

The Mathematics of Deep Learning: Can We Open the Black Box of Deep Neural Networks?

Gitta Kutyniok

(Technische Universität Berlin)

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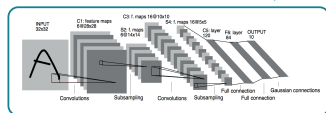


The Dawn of Deep Learning

Self-Driving Cars



Surveillance



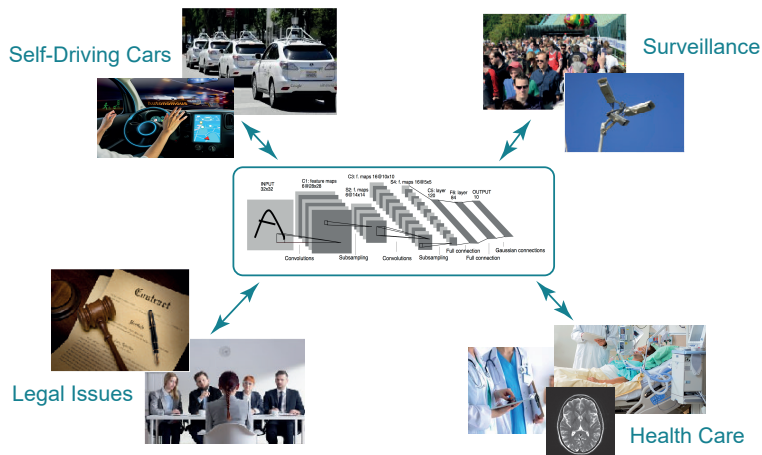
Legal Issues



Health Care



The Dawn of Deep Learning



Very few theoretical results explaining their success!

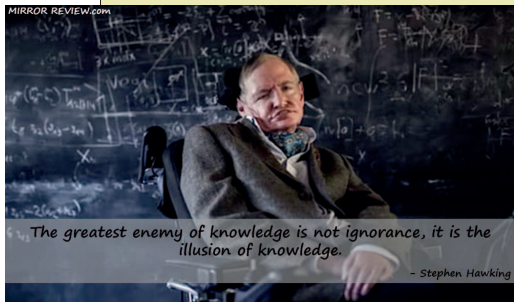
Deep Learning = Alchemy?



„Ali Rahimi, a researcher in artificial intelligence (AI) at Google in San Francisco, California, took a swipe at his field last December—and received a 40-second ovation for it. Speaking at an AI conference, Rahimi charged that **machine learning algorithms, in which computers learn through trial and error, have become a form of „alchemy.“** Researchers, he said, **do not know why some algorithms work and others don't, nor do they have rigorous criteria for choosing one AI architecture over another....“**

Science, May 2018

MIRROR REVIEW.com



The greatest enemy of knowledge is not ignorance, it is the illusion of knowledge.

- Stephen Hawking

Theoretical Foundations of Deep Learning

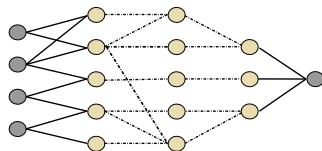


The Mathematics of Deep Neural Networks

Definition:

Assume the following notions:

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



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

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

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

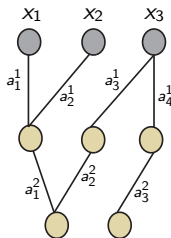
Affine Linear Maps and Weights

Remark: The affine linear map T_ℓ is defined by a matrix $A_\ell \in \mathbb{R}^{N_{\ell-1} \times N_\ell}$ and an affine part $b_\ell \in \mathbb{R}^{N_\ell}$ via

$$T_\ell(x) = A_\ell x + b_\ell.$$

$$A_1 = \begin{pmatrix} a_1^1 & a_2^1 & 0 \\ 0 & 0 & a_3^1 \\ 0 & 0 & a_4^1 \end{pmatrix}$$

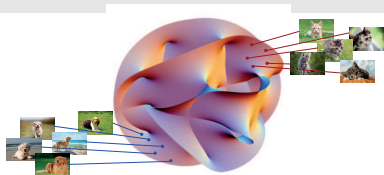
$$A_2 = \begin{pmatrix} a_1^2 & a_2^2 & 0 \\ 0 & 0 & a_3^2 \end{pmatrix}$$



Training of Deep Neural Networks

High-Level Set Up:

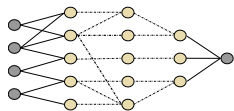
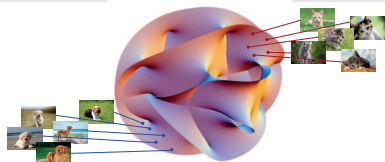
- ▶ Samples $(x_i, f(x_i))_{i=1}^m$ of a function such as $f : \mathcal{M} \rightarrow \{1, 2, \dots, K\}$.



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High-Level Set Up:

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- ▶ 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.



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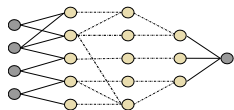
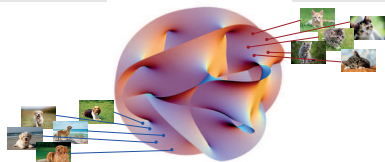
- ▶ Learn the affine-linear functions $(T_\ell)_{\ell=1}^L = (A_\ell \cdot + b_\ell)_{\ell=1}^L$ by

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

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

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

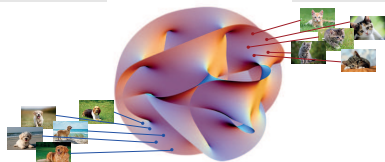
This is often done by stochastic gradient descent.



