Solving Mathematical Problems by Deep Learning: Partial Differential Equations

Gitta Kutyniok

(Technische Universität Berlin and University of Tromsø)

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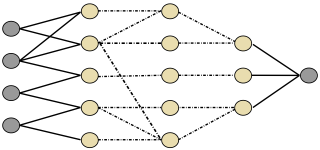
Mathematics of Deep Neural Networks

The Mathematics of Deep Neural Networks

Definition:

Assume the following notions:



- $d \in \mathbb{N}$: Dimension of input layer.
- L: Number of layers.
- N: Number of neurons.
- $\rho : \mathbb{R} \to \mathbb{R}$: (Non-linear) function called *activation function*.
- $T_\ell : \mathbb{R}^{N_{\ell-1}} \to \mathbb{R}^{N_\ell}$, $\ell = 1, \ldots, L$: Affine linear maps.

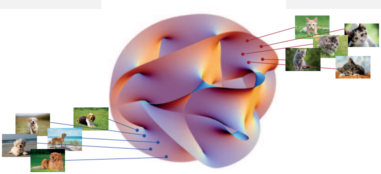
Then $\Phi : \mathbb{R}^d \to \mathbb{R}^{N_L}$ given by

$$\Phi(x) = T_L \rho(T_{L-1} \rho(\ldots \rho(T_1(x)))), \quad x \in \mathbb{R}^d,$$

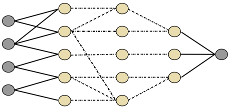
is called *(deep) neural network (DNN)*.

Training of Deep Neural Networks

High-Level Set Up:



- Samples $(x_i, f(x_i))_{i=1}^m$ of a function such as $f : \mathcal{M} \to \{1, 2, \ldots, K\}$.



- Select an architecture of a deep neural network, i.e., a choice of d, L, $(N_\ell)_{\ell=1}^L$, and ρ.
  Sometimes selected entries of the matrices $(A_\ell)_{\ell=1}^L$, i.e., weights, are set to zero at this point.
- Learn the affine-linear functions $(T_\ell)_{\ell=1}^L = (A_\ell \cdot + b_\ell)_{\ell=1}^L$ by

$$\min_{(A_\ell, b_\ell)_\ell} \sum_{i=1}^m \mathcal{L}(\Phi_{(A_\ell, b_\ell)_\ell}(x_i), f(x_i)) + \lambda \mathcal{R}((A_\ell, b_\ell)_\ell)$$

yielding the network $\Phi_{(A_\ell, b_\ell)_\ell} : \mathbb{R}^d \to \mathbb{R}^{N_L}$,

$$\Phi_{(A_\ell, b_\ell)_\ell}(x) = T_L \rho(T_{L-1} \rho(\ldots \rho(T_1(x)))).$$

This is often done by stochastic gradient descent.

Goal: $\Phi_{(A_\ell, b_\ell)_\ell} \approx f$

Fundamental Questions concerning Deep Neural Networks

- *Expressivity:*
  - How powerful is the network architecture?
  - Can it indeed represent the correct functions?

$\rightsquigarrow$ *Applied Harmonic Analysis, Approximation Theory, ...*

- *Learning:*
  - Why does the current learning algorithm produce anything reasonable?
  - What are good starting values?

$\rightsquigarrow$ *Differential Geometry, Optimal Control, Optimization, ...*

- *Generalization:*
  - Why do deep neural networks perform that well on data sets, which do not belong to the input-output pairs from a training set?
  - What impact has the depth of the network?

$\rightsquigarrow$ *Learning Theory, Optimization, Statistics, ...*

- *Interpretability:*
  - Why did a trained deep neural network reach a certain decision?
  - Which components of the input do contribute most?

$\rightsquigarrow$ *Information Theory, Uncertainty Quantification, ...*

What is Interpretability?

Main Questions: Given a trained deep neural network...

- Which input features contribute most to the decision?
- How can the outcome be explained?

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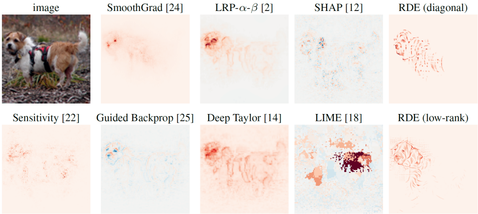
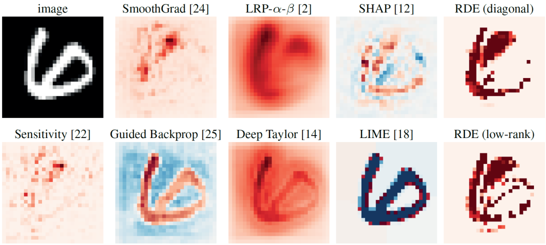
Some Recent Work:

- Sensitivity Analysis (Simonyan, Vedaldi, Zisserman; 2013)
- Layer-wise Relevance Propagation (Bach, Müller, Samek at al.; 2015)
- Deep Taylor Decompositions (Montavon, Samek, Müller; 2018)
- Rate Distortion Explanation (Waeldchen, Macdonald, Hauch, K; 2019)



Quality Measure of Interpretability

Classification of the Digit 6:



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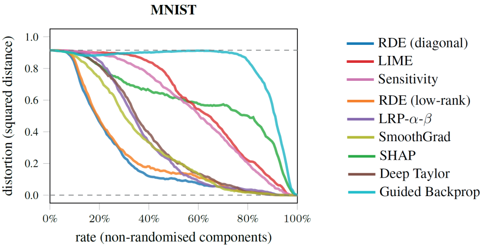

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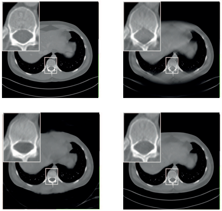
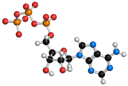
Impact of Deep Learning on Mathematics

Some Examples:

- Inverse Problems
  - ⇝ *Image denoising (Burger, Schuler, Harmeling; 2012)*
  - ⇝ *Superresolution (Klatzer, Soukup, Kobler, Hammernik, Pock; 2017)*
  - ⇝ *Limited-angle tomography (Bubba, K, Lassas, März, Samek, Siltanen, Srinivan; 2018)*
  - ⇝ *Edge detection (Andrade-Loarca, K, Öktem, Petersen; 2019)*



- Numerical Analysis of Partial Differential Equations
  - ⇝ *Schrödinger equation (Rupp, Tkatchenko, Müller, von Lilienfeld; 2012 –)*
  - ⇝ *Black-Scholes PDEs (Grohs, Hornung, Jentzen,von Wurstemberger; 2018)*
  - ⇝ *Parametric PDEs (Schwab, Zech; 2018)*
  - ⇝ *Parametric PDEs (K, Petersen, Raslan, Schneider; 2019)*



- Modelling
  - ⇝ *Learning equations from data (Sahoo, Lampert, Martius; 2018)*

Let's Now Enter the World of Parametric PDEs

Why Parametric PDEs?

Parameter dependent families of PDEs arise in basically any branch of science and engineering.

Some Exemplary Problem Classes:

- Complex design problems
- Inverse problems
- Optimization tasks
- Uncertainty quantification
- ...

The number of parameters can be

- finite (physical properties such as domain geometry, ...)
- infinite (modeling of random stochastic diffusion field, ...)

Parametric Map:

$$\mathcal{Y} \ni y \mapsto u_y \in \mathcal{H} \quad \text{such that} \quad \mathcal{L}(u_y, y) = f_y.$$

Parametric Partial Differential Equations

Our Setting: We will consider parameter-dependent equations of the form

$$b_y\left(u_y, v\right) = f_y(v), \qquad \text{for all } y \in \mathcal{Y},\ v \in \mathcal{H},$$

where

(i) $\mathcal{Y} \subseteq \mathbb{R}^p$ (p large) is the *compact parameter set*,

(ii) $\mathcal{H}$ is a Hilbert space,

(ii) $b_y : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ is a *symmetric, uniformally coercive, and uniformally continuous bilinear form*,

(iv) $f_y \in \mathcal{H}^*$ is the *uniformly bounded, parameter-dependent right-hand side*,

(v) $u_y \in \mathcal{H}$ is the *solution*.

We also assume the *solution manifold*

$$S(\mathcal{Y}) := \{u_y : y \in \mathcal{Y}\}$$

to be compact in $\mathcal{H}$.

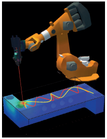
Multi-Query Situation

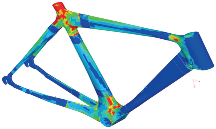
Many applications require solving the parametric PDE multiple times for different parameters:

$$\mathbb{R}^p \supset \mathcal{Y} \ni y = (y_1, \ldots, y_p) \quad \mapsto \quad u_y \in \mathcal{H}$$

Examples:

- Design optimization
- Optimal control
- Routine analysis
- Uncertainty quantification
- Inverse problems





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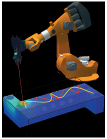

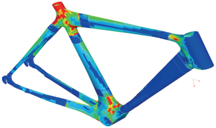

Curse of Dimensionality:

Computational cost often much too high!

High-Fidelity Approximations

Galerkin Approach: Instead of $b_y(u_y, v) = f_y(v)$, we solve

$$b_y\left(u_y^h, v\right) = f_y(v) \qquad \text{for all } v \in U^h,$$

where $U^h \subset \mathcal{H}$ with $D := \dim\left(U^h\right) < \infty$ is the *high-fidelity discretization* and $u_y^h \in U^h$ is the solution.

Cea's Lemma: u_y^h is (up to a constant) a best approximation of u_y by elements in U^h.

