Stable nonlinear manifold approximation using compositional networks

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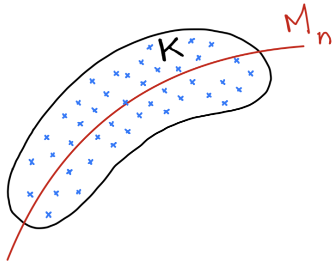
Joint works with Antoine Bensalah and Joel Soffo.

Introduction

We consider the problem of approximating a subset K of a normed space X by a low-dimensional set M_n, from samples in K.



A common setting (in statistics) if when K is the range of some vector or function-valued random variable.

Another classical setting is the solution of forward or inverse problems for parameter-dependent equations, where

$$K = \{u(y) : y \in Y\} \quad \text{with} \quad R(u(y); y) = 0.$$

Introduction

The approximating sets M_n can be

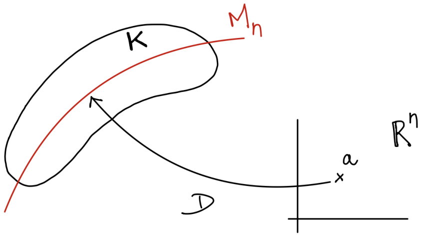
- constructed offline by manifold approximation methods, using samples from K,
- used online to compute approximations of elements in K with low computational complexity, or from limited information.

Encoder-Decoder

A large class of manifold approximation methods can be described by an encoder $E : K \to \mathbb{R}^n$ and a decoder $D : \mathbb{R}^n \to X$.

The decoder provides a parametrization of a n-dimensional "manifold"

$$M_n = \{D(a) : a \in \mathbb{R}^n\}.$$



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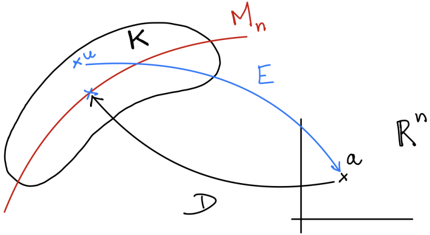

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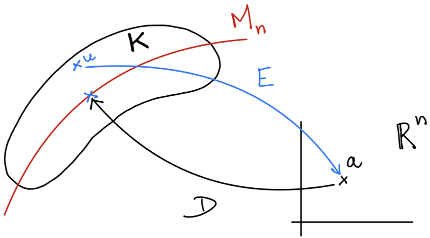

An element $u \in K$ is approximated by $D \circ E(u) \in M_n$.

This problem is equivalent to approximating the identity map on K by $D \circ E$ (auto-encoder of K).

Optimal performance

Manifold approximation methods can be classified in terms of the properties of their encoders and decoders.

The optimal performance of a given class $\mathcal{E}_n$ of encoders from X to $\mathbb{R}^n$ and a given class $\mathcal{D}_n$ of decoders from $\mathbb{R}^n \to X$ can be assessed in worst-case setting by

$$\inf_{D \in \mathcal{D}_n, E \in \mathcal{E}_n} \sup_{u \in K} \|u - D \circ E(u)\|_X.$$

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If the set K is equipped with a measure ρ, the optimal performance can be measured in average sense by

$$\inf_{D\in\mathcal{D}_n, E\in\mathcal{E}_n} \left(\int_K \|u - D\circ E(u)\|_X^p d\rho(u) \right)^{1/p}.$$

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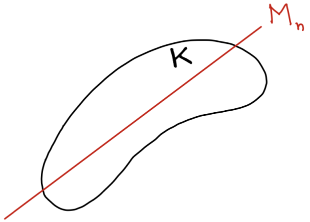
These errors define measures of complexity (widths) of K.

Linear approximation - Worst case setting

The range M_n of a **linear decoder** $D : \mathbb{R}^n \to X$ is a linear space with dimension at most n.



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Restricting the **decoder and encoder to be linear** yields the **approximation numbers** (linear widths)

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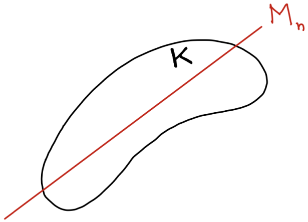
where the infimum is taken over all linear maps $A : X \to X$ with rank n.