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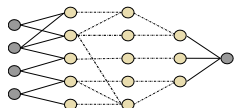
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This is often done by stochastic gradient descent.

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

Fundamental Questions concerning Deep Neural Networks

▶ *Expressivity:*

- ▶ How powerful is the network architecture?
- ▶ Can it indeed represent the correct functions?

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Impact of Deep Learning on Mathematics



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Some Examples:

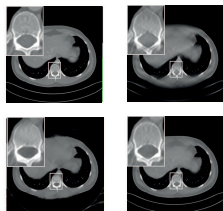
► Inverse Problems

~ Image denoising (Burger, Schuler, Harmeling; 2012)

~ Superresolution (Klatzer, Soukup, Kobler, Hammernik, Pock; 2017)

~ Limited-angle tomography (Bubba, K, Lassas, März, Samek, Siltanen, Srinivan; 2018)

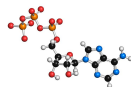
~ Edge detection (Andrade-Loarca, K, Öktem, Petersen; 2019)



► Numerical Analysis of Partial Differential Equations

~ Schrödinger equation (Rupp, Tkatchenko, Müller, von Lilienfeld; 2012 –)

~ Parametric PDEs (K, Petersen, Raslan, Schneider; 2019) (Geist, Petersen, Raslan, Schneider, K; 2020)



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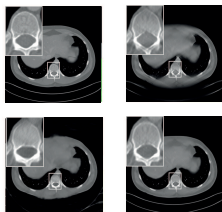
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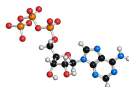
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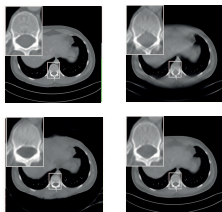
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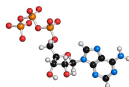
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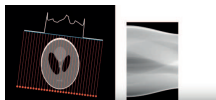
Deep Learning for Inverse Problems

Example: Limited-Angle Computed Tomography

A CT scanner samples the *Radon transform*

$$\mathcal{R}f(\phi, s) = \int_{L(\phi, s)} f(x) dS(x),$$

for $L(\phi, s) = \{x \in \mathbb{R}^2 : x_1 \cos(\phi) + x_2 \sin(\phi) = s\}$, $\phi \in [-\pi/2, \pi/2)$, and $s \in \mathbb{R}$.

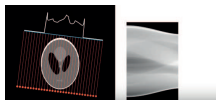


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Challenging inverse problem if $\mathcal{R}f(\cdot, s)$ is only sampled on $[-\phi, \phi]$, $\phi < \pi/2$

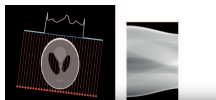
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Learn the Invisible (Bubba, K, Lassas, März, Samek, Siltanen, Srinivan; 2018):

Step 1: Use model-based methods as far as possible

- ▶ Solve with sparse regularization using shearlets.

Step 2: Use data-driven methods where it is necessary

- ▶ Use a deep neural network to recover the missing components.

Step 3: Carefully combine both worlds

- ▶ Combine outcome of Step 1 and 2.

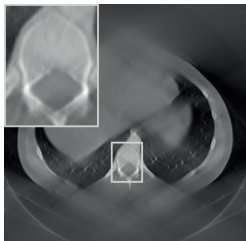


Learn the Invisible (Ltl)

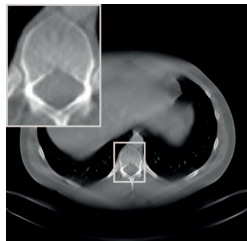
(Bubba, K, Lassas, März, Samek, Siltanen, Srinivan; 2018)



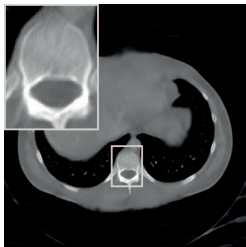
Original



Filtered Backprojection



Sparse Regularization with Shearlets



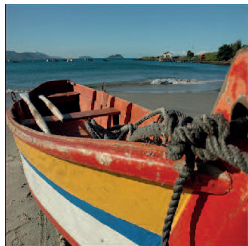
[Gu & Ye, 2017]



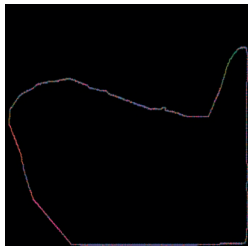
Learn the Invisible (Ltl)

Deep Network Shearlet Edge Extractor (DeNSE)

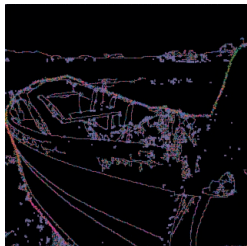
(Andrade-Loarca, K, Öktem, Petersen; 2019)



Original



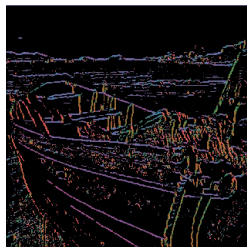
Human Annotation



SEAL [Yu et al; 2018]



CoShREM [Reisenhofer et al.; 2015]

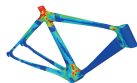


DeNSE

Deep Learning for (Parametric) PDEs

Parametric Map:

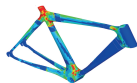
$\mathbb{R}^p \supset \mathcal{Y} \ni y \mapsto u_y \in \mathcal{H}$ such that $\mathcal{L}(u_y, y) = f_y$.



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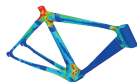


Curse of Dimensionality: Computational cost is exponential in p !

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Curse of Dimensionality: Computational cost is exponential in p !

