Deep Learning as a Mathematician

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Syllabus

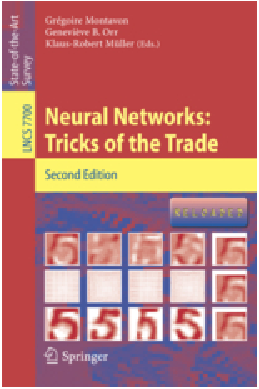
1 Why Mathematical Understanding?

Curiosity

It is the guiding principle of many applied mathematicians that if something mathematical works really well, there must be a good underlying mathematical reason for it, and we ought to be able to understand it.

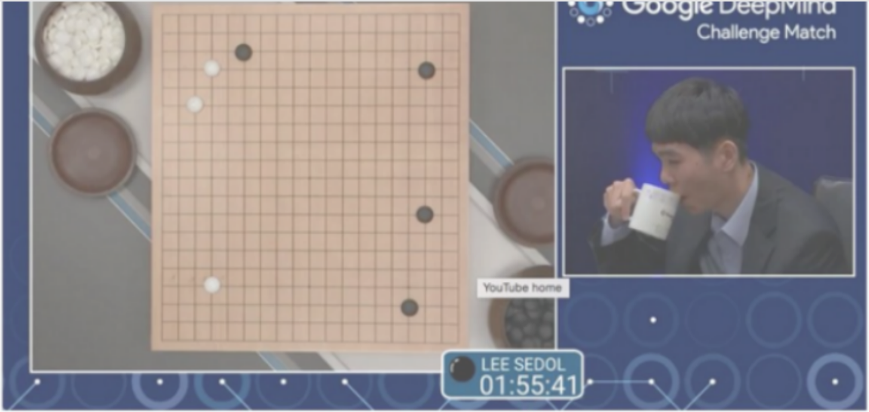
[Ingrid Daubechies. *Big Data's Mathematical Myteries*, Quanta Magazine (2015)]

Improve Usability/Availability



$\sim$ 800 page book explaining various ad-hoc tricks, which are necessary for good performance.

Be More Efficient



AlphaGO	Lee Se-dol
1202 CPUs, 176 GPUs, 100+ Scientists.	1 Human Brain, 1 Coffee.

Be More Efficient

Electricity bill for one game of AlphaGo:

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Electricity bill for one game of AlphaGo: $\sim$ 3000 USD

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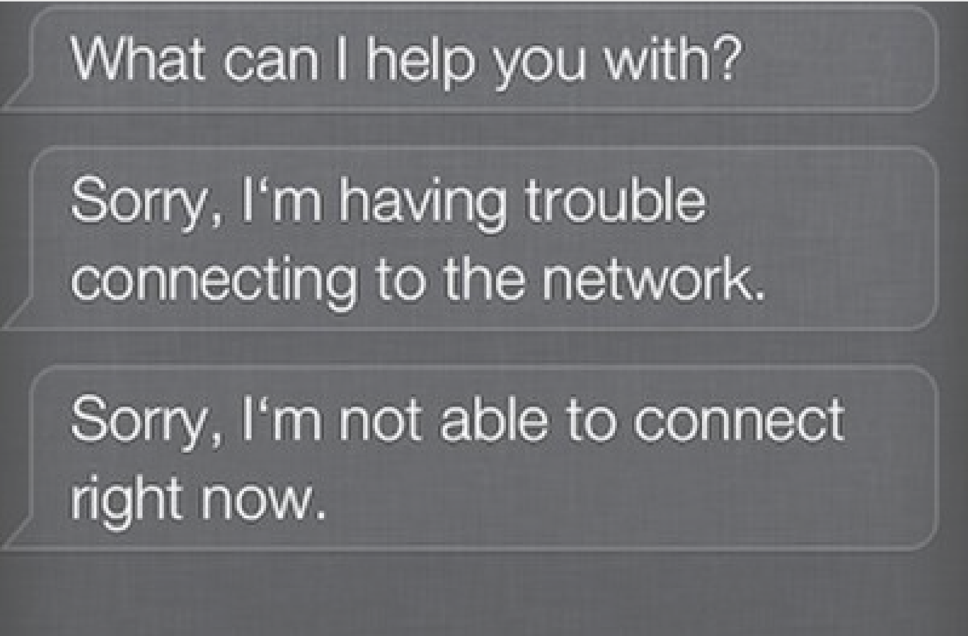

