Structured Nonlinear Dimension Reduction Using Gradient Evaluations

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Introduction

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

$$\mathcal{E}(\hat{u}) := \mathbb{E}\left[(u(X) - \hat{u}(X))^2\right]$$

where X has probability density μ_X.

- Given : Few costly point evaluations drawn from $\mu_X dx$,

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

- Remark : vector-valued u described in [ZCPM20, VPZ23]

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A first approach

- Gradient enhanced regression,

$$\min_{v \in \mathcal{U}_N} \frac{1}{n} \sum_{i=1}^{n} (u(x^{(i)}) - v(x^{(i)}))^2 + \|\nabla u(x^{(i)}) - \nabla v(x^{(i)})\|^2,$$

  taking $\mathcal{U}_N$ as polynomials, splines, Neural Nets, ...

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- Problem : large d and few samples $\Rightarrow$ ill-conditioned problem.

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Our approach

- Approximation of the form $\tilde{u} = f \circ g$.
- Example : if u is a QoI of some PDE discretized with d dofs, then Reduced Basis means taking $g(x) = U_r^T x$.
- 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** $f : \mathbb{R}^m \to \mathbb{R}$.

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- Step 2 : Parametric studies in $\mathbb{R}^m$ instead of $\mathbb{R}^d$.

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Profile map

- For a given g, the best profile function is

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

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

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Measuring the quality of g

What if $u = f \circ g$?

for some $g \in \mathcal{G}_m$ and some f.

If $u = f \circ g$

- Assume $u = f \circ g$ then $\nabla u(x) = J_g^T(x) J_f(g(x))$.Thus

$$\exists f \text{ s.t. } u = f \circ g \quad \Longrightarrow \quad \nabla u(x) \in \text{cspan}(J_g^T(x)), \forall x$$

- If $g^{-1}(z)$ is smoothly pathwise-connected for all $z \in \text{Im}(g)$,

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$$\exists f \text{ s.t. } u = f \circ g \qquad \Longleftrightarrow \qquad \mathcal{L}(g) = 0$$

- Define

$$\mathcal{L}(g) := \mathbb{E}\left[\|\nabla u(X) - P_{\mathsf{cspan} J_g^T(X)} \nabla u(X)\|^2\right]$$

$$= \mathbb{E}\left[\nabla u^T \nabla u - \nabla u^T J_g^T (J_g J_g^T)^{-1} J_g \nabla u\right]$$

Poincaré Inequality

Assuming that a.s. $J_g(X)$ has rank m then we can write

$$\mathcal{L}(g) := \mathbb{E}\left[\|\nabla u_{|\mathcal{M}_Z}(X)\|^2\right],$$

where $\mathcal{M}_z := g^{-1}(z)$ is a Riemannian submanifold of $\mathbb{R}^d$ endowed with euclidean metric.

Definition (Poincaré Inequality)

Given $z \in Im(g)$, let $C(\mu_{X|Z=z})$ the smallest constant such that for any $h \in \mathcal{C}^1(\mathcal{M}_z, \mathbb{R})$,

$$\mathbb{E}\left[(h(X) - \mathbb{E}\left[h(X)\right])^2 | Z = z\right] \leq C(\mu_{X|Z=z}) \mathbb{E}\left[\|\nabla h(X)\|^2 | Z = z\right],$$

If $C(\mu_{X|Z=z}) < \infty$ we say that $\mu_{X|Z=z}$ satisfies a Poincaré Inequality.

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Bounding the best error

(1) Assume $\text{rank}(J_g(X)) = m$ a.s., for all $g \in \mathcal{G}_m$.
(2) Assume $C(\mu_X, \mathcal{G}_m) < \infty$ where

$$C(\mu_X, \mathcal{G}_m) := \sup_{g \in \mathcal{G}_m} \sup_{z \in Im(g)} C(\mu_{X|Z=z}).$$

Proposition ([BMPZ22])

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

$$\mathbb{E}\left[(u(X) - f_g \circ g(X))^2\right] \leq C(\mu_X, \mathcal{G}_m)\mathcal{L}(g)$$

We now focus on

$$\min_{g \in \mathcal{G}_m} \mathcal{L}(g)$$

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Caveats:

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

Hopes:

- In practical cases the Poincaré bound is very pessimistic.
- Numerical experiments often showed a sharper bound.

