates multiple features
- ⑤ Numerical experiments
- ⑥ Conclusion and Perspectives

Introduction

$$u(x) = \sin(x_1 + 3x_2)$$

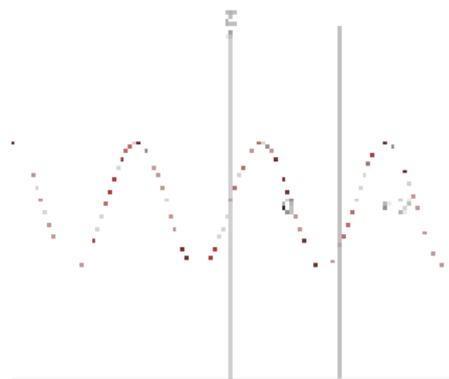


$$v(x) = \sin(x_1 + 3x_2 + 0.05x_1x_2)$$

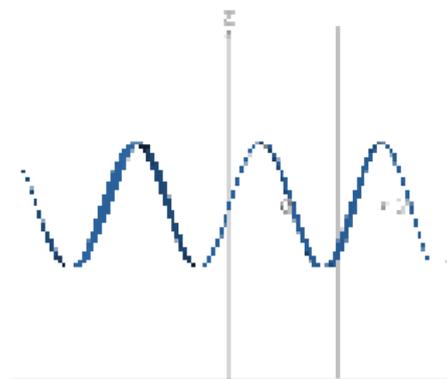


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- Goal : Approximate $u : \mathbb{R}^d \rightarrow \mathbb{R} \in \mathcal{C}^1$ with $d \gg 1$, i.e. minimize

$$\mathcal{E}(\tilde{u}) := \mathbb{E} [(u(\mathbf{X}) - \tilde{u}(\mathbf{X}))^2]$$

where \mathbf{X} has probability density $\mu_{\mathbf{X}}$.

- Given : Few costly point evaluations

$$\left(\mathbf{x}^{(i)}, u(\mathbf{x}^{(i)}), \nabla u(\mathbf{x}^{(i)}) \right)_{1 \leq i \leq n_s}.$$

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- Approximation of the form $\tilde{u} = f \circ g$.
- Step 1 : Learn a **feature map** $g \in \mathcal{G}_m \subseteq \mathcal{C}^1(\mathbb{R}^d, \mathbb{R}^m)$ with $m \leq d$, for some chosen **tractable** function class \mathcal{G}_m .
- Step 2 : Learn a profile map $f : \mathbb{R}^m \rightarrow \mathbb{R}$.

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- Step 2 : Learn a profile map $f : \mathbb{R}^m \rightarrow \mathbb{R}$.

- For a given g , the best profile map is

$$f_g(\mathbf{z}) := \mathbb{E} [u(\mathbf{X}) | \mathbf{Z} = \mathbf{z}],$$

where $\mathbf{Z} := g(\mathbf{X}) \in \mathbb{R}^m$. Problem : **not computable**.

- In practice : learn f^* via **regression**,

$$\inf_{f \in \mathcal{F}} \mathbb{E} [(u(\mathbf{X}) - f(\mathbf{Z}))^2]$$

- One can also consider gradient enhanced regression.

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The set \mathcal{G}_m

- [Constantine et al., 2014]
Linear $g(\mathbf{x}) = G^T \mathbf{x}$ with $G \in \mathbb{R}^{d \times m}$.
- [Bigoni et al., 2022, Romor et al., 2022]
Vector space $g(\mathbf{x}) = G^T \Phi(\mathbf{x})$ with $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^K$ and $G \in \mathbb{R}^{K \times m}$ with $K \geq d$.
- [Verdière et al., 2023, Zhang et al., 2019]
Diffeomorphism-based $g(\mathbf{x}) = (\psi_1(\mathbf{x}), \dots, \psi_m(\mathbf{x}))^T$ where $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a diffeomorphism.