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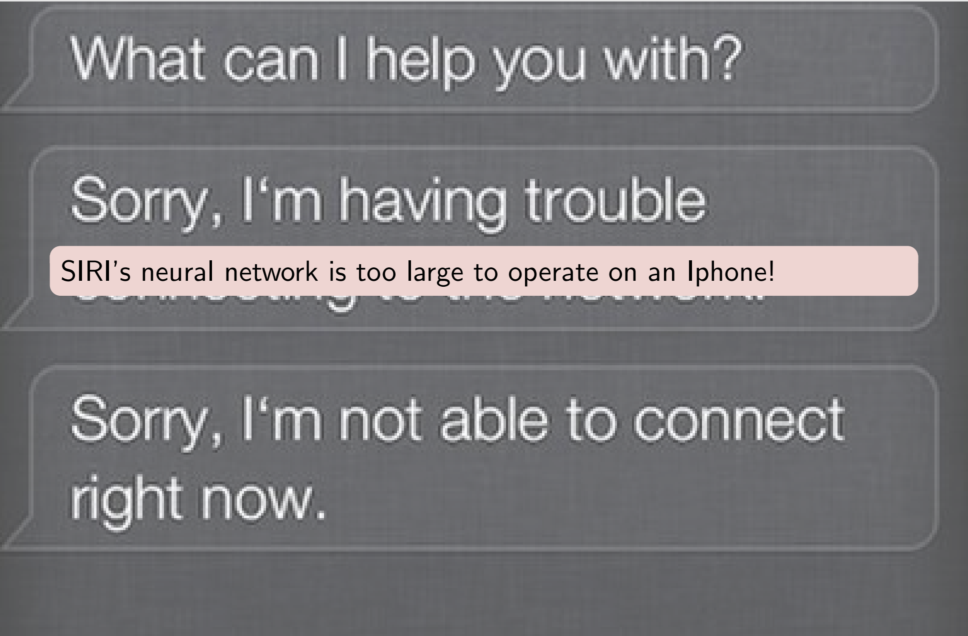

SIRI's neural network is too large to operate on an Iphone!

Today's Focus: Vanilla Neural Networks Regression

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Neural Network Hypothesis Class

Given $d, L, N_1, \ldots, N_L$ and σ define the associated hypothesis class

$$\mathcal{H}_{[d,N_1,\ldots,N_L],\sigma} :=$$
$$\left\{ A_L\sigma\left(A_{L-1}\sigma\left(\ldots\sigma\left(A_1(x)\right)\right)\right) : \; A_\ell : \mathbb{R}^{N_{\ell-1}} \to \mathbb{R}^{N_\ell} \text{ affine linear } \right\}.$$

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Simplest Regression/Classification Task

Given data $\mathbf{z} = ((x_i, y_i))_{i=1}^m \subset \mathbb{R}^d \times \mathbb{R}^{N_L}$, find the empirical regression function

$$f_{\mathbf{z}} \in \operatorname{argmin}_{f \in \mathcal{H}_{[d,N_1,\ldots,N_L],\sigma}} \sum_{i=1}^m \mathcal{L}(f, x_i, y_i),$$

where $\mathcal{L} : C(\mathbb{R}^d) \times \mathbb{R}^d \times \mathbb{R}^{N_L} \to \mathbb{R}_+$ is the *loss function* (in least squares problems we have $\mathcal{L}(f, x, y) = |f(x) - y|^2$).

