

**GRAN SASSO Science Institute, Intensive Trimester**  
**"Particles, Fluids and Patterns: Analytical and Computational Challenges"**  
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# High-dimensional approximation and sampling

## Part 3: Manifold approximation

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# Approximation of a function class

We consider the problem of approximating functions from a subset  $K$  of a normed vector space  $X$ .

We want to find a low-dimensional space or manifold  $M_n$  which approximates well the set  $K$ , or a sequence of models with increasing complexity  $(M_n)_{n \geq 1}$  that approximate  $K$  with a good rate of convergence.

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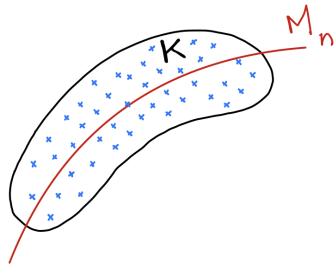
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- For more general sets  $K$  (application-dependent),  $M_n$  can be obtained by manifold approximation (or dimension reduction) methods.

# Approximation of a function class

In this part, we present methods for approximating a set  $K$  by low-dimensional sets  $M_n$ , using samples in  $K$ .



A common setting (in statistics) is 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

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



The approximating sets  $M_n$  can be

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

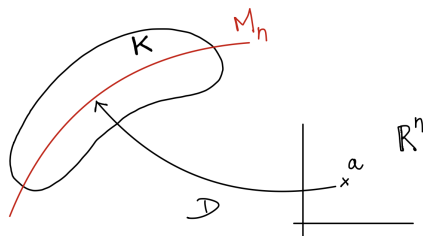
The offline construction may take into account the online approximation process.

# Encoder-Decoder

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

The decoder provides a parametrization of a  $n$ -dimensional “manifold”

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



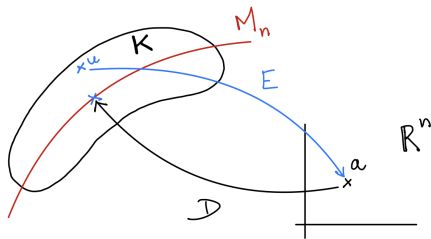
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The encoder is related to the approximation process (algorithm). It associates to  $u \in K$  a parameter value  $a = E(u) \in \mathbb{R}^n$ .



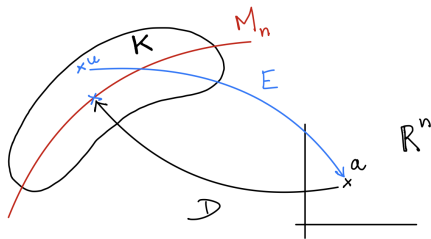
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An element  $u \in K$  is approximated by  $D \circ E(u) \in M_n$ .

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  $\mathbb{R}^n \rightarrow X$  can be assessed in **worst-case setting** by

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

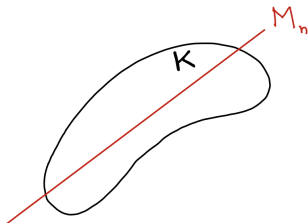
If the set  $K$  is equipped with a measure  $\rho$ , the optimal performance can be measured in **average sense** by

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

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

## Linear approximation - Worst case setting

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



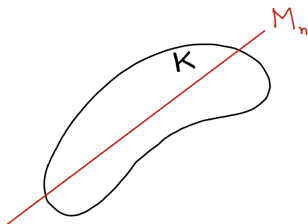
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Restricting the **decoder and encoder to be linear** yields the **approximation numbers**

$$a_n(K)_X = \inf_{\text{rank}(A)=n} \sup_{u \in K} \|u - Au\|_X,$$

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



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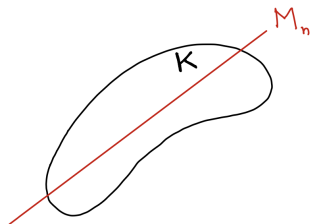
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Restricting **only the decoder to be linear** yields the **Kolmogorov  $n$ -width**

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





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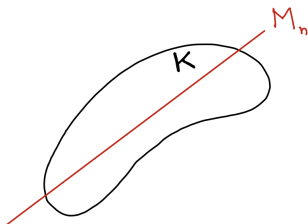
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For  $X$  a Hilbert space,  $a_n(K)_X = d_n(K)_X$  and an optimal auto-encoder  $D \circ E$  is given by the orthogonal projection  $P_{M_n}$  onto an optimal space  $M_n$ .