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Galerkin Solution: Let $(\varphi_i)_{i=1}^D$ be a basis for U^h. Then u_y^h satisfies

$$u_y^h = \sum_{i=1}^{D} (\mathbf{u}_y^h)_i \varphi_i \qquad \text{with} \qquad \mathbf{u}_y^h := \left(\mathbf{B}_y^h\right)^{-1} \mathbf{f}_y^h \in \mathbb{R}^D,$$

where $\mathbf{B}_y^h := (b_y(\varphi_j, \varphi_i))_{i,j=1}^D$ and $\mathbf{f}_y^h := (f_y(\varphi_i))_{i=1}^D$.

What about Deep Neural Networks?

Parametric Map:

$$\mathcal{Y} \ni y \mapsto \mathbf{u}_y^{\mathrm{h}} \in \mathbb{R}^D \quad \text{such that} \quad b_y\left(u_y^h, v\right) = f_y(v) \; \forall v \in U^h.$$

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Can a Neural Network Approximate the Parametric Map?

Advantages:

- After training, extremely rapid computation of the map.
- Flexible, universal approach.

Questions: Let $\varepsilon > 0$.

(1) Does there exist a neural network Φ such that

$$\|\Phi - \mathbf{u}_y^{\mathrm{h}}\| \le \varepsilon \qquad \text{for all } y \in \mathcal{Y}?$$

(2) How does the complexity of Φ depend on p and D?

Deep Learning Approaches to PDEs

Common Approach to Solve PDEs with Neural Networks:
Approximate the solution u of a PDE $\mathcal{L}(u) = f$ by a neural network Φ, i.e., solve

$$\mathcal{L}(\Phi) = f.$$

Key Idea: The size of the neural network does not depend exponentially on the underlying dimension.

Incomplete List:

- Lagaris, Likas, Fotiadis; 1998
- E, Yu; 2017
- Sirignano, Spiliopoulos; 2017
- Han, Jentzen, E; 2017
- Berner, Grohs, Jentzen; 2018
- Eigel, Schneider, Trunschke, Wolf; 2018
- Reisinger, Zhang; 2019
- ...

Solving Parametric PDEs

List of Deep Learning Approaches:

- K. Lee, K. Carlberg; 2018:
  Learn a parametrisation of $S(\mathcal{Y})$ represented by neural networks.
- J.S. Hesthaven, S. Ubbiali; 2018:
  Find reduced basis and then train neural networks to predict coeffcients of solution in that basis.
- Schwab, Zech; 2018:
  Assume that there is a reduced basis of polynomial chaos functions. These and the coefficients can be efficiently represented by neural networks.

Expressivity of Deep Neural Networks

Complexity of a Deep Neural Network

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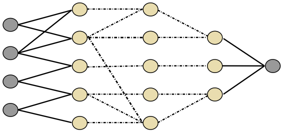

- $d \in \mathbb{N}$: Dimension of input layer.
- L: Number of layers.
- N: Number of neurons.
- $\rho : \mathbb{R} \to \mathbb{R}$: (Non-linear) function called *activation function*.
- $T_\ell : \mathbb{R}^{N_{\ell-1}} \to \mathbb{R}^{N_\ell}$, $\ell = 1, \ldots, L$: Affine linear maps $x \mapsto A_\ell x + b_\ell$.

Then $\Phi : \mathbb{R}^d \to \mathbb{R}^{N_L}$ given by

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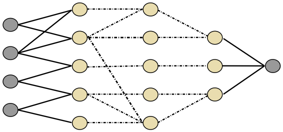

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Measure for Complexity: The *number of weights $W(\Phi)$* is defined by

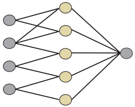
$$W(\Phi) := \sum_{\ell=1}^{L} \left(\|A_\ell\|_0 + \|b_\ell\|_0 \right).$$

We write $\Phi \in \mathcal{NN}_{L,W(\Phi),d,\rho}$.

One Size Fits All?

Universal Approximation Theorem (Cybenko, 1989)(Hornik, 1991):
Let $d \in \mathbb{N}$, $K \subset \mathbb{R}^d$ compact, $f : K \to \mathbb{R}$ continuous, $\rho : \mathbb{R} \to \mathbb{R}$ continuous and not a polynomial. Then, for each $\varepsilon > 0$, there exist $N \in \mathbb{N}$, $a_k, b_k \in \mathbb{R}, w_k \in \mathbb{R}^d$ such that

$$\|f - \sum_{k=1}^{N} a_k \rho(\langle w_k, \cdot \rangle - b_k)\|_\infty \le \varepsilon.$$



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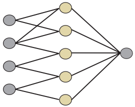

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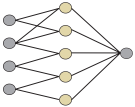