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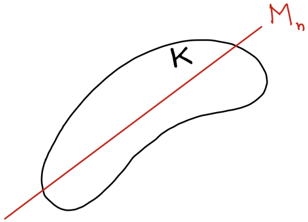

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Restricting **only the decoder to be linear** yields the **Kolmogorov n-width**

$$d_n(K)_X = \inf_{D \in L(\mathbb{R}^n;X)} \sup_{u \in K} \inf_{a \in \mathbb{R}^n} \|u - D(a)\|_X = \inf_{\dim M_n = n} \sup_{u \in K} \inf_{v \in M_n} \|u - v\|_X.$$

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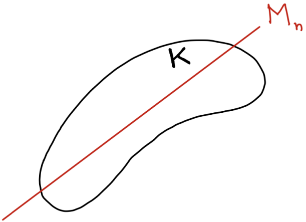

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For X a Hilbert space, $a_n(K)_X = d_n(K)_X$ and an optimal auto-encoder $D \circ E$ is given by the orthogonal projection P_{M_n} onto an optimal space M_n.

In practice optimal linear spaces in worst-case error are out of reach but near to optimal spaces M_n can be obtained by greedy algorithms, that generate an increasing sequence of spaces from samples in K [Buffa, Maday, Patera, Prud'homme, Turinici, Binev, Cohen, Dahmen, DeVore,...].

Linear approximation - Average setting

When X is a Hilbert space and the error is measured in average sense, it yields the **average Kolmogorov n-width**

$$d_n^{(p)}(K,\rho)_X^p = \inf_{D \in L(\mathbb{R}^n;X)} \int_K \inf_{a\in\mathbb{R}^n} \|u - D(a)\|_X^p d\rho(u) = \inf_{\dim M_n = n} \int_K \|u - P_{M_n} u\|_X^p d\rho(u).$$

For $p=2$ (mean-squared error), an optimal space M_n is given by a dominant eigenspace of the (compact) operator

$$T(v) = \int_K u(u,v)_X d\rho(u), \quad v \in X,$$

and

$$\int_K \|u - P_{M_n} u\|_X^2 d\rho(u) = d_n^{(2)}(K,\rho)_X^2 = \sum_{i>n} \lambda_i(T)$$

If ρ is a probability measure, assuming $\bar{u} = \int u \, d\rho(u) = 0$, T is the covariance operator of ρ and this corresponds to Principal Component Analysis (PCA).

Nonlinear continuous manifold approximation

Restricting both the **encoder and decoders to be continuous** (possibly nonlinear) yields the notion of **nonlinear manifold width** of [DeVore, Howard and Michelli 1989]

$$\delta_n(K)_X = \inf_{E \in C(X;\mathbb{R}^n)} \inf_{D \in C(\mathbb{R}^n;X)} \sup_{u \in K} \|u - D \circ E(u)\|_X.$$

Further restricting **encoders and decoders to be Lipschitz continuous** yields the notion of **stable manifold width** [Cohen et al 2022]

$$\delta_n^L(K)_X = \inf_{Lip(E) \leq L} \inf_{Lip(D) \leq L} \sup_{u \in K} \|u - D \circ E(u)\|_X.$$

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Lipschitz continuity ensures stability of the approximation process, a crucial property in practice.

However, implementation of optimal nonlinear encoders may be difficult or even infeasible, e.g. associated with NP-hard optimization problems.

Linear encoder and nonlinear decoder

Restricting the **encoder to be linear and continuous** yields the **n-th minimal error of linear information** (sometimes called sensing numbers)

$$e_n(K)_X = \inf_{D} \inf_{\ell_1,\dots,\ell_n} \sup_{u\in K} \|u - D(\ell_1(u),\dots,\ell_n(u))\|_X$$

where the infimum is taken over all linear forms $\ell_1,\dots,\ell_n$ and all nonlinear maps D.

This benchmark are relevant in many applications where the available information $E(u) = (\ell_1(u),\dots,\ell_n(u))$ is linear in u (point evaluations of functions, local averages of functions or more general linear functionals).