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  $K$  [ DeVore et al 2013].



## Greedy algorithms (for linear approximation)

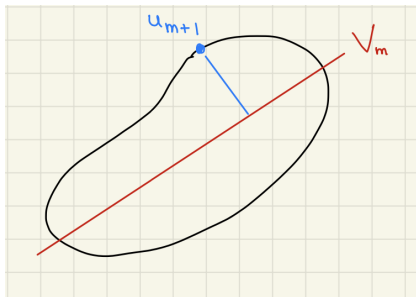
Greedy algorithms can be used for the construction of a hierarchical sequence of spaces  $(V_n)_{n \geq 1}$  using samples (snapshots) from  $K$ . Spaces are defined by  $V_n = \text{span}\{u_1, \dots, u_n\}$  where  $(u_n)_{i \geq 1}$  is a sequence from  $K$  selected greedily.

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Given  $V_n$ ,  $u_{n+1}$  is the element which provides the highest error of approximation by  $V_n$

$$E(u_{n+1}, V_n)_X = \max_{u \in K} E(u, V_n)_X$$



## Greedy algorithms (for linear approximation)

When  $K = \{u(y) : y \in Y\}$ ,  $u_{n+1} = u(y_{n+1})$  where the parameter value  $y_{n+1}$  is such that

$$y_{n+1} \in \arg \max_{y \in Y} E(u(y), V_n)_X$$

In practice, for a computationally feasible algorithm,  $E(u(y), V_n)_X$  is replaced by some error estimate  $\Delta(u(y), V_n)$ , and the maximum is taken over a finite training set in  $Y$  (possibly random [Cohen et al 2020]).

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A typical setting is when  $K = \{u(y) : y \in Y\} \subset X$  is the solution of some parameter dependent equation

$$R(u(y); y) = 0$$

Here  $\Delta(u(y), V_m)$  is typically defined as some residual norm

$$\Delta(u(y), V_n) = \|R(u_n(y); y)\|$$

with  $u_n(y)$  a Galerkin projection of  $u(y)$  onto  $V_n$  (Galerkin encoder).

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Randomized linear algebra can be used for an efficient and stable estimation of residual norms [Balabanov and Nouy 2021a], and for the construction of preconditioners [Balabanov and Nouy 2021b].

## Greedy algorithms (for linear approximation)

This yields a suboptimal selection of  $u_{n+1}$  satisfying

$$E(u_{n+1}, V_n)_X \geq \gamma \max_{u \in K} E(u, V_n)_X, \quad \gamma \leq 1.$$

This algorithm therefore generates a suboptimal sequence of spaces yielding a worst case error

$$\sigma_n(K)_X := \sup_{u \in K} E(u, V_n)_X \geq d_n(K)_X$$

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Assuming  $\gamma \geq 1$  is independent of  $n$ , the algorithm is a weak greedy algorithm for which results have been obtained in [ DeVore et al 2013 ].

For  $X$  a Hilbert space, it holds

- $\sigma_{2n}(K)_X \leq \sqrt{2} \gamma^{-1} \sqrt{d_n(K)_X}$
- If  $d_n(K)_X \leq C_0 n^{-\alpha}$  then  $\sigma_n(K)_X \leq C_1 n^{-\alpha}$
- If  $d_n(K)_X \leq C_0 e^{-c_0 n^\alpha}$  then  $\sigma_n(K)_X \leq C_1 e^{-c_1 n^\alpha}$

For  $X$  a Banach space, similar but slightly worse results hold.