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The class $\mathcal{G}_m$

- [CDW14] Linear $g(x) = A^T x$ with $A \in \mathbb{R}^{d\times m}$.
  - $+$ Known bounds on $C(\mu_X, \mathcal{G}_m)$ for some classical μ_X.
  - $+$ Easy to minimize $\mathcal{L}$, i.e. to find the best A.
  - $-$ Restricted class.
- [VPZ23] Diffeomorphism-based $g(x) = (\psi_1(x), \cdots, \psi_m(x))^T$ where $\psi : \mathbb{R}^d \to \mathbb{R}^d$ is a diffeomorphism .
  - $+$ Allow penalization for better control on $C(\mu_{X|Z=z})$.
  - $-$ Learning ψ can be difficult.
- [BMPZ22] Linear in features $g(x) = G^T \phi(x)$ with $\phi : \mathbb{R}^d \to \mathbb{R}^K$ and $G \in \mathbb{R}^{K\times m}$ with $K \geq d$.
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Minimizing $\mathcal{L}$

- Choose $\phi : \mathbb{R}^d \to \mathbb{R}^K$ with $K \geq d$, e.g. multivariate polynomials or splines.
- Tackle the following problem

$$\min_{\substack{G \in \mathbb{R}^{K \times m} \\ \text{constrains}(G)}} \quad \mathcal{L}(G^T \phi)$$

- [BMPZ22] Use a quasi-Newton method and go greedy on polynomial degree for ϕ.
- Questions :
  - Simpler way of building a good G ?
  - Other approach to build ϕ ?

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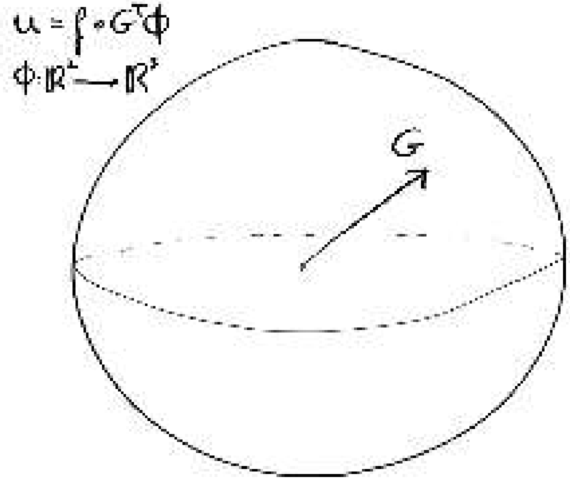
What if $u = f \circ G^T \phi$ and $m = 1$?

for some $\phi : \mathbb{R}^d \to \mathbb{R}^K$, some $G \in \mathbb{R}^{K \times m}$

If $u = f \circ G^T \phi$ and $m = 1$



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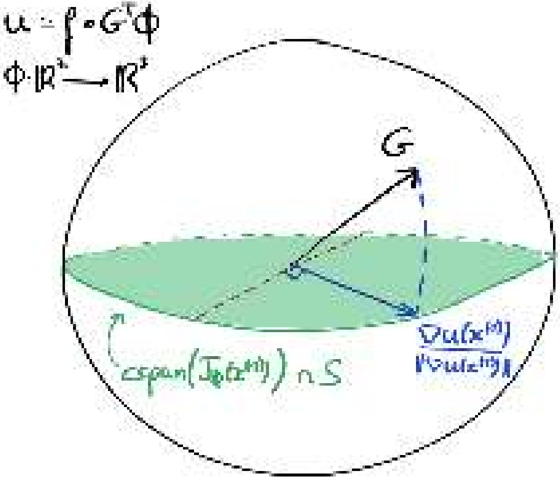

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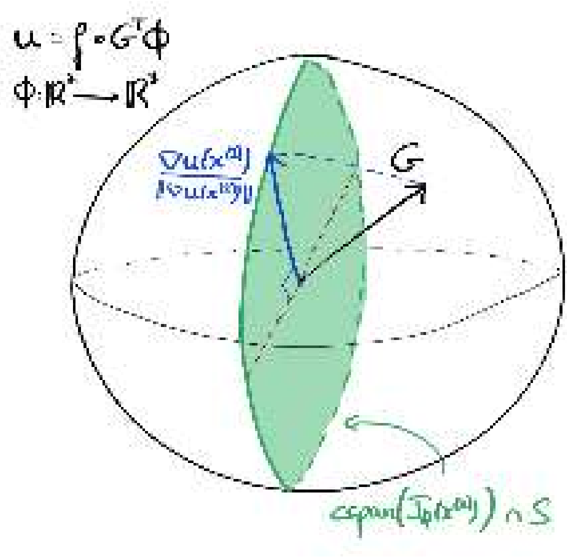