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Poincaré Inequality

- Assuming $\nabla g(\mathbf{X})$ has rank m a.s., then $\mathcal{M}_{\mathbf{Z}} := g^{-1}(\mathbf{Z})$ is a smooth submanifold of \mathbb{R}^d .
- Let $C_{\mathbf{Z}}$ the smallest constant such that for any $h \in \mathcal{C}^1(\mathcal{M}_{\mathbf{Z}}, \mathbb{R})$ with mean 0,

$$\mathbb{E} [h(\mathbf{X})^2 | \mathbf{Z} = \mathbf{z}] \leq C_{\mathbf{Z}} \mathbb{E} [\|\nabla h(\mathbf{X})\|_2^2 | \mathbf{Z} = \mathbf{z}].$$

If $C_{\mathbf{Z}} < \infty$ we say that $\mu_{\mathbf{X}|\mathbf{Z}=\mathbf{z}}$ satisfies a **Poincaré Inequality**.

- Apply to $h = (u - f_g \circ g)|_{\mathcal{M}_{\mathbf{z}}}$ for $\mathbf{x} \in \mathcal{M}_{\mathbf{z}}$,

$$\|\nabla h(\mathbf{x})\|_2^2 = \|\Pi_{\nabla g(\mathbf{x})}^\perp \nabla u(\mathbf{x})\|_2^2 = \|\nabla u(\mathbf{x})\|_2^2 - \|\Pi_{\nabla g(\mathbf{x})} \nabla u(\mathbf{x})\|_2^2$$

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Poincaré-based upper-bound

For $g \in \mathcal{G}_m$ define

$$\mathcal{J}(g) := \mathbb{E} \left[\|\Pi_{\nabla g(\mathbf{X})}^\perp \nabla u(\mathbf{X})\|_2^2 \right]$$

- (1) Assume $\text{rank}(\nabla g(\mathbf{x})) = m$ for all $\mathbf{x} \in \mathcal{X}$ and all $g \in \mathcal{G}_m$.
- (2) Assume $C(\mathbf{X}|\mathcal{G}_m) < \infty$ where

$$C(\mathbf{X}|\mathcal{G}_m) := \sup_{g \in \mathcal{G}_m} \sup_{\mathbf{z} \in g(\mathcal{X})} C_{\mathbf{z}}.$$

Proposition ([Bigoni et al., 2022])

Under assumptions (1) and (2), it holds

$$\min_{f: \mathbb{R}^m \rightarrow \mathbb{R}} \mathbb{E} [(u(\mathbf{X}) - f \circ g(\mathbf{X}))^2] \leq C(\mathbf{X}|\mathcal{G}_m) \mathcal{J}(g)$$

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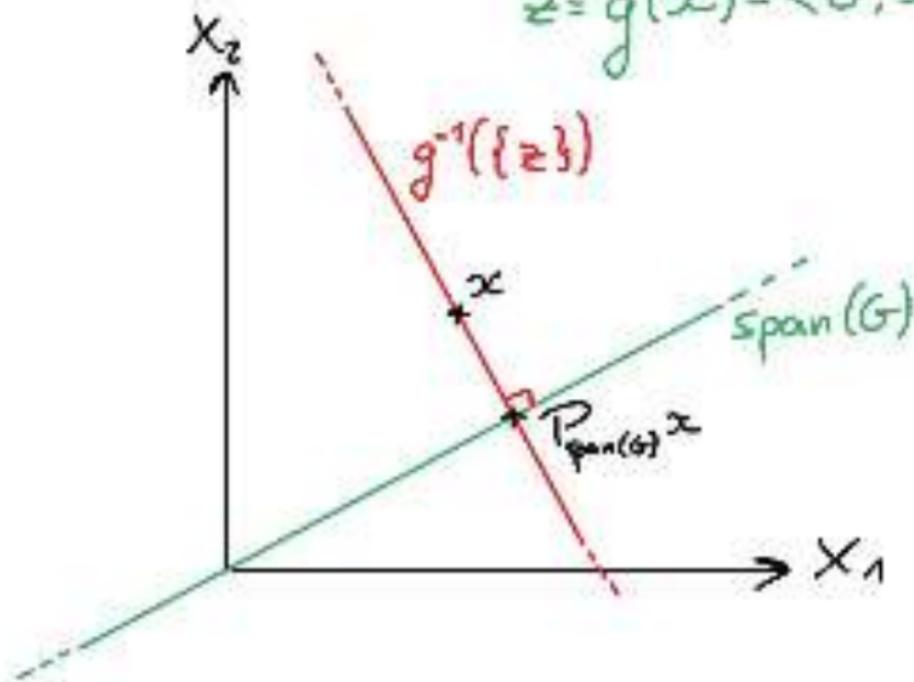
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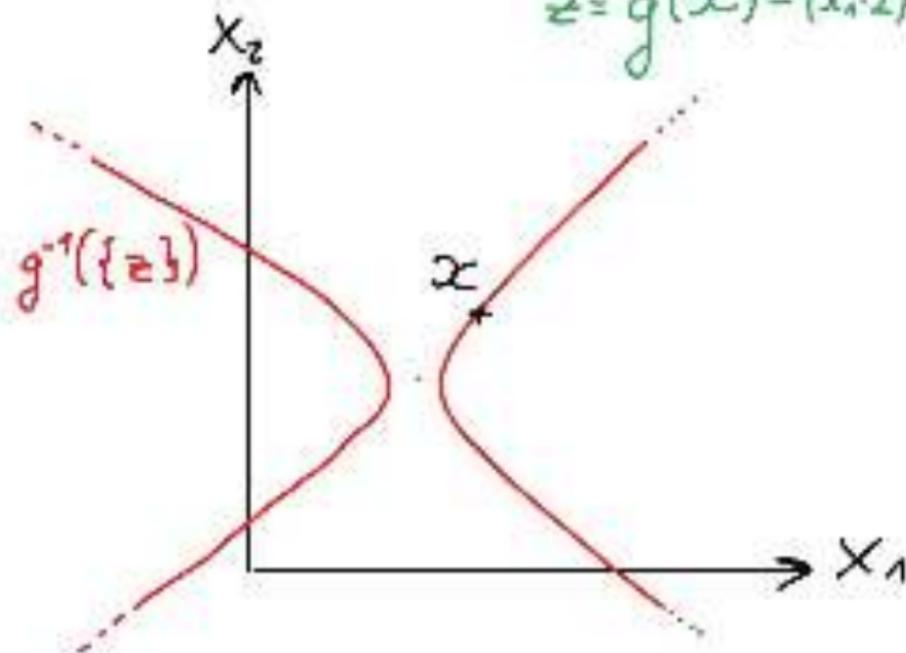
Linear level sets