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Theorem (Yarotsky; 2017): For all $f \in \mathcal{C} = C^s([0,1]^d)$ and ρ the *ReLU (Rectifiable Linear Unit $\rho(x) = \max\{0, x\}$)*, there exist neural networks $(\Phi_n)_{n \in \mathbb{N}}$ with $L(\Phi_n) \approx \log(n)$ such that

$$\|f - \Phi_n\|_\infty \lesssim W(\Phi_n)^{-\frac{s}{d}} \to 0 \quad \text{as } n \to \infty.$$

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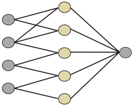

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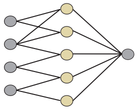

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Correct Function Spaces? (Gribonval, K, Nielsen, Voigtlaender; 2019)

A Fundamental Lower Bound

Key Ingredient from Information Theory:

Given $\mathcal{C} \subseteq L^2(\mathbb{R}^d)$. With $E : L^2(\mathbb{R}^d) \to \{0,1\}^\ell$, $D : \{0,1\}^\ell \to L^2(\mathbb{R}^d)$, set

$$L(\varepsilon, \mathcal{C}) := \min\{\ell \in \mathbb{N} : \exists (E, D) \in \mathfrak{E}^\ell \times \mathfrak{D}^\ell : \sup_{f \in \mathcal{C}} \|D(E(f)) - f\|_{L^2(\mathbb{R}^d)} \leq \varepsilon\}.$$

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Theorem (Bölcskei, Grohs, K, and Petersen; 2017):
Let $d \in \mathbb{N}$, $\rho : \mathbb{R} \to \mathbb{R}$, and let $\mathcal{C} \subset L^2(\mathbb{R}^d)$. Assume that

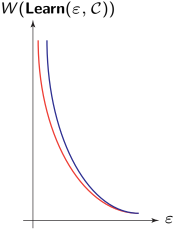
$$\mathbf{Learn} : (0,1) \times \mathcal{C} \to \mathcal{NN}_{\infty,\infty,d,\rho}$$

satisfies that, for each $f \in \mathcal{C}$ and $0 < \varepsilon < 1$

$$\sup_{f \in \mathcal{C}} \|f - \mathbf{Learn}(\varepsilon, f)\|_{L^2(\mathbb{R}^d)} \leq \varepsilon.$$

Then, for all $\gamma < \gamma^*(\mathcal{C})$, there is no $C > 0$ with

$$\sup_{f \in \mathcal{C}} W(\mathbf{Learn}(\varepsilon, f)) \leq C\varepsilon^{-\gamma} \quad \text{for all } \varepsilon > 0$$



A Fundamental Lower Bound

Key Ingredient from Information Theory:
Given $\mathcal{C} \subseteq L^2(\mathbb{R}^d)$. With $E : L^2(\mathbb{R}^d) \to \{0,1\}^\ell$, $D : \{0,1\}^\ell \to L^2(\mathbb{R}^d)$, set

$$L(\varepsilon, \mathcal{C}) := \min\{\ell \in \mathbb{N} : \exists (E,D) \in \mathfrak{E}^\ell \times \mathfrak{D}^\ell : \sup_{f \in \mathcal{C}} \|D(E(f)) - f\|_{L^2(\mathbb{R}^d)} \leq \varepsilon\}.$$

Then the optimal exponent $\gamma^*(\mathcal{C})$ is $\gamma^*(\mathcal{C}) := \inf\{\gamma \in \mathbb{R} : L(\varepsilon, \mathcal{C}) = O(\varepsilon^{-\gamma})\}$.

Theorem (Bölcskei, Grohs, K, and Petersen; 2017):
Let $d \in \mathbb{N}$, $\rho : \mathbb{R} \to \mathbb{R}$, and let $\mathcal{C} \subset L^2(\mathbb{R}^d)$. Assume that

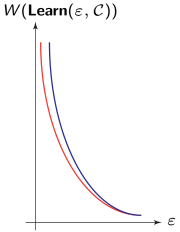
$$\mathbf{Learn} : (0,1) \times \mathcal{C} \to \mathcal{NN}_{\infty,\infty,d,\rho}$$

satisfies that, for each $f \in \mathcal{C}$ and $0 < \varepsilon < 1$

$$\sup_{f \in \mathcal{C}} \|f - \mathbf{Learn}(\varepsilon, f)\|_{L^2(\mathbb{R}^d)} \leq \varepsilon.$$

Then, for all $\gamma < \gamma^*(\mathcal{C})$, there is no $C > 0$ with

$$\sup_{f \in \mathcal{C}} W(\mathbf{Learn}(\varepsilon, f)) \leq C\varepsilon^{-\gamma} \quad \text{for all } \varepsilon > 0$$



What happens for $\gamma = \gamma^*(\mathcal{C})$?