Theoretical Approach (K, Petersen, Raslan, Schneider; 2019):

Expressivity

- ▶ We show the existence of a neural network Φ which approximates the parametric map, i.e.,
$$\|\Phi - u_y\| \leq \epsilon \quad \text{for all } y \in \mathcal{Y}.$$

Complexity Analysis

- ▶ We prove that the complexity of the neural network Φ does not suffer from the curse of dimensionality.



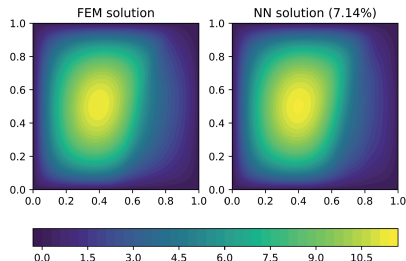
Numerical Results

(Geist, Petersen, Raslan, Schneider, K; 2020)

Set-Up:

- ▶ Parametric diffusion equation with various parametrizations
- ▶ **Fixed neural network**: 11 layers and 0.2-LReLU
- ▶ Training set: 20000 i.i.d. parameter samples

Example ($\rho = 91$):



The performance does not suffer from the curse of dimensionality!

Data-Driven Versus Model-Based Approaches?



Optimal balancing of
data-driven and model-based approaches!

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Expressivity



Main Research Goal

Some Questions:

- ▶ Which architecture to choose for a particular application?
- ▶ What is the expressive power of a given architecture?
- ▶ What effect has the depth of a neural network in this respect?
- ▶ What is the complexity of the approximating neural network?
- ▶ Can deep neural networks beat the curse of dimensionality?

General Mathematical Problem:

Given a **function class** \mathcal{C} and $f \in \mathcal{C}$ as well as an **accuracy** $\varepsilon > 0$, does there exist a **neural network** Φ such that

$$\|\Phi - f\| \leq \varepsilon,$$

and which **complexity** does Φ have?

Function Approximation in a Nutshell

Goal: Given $\mathcal{C} \subseteq L^2(\mathbb{R}^d)$ and $(\varphi_i)_{i \in I} \subseteq L^2(\mathbb{R}^d)$. Measure the suitability of $(\varphi_i)_{i \in I}$ for uniformly approximating functions from \mathcal{C} .

Definition: The *error of best N -term approximation* of some $f \in \mathcal{C}$ is given by

$$\|f - f_N\|_2 := \inf_{I_N \subset I, \#I_N=N, (c_i)_{i \in I_N}} \|f - \sum_{i \in I_N} c_i \varphi_i\|_2.$$

The largest $\gamma > 0$ such that

$$\sup_{f \in \mathcal{C}} \|f - f_N\|_2 = O(N^{-\gamma}) \quad \text{as } N \rightarrow \infty$$

determines the *optimal (sparse) approximation rate* of \mathcal{C} by $(\varphi_i)_{i \in I}$.

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*Approximation accuracy \leftrightarrow Complexity of approximating system
in terms of sparsity*



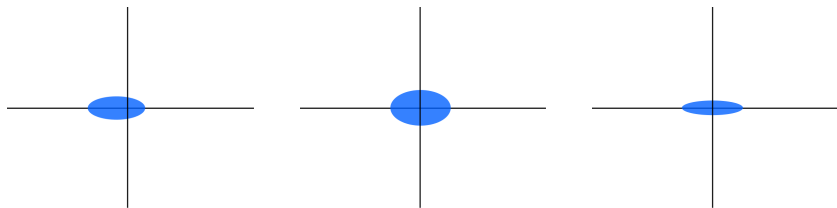
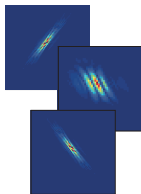
Example: Shearlet Systems

Definition (K, Labate; 2006):

$$A_j := \begin{pmatrix} 2^j & 0 \\ 0 & 2^{j/2} \end{pmatrix}, \quad S_k := \begin{pmatrix} 1 & k \\ 0 & 1 \end{pmatrix}, \quad j, k \in \mathbb{Z}.$$

Then

$$\psi_{j,k,m} := 2^{\frac{3j}{4}} \psi(S_k A_j \cdot -m).$$



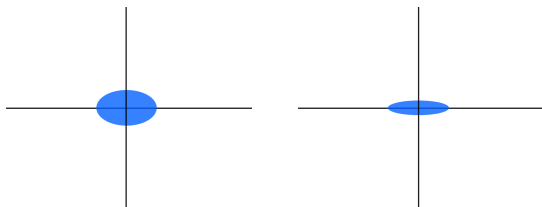
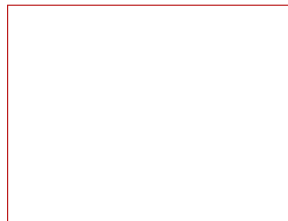
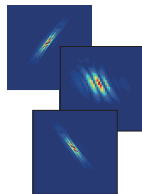
Example: Shearlet Systems

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$$A_j := \begin{pmatrix} 2^j & 0 \\ 0 & 2^{j/2} \end{pmatrix}, \quad S_k := \begin{pmatrix} 1 & k \\ 0 & 1 \end{pmatrix}, \quad j, k \in \mathbb{Z}.$$