## Linear approximation - Average setting

When  $X$  is a Hilbert space and the error is measured in average sense, optimal linear decoders are related to 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

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

where  $\{\lambda_i(T)\}_{i \geq 1}$  are the eigenvalues of  $T$ , sorted by decreasing value. This is related to the **singular value decomposition** of the map

$$U : v \in X \mapsto (u, v)_X \in L_\rho^2$$

such that  $T = U^* U$ .

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

If  $\rho$  has mean  $\bar{u} \neq 0$ , we can consider the covariance operator  $Tv = \int_K (u - \bar{u})(u - \bar{u}, v)_X d\rho(u)$ , and  $u \in K$  is approximated by  $\bar{u} + P_{M_n}(u - \bar{u})$ , with  $M_n$  the dominant eigenspace of  $T$ .

Given samples  $u_1, \dots, u_m$  in  $K$ , an estimation  $M_n$  of the optimal space is given by solving

$$\min_{\dim(M_n)=n} \sum_{i=1}^m w_i \|u_i - P_{M_n} u_i\|_X^2$$

that is empirical PCA (up to centering).

The solution is the dominant eigenspace of the operator

$$T_m : v \mapsto \sum_{i=1}^m w_i u_i (u_i, v)_X.$$

For an analysis of empirical PCA, see e.g.

[Reiss and Wahl 2020, Milbradt and Wahl 2020].

Assuming  $X = \mathbb{R}^N$ ,  $M_n$  is given by the dominant eigenvectors of the matrix

$$\sum_{i=1}^m w_i u_i u_i^T \in \mathbb{R}^{N \times N}.$$

This is equivalent to compute the dominant left singular vectors of the matrix

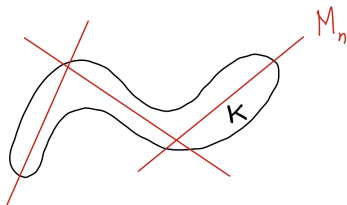
$$A = (u_1, \dots, u_m) \in \mathbb{R}^{N \times m}$$

An important question is how to optimally sample from  $K$  ? If  $\rho$  is a probability measure, i.i.d. sampling from  $\rho$  and  $w_i = \frac{1}{m}$  (standard Monte-Carlo) is in general not optimal. Optimal sampling requires an estimation of singular vectors.

# Multi-space approximation

$M_n$  can be chosen as a union of  $N$  linear spaces of dimension  $n$

$$M_n = \bigcup_{k=1}^N V_k$$



A related measure of complexity is the **nonlinear Kolmogorov width** or **library width**

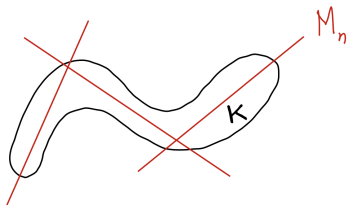
$$d_n(K, N)_X = \inf_{\#\mathcal{L}_{N,n}=N} \sup_{u \in K} \inf_{V \in \mathcal{L}_{N,n}} \|u - P_V u\|_X \quad [\text{Temlyakov 1998}]$$

where the infimum is taken over all libraries  $\mathcal{L}_{N,n}$  of  $N$  linear spaces of dimension  $n$ .

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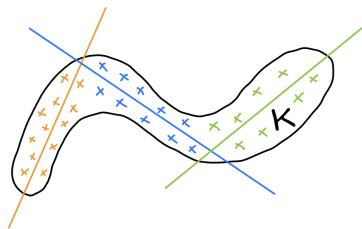
An **encoder-decoder view** is

$$E : K \rightarrow \mathbb{R}^n \times \{1, \dots, N\}, \quad D : \mathbb{R}^n \times \{1, \dots, N\} \rightarrow X \quad \text{with} \quad \text{Range}(D(\cdot, k)) = V_k$$

An optimal encoding requires a **selection of a subspace**  $V_k$  and a **projection** onto  $V_k$ .