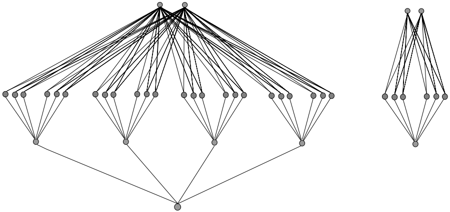
DNNs and Representation Systems, I

Observation: Assume a system $(\varphi_i)_{i \in I} \subset L^2(\mathbb{R}^d)$ satisfies:

- For each $i \in I$, there exists a neural network Φ_i with at most $C > 0$ edges such that $\varphi_i = \Phi_i$.

Then we can construct a network Φ with $O(M)$ edges with

$$\Phi = \sum_{i \in I_M} c_i \varphi_i, \quad \text{if } |I_M| = M.$$



DNNs and Representation Systems, II

Observation: Assume a system $(\varphi_i)_{i\in I} \subset L^2(\mathbb{R}^d)$ satisfies:

- For each $i \in I$, there exists a neural network Φ_i with at most $C > 0$ edges such that $\varphi_i = \Phi_i$.
- There exists $\tilde{C} > 0$ such that, for all $f \in \mathcal{C} \subset L^2(\mathbb{R}^d)$, there exists $I_M \subset I$ with
$$\|f - \sum_{i\in I_M} c_i\varphi_i\| \leq \tilde{C} M^{-1/\gamma^*(\mathcal{C})}.$$

Then every $f \in \mathcal{C}$ can be approximated up to an error of ε by a neural network with only $O(\varepsilon^{-\gamma^*(\mathcal{C})})$ edges.

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Recall: Then, for all $\gamma < \gamma^*(\mathcal{C})$, there is no $C > 0$ with

$$\sup_{f \in \mathcal{C}} W(\textbf{Learn}(\varepsilon, f)) \leq C\varepsilon^{-\gamma} \qquad \text{for all } \varepsilon > 0.$$

Road Map

General Approach:

(1) Determine a class of functions $\mathcal{C} \subseteq L^2(\mathbb{R}^2)$.

(2) Determine an associated representation system with the following properties:

- The elements of this system can be realized by a neural network with controlled number of edges.
- This system provides optimally sparse approximations for $\mathcal{C}$.

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- The elements of this system can be realized by a neural network with controlled number of edges.
  $\rightsquigarrow$ *Still to be analyzed!*
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Affine Transforms

Building Principle:

Many systems from applied harmonic analysis such as

- wavelets,
- ridgelets,
- shearlets,

constitute affine systems:

$$\{|\det A|^{d/2}\psi(A\,\cdot\,-t) : A \in G \subseteq GL(d),\ t \in \mathbb{Z}^d\}, \quad \psi \in L^2(\mathbb{R}^d).$$

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Realization by Neural Networks:

The following conditions are equivalent:

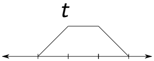
(i) $|\det A|^{d/2}\psi(A\,\cdot\,-t)$ can be realized by a neural network Φ_1.

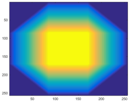
(ii) ψ can be realized by a neural network Φ_2.

Also, Φ_1 and Φ_2 have the same number of edges up to a constant factor.

Construction of Generators

Wavelet generators (LeCun; 1987), (Shaham, Cloninger, Coifman; 2017):

- Assume activation function $\rho(x) = \max\{x, 0\}$ (ReLUs).
- Define
$$t(x) := \rho(x) - \rho(x-1) - \rho(x-2) + \rho(x-3).$$


  $\rightsquigarrow$ *t can be constructed with a 2 layer network.*
- Observe that
$$\phi(x_1, x_2) := \rho(t(x_1) + t(x_2) - 1)$$


  yields a 2D bump function.
- Summing up shifted versions of ϕ yields a function ψ with vanishing moments.

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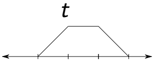

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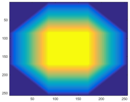

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This cannot yield differentiable functions ψ!

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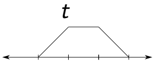

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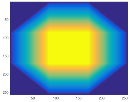

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Our Construction: Use a smoothed version of a ReLU.

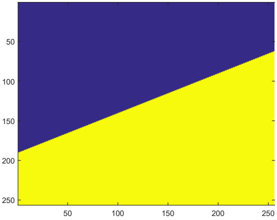
$\rightsquigarrow$ *Leads to appropriate shearlet generators!*

Optimal Approximation

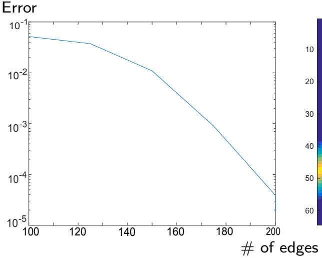
Theorem (Bölcskei, Grohs, K, and Petersen; 2017): Let ρ be an admissible smooth rectifier, and let $\varepsilon > 0$. Then there exist $C_\varepsilon > 0$ such that, for all cartoon-like functions f and $N \in \mathbb{N}$, we can construct a neural network $\Phi \in \mathcal{NN}_{3,O(N),2,\rho}$ satisfying

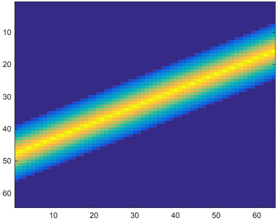
$$\|f - \Phi\|_{L^2(\mathbb{R}^2)} \leq C_\varepsilon N^{-1+\varepsilon}.$$

Function classes which are optimal representable by affine systems are also optimally approximated by sparsely connected neural networks!