$$z = g(x) = \langle G, x \rangle$$



Nonlinear level sets

$$z = g(x) = (x_1 + 2)^2 - (x_2 - 2)^2$$



The Poincaré Constant

Caveats:

- For general classes \mathcal{G}_m bounding $C(\mathcal{G}_m)$ is an open problem.
- Worse : if $g^{-1}(\{z\})$ is not connected then $C_z = \infty$.

Hopes:

- Poincaré-like bounds are pessimistic.
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The function \mathcal{J}

- Recall that

$$\mathcal{J}(g) = \mathbb{E} [\|\nabla u(\mathbf{X})\|_2^2] - \mathbb{E} [\|\Pi_{\nabla g(\mathbf{X})} \nabla u(\mathbf{X})\|_2^2]$$

- For $g(\mathbf{x}) = G^T \mathbf{x}$ with $G^T G = I_m$,

$$\Pi_{\nabla g(\mathbf{X})} = G G^T,$$

thus $G \mapsto \mathcal{J}(G^T)$ is **quadratic** and can be **explicitly minimized**.

- For $g(\mathbf{x}) = G^T \Phi(\mathbf{x})$ with fixed $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^K$,

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The set \mathcal{G}_m

- Linear $g(\mathbf{x}) = G^T \mathbf{x}$ with $G \in \mathbb{R}^{d \times m}$.
 - + Known bounds on $C(\mathbf{X}|\mathcal{G}_m)$ for some classical $\mu_{\mathbf{X}}$.
 - + Easy to minimize \mathcal{J} , i.e. to find the best A .
 - Restricted class.
- Vector space $g(\mathbf{x}) = G^T \Phi(\mathbf{x})$ with $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}^K$ and $G \in \mathbb{R}^{K \times m}$ with $K \geq d$.
 - + Learning G is more reasonable (\mathcal{J} non-convex but \mathcal{G}_m convex).
 - Cannot say much on $C_{\mathbf{z}}$.
- Diffeomorphism-based $g(\mathbf{x}) = (\psi_1(\mathbf{x}), \dots, \psi_m(\mathbf{x}))^T$ where $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a diffeomorphism .
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Surrogate one feature: definition