# Multi-space approximation

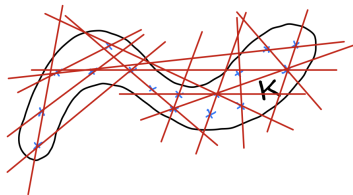
From samples from  $K$ , spaces can be obtained by a clustering/partitioning approach (h-p method) [Eftang et al 2010][Bonito et al 2021][Guignard and Mula 2024]



# Multi-space approximation

Spaces can be generated from a dictionary  $\mathcal{D} = \{u_1, \dots, u_m\}$  of samples from  $K$  [Balabanov and Nouy 2021a, Nouy and Pasco 2024]. By considering subspaces with dimension less than  $n$ , this yields the model class

$$M_n = \bigcup_{\alpha \in \{1, \dots, m\}^n} V_\alpha, \quad V_\alpha = \text{span}\{u_{\alpha_1}, \dots, u_{\alpha_n}\}$$



This is equivalent to  $n$ -term approximation

$$M_n = \left\{ \sum_{i=1}^m c_i u_i : c \in \mathbb{R}^m, \|c\|_0 \leq n \right\} := \left\{ D(a, \alpha) = \sum_{i=1}^n a_i u_{\alpha_i} : a \in \mathbb{R}^n, \alpha \in \{1, \dots, m\}^n \right\}.$$

The dictionary (samples) can be taken arbitrarily or generated with a greedy procedure proposed in [Balabanov and Nouy 2021a], using randomized linear algebra for handling large dictionaries.



# Nonlinear manifold approximation

We now consider methods for the approximation of a set  $K$  by a parametrized nonlinear manifold

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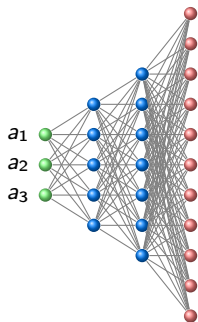
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For a finite dimensional space  $X$  identified with  $\mathbb{R}^N$ , a neural network representation can be used for  $D : \mathbb{R}^n \rightarrow \mathbb{R}^N$ .



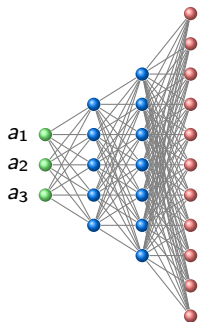
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However, the problem of finding an optimal parameter value  $a$  to approximate  $u \in K$  (optimal encoding) may be ill-posed or NP-hard.

This suggests to look for a "reasonable" encoder-decoder pair.

# Nonlinear manifold approximation

An encoder  $E$  and decoder  $D$  can be learned from samples in  $K$  by minimizing

$$\min_{D,E} \sum_{i=1}^m \|u_i - D \circ E(u_i)\|$$

over some restricted classes of maps. Optimal continuous encoder-decoder pairs are related to the notion of **nonlinear manifold width** of [ DeVore, Howard and Micchelli 1989]

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

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An encoder  $E$  and decoder  $D$  can be learned from samples in  $K$  by minimizing

$$\min_{D,E} \sum_{i=1}^m \|u_i - D \circ E(u_i)\|$$

over some restricted classes of maps. Optimal continuous encoder-decoder pairs are related to the notion of **nonlinear manifold width** of [ DeVore, Howard and Micchelli 1989]

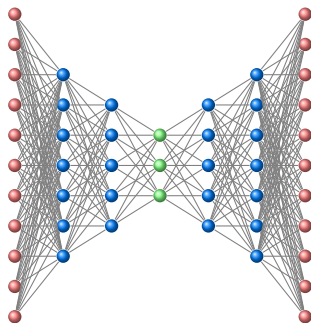
$$\delta_n(K)_X = \inf_{E \in C(X; \mathbb{R}^n), D \in C(\mathbb{R}^n; X)} \sup_{u \in K} \|u - D \circ E(u)\|_X.$$

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

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

# Nonlinear manifold approximation

Neural networks can be used for both the encoder  $E : \mathbb{R}^N \rightarrow \mathbb{R}^n$  and decoder  $D : \mathbb{R}^n \rightarrow \mathbb{R}^N$ .