Example: Handwritten Digits

MNIST Database for handwritten digit recognition http://yann.lecun.com/exdb/mnist/

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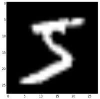

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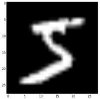

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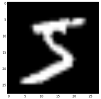

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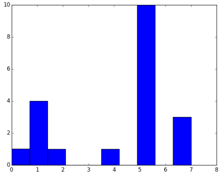

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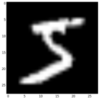

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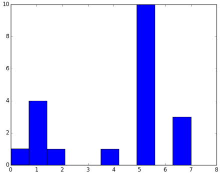

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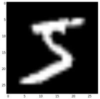

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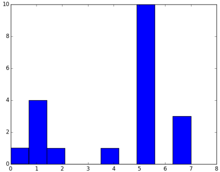

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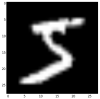

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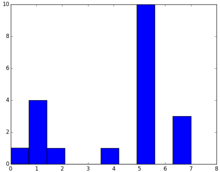

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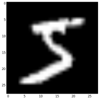

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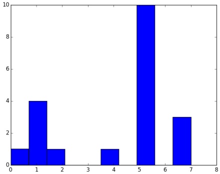

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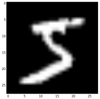

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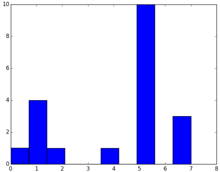

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- Typically solved by stochastic first order approximation methods.

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4. Invariances and Discriminatory Properties

This Talk

1. Approximation Power of (Convolutional) Neural Networks
2. Convergence Properties of Stochastic Optimization Algorithms
3. Generalization of Neural Networks
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1. Approximation Power

Universal Approximation Theorem

Theorem [Cybenko (1989), Hornik (1991)]

Suppose that $\sigma : \mathbb{R} \to \mathbb{R}$ continuous is not a polynomial and fix $d \geq 1, L \geq 2, N_L \geq 1 \in \mathbb{N}$ and a compact subset $K \subset \mathbb{R}^d$. Then for any continuous $f : \mathbb{R}^d \to \mathbb{R}^{N_L}$ and any $\varepsilon > 0$ there exist $N_1, \ldots, N_{L-1} \in \mathbb{N}$ and affine linear maps $A_\ell : \mathbb{R}^{N_{\ell-1}} \to \mathbb{R}^{N_\ell}$, $1 \leq \ell \leq L$ such that the neural network

$$\Phi(x) = A_L \sigma \left(A_{L-1} \sigma \left(\ldots \sigma \left(A_1(x) \right) \right) \right), \quad x \in \mathbb{R}^d,$$

approximates f to within accuracy ε, i.e.,

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Does not imply any quantitative results (e.g., how many nodes to achieve a desired accuracy?).

A Quantitative Universal Approximation Theorem

Theorem [Maiorov - Pinkus (1999)]

There exists an activation function $\sigma : \mathbb{R} \to \mathbb{R}$ that is smooth, monotone increasing and sigmoidal ($\lim_{t\to\infty} \sigma(t) = 1$ and $\lim_{t\to-\infty} \sigma(t) = 0$) with the following property: For any $\varepsilon > 0$, any $d \geq 1$, any compact subset $K \subset \mathbb{R}^d$ and any continuous $f : \mathbb{R}^d \to \mathbb{R}^{N_L}$ there exist affine linear maps $A_1 : \mathbb{R}^d \to \mathbb{R}^{3d}$, $A_2 : \mathbb{R}^{3d} \to \mathbb{R}^{6d+3}$, $A_2 : \mathbb{R}^{6d+3} \to \mathbb{R}^{N_L}$ such that the neural network

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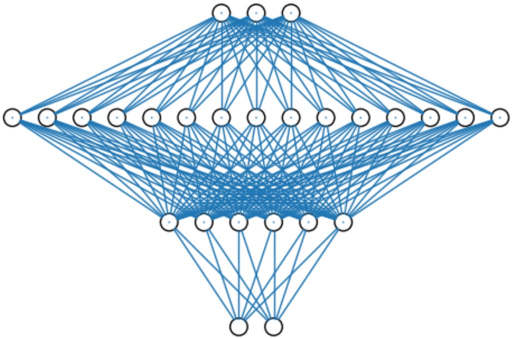
In other words, we can approximate *any* function up to *any* accuracy with a *fixed* number of coefficients????