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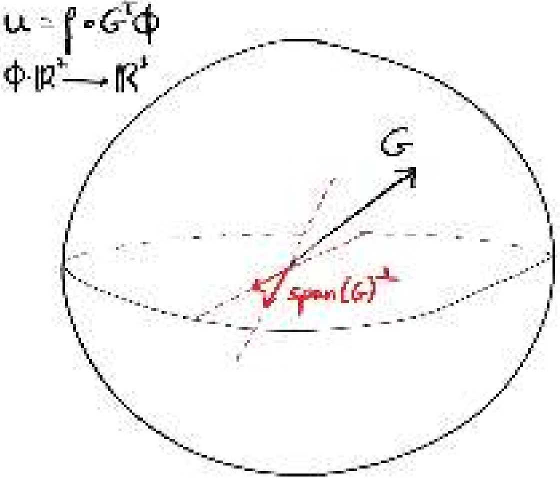

Case $m = 1$

- Define

$$\mathcal{J}(g) := \mathbb{E}\left[\|\nabla g(X) - P_{\mathsf{span}\nabla u(X)} \nabla g(X)\|^2\right].$$

which satisfies $\mathcal{J}(g) = 0 \iff \mathcal{L}(g) = 0$.

- Using $g = G^T \phi$ we can define some $H \in \mathbb{R}^{K \times K}$ s.t.

$$\mathcal{J}(g) = G^T H G.$$

$\rightarrow$ We can minimize $\mathcal{J}$ by solving an eigen-value problem !

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- If $m > 1$ then $\mathcal{J}(g) = 0 \not\Leftrightarrow \mathcal{L}(g) = 0$
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Structured approach

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- See $X = (S, T)$ consider g of the form

$$g(X) = G_3^T \phi_3\big(\, G_1^T \phi_1(S), G_2^T \phi_2(T)\,\big),$$

  for some chosen ϕ_i.

- First fit G_1 and G_2 independently, then fit G_3.

- Go further and consider a tree structure for g.

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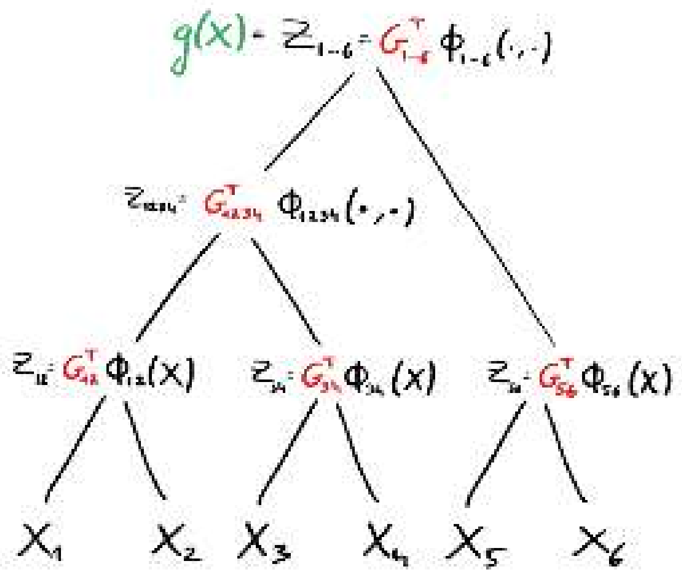

Structured approach

+ Better learning than Neural Nets while more expressive than Tensor Nets.

+ Several low-dim problems instead of one high-dim problem.

+ Under assumptions, we can use the approach from the case $m = 1$ to fit $G_1 \in \mathbb{R}^{K_1 \times m_1}$ and $G_2 \in \mathbb{R}^{K_2 \times m_2}$ with $m_1, m_2 > 1$.

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+ Under assumptions, we can use the approach from the case $m = 1$ to fit $G_1 \in \mathbb{R}^{K_1 \times m_1}$ and $G_2 \in \mathbb{R}^{K_2 \times m_2}$ with $m_1, m_2 > 1$.

- Good choice for the structure and for ϕ_i ?