However, learning  $D$  and  $E$  is a highly nonlinear optimization problem. Also, controlling the stability is not easy task.

Restricting the **encoder to be linear and continuous** simplifies its estimation and the control of its stability.

This is related to the notion of **sensing numbers**

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

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

This benchmark is 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/affine encoder and nonlinear decoder

The class of decoders should admit a feasible implementation. A practical approach consists in restricting  $D$  to take values in some linear/affine space  $\bar{u} + X_N$  with dimension  $N \geq n$ .

Given a basis  $\varphi_1, \dots, \varphi_N$  of  $X_N$ , the decoder can be written in the form

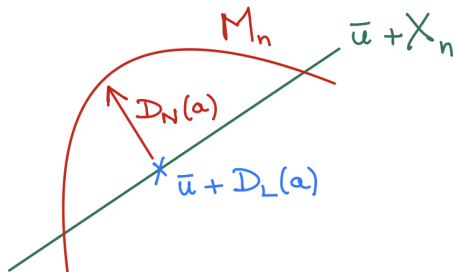
$$D(a) = \bar{u} + \sum_{i=1}^n a_i \varphi_i + \sum_{i=n+1}^N g_i(a) \varphi_i := \bar{u} + D_L(a) + D_N(a)$$

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

$D_L$  is a linear operator from  $\mathbb{R}^n$  to  $X_n := \text{span}\{\varphi_1, \dots, \varphi_n\}$ .

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

The range of  $D$  is a nonlinear manifold  $M_n \subset \bar{u} + X_N$ .





The space  $X_N$  and its subspace  $X_n$  can be optimized (highly nonlinear problem).

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].

The structure of the decoder relies on the fact that for

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

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]
- Neural networks or random forests [Barnett, Farhat and Maday 2023], [Cohen et al 2023]

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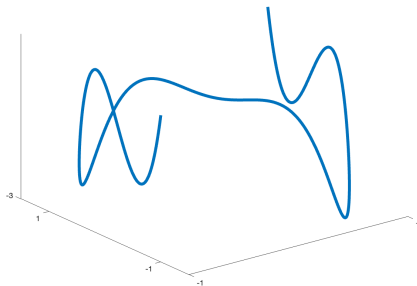
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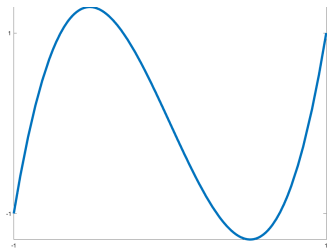
The relation between  $a_i(u)$  and  $E(u)$  may be highly nonlinear. Even highly expressive approximation tools may result in poor accuracy, due to the difficulty of learning with limited data.

## Linear/affine 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  $n < j < i$ .



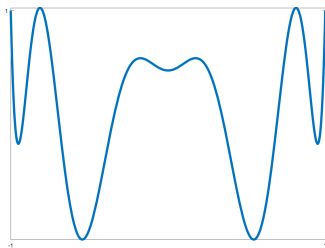
(a)  $K = \{(a_1(t), a_2(t), a_3(t)) : t \in [0, 1]\}$



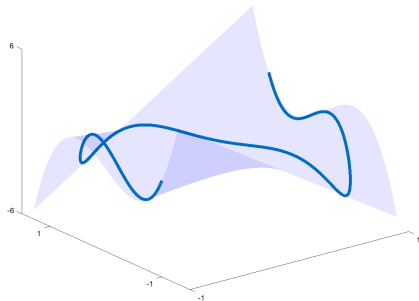
(b)  $a_2$  as function of  $a_1$

## Linear/affine 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  $n < j < i$ .



(c)  $a_3$  as function of  $a_1$



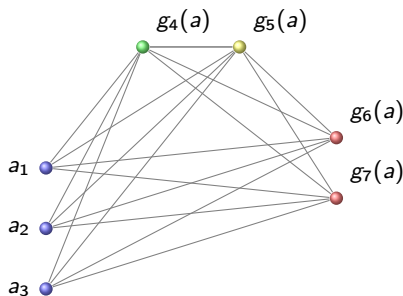
(d)  $a_3$  as function of  $(a_1, a_2)$