A Universal Architecture



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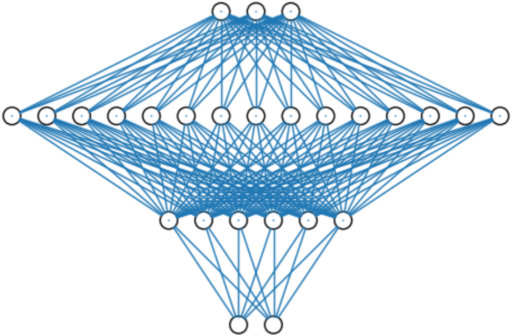

Where is the catch?

A Meaningful Notion of Approximation

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Definition [Bölcskei-G-Kutyniok-Petersen (2017)]

A regression problem class $\mathcal{C}$ has effective approximation rate γ if there exists a constant $C > 0$ and a polynomial π with

$$\sup_{f \in \mathcal{C}} \inf_{\Phi \in \mathcal{NN}_{M,\sigma,\pi(M)}} \|f - \Phi\|_{L^2(K)} \leq C \cdot M^{-\gamma}.$$

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Theorem ([Bölcskei-G-Kutyniok-Petersen (2017)] Informal Version)

Let $s(\mathcal{C})$ be the Kolmogorov entropy of $\mathcal{C}$ (a measure of complexity that can be computed). Then $\gamma \leq 1/s(\mathcal{C})$. In particular, this scaling between accuracy and complexity has to be obeyed by all learning algorithms!

...or more formally...

Theorem [Bölcskei-G-Kutyniok-Petersen (2017)]

Consider *any* learning algorithm **Learn** : $(0,1) \times \mathcal{C} \to \mathcal{NN}$ ($\mathcal{NN}$ being the class of neural networks) which satisfies

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Coefficients in Pinkus' network are so large that they cannot be stored!

...we can finally ask a meaningful question

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- What architectures (deep, shallow,...) are good for which regression problem classes?

What is Known

Theorem ([Bölcskei-G-Kutyniok-Petersen (2017)] Informal Version)

Let $\mathcal{C}$ be a ball of any classical approximation space (for example Sobolev, Besov, Shearlet, Kernel Approximation Space, piecewise smooth functions on submanifolds, ...). Then neural networks are optimal for $\mathcal{C}$.

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- This means neural networks are as good as all classical 'linear' methods combined!
- They are even better: Result remains true if signal class is defined on a submanifold and/or is warped by a smooth diffeomorphism.

A Detour: Sparse Coding

- Given a dictionary $\mathcal{D} = (\varphi_i)_{i \in \mathbb{N}} \subset L^2(\Gamma)$, approximate every $F \in \mathcal{C}$ by *optimally sparse* linear combinations of $\mathcal{D}$, i.e.

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- Examples: Textures $\leftrightarrow$ Gabor frames (JPEG), point singularities $\leftrightarrow$ wavelets (JPEG2000), line/hyperplane singularities $\leftrightarrow$ ridgelets, curved/hypersurface singularities $\leftrightarrow$ (α-)curvelets.

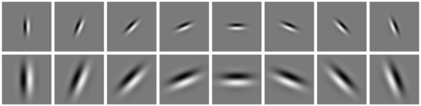
A Detour: Sparse Coding

- Given a dictionary $\mathcal{D} = (\varphi_i)_{i\in\mathbb{N}} \subset L^2(\Gamma)$, approximate every $F \in \mathcal{C}$ by *optimally sparse* linear combinations of $\mathcal{D}$, i.e.

$$\sum_{i\in J} c_i\varphi_i$$

  with $|J|$ as small as possible.