- The loss function \mathcal{J} now writes

$$\begin{aligned}\mathcal{J}(g) &= \mathbb{E} \left[\|\nabla u(\mathbf{X})\|_2^2 - \frac{(\nabla g(\mathbf{X})^T \nabla u(\mathbf{X}))^2}{\|\nabla g(\mathbf{X})\|_2^2} \right] \\ &= \mathbb{E} \left[\frac{1}{\|\nabla g(\mathbf{X})\|_2^2} \underbrace{\|\nabla u(\mathbf{X})\|_2^2 \|\Pi_{\nabla u(\mathbf{X})}^\perp \nabla g(\mathbf{X})\|_2^2}_{\text{Quadratic wrt } g} \right]\end{aligned}$$

- Controlling $\|\nabla g(\mathbf{X})\|_2^2$ allows to control $\mathcal{J}(g)$ by a **quadratic** surrogate,

$$\mathcal{L}_1(g) := \mathbb{E} \left[\|\nabla u(\mathbf{X})\|_2^2 \|\Pi_{\nabla u(\mathbf{X})}^\perp \nabla g(\mathbf{X})\|_2^2 \right].$$

- Problem : control should be **uniform** on \mathcal{G}_1 .

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Surrogate one feature: Uniform control

- Uniformly bi-Lipschitz (ideal setting), i.e

$$\forall g \in \mathcal{G}_1, \quad 0 < c \leq \|\nabla g(\mathbf{X})\|_2^2 \leq C < +\infty$$

- + Possible when : linear or diffeomorphism-based.
- Not possible when : vector space of dimension $K > d$.

- Deviation inequalities, i.e rate of convergence of

$$\forall g \in \mathcal{G}_1, \quad \underbrace{\mathbb{P} [\|\nabla g(\mathbf{X})\|_2^2 \leq \beta^{-1}]}_{\text{Small deviations}}, \underbrace{\mathbb{P} [\|\nabla g(\mathbf{X})\|_2^2 \geq \beta]}_{\text{Large deviations}} \xrightarrow{\beta \rightarrow +\infty} 0$$

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Surrogate one feature: Deviation inequalities

Consider $h : \mathbb{R}^d \rightarrow \mathbb{R}$. Assume that

- (1) \mathbf{X} has s -concave, $s \in (0, 1/d]$, proba law (implies compactly supported on a convex set).
- (2) For any bounded line $J \subset \mathbb{R}^d$ and any measurable $I \subset J$,

$$\sup_{\mathbf{x} \in J} |h(\mathbf{x})| \leq \left(\frac{A_h |J|}{|I|} \right)^{k_h} \sup_{\mathbf{x} \in I} |h(\mathbf{x})|,$$

e.g. $A_h = 4$ and $k_h = k$ for polynomial with total degree $\leq k$.

Proposition (Direct consequence of [Fradelizi, 2009])

Under (1) and (2) and for some η_h , it holds for all $\beta > 0$,

$$\mathbb{P} [|h(\mathbf{X})| \leq \beta^{-1}] \lesssim \beta^{-1/k_h}, \quad \mathbb{P} [|h(\mathbf{X})| \geq \beta^{-1}] \lesssim 1_{\beta \leq \eta_h}.$$

For $s \in [-\infty, 0]$, still holds but slower decay for large deviations.

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$$\mathbb{P} [|h(\mathbf{X})| \leq \beta^{-1}] \lesssim \beta^{-1/k_h}, \quad \mathbb{P} [|h(\mathbf{X})| \geq \beta^{-1}] \lesssim 1_{\beta \leq \eta_h}.$$

For $s \in [-\infty, 0]$, still holds but slower decay for large deviations.

Surrogate one feature: Deviation inequalities

Consider $h : \mathbb{R}^d \rightarrow \mathbb{R}$. Assume that

- (1) \mathbf{X} has s -concave, $s \in (0, 1/d]$, proba law (implies compactly supported on a convex set).
- (2) For any bounded line $J \subset \mathbb{R}^d$ and any measurable $I \subset J$,

$$\sup_{\mathbf{x} \in J} |h(\mathbf{x})| \leq \left(\frac{A_h |J|}{|I|} \right)^{k_h} \sup_{\mathbf{x} \in I} |h(\mathbf{x})|,$$

e.g. $A_h = 4$ and $k_h = k$ for polynomial with total degree $\leq k$.

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Surrogate one feature: Suboptimality result

- If \mathcal{G}_1 contains only non-constant polynomials of total degree at most $\ell + 1$, then the previous deviation inequalities hold uniformly on \mathcal{G}_1 with $k = 2\ell$ and $A = 4$.