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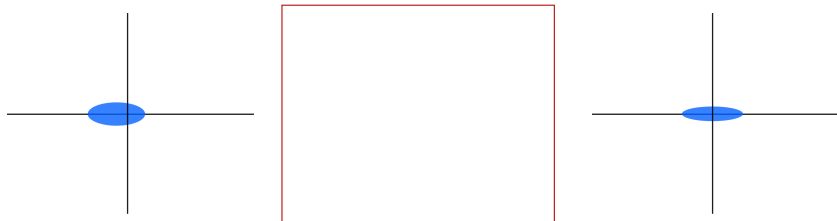
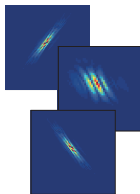
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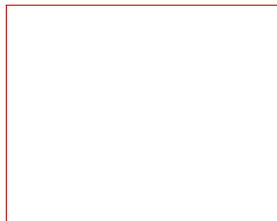
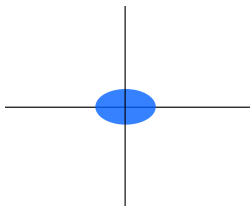
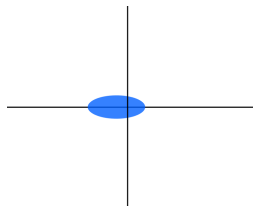
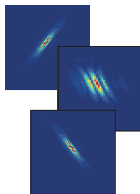
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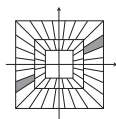
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The (cone-adapted) discrete shearlet system $\mathcal{SH}(c; \phi, \psi, \tilde{\psi})$, $c > 0$, generated by $\phi \in L^2(\mathbb{R}^2)$ and $\psi, \tilde{\psi} \in L^2(\mathbb{R}^2)$ is the union of

$$\{\phi(\cdot - cm) : m \in \mathbb{Z}^2\},$$

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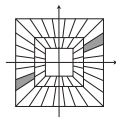
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Theorem (K, Lim; 2011):

Let $\phi, \psi, \tilde{\psi} \in L^2(\mathbb{R}^2)$ be compactly supported, and let $\hat{\psi}, \hat{\tilde{\psi}}$ satisfy certain decay condition. Then $\mathcal{SH}(\phi, \psi, \tilde{\psi})$ provides an **optimally sparse approximation** of cartoon-like functions f , i.e.,

$$\|f - f_N\|_2 \leq C \cdot N^{-1} \cdot (\log N)^{3/2}, \quad N \rightarrow \infty.$$



Function Approximation in a Nutshell

Goal: Given $\mathcal{C} \subseteq L^2(\mathbb{R}^d)$ and $(\varphi_i)_{i \in I} \subseteq L^2(\mathbb{R}^d)$. Measure the suitability of $(\varphi_i)_{i \in I}$ for uniformly approximating functions from \mathcal{C} .

Definition: The *error of best N -term approximation* of some $f \in \mathcal{C}$ is given by

$$\|f - f_N\|_2 := \inf_{I_N \subset I, \#I_N=N, (c_i)_{i \in I_N}} \left\| f - \sum_{i \in I_N} c_i \varphi_i \right\|_2.$$

The largest $\gamma > 0$ such that

$$\sup_{f \in \mathcal{C}} \|f - f_N\|_2 = O(N^{-\gamma}) \quad \text{as } N \rightarrow \infty$$

determines the *optimal (sparse) approximation rate* of \mathcal{C} by $(\varphi_i)_{i \in I}$.

*Approximation accuracy \leftrightarrow Complexity of approximating system
in terms of sparsity*



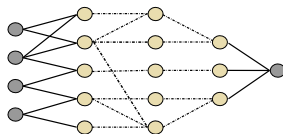
Complexity of a Deep Neural Network



Complexity of a Deep Neural Network

Recall:

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



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

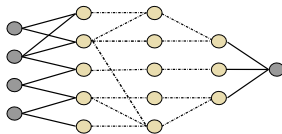
$$\Phi(x) = T_L \rho(T_{L-1} \rho(\dots \rho(T_1(x)))) , \quad x \in \mathbb{R}^d ,$$

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

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

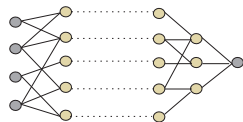
$$W(\Phi) := \sum_{\ell=1}^L (\|A_\ell\|_0 + \|b_\ell\|_0) .$$

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

Sparsely Connected Deep Neural Networks

Key Problem:

- ▶ Deep neural networks employed in practice often consist of **hundreds of layers**.
- ▶ Training and storage of such networks pose **formidable (computational) challenge**.



→ *Employ deep neural networks with **sparse connectivity!***

Example of Speech Recognition:

- ▶ Typically speech recognition is performed in the cloud (e.g. SIRI).
- ▶ New speech recognition systems (e.g. Android) can operate offline and are based on a **sparsely connected deep neural network**.

Key Challenge:

*Approximation accuracy \leftrightarrow Complexity of approximating DNN
in terms of sparse connectivity!*

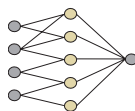


One Size Fits All?

Universal Approximation Theorem (Cybenko, 1989)(Hornik, 1991):

Let $d \in \mathbb{N}$, $K \subset \mathbb{R}^d$ compact, $f : K \rightarrow \mathbb{R}$ continuous, $\rho : \mathbb{R} \rightarrow \mathbb{R}$ continuous and not a polynomial. Then, for each $\epsilon > 0$, there exist $N \in \mathbb{N}$, $a_k, b_k \in \mathbb{R}$, $w_k \in \mathbb{R}^d$ such that

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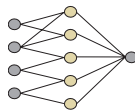


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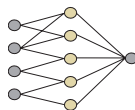
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Theorem (Yarotsky; 2017): For all $f \in \mathcal{C} = C^s([0, 1]^d)$ and ρ the *ReLU* (*Rectifiable Linear Unit* $\rho(x) = \max\{0, x\}$), there exist neural networks $(\Phi_n)_{n \in \mathbb{N}}$ with $L(\Phi_n) \approx \log(n)$ such that

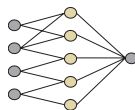
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This result is not optimal!



