Deep Neural Networks Are Effective At Learning High-Dimensional Hilbert-Valued Functions From Limited Data

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Motivation

Multivariate function recovery

Approximate $f : \mathcal{U} \to \mathcal{V}$, a Hilbert-valued function, from its evaluations at $m \in \mathbb{N}$ sample points $y_1, \ldots, y_m \in \mathcal{U}$:

$$d_i = f(y_i) + n_i \in \mathcal{V}_h, \quad i = 1, \ldots, m.$$
Main motivation

**Parametric PDE**

A parametric PDE takes the form

\[ \mathcal{L}_y[u(\cdot, y)] = 0 \]

with suitable boundary conditions.

- Parametric variables \( y \in \mathcal{U} \).
- Physical variables \( x \in \Omega \).
- \( \mathcal{L}_y \) is an operator depending on the parameters \( y \) (e.g. differentiation wrt \( x \)).
- \( u(\cdot, y) \) is an element of some Banach or Hilbert space \( \mathcal{V} \).

Example:

\[ -\nabla_x \cdot (a(x, y)\nabla_x u(x, y)) = g(x) \quad \text{in} \quad \Omega, \]

and BC.
Main challenges

1. **High-dimensional models**: Often $d \gg 1$ or even $d = \infty$.

2. **The space $V$ is infinite dimensional (Hilbert or Banach)**:
   Needs discretization $V_h$ over $\Omega \rightarrow$ induces a discretization error.

3. **Corrupted data (unknown errors)**:
   Modelling errors, numerical error, random noise in the measurements.

4. **Generating data is expensive**:
   Example: generating multiple solutions of a particular PDE using a **black-box** numerical PDE solver.
Holomorphy assumption

For $d \geq 1$, let $\rho \in \mathbb{R}^d$ with $\rho > 1$. The Bernstein polyellipse of polyradius $\rho$ is

$$E_{\rho} = E_{\rho_1} \times E_{\rho_2} \times \cdots E_{\rho_d} \subset \mathbb{C}^d.$$ 

where

$$E_{\rho} = \left\{ \frac{1}{2} (z + z^{-1}) : z \in \mathbb{C}, 1 \leq |z| \leq \rho \right\} \subset \mathbb{C}$$

**Assumption**

The function $f$ has a **holomorphic extension** from $[-1, 1]^d$ to some Bernstein polyellipse $E_{\rho}$.

- Many parametric DEs provably satisfy this assumption, including elliptic diffusion equations, parametric IVPs,...

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Deep Neural Network (DNN) \( \Phi : \mathbb{R}^d \rightarrow \mathbb{R}^K \)

\[ z^{(1)} = \sigma \left( W^{(1)} y + b^{(1)} \right), \]

\[ z^{(\ell)} = \sigma \left( W^{(\ell)} z^{(\ell-1)} + b^{(\ell)} \right), \quad \ell = 2, \ldots, L - 1 \]

\[ \Phi(y) = W^{(L)} z^{(L-1)} + b^{(L)}. \]

- \( W^{(\ell)} \in \mathbb{R}^{N_{\ell} \times N_{\ell-1}} \) are the weights.
- \( b^{(\ell)} \in \mathbb{R}^{N_{\ell}} \) are the biases.
- \( \sigma \) is the activation function, e.g., \( \sigma(t) = \max\{0, t\} \) (ReLU).
Why DNN?

DNNs are capable of efficiently approximating functions from a wide variety of classes:

- Smooth functions, piecewise smooth functions, $H^k$ functions, ...


- There are existence theorems about DNNs approximating holomorphic functions.

- These DNNs can achieve the same error bound as the best $s$-term polynomial approximation.

- Specifically, they can obtain an error proportional to $\exp\left(-\gamma s^{1/d}\right)$, where $\gamma$ depends on the region of holomorphy.

- The size and depth of these DNNs are bounded in terms of $s$ and $d$.

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Input

- Each $d_i$ is uniquely represented as

$$d_i = f(y_i) + n_i = \sum_{k=1}^{K} d_{i,k} \varphi_k \in \mathcal{V}_h, \quad i = 1, \ldots, m.$$  

- The values $\{(y_i, d_i)\}_{i=1}^m$ are the input.

Output

- Let $\{\Psi_i\}_{i=1}^N$ be a basis for $\mathcal{P}_\Lambda$, where $N = |\Lambda|$. Then we may write

$$\hat{f}_{\Lambda,h} : y \mapsto \sum_{i=1}^{N} \left( \sum_{k=1}^{K} \hat{c}_{i,k} \varphi_k \right) \Psi_i(y),$$

where $\hat{c}_{i,k} \in \mathbb{R}$.