Proposition

Under (1), with \mathcal{G}_1 as above, it holds

$$\forall g \in \mathcal{G}_1, \quad \gamma_1 \mathcal{L}_1(g) \leq \mathcal{J}(g) \leq \gamma_2 \mathcal{L}_1(g)^{\frac{1}{1+2\ell}},$$

for some $0 < \gamma_1, \gamma_2 < +\infty$. In particular, for some $0 < \gamma_3 < +\infty$,

$$\mathcal{J}(g^*) \leq \gamma_3 \inf_{\mathcal{G}_1} \mathcal{J}^{\frac{1}{1+2\ell}}$$

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Similar results hold for $s \in [-\infty, 0]$.

Surrogate one feature: Vector space

- For assumptions to hold, we consider a sym pd $R \in \mathbb{R}^{K \times K}$,

$$\mathcal{G}_1 := \left\{ g : \mathbf{x} \mapsto G^T \Phi(\mathbf{x}) : G \in \mathbb{R}^K, G^T R G = 1 \right\},$$

- [Bigoni et al., 2022] Invariance property of \mathcal{J} implies

$$\inf_{g \in \text{span}\{\Phi_1, \dots, \Phi_K\}} \mathcal{J}(g) = \inf_{g \in \mathcal{G}_1} \mathcal{J}(g)$$

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$$\min_{g \in \mathcal{G}_1} \mathcal{L}_1(g) = \min_{\substack{G \in \mathbb{R}^K \\ G^T R G = 1}} G^T H G,$$

where $H := H^{(1)} - H^{(2)} \in \mathbb{R}^{K \times K}$ is sym psd and

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Surrogates multiple features: Quick overview

- With similar reasoning, we define for $1 \leq j \leq m$,

$$\mathcal{L}_{m,j}(g) := \mathbb{E} \left[\|v_{g,j}(\mathbf{X})\|_2^2 \|\Pi_{v_{g,j}(\mathbf{X})}^\perp \Pi_{\nabla g_j(\mathbf{X})}^\perp \nabla g_j(\mathbf{X})\|_2^2 \right],$$

with $v_{g,j}(\mathbf{x}) := \Pi_{\nabla g_j(\mathbf{x})}^\perp \nabla u(\mathbf{x})$.

- For fixed $g_{-j} : \mathbb{R}^d \rightarrow \mathbb{R}^{m-1}$, we use $h \mapsto \mathcal{L}_{m,j}((g_{-j}, h))$ as a quadratic surrogate to $h \mapsto \mathcal{J}((g_{-j}, h))$.
- Now need deviation inequalities on $\mathbf{x} \mapsto \|\Pi_{\nabla g_j(\mathbf{x})}^\perp \nabla g_j(\mathbf{x})\|_2^2$.

Proposition

Assume the law of \mathbf{X} is s -concave with $s \in (0, 1/d]$. Assume \mathcal{G}_m is a compact set of polynomial with total degree at most $\ell + 1$ with full rank gradients a.s. For a fixed g_{-j} , it holds

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Settings

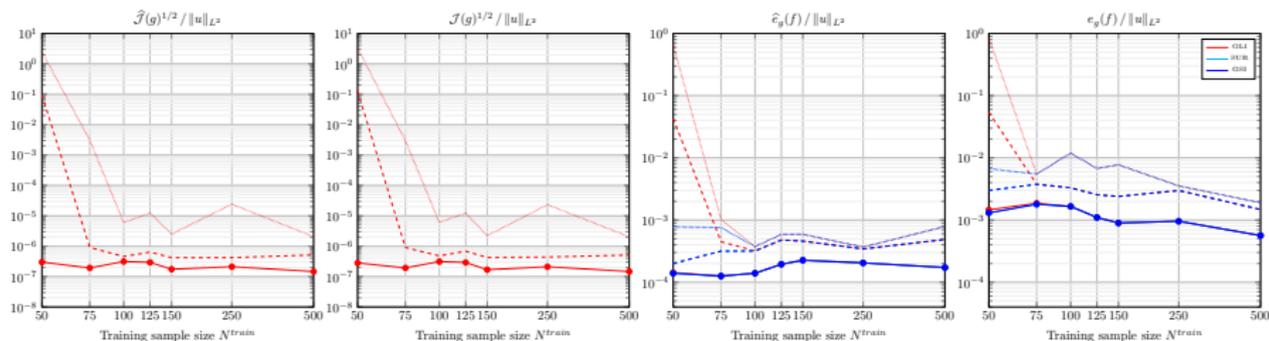
- Feature: Tensorized polynomial basis $\Phi(\mathbf{x}) = (\phi_\alpha(\mathbf{x}))_{\alpha \in \Lambda_{p,k}}$ with