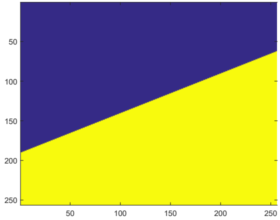
Linear Singularity





Subnetworks: Ridgelets!

Numerical Experiments (with ReLUs & Backpropagation)



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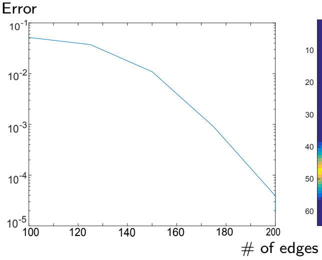

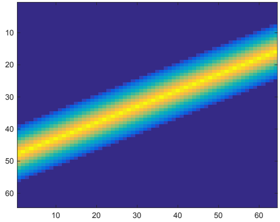

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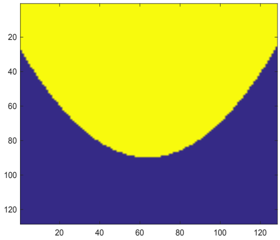
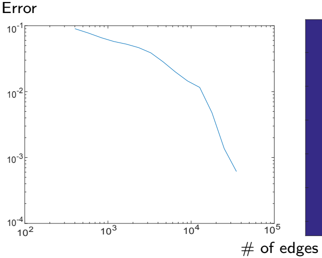
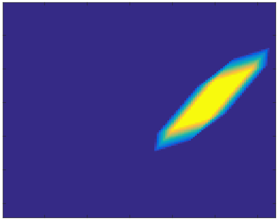


Curvilinear Singularity





Subnetworks: $\approx$ Shearlets!

Deep Learning for Parametric PDEs

or

How to Beat the Curse of Dimensionality

Parametric Partial Differential Equations

Our Setting: We will consider parameter-dependent equations of the form

$$b_y(u_y, v) = f_y(v), \quad \text{for all } y \in \mathcal{Y},\ v \in \mathcal{H},$$

where

(i) $\mathcal{Y} \subseteq \mathbb{R}^p$ (p large) is the *compact parameter set*,

(ii) $\mathcal{H}$ is a Hilbert space,

(ii) $b_y : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ is a *symmetric, uniformally coercive, and uniformally continuous bilinear form*,

(iv) $f_y \in \mathcal{H}^*$ is the *uniformly bounded, parameter-dependent right-hand side*,

(v) $u_y \in \mathcal{H}$ is the *solution*.

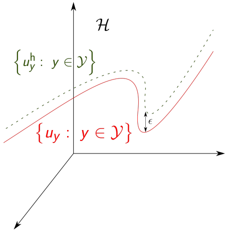
We also assume the *solution manifold*

$$S(\mathcal{Y}) := \{u_y : y \in \mathcal{Y}\}$$

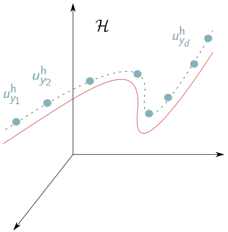
to be compact in $\mathcal{H}$.

Reduced Basis Method: Key Idea

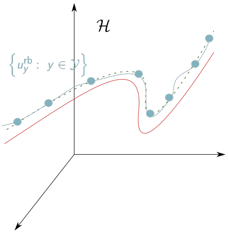
High-Fidelity Discretization:



Key Idea:



Offline (slow):
Compute snap shots



Online (fast):
Compute solutions for new parameters

Reduced Basis Method: Details

Assumption: For all $\varepsilon > \varepsilon_0$, there exists $U^{\mathrm{rb}} \subset \mathcal{H}$, $d(\varepsilon) \coloneqq \dim\left(U^{\mathrm{rb}}\right) \ll D$ such that

$$\sup_{y\in\mathcal{Y}} \inf_{w\in U^{\mathrm{rb}}} \|u_y - w\|_{\mathcal{H}} \leq \varepsilon.$$

$\rightsquigarrow$ Optimality through *Kolmogorov N-width*!

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Transfer to Reduced Basis:

- Let $U^{\mathrm{rb}} := \mathrm{span}\,(\psi_i)_{i=1}^{d(\varepsilon)}$ with $(\psi_i)_{i=1}^{d(\varepsilon)} = \left(\sum_{j=1}^{D} \mathbf{V}_{j,i}\varphi_j\right)_{i=1}^{d(\varepsilon)}$.