- For most known $\mathcal{C}$ there exists a specific *optimal* dictionary that achieves the optimal tradeoff between sparsity ($\sim$ codelength!) and approximation error, as dictated by $\gamma^*(\mathcal{C})$.
- Examples: Textures $\leftrightarrow$ Gabor frames (JPEG), point singularities $\leftrightarrow$ wavelets (JPEG2000), line/hyperplane singularities $\leftrightarrow$ ridgelets, curved/hypersurface singularities $\leftrightarrow$ (α-)curvelets.



Transferring Optimality

Definition [Bölcskei-G-Kutyniok-Petersen (2017)]

A dictionary $\mathcal{D} = (\varphi_i)_{i \in \mathbb{N}}$ is representable by neural networks if for all $\epsilon > 0$ and $i \in \mathbb{N}$ there is $\Phi_{i,\epsilon} \in \mathcal{NN}$ with $O(1)$ nonzero weights, growing at most polynomially in $i \cdot \epsilon^{-1}$ with

$$\|\varphi_i - \Phi_{i,\epsilon}\| \leq \epsilon.$$

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$$\|\varphi_i - \Phi_{i,\epsilon}\| \leq \epsilon.$$

Theorem [Bölcskei-G-Kutyniok-Petersen (2017)]

Suppose that the dictionary $\mathcal{D}$ is optimal for the class $\mathcal{C}$ and suppose that $\mathcal{D}$ is representable by neural networks. Then neural networks are optimal for the regression class $\mathcal{C}$.

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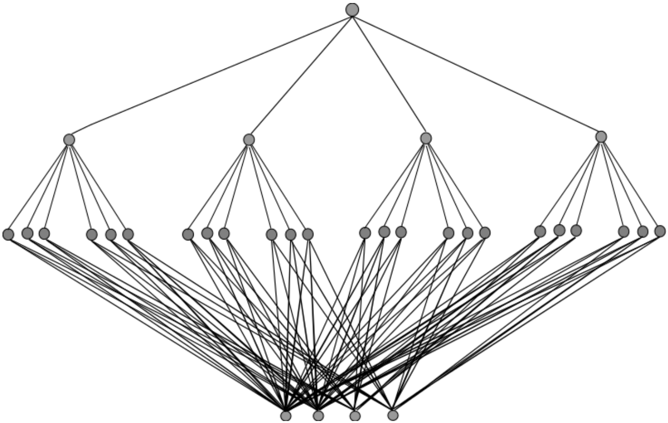

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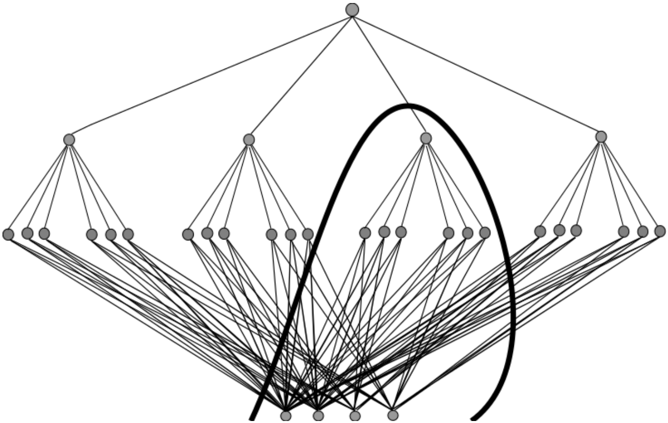

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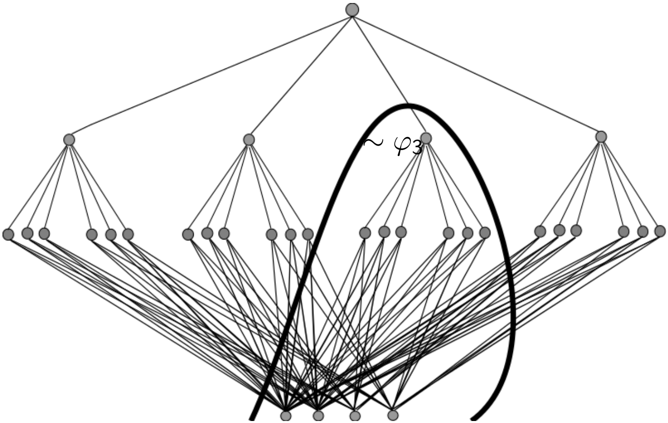

