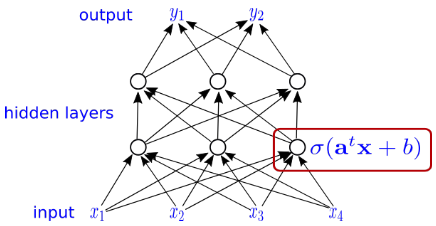
Statistical theory for deep neural networks

Lectures 1 & 2



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The problem

general belief that no or little theory can be developed for modern deep network architectures

- complex data structures $\rightsquigarrow$ no available statistical models
- combination of intricate network architectures with various regularization methods
- fitting a network is a non-linear problem in the network parameters
- non-convex function class
- ...

Why theory?

What is the use of theoretical results in a field that is (successfully) driven by trial and error?

- understand why deep learning works
- deep learning is a chaotic field (thousands of publications) $\rightsquigarrow$ mathematical theory can be useful to extract key concepts
- comparison with other methods
- selection of tuning parameters
- detecting limitations of deep learning
- improvements
- hybrid methods

organization of the course

Lectures:

- Theory for shallow networks
- Advantages of additional layers
- Statistical theory for deep ReLU networks
- Energy landscape and open problems

Shallow networks

- shallow neural network with one output is a function $f : \mathbb{R}^d \to \mathbb{R}$ of the form

$$f(\mathbf{x}) = \sum_{j=1}^{m} c_j \sigma\left(\mathbf{w}_j^\top \mathbf{x} + v_j\right), \quad \mathbf{w}_j \in \mathbb{R}^d,\ v_j, c_j \in \mathbb{R}.$$

- activation function $\sigma : \mathbb{R} \to \mathbb{R}$

Feedforward neural networks

- for $\mathbf{v} = (v_1, \ldots, v_r)^\top, \mathbf{y} = (y_1, \ldots, y_r)^\top \in \mathbb{R}^r$, define the shifted activation function $\sigma_{\mathbf{v}} : \mathbb{R}^r \to \mathbb{R}^r$ as

$$\sigma_{\mathbf{v}} = (\sigma(y_1 - v_1), \ldots, \sigma(y_r - v_r))^\top.$$

- network architecture $(L, \mathbf{p})$
  - positive integer L called number of hidden layers/depth
  - width vector $\mathbf{p} = (p_0, \ldots, p_{L+1}) \in \mathbb{N}^{L+2}$

Neural network with architecture $(L, \mathbf{p})$ is

$$f(\mathbf{x}) = W_L \sigma_{\mathbf{v}_L} W_{L-1} \sigma_{\mathbf{v}_{L-1}} \cdots W_1 \sigma_{\mathbf{v}_1} W_0 \mathbf{x},$$

- W_i is a $p_i \times p_{i+1}$ weight matrix
- $\mathbf{v}_i \in \mathbb{R}^{p_i}$ is a shift vector

Feedforward neural networks

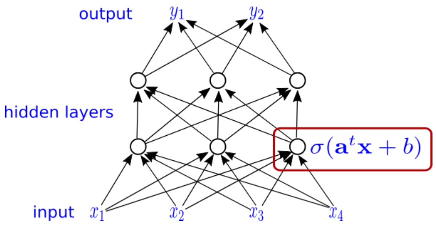
Neural network:

$$f(\mathbf{x}) = W_L \sigma_{\mathbf{v}_L} W_{L-1} \sigma_{\mathbf{v}_{L-1}} \cdots W_1 \sigma_{\mathbf{v}_1} W_0 \mathbf{x},$$

Comments:

- feedforward $\rightsquigarrow$ information is passed in one direction through the network
- network functions are build by alternating matrix-vector multiplications with the action of the non-linear activation function σ
- network architecture is given
- parameters generating the underlying function class are the matrices $W_0, \ldots, W_L$ and the shift bectors $v_1, \ldots, v_L$

Graph representation



- in CS, neural networks are introduced via graph representation
- nodes in the graph (also called *units*) are arranged in layers
- input layer is the first layer and the output layer the last layer
- layers that lie in between are called hidden layers
- number of hidden layers corresponds to L and the number of units in each layer generates the width vector $\mathbf{p}$
- Each node/unit in the graph representation stands for operation $\sigma(\mathbf{a}^t \cdot + b)$