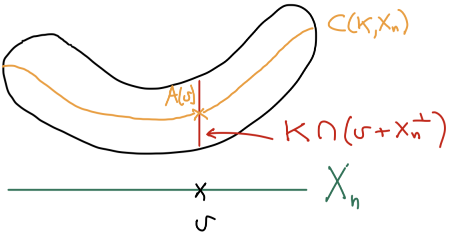
Linear encoder and nonlinear decoder

In a Hilbert setting and worst case setting, this corresponds to

$$\inf_{\dim(X_n)=n} \inf_{A:X_n\to X} \sup_{u\in K} \|u - A(P_{X_n}u)\|_X$$

For a given X_n, an optimal algorithm $A : X_n \to X$ is such that $A(v)$ is the Chebychev center of the slice

$$K \cap (v + X_n^\perp) = \{u \in K : P_{X_n}u = v\}.$$



This yields an optimal n-dimensional manifold

$$M_n = C(K, X_n) := \{cen(K \cap (v + X_n^\perp)) : v \in P_{X_n}K\}.$$

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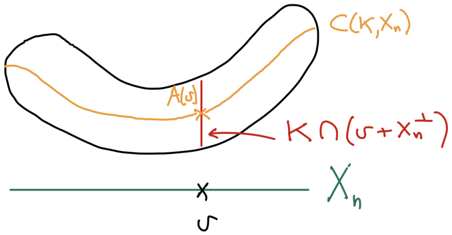

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In average setting, an average minimal error can be defined, and optimal manifold is obtained by averaging over slices.

Linear encoder and nonlinear decoder

With $(\varphi_i)_{i\geq 1}$ an orthonormal basis of X and $X_n = span\{\varphi_1, \dots, \varphi_n\}$, this is associated with the linear encoder

$$E(u) = ((u, \varphi_i))_{i=1}^n$$

and a decoder of the form

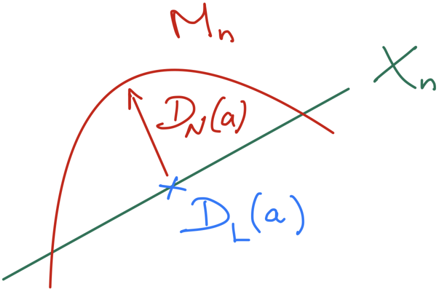
$$D(a) = A(\sum_{i=1}^n a_i \varphi_i) = \sum_{i=1}^n a_i \varphi_i + \sum_{i>n} g_i(a)\varphi_i = D_L(a) + D_N(a),$$

where the functions $g_i : \mathbb{R}^n \to \mathbb{R}$ are nonlinear maps.

D_L is a linear operator from $\mathbb{R}^n$ to $X_n := span\{\varphi_1, \dots, \varphi_n\}$ such that $D_L(E(u)) = P_{X_n} u$.

D_N maps $\mathbb{R}^n$ to the complementary space of X_n in X.

For a feasible implementation, we truncate to the first N terms, so that the range of D is a nonlinear manifold $M_n \subset X_N = span\{\varphi_1, \dots, \varphi_N\}$.



Linear encoder and nonlinear decoder

The structure of the decoder relies on the fact that for

$$u = \sum_{i=1}^{n} a_i(u)\varphi_i + \sum_{i>n} a_i(u)\varphi_i \in K,$$

the coefficients $a_i(u)$ for $i > n$ may be well approximated as functions $g_i(E(u))$ of the first few coefficients $E(u) = (a_i(u))_{i=1}^{n}$.

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Natural choices for functions g_i are

- Quadratic polynomials [Barnett and Farhat 2022][Geelen et al 2023]
- Sums of univariate high-order polynomials [Geelen et al 2024]
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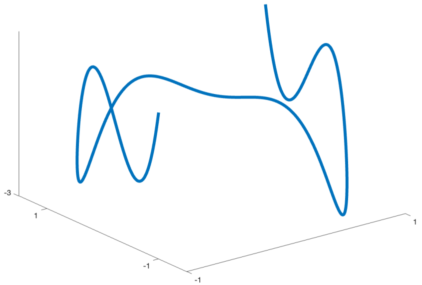
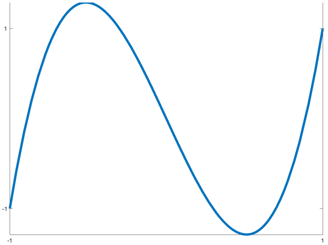
The relation between $a_i(u)$ and $E(u)$ may be highly nonlinear. Even highly expressive approximation tools may result in poor accuracy, due to the difficulty of learning with limited data.