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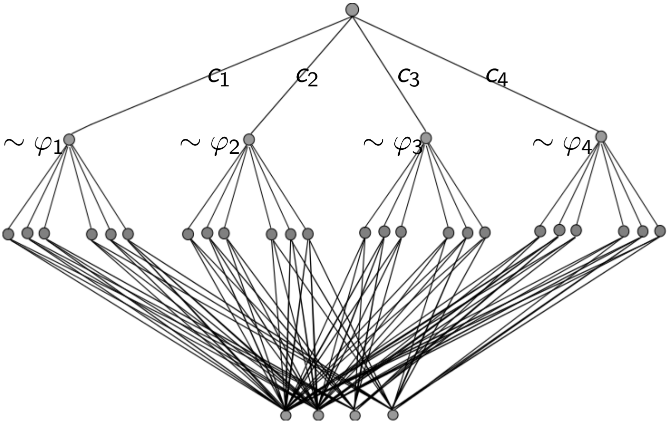

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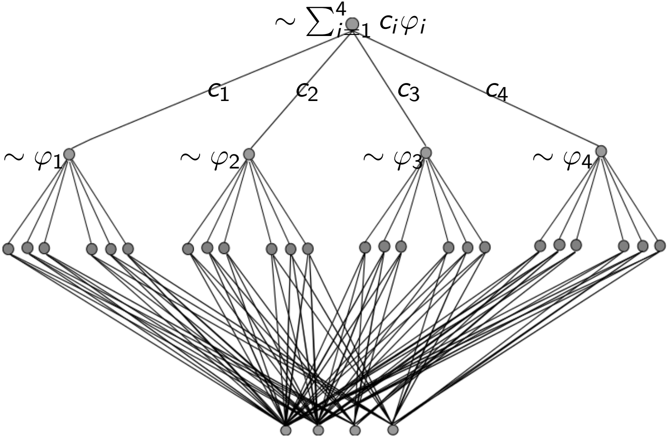

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Theorem ([Bölcskei-G-Kutyniok-Petersen (2017)] informal version)

All known (affine) dictionaries are representable by (shallow) neural networks (under weak assumptions on the activation function).

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All known (affine) dictionaries are representable by (shallow) neural networks (under weak assumptions on the activation function).

 Neural network regression is as powerful as regression with all known dictionaries, combined and in particular optimal for all corresponding problem classes!

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Big Question 2

Why are neural networks so good at approximating high-dimensional functions?

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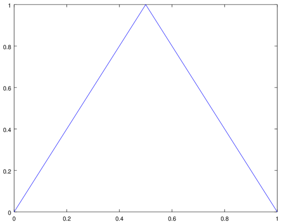

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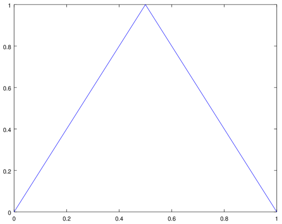

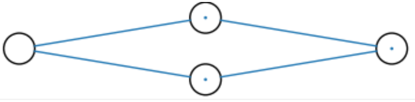

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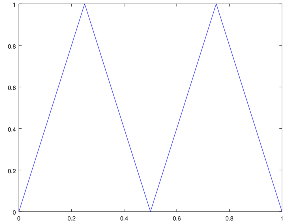

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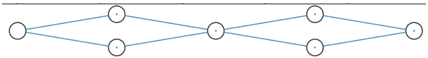

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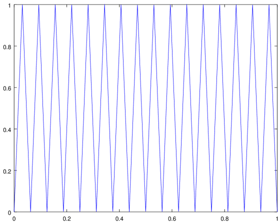

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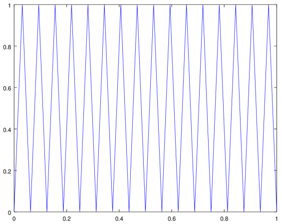

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High-frequency oscillations can be represented by deep neural networks!