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Galerkin Solution: $\left(\sup_{y \in \mathcal{Y}} \|u_y - u_y^{\mathrm{rb}}\|_{\mathcal{H}} \leq C\varepsilon\right)$

$$u_y^{\mathrm{rb}} =$$

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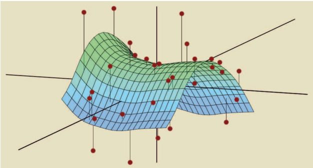
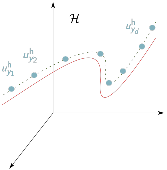
Our Analysis

Statistical Learning Problem = Parametric Problem?

Comparison/Similarities:

Statistical Learning Problem	Parametric Problem
Learn $f : X \to Y$	
Distribution on $X \times Y$	
Loss function $\mathcal{L}\colon Y \times Y \to \mathbb{R}^+$	
Training data $(\mathbf{x}_i, \mathbf{y}_i)_{i=1}^N$	
Training phase $\sum_{i=1}^N \mathcal{L}(f(\mathbf{x}_i), \mathbf{y}_i)$	





Statistical Learning Problem = Parametric Problem?

Comparison/Similarities:

Statistical Learning Problem	Parametric Problem
Learn $f : X \to Y$	Learn $\mathcal{Y} \ni y \mapsto u_y \in \mathcal{H}$
Distribution on $X \times Y$	
Loss function $\mathcal{L}$: $Y \times Y \to \mathbb{R}^+$	
Training data $(\mathbf{x}_i, \mathbf{y}_i)_{i=1}^N$	
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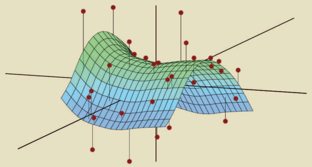

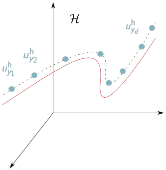

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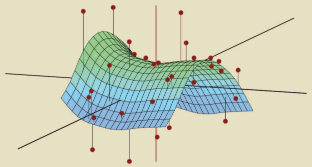

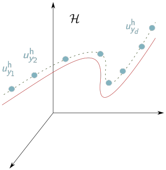

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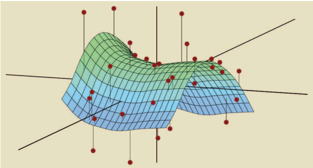

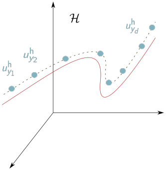

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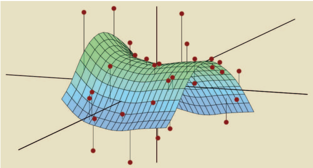
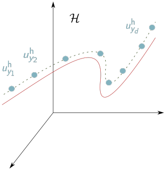
Training phase $\sum_{i=1}^N \mathcal{L}(f(\mathbf{x}_i), \mathbf{y}_i)$	





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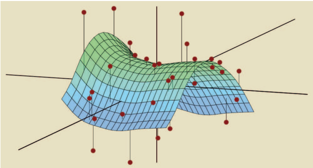
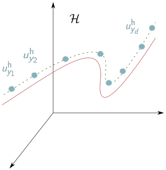
Training phase $\sum_{i=1}^N \mathcal{L}(f(\mathbf{x}_i), \mathbf{y}_i)$	Offline phase





Our Results: Discrete Version

Theorem (K, Petersen, Raslan, Schneider; 2019):
We assume the following:

- For all $\varepsilon > 0$, there exists $d(\varepsilon) \ll D$, $\mathbf{V} \in \mathbb{R}^{D \times d(\varepsilon)}$, such that for all $y \in \mathcal{Y}$ there exists $\mathbf{B}_y^{\mathrm{rb}} \in \mathbb{R}^{d(\varepsilon) \times d(\varepsilon)}$ with
$$\|\mathbf{V}(\mathbf{B}_y^{\mathrm{rb}})^{-1} V^T \mathbf{f}_y^{\mathrm{h}} - \mathbf{u}_y^{\mathrm{h}}\| \leq \varepsilon.$$
- There exist ReLU neural networks Φ^B and Φ^f of size $O(\mathrm{poly}(p) d(\varepsilon)^2 \mathrm{polylog}(\varepsilon))$ such that, for all $y \in \mathcal{Y}$,
$$\|\Phi^B - \mathbf{B}_y^{\mathrm{rb}}\| \leq \varepsilon \quad \text{and} \quad \|\Phi^f - V^T \mathbf{f}_y^{\mathrm{h}}\| \leq \varepsilon.$$

Then there exists a ReLU neural network Φ of size $O(d(\varepsilon)^3 \mathrm{polylog}(\varepsilon) + D + \mathrm{poly}(p) d(\varepsilon)^2 \mathrm{polylog}(\varepsilon))$ such that
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Extremely fast computation of the parametric map,
while beating the curse of dimensionality!