Linear encoder and nonlinear decoder

In many applications, a coefficient $a_i(u)$ for $i > n$ may have a highly nonlinear relation with the first n coefficients $a = E(u)$ but a much smoother relation when expressed in terms of a and additional coefficients $a_j(u)$ with $n < j < i$.



(a) $K = \{(a_1(t), a_2(t), a_3(t)) : t \in [0, 1]\}$



(b) a_2 as function of a_1

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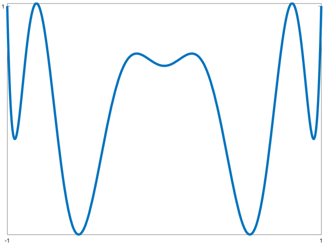
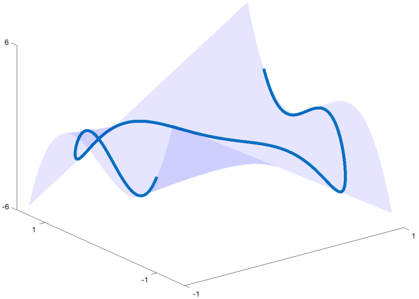


(c) a_3 as function of a_1



(d) a_3 as function of (a_1, a_2)

Decoder based on compositional polynomial network (CPN)

This suggests the following compositional structure of the decoder's functions

$$g_i(a) = f_i(a, (g_j(a))_{n<j\leq n_i}),$$

where the f_i are polynomial functions.

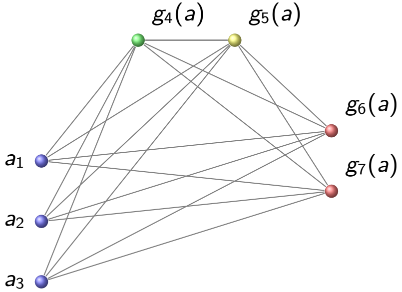


Figure: A compositional polynomial network (CPN) with $N = 7$ and $n = 3$, maximum number of compositions 3.

Decoder based on compositional polynomial network (CPN)

The variables $(a, (g_j(a))_{n<j\leq n_i})$ take values in a set of measure zero in $\mathbb{R}^{n_i}$, but it is still possible to learn polynomial functions f_i from a limited training set.

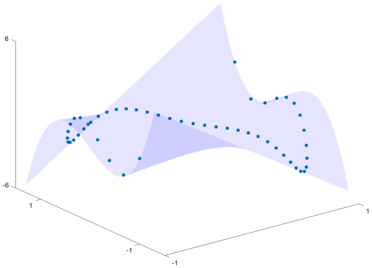


Figure: Learning a_3 as function of (a_1, a_2)

In practice, for high-dimensional approximation of $f_i : \mathbb{R}^{n_i} \to \mathbb{R}$ from samples, use of sparse polynomial approximation (CPN-S) or low-rank approximation (tensor networks) (CPN-LR) in $\mathbb{P}_p^{\otimes n_i}$.

Control of error (mean-squared setting)

Assume X is a Hilbert space and consider $D : \mathbb{R}^n \to X_N$, with X_N the subspace with orthonormal basis $\varphi_1, \dots, \varphi_N$.

The mean squared error

$$e_2(D \circ E)^2 := \|id - D \circ E\|_2^2 := \int_K \|u - D(E(u))\|_X^2 d\rho(u)$$

$$\text{satisfies} \quad e_2(D \circ E)^2 = \sum_{i=n+1}^{N} \epsilon_{i,2}^2 + \|id - P_{X_N}\|_2^2, \quad \epsilon_{i,2} = \|a_i - g_i \circ a\|_2$$

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Given a prescribed precision $0 < \epsilon < 1$, it holds

$$\boxed{e_2(D \circ E) \le \epsilon \, e_2(0)}$$

whenever

$$\|id - P_{X_N}\|_2^2 \le \beta \epsilon^2 e_2(0)^2 \tag{1}$$

$$\epsilon_{i,2}^2 \le \bar{\epsilon}_{i,2}^2 := \omega_i (1 - \beta) \epsilon^2 e_2(0)^2, \quad \forall i > n \tag{2}$$

where $0 < \beta < 1$ and $(\omega_i)_{i=n+1}^N$ are such that $\sum_{i=1}^N \omega_i = 1$.