Structured approach

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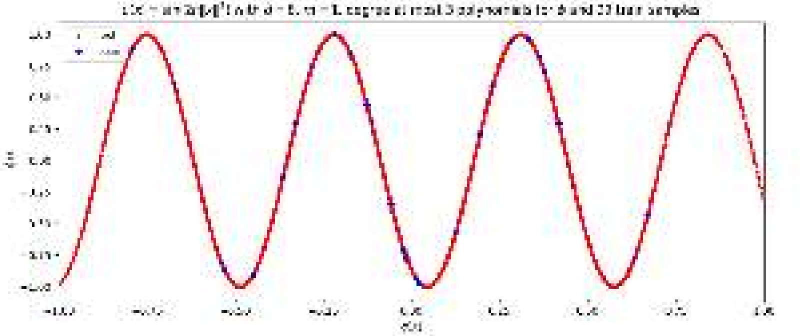
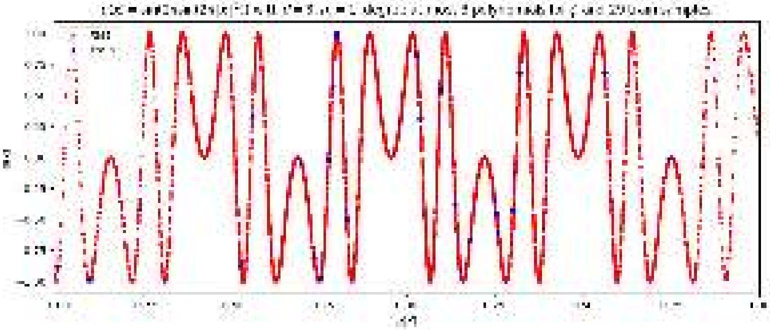
Numerical experiments

Structured approach



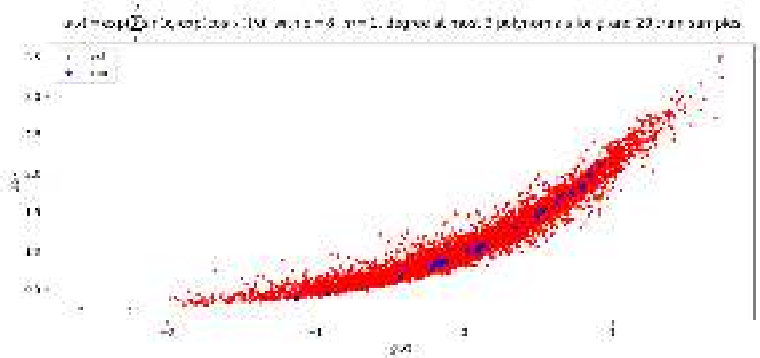
$$u(x) = \sin(2\pi\|x\|^2)$$

29 train samples



$$u(x) = \sin(2\pi \sin(2\pi \|x\|^2))$$

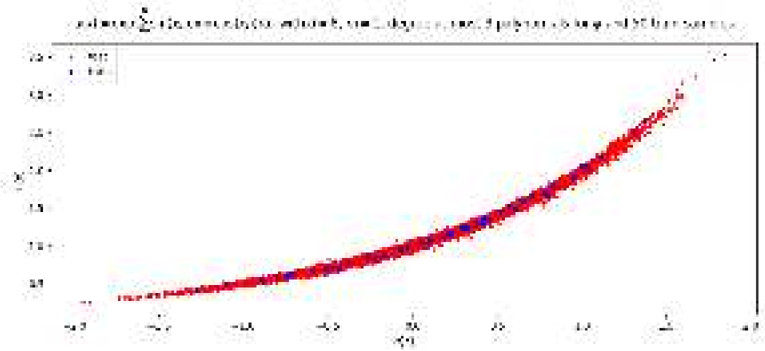
29 train samples



$$u(x) = \exp\big(\frac{1}{d}\sum_{i=1}^{d}\sin(x_i)\exp(\cos(x_i))\big)$$

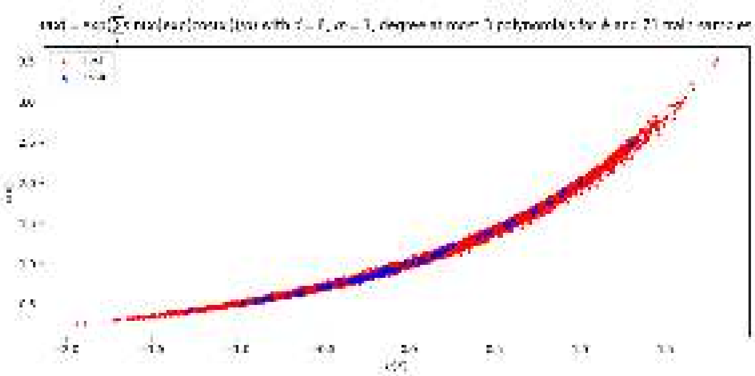
29 train samples

Structured approach



$$u(x) = \exp\Big(\frac{1}{d}\sum_{i=1}^{d}\sin(x_i)\exp(\cos(x_i))\Big)$$

50 train samples



$$u(x) = \exp\Big(\frac{1}{d}\sum_{i=1}^{d}\sin(x_i)\exp(\cos(x_i))\Big)$$

71 train samples

Conclusion and Perspectives

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- Structured way of fitting the feature map

$\rightarrow$ Investigate $\mathcal{L}(g)$ VS $\mathcal{J}(g)$

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Thank you !

Appendix

References I

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