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Let $(\psi_i)_{i=1}^{d(\varepsilon)}$ denote the reduced basis. We assume in addition the following:

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Remark: The hypotheses are fulfilled, for example, by

- Diffusion equations,
- Linear elasticity equations.

Key Idea of the Proof

Main Task: Approximate $\mathbf{V}(\mathbf{B}_y^{\mathrm{rb}})^{-1}\mathbf{V}^T\mathbf{f}_y^{\mathrm{h}}$ by a ReLU neural network and control its size!

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For $g(x) := \min\{2x, 2-2x\}$ and $g_s := g \circ \ldots \circ g$ (s times), we have

$$x^2 = \lim_{n\to\infty} x - \sum_{s=1}^{n} \frac{g_s(x)}{2^{2s}} \quad \text{for all } x \in [0,1].$$

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Moreover,

$$xz = 1/4((x+z)^2 - (x-z)^2) \quad \text{for all } x, z \in \mathbb{R}.$$

$\Longrightarrow$ *Scalar multiplication on $[-1,1]^2$ can be ε-approximated by a neural network of size $\mathcal{O}(\log_2(1/\varepsilon))$.*

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Step 2 (Multiplication):

A matrix multiplication of two matrices of size $d \times d$ can be performed by d^3 scalar multiplications.

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Step 3 (Inversion):

- Neural networks can approximate matrix polynomials.
- Neural networks can the inversion operator $\mathbf{A} \mapsto \mathbf{A}^{-1}$ using

$$\sum_{s=0}^{m} \mathbf{A}^s \longrightarrow (\mathbf{Id}_{\mathbb{R}^d} - \mathbf{A})^{-1} \quad \text{as } m \to \infty.$$

$\Longrightarrow$ *Matrix inversion can be ε-approximated by a neural network of size $\mathcal{O}(d(\varepsilon)^3 \log_2^q(1/\varepsilon))$ for a constant $q > 0$.*

Key Idea of the Proof

Step 4 (Discrete Parametric Map w.r.t Reduced Basis):

- Now use the assumptions on $\mathbf{B}_y^{\mathrm{rb}}$ and $\mathbf{f}_y^{\mathrm{rb}}$.

$\Longrightarrow$ *The map* $y \mapsto (\mathbf{B}_y^{\mathrm{rb}})^{-1}\mathbf{f}_y^{\mathrm{rb}}$ *can be* ε*-approximated by a neural network* Φ^{rb} *of size* $\mathcal{O}(d(\varepsilon)^3 \log_2^q(1/\varepsilon) + poly(p) d(\varepsilon)^2 \log_2^q(1/\varepsilon))$.

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For Theorem 1:

- Now use the assumption that every element from the reduced basis can be approximately represented in the high-fidelity basis.
- Consider then $\mathbf{V} \circ \Phi^{\mathrm{rb}}$.

$\Longrightarrow$ *The discrete parametric map can be ε-approximated by a neural network of size $\mathcal{O}(d(\varepsilon)^3 \log_2^q(1/\varepsilon) + d(\varepsilon)D + poly(p)d(\varepsilon)^2 \log_2^q(1/\varepsilon))$.*

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For Theorem 2:

- Now use the assumption that neural networks can approximate each element of the reduced basis.

$\Longrightarrow$ *The continuous parametric map can be ε-approximated by a neural network of size $\mathcal{O}(d(\varepsilon)^3 \log_2^q(1/\varepsilon) + poly(p)d(\varepsilon)^2 \log_2^q(1/\varepsilon))$.*

Conclusions

What to take Home...?

Deep Learning:

- Impressive performance in combination with classical model-based methods (Inverse Problems, PDEs, ...) $\rightsquigarrow$ Limited-Angle CT.
- Theoretical foundation of neural networks almost entirely missing: Expressivity, Learning, Generalization, and Explainability.

Expressivity of Deep Neural Networks:

- We derive a fundamental lower bound on the complexity, which each learning algorithm has to obey.
- Neural networks are as powerful approximators as classical affine systems such as wavelets, shearlets, ...

Deep Neural Networks for Parametric PDEs:

- We theoretically show that in this setting neural networks beat the curse of dimensionality by explicably constructing such networks.
- Once the network is trained, the parametric map can be computed extremely fast.

THANK YOU!

References available at:

www.math.tu-berlin.de/∼kutyniok

Code available at:

www.ShearLab.org

Related Books:

- Y. Eldar and G. Kutyniok
  Compressed Sensing: Theory and Applications
  Cambridge University Press, 2012.
- G. Kutyniok and D. Labate
  Shearlets: Multiscale Analysis for Multivariate Data
  Birkhäuser-Springer, 2012.
- P. Grohs and G. Kutyniok
  Theory of Deep Learning
  Cambridge University Press (in preparation)