A Fundamental Lower Bound

Complexity of a Function Class:

The **optimal exponent** $\gamma^*(\mathcal{C})$ measures the complexity of $\mathcal{C} \subset L^2(\mathbb{R}^d)$.

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Theorem (Bölcskei, Grohs, K, and Petersen; 2019):

Let $d \in \mathbb{N}$, $\rho : \mathbb{R} \rightarrow \mathbb{R}$, and let $\mathcal{C} \subset L^2(\mathbb{R}^d)$. Further, let

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

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

$$\sup_{f \in \mathcal{C}} \|f - \mathbf{Learn}(\epsilon, f)\|_2 \leq \epsilon.$$

Then, for all $\gamma < \gamma^*(\mathcal{C})$,

$$\epsilon^\gamma \sup_{f \in \mathcal{C}} W(\mathbf{Learn}(\epsilon, f)) \rightarrow \infty, \quad \text{as } \epsilon \rightarrow 0.$$

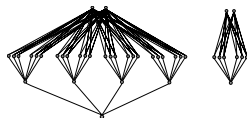
Conceptual bound independent on the learning algorithm!



Optimally Memory Efficient Neural Networks

Key Ideas:

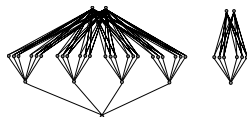
- ▶ Consider a representation system which provides an optimal approximation rate of a specific function class.
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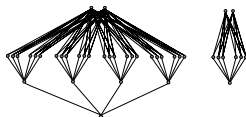
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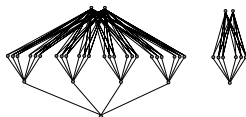
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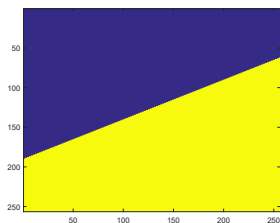
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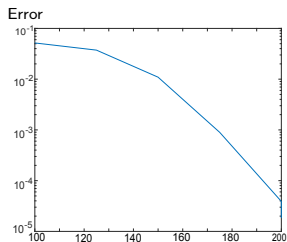
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DNNs achieve optimal approx. properties of all affine systems combined

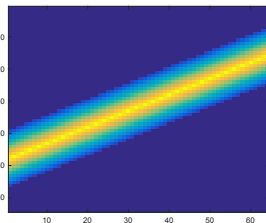
Numerical Experiments (with ReLUs & Backpropagation)



Linear Singularity

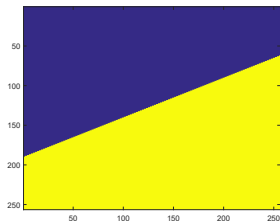


of edges

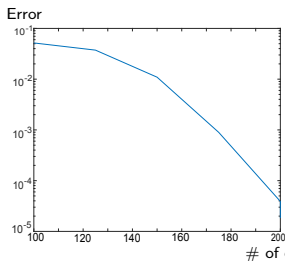


Subnetworks: Ridgelets!

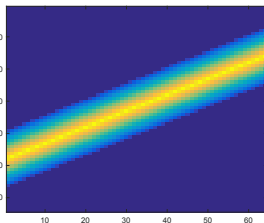
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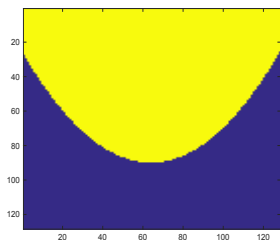
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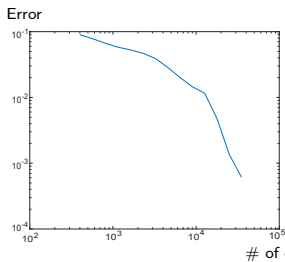
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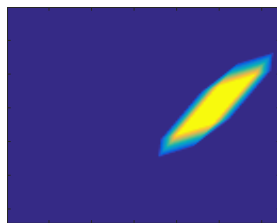
Subnetworks: Ridgelets!



Curvilinear Singularity



of edges



Subnetworks: \approx Shearlets!

Mathematics of Deep Neural Networks

▶ *Expressivity:*

- ▶ How powerful is the network architecture?
- ▶ Can it indeed represent the correct functions?

↪ *Applied Harmonic Analysis, Approximation Theory, ...*

▶ *Learning:*

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

↪ *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?

↪ *Learning Theory, Optimization, Statistics, ...*

▶ *Interpretability:*

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

↪ *Information Theory, Uncertainty Quantification, ...*



Interpretability

General Problem Setting

Question:

- ▶ Given a trained neural network.
- ▶ We don't know what the training data was nor how it was trained.

~> *Can we determine how it operates?*

Opening the Black Box!



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- ▶ Assume a job application is rejected.
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Holy Grail: 

- ▶ Explanation of a decision indistinguishable from a human being!