$$\phi_\alpha(\mathbf{x}) := \prod_{\nu=1}^d \phi_{\alpha_\nu}^\nu(x_\nu), \quad \Lambda_{p,k} := \{\alpha \in \mathbb{N}^d : \|\alpha\|_p \leq k\} \setminus \{0\},$$

where (k, p) are hyperparameters learnt by 5-fold cross-validation.

- Regression: Kernel regression with gaussian kernel and Ridge regularization, whose hyperparameters are learnt by 10-fold cross-validation.

Numerical experiments: one feature



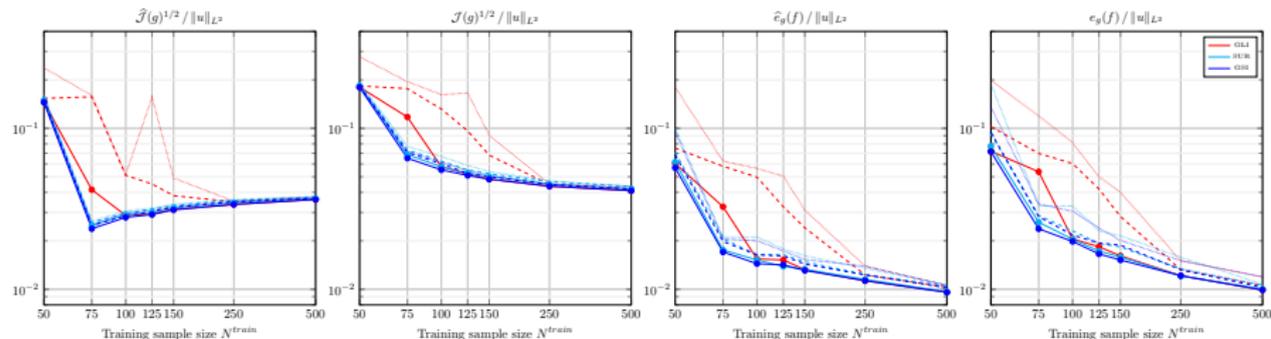
$$u(x) = \sin\left(\frac{4}{\pi^2} \|x\|^2\right), \quad d = 8, \quad m = 1$$

50%, 90% and 100% quantiles over 20 realizations.

Left plots : train and test estimations of $\mathcal{J}(g) / \|u\|_{L^2}$.

Right plots : train and test estimations of $\|u - f \circ g\|_{L^2} / \|u\|_{L^2}$.

Numerical experiments: one feature



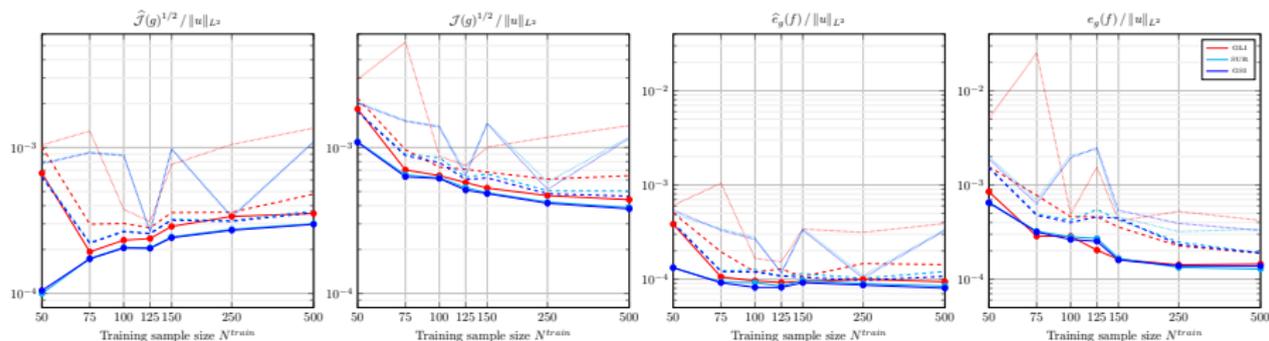
$$u(x) = \exp\left(\frac{1}{d} \sum_{i=1}^d \sin(x_i) e^{\cos(x_i)}\right), \quad \mathbf{X} \sim \mathcal{U}\left(\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]^8\right) \quad m = 1$$

50%, 90% and 100% quantiles over 20 realizations.