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(1) is achieved by using PCA to define X_N, with a suitable selection of $N = N(\epsilon)$.
(2) is achieved by a control of the approximation of a_i by $f_i((g_j(a))_{j=1}^{n_i})$, using validation.

Control of stability

Given an orthonormal basis $\varphi_1, \dots, \varphi_N$, the encoder $E : X \to \mathbb{R}^n$ is 1-Lipschitz

$$\boxed{\|E(u) - E(u')\|_2 = \|P_{X_n}(u - u')\|_X \leq \|u - u'\|_X}$$

Given $\gamma = (\gamma_i)_{i=n+1}^N$, we equip $\mathbb{R}^{n_i}$ with the norm

$$\|b\|_{i,\gamma} = \max\{\|(b_j)_{j=1}^n\|_2, \max_{n<j\leq n_i} \gamma_j^{-1}|b_j|\}$$

and define the corresponding Lipschitz norm (estimated from samples)

$$\|f_i\|_{i,\gamma} = \max_{b,b'} \frac{|f_i(b) - f_i(b')|}{\|b - b'\|_{i,\gamma}}$$

Given a prescribed Lipschitz constant $L \geq 1$, letting $\|f_i\|_{i,\gamma} = \gamma_i$ and assuming $\gamma_i^2 \leq \bar{\gamma}_i^2$ with $\sum_{i=n+1}^n \bar{\gamma}_i^2 \leq L^2 - 1$, it holds

$$\boxed{\|D(a) - D(a')\|_X \leq L\|a - a'\|_2}$$

Adaptive algorithm

The prescribed bounds for errors

$$\epsilon_{i,p} \leq \bar{\epsilon}_{i,p}$$

or Lipschitz constants

$$\gamma_i = \|f_i\|_{i,\gamma} \leq \bar{\gamma}_i$$

may not be satisfied for some indices $i \in \{1, \ldots, N\}$.

This requires to progressively adapt the set of indices $\{1, \ldots, n\}$ associated with the encoder.

Prescribed upper bounds $\bar{\epsilon}_{i,p}$ and $\bar{\gamma}_i$ can be updated during the algorithm in order to obtain a sharper control of error and stability.

Numerical illustration: KdV

We consider the Korteweg-de Vries (KdV) equation

$$\frac{\partial u}{\partial t} + 4u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0 \quad on \quad [-\pi, \pi] \times [0, 1]$$

with periodic boundary conditions and some initial condition. We consider the manifold

$$K = \{u(\cdot, t) : t \in [0, 1]\}$$

We use 5000 samples $u_i = u(\cdot, t_i)$ as training samples.

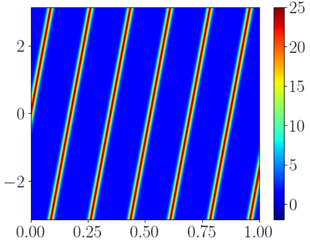


Figure: Function $u(x, t)$.

Method	p	n	N	$\mathbf{RE}_{\text{train}}$	$\mathbf{RE}_{\text{test}}$
Linear	/	5	5	0.435	0.450
Quadratic	2	5	20	0.094	0.099
Additive + AM	5	5	43	0.081	0.084
Sparse	5	5	43	0.013	0.014
CPN-S ($\varepsilon = 10^{-4}$)	5	5	43	0.000072	0.000074

Table: Comparison of methods for the same manifold dimension $n = 5$. CPN-S with sparse polynomials of degree $p = 5$.

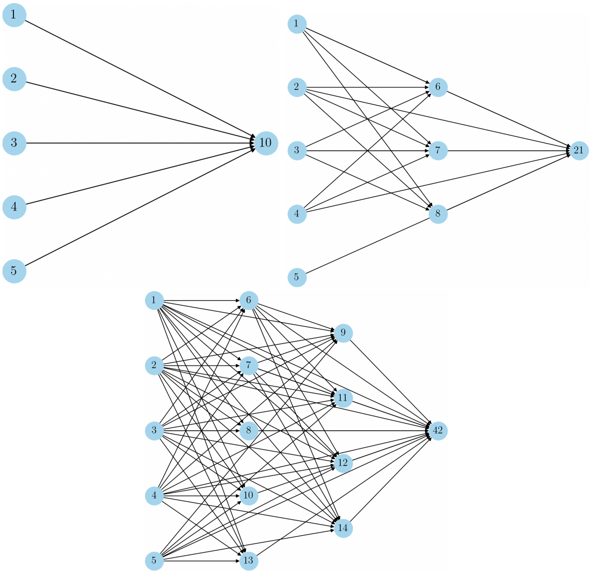


Figure: Compositional networks for g_{10}, g_{21} and g_{42} ($\epsilon = 10^{-4}$, $p = 5$)