- The values $(\hat{c}_{i,k})_{N,K}^{n,k}$ are the output.
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**Practical DNN existence theorem for Hilbert-valued functions:**

Let $f : \mathcal{U} \rightarrow \mathcal{V}$ be holomorphic in a suitable region, and $\tilde{m} = cm/(\log^3(m) \log(d))$. Then there exists

1. a class of ReLU DNNs,
2. a loss function (regularized $\ell^2$-loss),
3. a choice of $m$ sample points $y_1, \ldots, y_m$,

such that any DNN $\Phi$ trained from the input $\{(y_i, d_i)\}_{i=1}^m$ gives an approximation $f_\Phi$ satisfying

$$\|f - f_\Phi\|_{L^2(\mathcal{U}; \mathcal{V})} \lesssim (E_1 + E_2 + E_3),$$

$$E_1 = \exp\left(-\gamma \frac{1}{2d} \frac{1}{\tilde{m}^{1/(2d)}}\right), \quad E_2 = \left(\frac{1}{m} \sum_{i=1}^m \|n_i\|^2_{\mathcal{V}}\right)^{1/2}, \quad E_3 = \|f - \mathcal{P}_h(f)\|_{L^\infty(\mathcal{U}; \mathcal{V})}.$$

- $E_1$ is the **approximation error**: quantifies how well $f$ is approximated by a DNN in terms of $\tilde{m}$.
- $E_2$ is the **measurement error**: quantifies the error in the pointwise evaluations of $f$ at the points $y_i$.
- $E_3$ is the **discretization error**: since we work with $\mathcal{V}_h$ instead of $\mathcal{V}$.

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Orthogonal polynomials

- $\mathcal{U} = [-1, 1]^d$ the unit hypercube.
- $d\varrho(y) = 2^{-d} \, dy$ be the uniform measure on $\mathcal{U}$.
- $\{\Psi_\nu\}_{\nu \in \mathbb{N}_0^d}$ be the tensor-product, orthonormal Legendre polynomial basis of $L^2_\varrho(\mathcal{U})$.

Let $L^2_\varrho(\mathcal{U}; \mathcal{V})$ the Lebesgue-Bochner space of Hilbert-valued functions $f : \mathcal{U} \to \mathcal{V}$.

**Polynomial expansion:** if $f \in L^2_\varrho(\mathcal{U}; \mathcal{V})$, then

$$f = \sum_{\nu \in \mathbb{N}_0^d} c_\nu \Psi_\nu, \quad c_\nu = \int_{\mathcal{U}} f(y) \Psi_\nu(y) \, d\varrho(y) \in \mathcal{V}.$$ 

**Sequence in $\ell^p(\Lambda; \mathcal{V})$:** For $1 \leq p < \infty$ and $c \in \ell^p(\Lambda; \mathcal{V})$, define

$$\|c\|_{\ell^p_{\mathcal{V}}} = \sum_{\nu \in \Lambda} \|c_\nu\|_{\mathcal{V}}^p.$$
Polynomial approximation as a compressed sensing problem

Let $\Lambda$ be a finite index set with $|\Lambda| = N$. Define the normalized measurement matrix

$$A = \left( \frac{\psi_{v_j}(y_i)}{\sqrt{m}} \right)_{i,j=1}^{m,N} \in \mathbb{R}^{m \times N},$$

and the normalized measurement and error vectors

$$b = \frac{1}{\sqrt{m}} (f(y_i) + n_i)_{i=1}^m \in \mathcal{V}_h^m, \quad \text{and} \quad e = \frac{1}{\sqrt{m}} (n_i)_{i=1}^m \in \mathcal{V}^m.$$

Hence, the recovery of the polynomial coefficients $c_{\Lambda} = (c_{v})_{v \in \Lambda}$ of $f$ is equivalent to solving the noisy linear system

$$Ac_{\Lambda} + e + e' = b,$$

where

$$e' = \frac{1}{\sqrt{m}} (f(y_i) - f_{\Lambda}(y_i))_{i=1}^m.$$

Consider the Square Root LASSO problem

$$\min_{z \in \mathcal{V}_N^h} \lambda \| z \|_{\mathcal{V},1} + \| Az - b \|_{\mathcal{V},2}.$$
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Emulation as a DNN training problem

Key insight: approximating polynomials as DNNs

For any $\delta > 0$, there exists a DNN $\Gamma : \mathbb{R}^d \to \mathbb{R}^{|\Lambda|}$ (of size and depth depending on $d$, $|\Lambda|$ and $\delta$) such that

$$\|\Psi_{\nu} - \Psi_{\nu,\delta}\|_{L^\infty(U)} \leq \delta,$$

where $\Gamma(y) = (\Psi_{\nu,\delta}(y))_{\nu \in \Lambda}$.