# Decoder based on compositional polynomial network

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

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

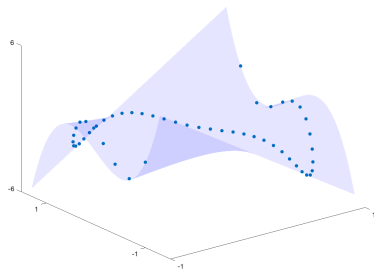
where the  $f_i$  are polynomial functions [Bensalah, Nouy and Soffo 2025].



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

# Decoder based on compositional polynomial network

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  $f_i : \mathbb{R}^{n_i} \rightarrow \mathbb{R}$  from samples, use of **sparse polynomial approximation** or **tensor networks (low-rank approximation)** in  $\mathbb{P}_p^{\otimes n_i}$ .



## Control of error (mean-squared setting)

The mean squared error

$$e_2(D \circ E) := \|id - D \circ E\|_2 := \left( \int_K \|u - D(E(u))\|_X^2 d\rho(u) \right)^{1/2}$$

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

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

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

whenever

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

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

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

(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  $E : X \rightarrow \mathbb{R}^n$  is 1-Lipschitz

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

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  $\gamma_i^2 \leq \tilde{\gamma}_i^2$  with  $\sum_{i=n+1}^n \tilde{\gamma}_i^2 \leq L^2 - 1$ , it holds

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

# Adaptive algorithm

Satisfying the prescribed bounds for precisions

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

or Lipschitz constants

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

may be a difficult task for some indices  $i \in \{1, \dots, N\}$ .

This requires to progressively adapt the set of indices  $\{1, \dots, n\}$  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

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

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.

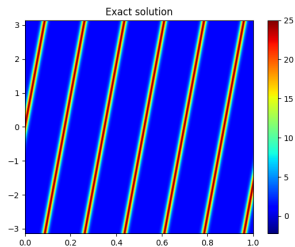
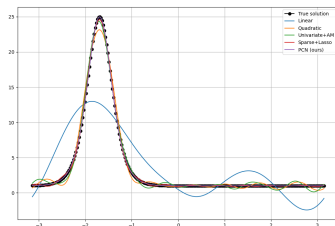
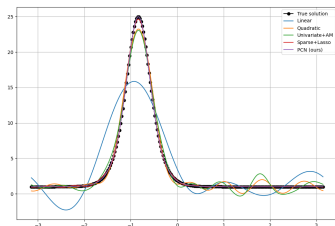


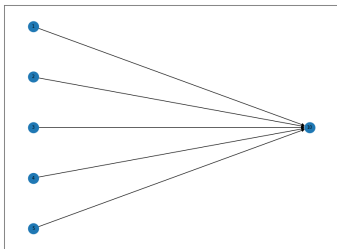
Figure: Function  $u(x, t)$ .

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

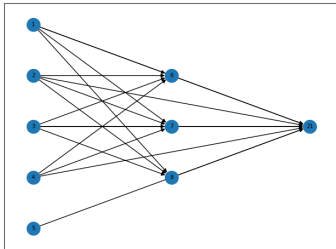
**Table:** Comparison of methods for the same manifold dimension  $n = 5$ .



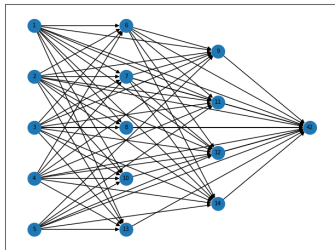
**Figure:** Comparison of methods for predicting  $u(\cdot, t)$  at  $t = 0.5$  (left) and  $t = 1$  (right). Same dimension  $n = 5$ .