Tolerance	n	N	$\mathbf{RE}_{\text{train}}$	$\mathbf{RE}_{\text{test}}$
$\varepsilon = 10^{-1}$	2	15	6.2×10^{-2}	6.4×10^{-2}
$\varepsilon = 10^{-2}$	2	25	6.67×10^{-3}	6.84×10^{-3}
$\varepsilon = 10^{-3}$	3	34	6.83×10^{-4}	7×10^{-4}
$\varepsilon = 10^{-4}$	5	43	7.170×10^{-5}	7.367×10^{-5}
$\varepsilon = 10^{-5}$	6	52	6.76×10^{-6}	6.916×10^{-6}
$\varepsilon = 10^{-6}$	11	61	7.689×10^{-7}	7.885×10^{-7}

Table: Results of CPN-S for $p = 5$ and different target precisions ε.

p	n	N	$\mathbf{RE}_{\text{train}}$	$\mathbf{RE}_{\text{test}}$
3	9	43	7.401×10^{-5}	7.574×10^{-5}
4	7	43	7.524×10^{-5}	7.720×10^{-5}
5	5	43	7.170×10^{-5}	7.367×10^{-5}

Table: Results of CPN-S with different degrees p for $\epsilon = 10^{-4}$

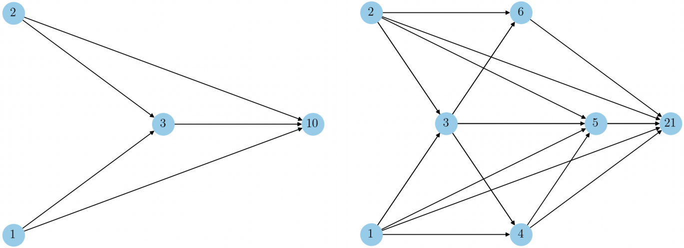


Figure: Compositional networks for g_{10} and g_{21} ($\epsilon = 10^{-2}$, $p = 5$)

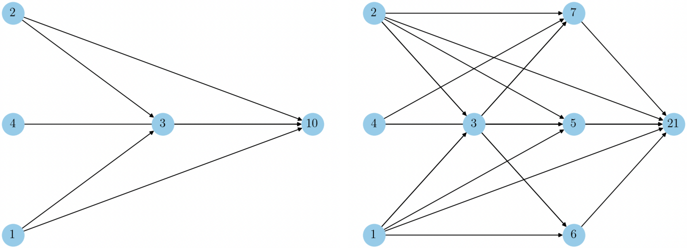


Figure: Compositional networks for g_{10} and g_{21} ($\epsilon = 10^{-3}$, $p = 5$)

Method	p	n	N	$\mathbf{RE}_{\text{train}}$	$\mathbf{RE}_{\text{test}}$
Linear	/	2	/	6.63×10^{-1}	6.91×10^{-1}
Quadratic	2	2	5	5.33×10^{-1}	5.66×10^{-1}
Additive-AM	5	2	43	2.10×10^{-1}	5.47×10^{-1}
Sparse	5	2	43	1.73×10^{-1}	1.85×10^{-1}
Low-Rank	5	2	43	7.47×10^{-2}	7.94×10^{-2}
CPN-LR ($\epsilon = 10^{-4}$)	5	2	43	6.85×10^{-5}	7.06×10^{-5}

Table: Comparison of methods for the same manifold dimension $n = 5$. CPN-LR uses low-rank polynomials with degree $p = 5$ (tensor train format).