We can use this result to emulate the polynomial approximation problem as a DNN training problem:

$$A = \left(\frac{\Psi_{\nu_j}(y_i)}{\sqrt{m}}\right)_{i,j=1}^{m,N} \in \mathbb{R}^{m \times N} \quad \sim \quad A' = \left(\frac{\Psi_{\nu_j,\delta}(y_i)}{\sqrt{m}}\right)_{i,j=1}^{m,N} \in \mathbb{R}^{m \times N}$$

Carefully balancing the error due to this approximation and accounting for all other sources of errors leads to the main result.
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Parametric PDE approximation

A practical example:

- $\Omega = (0, 1)^2$ physical domain with discretization $\Omega_h$.
- $\mathcal{U} = [-1, 1]^d$ parametric domain with uniform probability measure.
- We seek a function $u : \Omega \times \mathcal{U} \to \mathbb{R}$ satisfying
  $$-\nabla_x \cdot (a(x, y) \nabla_x u(x, y)) = g(x) \quad \text{in} \quad \Omega, \quad \text{and BC}.$$ 

**Compute:** Approximation $u_{\Phi, h} : \mathcal{U} \to \mathcal{V}_h$ with a DNN $\Phi : \mathbb{R}^d \to \mathbb{R}^K$, of the form
  $$u_{\Phi, h}(x, y) = \sum_{k=1}^{K} (\Phi(y))_k \varphi_k(x).$$

**Note:** we do not implement the training strategy from the theorem.
Training: Given data \( \{(y_i, d_i)\}_{i=1}^{m}, d_i = (c_k (y_i))_{k=1}^{K} \) from a fixed FE discretization, minimize the loss function

\[
\text{MSE}(y) := \frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} (c_k (y_i) - (\Phi (y_i))_k)^2,
\]
or

\[
\text{MVNSE}(y) := \frac{1}{m} \sum_{i=1}^{m} \| u_h (y_i) - u_{\Phi, h} (y_i) \|_V^2.
\]

Testing: We compare the testing error in \( L^2_{\varrho} (\mathcal{U}; L^2 (\Omega)) \) and \( L^2_{\varrho} (\mathcal{U}; H^1_0 (\Omega)) \) norm.

- We use deterministic high-order sparse grid stochastic collocation method.
Effective architectures and loss functions

- DNN architectures with MVNSE underperform identical architectures trained with the MSE.
- Big difference between in the $L^2(\Omega)$-norm (right) for tanh, ReLU and Leaky-ReLU $5 \times 50$ DNNs.
Prediction for $u_h(x, y)$ from a tanh $5 \times 50$ DNN at $y = [0.995, 0]^t$:
- Early training: after 2 epochs of Adam (MSE 6.4255).
- At the end of the training: after 2045 epochs (MSE $4.879 \cdot 10^{-7}$).
Comparison with Simultaneous Compressed Sensing (SCS)

- Elliptic PDE with \( d=30 \) dimensional log-affine parametric diffusion.
- DNNs can outperform state-of-art polynomial-based CS methods.

![Graph showing comparison with SCS](image)
A mixed formulation

Define $K = \text{diag}(a_1, a_2)$ and

$-\nabla \cdot (K(x, y) \nabla u(x, y)) = f(x, y)$ \quad x \in \Omega, y \in U,

$u(x, y) = h(x, y)$ \quad x \in \Gamma_D, y \in U,

$\nabla u(x, y) \cdot n = 0$ \quad x \in \Gamma_N, y \in U.

Given $y \in U$, find $(u(y), \sigma(y)) \in [L^2(\Omega)] \times H^1_\text{N}(\text{div}; \Omega)$ such that

$\langle \sigma, \tau \rangle_{L^2(\Omega)} + \langle u, \nabla \cdot \tau \rangle_{L^2(\Omega)} = \langle \tau \cdot n, h \rangle_{\Gamma_D}$

$\langle \nabla K \cdot \sigma, v \rangle_{L^2(\Omega)} + \langle K v, \nabla \cdot \sigma \rangle_{L^2(\Omega)} = -\langle f, v \rangle_{L^2(\Omega)}$

Here $\sigma(y) = \nabla u(y) \in H^1_\text{N}(\text{div}; \Omega)$. 
Testing errors for $u$ are substantially smaller than those for its gradient $\nabla u$.

DNNs can be used as well to approximate parametric PDEs with mixed boundary conditions.
Conclusions

- Deep learning is capable of approximating Hilbert-valued functions from limited data.
- There exists a DNN architecture and training procedure that performs as well as current best-in-class schemes.
- DNN can be used to approximate mixed formulations.
- Using the MSE loss function leads to better and faster approximations.
- In practice DNNs can outperform or match best current methods.
References