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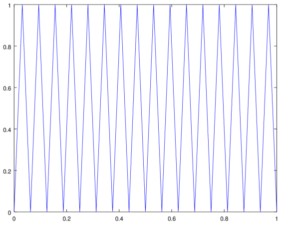

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Exercise (see also [Telgarsky (2015)])

Shallow networks cannot represent high-frequency oscillations: one needs $\gtrsim j$ layers to capture frequencies oscillating at scale 2^{-j}

Related Results

[Montufar (2014)] shows that the number of linear regions in ReLU networks grows exponentially for deep networks and only polynomially for shallow networks

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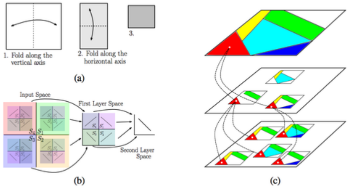

Figure 2: (a) Space folding of 2-D Euclidean space along the two coordinate axes. (b) An illustration of how the top-level partitioning (on the right) is replicated to the original input space (left). (c) Identification of regions across the layers of a deep model.

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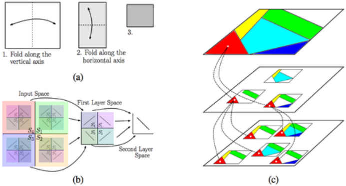

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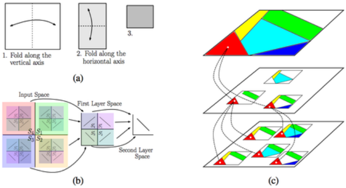

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It seems that deep networks are better at approximating highly oscillating textures with fractal structure, but no precise characterization yet!

High-Dimensional PDEs

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Consider for example the Black-Scholes equation where we want to compute the prize $V(0, x)$ of an option depending on a financial portfolio $x \in \mathbb{R}^d$ subject to

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where g models the prize of of the option g at terminal time T. Typical options (maximum call) are of the form

$$g(x) = \max(\max_{i=1}^{d} x_i - X, 0).$$

Deep DBSE Solver

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Question

Why does this work so well? Can we establish a neural network approximation theory for solutions of PDEs?

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The maximum call option can be expressed by neural networks with $\sim \log_2(d)$ and nodes!

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Depth is Necessary!

One can show that high-dimensional options cannot be approximated well by shallow networks (related methods for circuits in [Hastad (1986)] and [Kane-Williams (2016)])!

Related Work

[Mhaskar, Liao, Poggio (2014)] consider *compositional functions* for example of the form

$$f(x_1, \ldots, x_8) = \\ h_3\left(h_{21}\left(h_{11}(x_1, x_2), h_{12}(x_3, x_4)\right), h_{22}\left(h_{13}(x_5, x_6), h_{14}(x_7, x_8)\right)\right),$$

with h_{ij} smooth.

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2. Stochastic Optimization Algorithms

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🙁 In general nothing can be said about global convergence.

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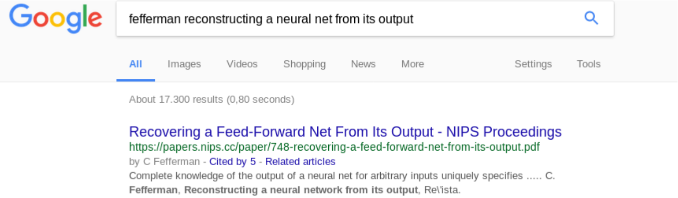

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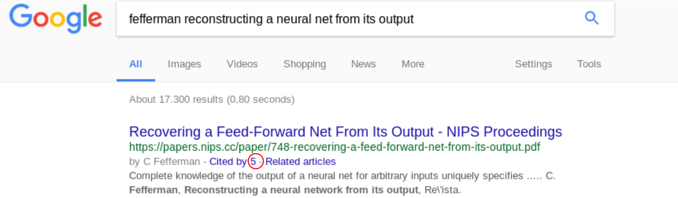

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Thank You!

Questions?