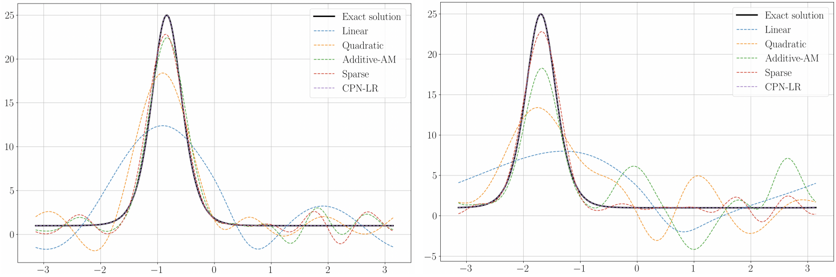
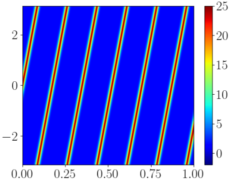
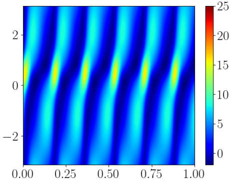


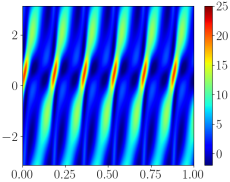
Figure: Comparison of methods for predicting $u(\cdot, t)$ at $t = 0.5$ (left) and $t = 1$ (right). Same dimension $n = 5$.



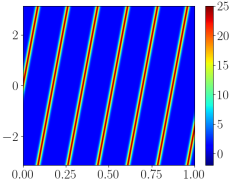
(a) Exact solution



(b) Linear



(c) Quadratic



(d) CPN-LR

Figure: Predictions for different methods, with manifold dimension $n = 2$.

Optimal linear encoders and associated spaces

The encoder (or associated space X_n) can be optimized.

A natural choice is to consider the optimal or near-optimal spaces of linear methods, given by principal component analysis (optimal in mean-squared error) or greedy algorithms (close to optimal in worst case error) [Barnett and Farhat 2022, Geelen et al 2023, Barnett, Farhat and Maday 2023, Geelen et al 2024].

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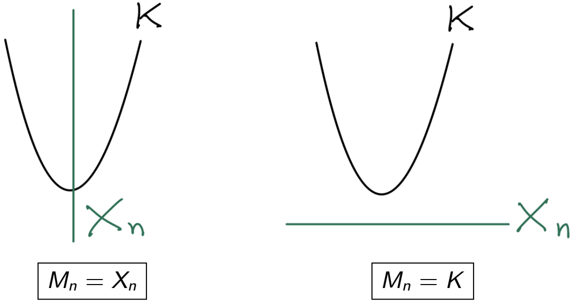

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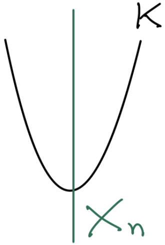
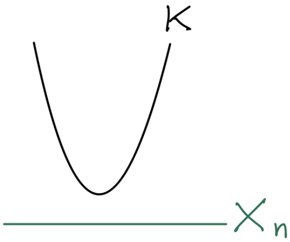


$\boxed{M_n = X_n}$



$\boxed{M_n = K}$

In [Schwerdtner and Peherstorfer 2024], greedy algorithm for a (near to) optimal construction of X_n for quadratic manifold approximation (quadratic decoder).

Optimal spaces guided by Lipschitz stability (worst case setting)

The benchmark for a linear encoder and a Lipschitz stable decoder is

$$e_n^L(K)_X = \inf_{Lip(E) \leq 1} \inf_{Lip(D) \leq L} \sup_{u \in K} \|u - D(E(u))\|_X$$

where the infimum is taken over linear 1-Lipschitz encoders and L-Lipschitz decoders.

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Equivalently

$$e_n^L(K)_X = \inf_{\dim(X_n)=n} \inf_{Lip(A)\leq L} \sup_{u\in K} \|u - A(P_{X_n}u)\|_X$$

where

$$Lip(A) = \sup_{\substack{u,v\in K \\ P_{X_n}(u-v)\neq 0}} \frac{\|A(P_{X_n}u) - A(P_{X_n}u)\|_X}{\|P_{X_n}u - P_{X_n}v\|_X} \leq L$$

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A dual version is

$$\tilde{e}_n^\eta(K)_X = \inf_{\dim(X_n)=n} \inf_{A} Lip(A)$$

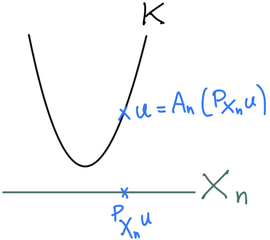
where the infimum is taken over maps A such that

$$\sup_{u\in K} \|u - A(P_{X_n}u)\|_X \leq \eta$$

$e_n^L(K)_X$ or $\tilde{e}_n^\eta(K)_X$ can be seen as notions of "Lipschitz widths" of K, using linear encoder. See related notion in [Petrova and Wojtaszczyk 2023] with arbitrary encoders.