(a)  $g_{10}$



(b)  $g_{21}$



(c)  $g_{42}$

Figure: Compositional networks for different coefficients

Tolerance	$n$	$N$	Max comp.	$RE_{\text{train}}$	$RE_{\text{test}}$
$\varepsilon = 10^{-1}$	2	15	2	0.062	0.064
$\varepsilon = 10^{-2}$	3	25	5	$6.67 \times 10^{-3}$	$6.84 \times 10^{-3}$
$\varepsilon = 10^{-3}$	3	34	8	$6.83 \times 10^{-4}$	$7 \times 10^{-4}$
$\varepsilon = 10^{-4}$	5	43	8	$7.170 \times 10^{-5}$	$7.367 \times 10^{-5}$
$\varepsilon = 10^{-5}$	6	52	11	$6.76 \times 10^{-6}$	$6.916 \times 10^{-6}$
$\varepsilon = 10^{-6}$	11	61	10	$7.689 \times 10^{-7}$	$7.885 \times 10^{-7}$

**Table:** Results of CPN for  $p = 5$  and different target precisions  $\varepsilon$ .

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

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



# Online approximation

Consider a parametrized manifold

$$K = \{u(y) : y \in Y\}$$

From samples  $(y_i, u(y_i))$ , we compute **offline** the decoder  $D$  and also an approximation

$$\tilde{a}(y) \approx a(y) := E(u(y)) \quad \left( \begin{array}{c} y \\ \text{5 purple nodes} \\ \text{3 green nodes} \\ \text{4 blue nodes} \\ \tilde{a}(y) \end{array} \right)$$

**Online**, for a parameter value  $y \in Y$ , we predict

$$\tilde{u}(y) = D(\tilde{a}(y)) \quad \left( \begin{array}{c} \tilde{a}_1(y) \\ \tilde{a}_2(y) \\ \tilde{a}_3(y) \\ \text{2 green nodes} \\ g_4(\tilde{a}(y)) \quad g_5(\tilde{a}(y)) \\ \text{3 red nodes} \\ g_6(\tilde{a}(y)) \\ g_7(\tilde{a}(y)) \end{array} \right)$$

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**Online**, for a parameter value  $y \in Y$ , we predict

$$\tilde{u}(y) = D(\tilde{a}(y)) \quad \left( \begin{array}{c} \text{Diagram of a neural network with 3 input nodes (blue) labeled } \tilde{a}_1(y), \tilde{a}_2(y), \tilde{a}_3(y); \text{ 2 hidden nodes (green and yellow) labeled } g_4(\tilde{a}(y)), g_5(\tilde{a}(y)); \text{ and 3 output nodes (red) labeled } g_6(\tilde{a}(y)), g_7(\tilde{a}(y)). \\ \tilde{a}_1(y) \quad \tilde{a}_2(y) \quad \tilde{a}_3(y) \qquad \qquad \qquad g_6(\tilde{a}(y)) \quad g_7(\tilde{a}(y)) \end{array} \right)$$

The error satisfies

$$\|\tilde{u}(y) - u(y)\|_x \leq \|u(y) - D(E(u(y)))\|_x + L\|\tilde{a}(y) - a(y)\|_2.$$

The error  $\|\tilde{a}(y) - a(y)\|_2$  should be of the order of  $\|u(y) - D(E(u(y)))\|_x / L$ .

Even if the constructed manifold  $M_n = \{D(a) : a \in \mathbb{R}^n\}$  approximates well  $K$ , an approximation/perturbation of the encoding may result in a significant loss of accuracy. Ideally, we would like an element of best approximation

$$\min_{v \in M_n} \|u - v\|_X = \min_{a \in \mathbb{R}^n} \|u - D(a)\|_X$$

This is not achievable using limited information, but a reasonable approximation can be obtained by using advanced learning/optimization strategy (next part).

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