Left plots : train and test estimations of $\mathcal{J}(g)/\|u\|_{L^2}$.

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Numerical experiments: one feature



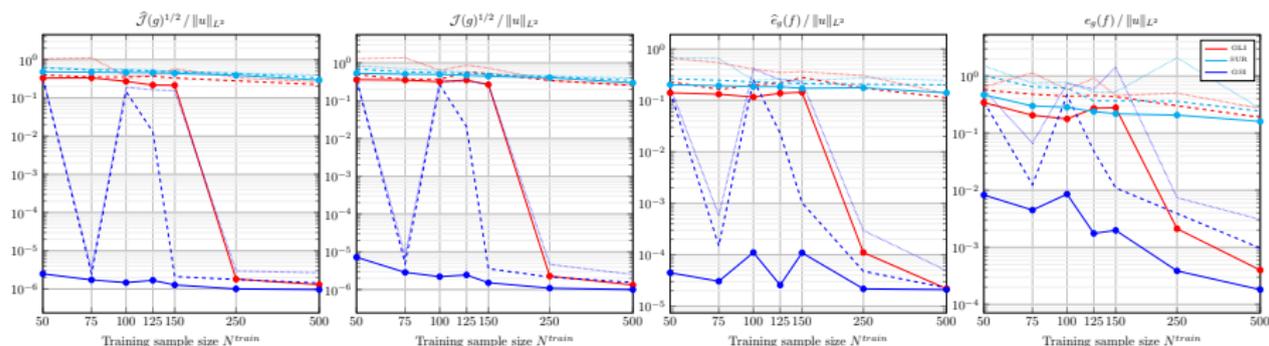
$$u(x) = \text{borehole}, \quad d = 8, \quad m = 1$$

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Right plots : train and test estimations of $\|u - f \circ g\|_{L^2}/\|u\|_{L^2}$.

Numerical experiments: multiple features



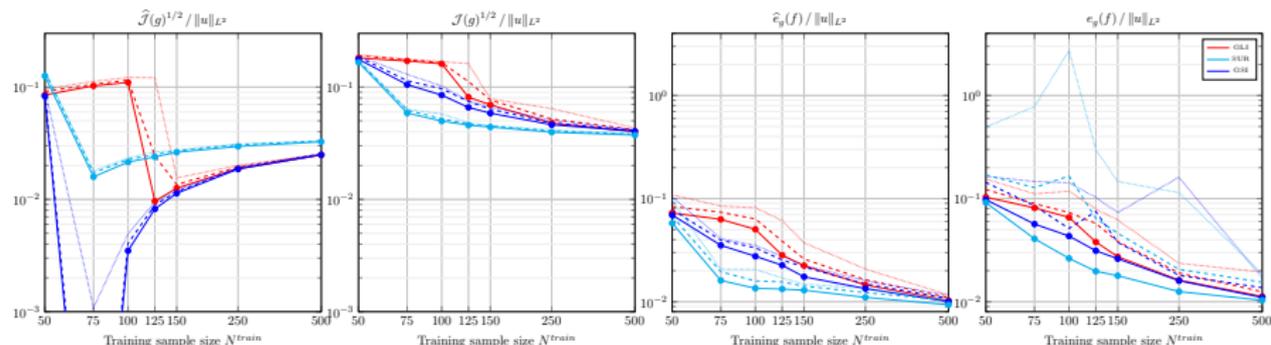
$$u(x) := \cos\left(\frac{1}{2}x^T x\right) + \sin\left(\frac{1}{2}x^T Mx\right), \quad \mathbf{X} \sim \mathcal{U}\left(\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]^8\right) \quad m = 2$$

50%, 90% and 100% quantiles over 20 realizations.

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Conclusion and Perspectives

- Quadratic surrogates with controlled suboptimality
- Works well for $m = 1$, more mitigated for $m > 1$.

→ Structured approach in a Tensor-Network fashion.

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→ Optimal sampling for f , oblivious to g .

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Thank you !

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