Optimal spaces guided by Lipschitz stability (worst case setting)

Consider $\eta = 0$, assuming the existence of an exact recovery map A_n for some X_n. This requires K to be a n-dimensional manifold, and A_n is a global chart associated to X_n.



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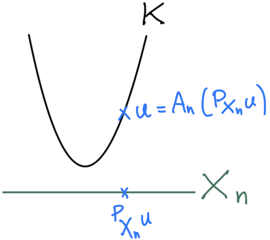


Then we obtain a measure of Lipschitz regularity of K related to X_n as

$$Lip(A_n) = \sup_{\substack{u,v\in K \\ P_{X_n}(u-v)\neq 0}} \frac{\|u-v\|_X}{\|P_{X_n}(u-v)\|_X} =: Lip(K, X_n)_X$$

and the corresponding notion of Lipschitz width of K

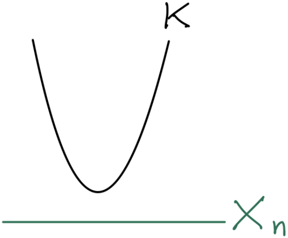
$$L_n(K)_X := \inf_{\dim(X_n)=n} Lip(K, X_n)_X$$

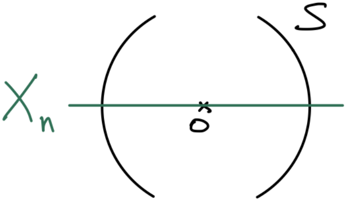
which defines an optimal space X_n in terms of stability of the corresponding chart A_n.

Optimal spaces guided by Lipschitz stability (worst case setting)

It holds

$$L_n(K)_X = \frac{1}{1 - d_n(S)_X} \quad \text{with} \quad S = \{\frac{z}{\|z\|_X} : z \in (K - K) \setminus \{0\}\}.$$





$$\boxed{L_n(K)_X = \min_{X_n} Lip(K, X_n)_X} \quad \Longleftrightarrow \quad \boxed{d_n(S)_X = \min_{X_n} d(S, X_n)_X}$$

Close to optimal spaces can be obtained by greedy algorithms.

Optimal spaces guided by Lipschitz stability (average setting)

In the average setting, possible relaxation by considering the average width $d^{(2)}(S,\pi)_X$, with π the push-forward measure on S of $\rho \otimes \rho$ through the map $(u,v) \mapsto (u-v)/\|u-v\|_X$.

Instead of

$$d_n(S) = \inf_{\dim(X_n)=n} \sup_{z \in S} \|z - P_{X_n} z\|_X$$

we consider

$$d^{(2)}(S,\pi)_X = \inf_{\dim(X_n)=n} \int_S \|z - P_{X_n} z\|_X^2 d\pi(z)$$

that is an eigenvalue problem.

In practice, we introduce estimators from finitely many samples in K.

Optimal spaces guided by Lipschitz stability

Previous notions may not be well defined for sets K that are not smooth n-dimensional manifolds described by global chart.

This requires to consider relaxations $\tilde{e}_n^{\eta}(K)_X$ that balance Lipschitz stability and approximation error, or n-dimensional approximations of the set K.

The design of practical strategies using samples from K is a challenging problem.

Conclusions

- Nonlinear manifold approximation method with linear encoder and nonlinear decoder based on compositional polynomial networks, with control of error and stability [1].

Reference
[1] A. Bensalah, A. Nouy, and J. Soffo. Nonlinear manifold approximation using compositional polynomial networks. arXiv e-prints arXiv:2502.05088, Feb. 2025.

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Conclusions

- Nonlinear manifold approximation method with linear encoder and nonlinear decoder based on compositional polynomial networks, with control of error and stability [1].
- Optimal spaces/encoders based on Lipschitz stability of decoders.
- Some challenging problems related to online approximation with nonlinear manifolds: optimization and sampling/discretization.

Reference

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THANK YOU FOR YOUR ATTENTION

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