History of the Field

Previous Relevance Mapping Methods:

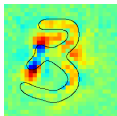
- ▶ Gradient based methods:
 - ▶ **Sensitivity Analysis** (Baehrens, Schroeter, Harmeling, Kawanabe, Hansen, Müller, 2010)
 - ▶ **SmoothGrad** (Smilkov, Thorat, Kim, Viégas, Wattenberg, 2017)
- ▶ Backwards propagation based methods:
 - ▶ **Guided Backprop** (Springenberg, Dosovitskiy, Brox, Riedmiller, 2015)
 - ▶ **Layer-wise Relevance Propagation** (Bach, Binder, Montavon, Klauschen, Müller, Samek, 2015)
 - ▶ **Deep Taylor** (Montavon, Samek, Müller, 2018)
- ▶ Surrogate model based methods:
 - ▶ **LIME (Local Interpretable Model-agnostic Explanations)** (Ribeiro, Singh, Guestrin, 2016)
- ▶ Game theoretic methods:
 - ▶ **Shapley values** (Shapley, 1953), (Kononenko, Štrumbelj, 2010)
 - ▶ **SHAP (Shapley Additive Explanations)** (Lundberg, Lee, 2017)



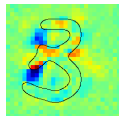
What is Relevance?

Main Goal: We aim to **understand** decisions of “black-box” predictors!

map for digit 3



map for digit 8



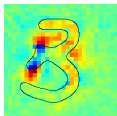
Challenges:

- ▶ What **exactly** is relevance in a mathematical sense?
- ▶ What is a **good** relevance map?
- ▶ How to **compare** different relevance maps?

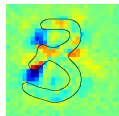
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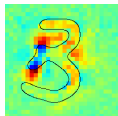
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 \leadsto *Rigorous definition of relevance by information theory.*
- ▶ What is a **good** relevance map?

- ▶ How to **compare** different relevance maps?

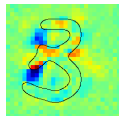
What is Relevance?

Main Goal: We aim to **understand** decisions of “black-box” predictors!

map for digit 3



map for digit 8



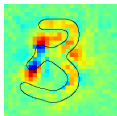
Challenges:

- ▶ What **exactly** is relevance in a mathematical sense?
~> *Rigorous definition of relevance by information theory.*
- ▶ What is a **good** relevance map?
~> *Formulation of interpretability as optimization problem.*
~> *Theoretical analysis of complexity.*
- ▶ How to **compare** different relevance maps?

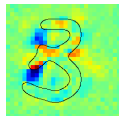
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Challenges:

- ▶ What **exactly** is relevance in a mathematical sense?
~ *Rigorous definition of relevance by information theory.*
- ▶ What is a **good** relevance map?
~ *Formulation of interpretability as optimization problem.*
~ *Theoretical analysis of complexity.*
- ▶ How to **compare** different relevance maps?
~ *Canonical framework for comparison.*

The Relevance Mapping Problem

The Relevance Mapping Problem

The Setting: Let

- ▶ $\Phi: [0, 1]^d \rightarrow [0, 1]$ be a **classification function**,
- ▶ $x \in [0, 1]^d$ be an **input signal**.

The Task:

- ▶ Determine the **most relevant components** of x for the prediction $\Phi(x)$.
- ▶ Choose $S \subseteq \{1, \dots, d\}$ of components that are considered **relevant**.
- ▶ S should be small (usually not everything is relevant).
- ▶ S^c is considered **non-relevant**.



Original image x

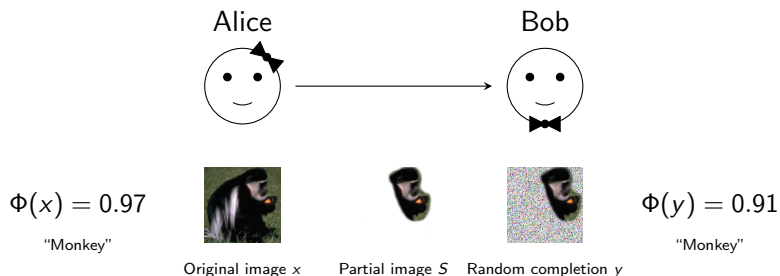


Relevant components S



Non-relevant components S^c

Rate-Distortion Viewpoint



Obfuscation: Let

- ▶ $n \sim \mathcal{V}$ be a **random noise vector**, and
- ▶ y be a random vector defined as $y_S = x_S$ and $y_{S^c} = n_{S^c}$.

Rate-Distortion Viewpoint

Recall: Let

- ▶ $\Phi: [0, 1]^d \rightarrow [0, 1]$ be a **classification function**,
- ▶ $x \in [0, 1]^d$ be an **input signal**,
- ▶ $n \sim \mathcal{V}$ be a **random noise vector**, and
- ▶ y be a random vector defined as $y_S = x_S$ and $y_{S^c} = n_{S^c}$.

Expected Distortion:

$$D(S) = D(\Phi, x, S) = \mathbb{E} \left[\frac{1}{2} (\Phi(x) - \Phi(y))^2 \right]$$

Rate-Distortion Function:

$$R(\epsilon) = \min_{S \subseteq \{1, \dots, d\}} \{|S| : D(S) \leq \epsilon\}$$

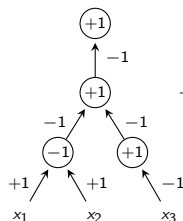
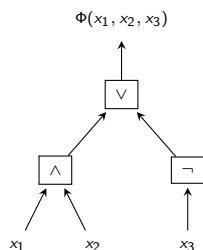
\leadsto *Use this viewpoint for the definition of a relevance map!*



*Finding a minimizer of $R(\epsilon)$
or even approximating it is very hard!*

Hardness Results

Boolean Functions as ReLU Neural Networks:

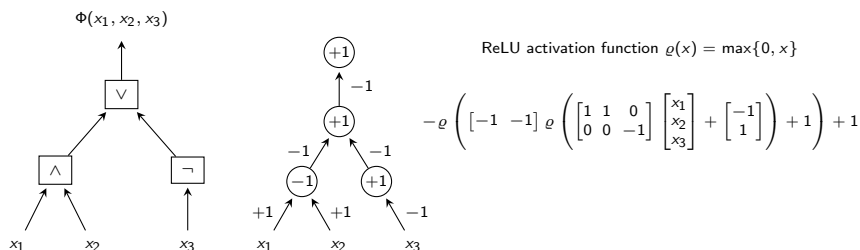


ReLU activation function $\varrho(x) = \max\{0, x\}$

$$-\varrho\left(\left[-1 \ -1\right] \varrho\left(\left[\begin{array}{ccc} 1 & 1 & 0 \\ 0 & 0 & -1 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} -1 \\ 1 \end{bmatrix}\right) + 1\right) + 1$$

Hardness Results

Boolean Functions as ReLU Neural Networks:



The Binary Setting: Let

- ▶ $\Phi: \{0, 1\}^d \rightarrow \{0, 1\}$ be **classifier functions**,
- ▶ $x \in \{0, 1\}^d$ be **signals**, and
- ▶ $\mathcal{V} = \mathcal{U}(\{0, 1\}^d)$ be a **uniform distribution**.

Hardness Results

We consider the binary case.

Theorem (Wäldchen, Macdonald, Hauch, K, 2019):

Given Φ , x , $k \in \{1, \dots, d\}$, and $\epsilon < \frac{1}{4}$. Deciding whether $R(\epsilon) \leq k$ is NP^{PP} -complete.

Finding a minimizer of $R(\epsilon)$ is hard!

Theorem (Wäldchen, Macdonald, Hauch, K, 2019):

Given Φ , x , and $\alpha \in (0, 1)$. Approximating $R(\epsilon)$ to within a factor of $d^{1-\alpha}$ is NP-hard.

Even the approximation problem of it is hard!

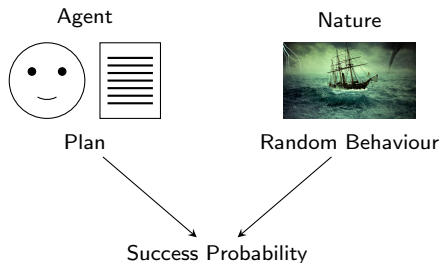
What is NP^{PP} ?

The Complexity Class NP^{PP} :

Many important problems in artificial intelligence belong to this class.

Some Examples:

- ▶ Planning under uncertainties
- ▶ Finding maximum a-posteriori configurations in graphical models
- ▶ Maximizing utility functions in Bayesian networks



Our Method:

Rate-Distortion Explanation (RDE)

Problem Relaxation

	Discrete problem	Continuous problem
Relevant set	$S \subseteq \{1, \dots, d\}$	
Obfuscation	$y_S = x_S, y_{S^c} = n_{S^c}$	
Distortion	$D(S)$	
Rate/Size	$ S $	

Problem Relaxation

	Discrete problem	Continuous problem
Relevant set	$S \subseteq \{1, \dots, d\}$	$s \in [0, 1]^d$
Obfuscation	$y_S = x_S, y_{S^c} = n_{S^c}$	$y = s \odot x + (1 - s) \odot n$
Distortion	$D(S)$	$D(s)$
Rate/Size	$ S $	$\ s\ _1$

Problem Relaxation

	Discrete problem	Continuous problem
Relevant set	$S \subseteq \{1, \dots, d\}$	$s \in [0, 1]^d$
Obfuscation	$y_S = x_S, y_{S^c} = n_{S^c}$	$y = s \odot x + (1 - s) \odot n$
Distortion	$D(S)$	$D(s)$
Rate/Size	$ S $	$\ s\ _1$

Resulting Minimization Problem:

$$\text{minimize } D(s) + \lambda \|s\|_1 \quad \text{subject to } s \in [0, 1]^d$$

Numerical Experiments

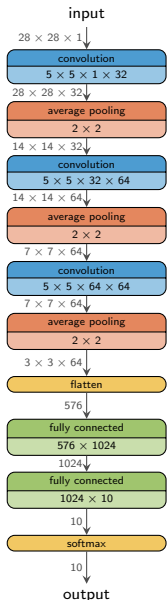
MNIST Experiment

6 8 3 4

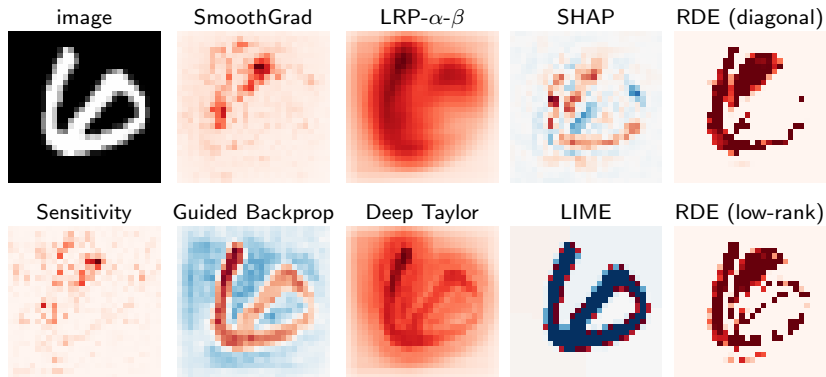
Data Set

Image size	$28 \times 28 \times 1$
Number of classes	10
Training samples	50000

Test accuracy: 99.1%

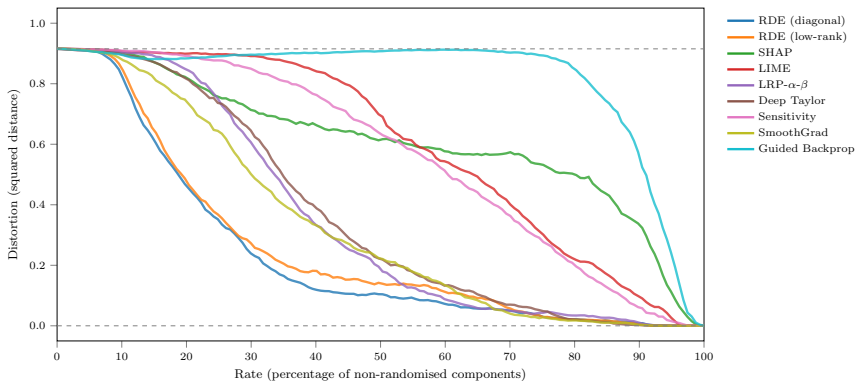


MNIST Experiment



SmoothGrad (Smilkov, Thorat, Kim, Viégas, Wattenberg, 2017), Layer-wise Relevance Propagation (Bach, Binder, Montavon, Klauschen, Müller, Samek, 2015), SHAP (Lundberg, Lee, 2017), Sensitivity Analysis (Simonyan, Vedaldi, Zisserman, 2013), Guided Backprop (Springenberg, Dosovitskiy, Brox, Riedmiller, 2015), Deep Taylor Decompositions (Montavon, Samek, Müller, 2016), LIME (Ribeiro, Singh, Guestrin, 2016)

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STL-10 Experiment

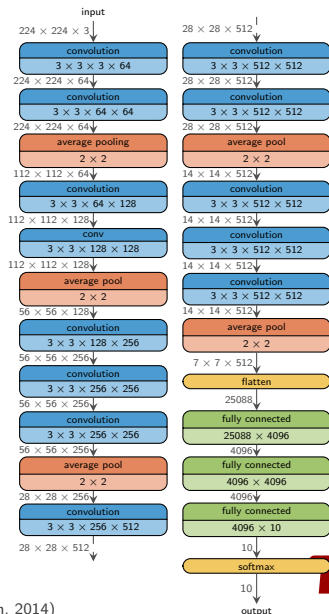


Data Set

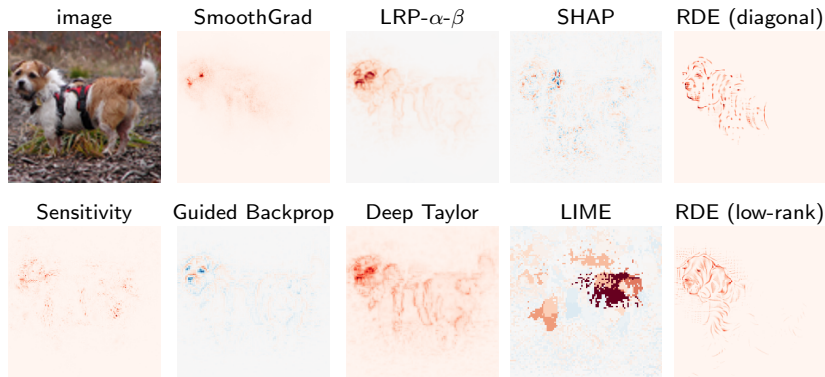
Image size	$96 \times 96 \times 3$ ($224 \times 224 \times 3$)
Number of classes	10
Training samples	4000

Test accuracy: 93.5%

(VGG-16 convolutions pretrained on Imagenet)

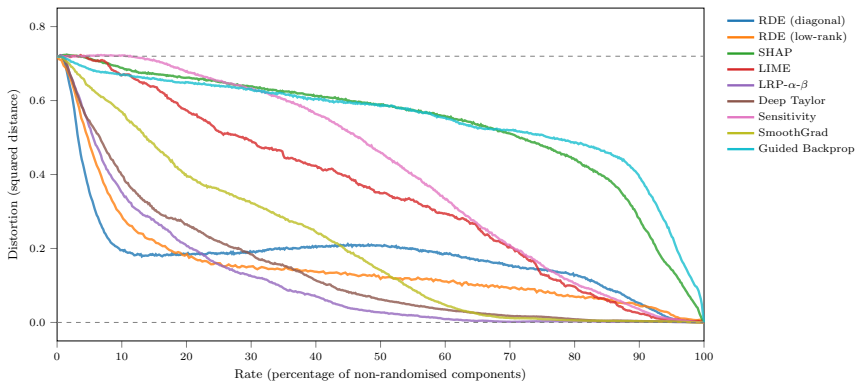


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Conclusions

What to take Home...?

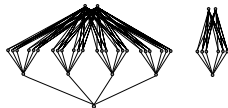
Deep Learning:

- ▶ Impressive performance *in combination with classical mathematical methods* (Inverse Problems, PDEs, ...).
- ▶ A theoretical foundation of neural networks is largely missing: *Expressivity, Learning, Generalization, and Interpretability.*



Expressivity:

- ▶ Fundamental lower bound on the complexity, leading to the construction of *optimally memory-efficient networks*.
- ▶ Neural networks are as *powerful approximators* as classical affine systems such as wavelets, shearlets, ...



Interpretability:

- ▶ We provide a precise mathematical notion for *relevance* based on *rate-distortion theory*.
- ▶ We show that solving the optimization problem is *hard*.
- ▶ *RDE considers a relaxed version* and *outperforms current methods*.



THANK YOU!

References available at:

`www.math.tu-berlin.de/~kutyniok`

Related Book:

- ▶ P. Grohs and G. Kutyniok
Theory of Deep Learning
Cambridge University Press (in preparation)