Special types

Neural network:

$$f(\mathbf{x}) = W_L \sigma_{\mathbf{v}_L} W_{L-1} \sigma_{\mathbf{v}_{L-1}} \cdots W_1 \sigma_{\mathbf{v}_1} W_0 \mathbf{x},$$

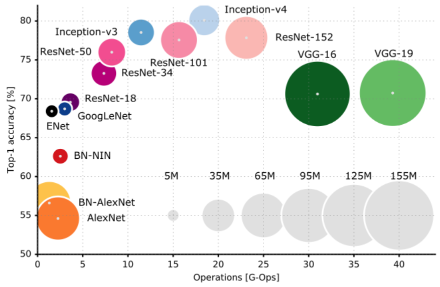
Comments:

- network is called sparse if W_i are sparse matrices
- i-th layer is fully connected $\rightsquigarrow$ W_i is dense
- for $L = 1$ network coincides with shallow networks
- if $L > 1$, network is called deep

Depth

- Networks are deep
  - version of ResNet with 152 hidden layers
  - networks become deeper

High-dimensionality



Source: arxiv.org/pdf/1605.07678.pdf

- Number of network parameters is larger than sample size
  - AlexNet uses 60 million parameters for 1.2 million training samples

functions generated by shallow networks

Consider function class

$$\mathcal{F}_{m,\sigma} := \left\{ f = \sum_{j=1}^{m} c_j \sigma\left(\mathbf{w}_j^\top \cdot + v_j\right) \ : \ \mathbf{w}_j \in \mathbb{R}^d, v_j, c_j \in \mathbb{R} \right\}.$$

problems:

- how large is this class?
- how well can we approximate functions of a specific smoothness?
- or the function $f(x_1, x_2) = x_1 x_2$?

universal approximation

$$\mathcal{F}_{m,\sigma} := \left\{ f = \sum_{j=1}^{m} c_j \sigma\left(\mathbf{w}_j^\top \cdot + v_j\right) \ : \ \mathbf{w}_j \in \mathbb{R}^d, v_j, c_j \in \mathbb{R} \right\}.$$

- functions in the class $\mathcal{F}_{m,\sigma}$ have $m(d+2)$ real parameters
- nested spaces, e.g. $\mathcal{F}_{m,\sigma} \subseteq \mathcal{F}_{m',\sigma}$ whenever $m' \geq m$.

Universal approximation property: Shallow networks with activation function σ have the universal approximation property if for any $\varepsilon > 0$ and any continuous function f on $[0,1]^d$, there exists an integer $m = m(f, \varepsilon)$, such that

$$\inf_{g \in \mathcal{F}_{m,\sigma}} \|f - g\|_{L^\infty([0,1]^d)} \leq \varepsilon.$$

reduction to ridge functions

- many proofs first show universal approximation in dimension one
- univariate functions $\{\sigma(w \cdot + v) : w, v \in \mathbb{R}\}$ span the space of continuous functions
- statement does not involve scalar products anymore

afterwards, it is enough to show that the function space spanned by so called ridge functions

$$f = \sum_{j=1}^{m} g_j(\mathbf{w}_j^\top \cdot)$$

with g_j univariate and continuous has the universal approximation property

universal approximation for univariate functions

Theorem: Shallow networks with smooth activation function that is not a polynomial have universal approximation property for $d = 1$.

Proof:

- $\Delta_h^1 \sigma(t) := (\sigma(t + xh) - \sigma(t))/h$
- $\Delta_h^k \sigma(t) := \Delta_h^1 (\Delta_h^{k-1} \sigma)(t)$
- definition of the k-th derivative $\rightsquigarrow$

$$\left| \frac{\Delta_h^k \sigma(t)}{x^k} - \sigma^{(k)}(t) \right| \to 0, \quad \text{as } h \to 0$$

universal approximation for univariate functions (ctd.)

- σ not a polynomial $\rightsquigarrow$ there exists for each k a real number t_k with $\sigma^{(k)}(t_k) \neq 0$
- multiplying with x^k and division $\sigma^{(k)}(t_k)$ yields

$$\left| \frac{\Delta_h^k \sigma(t_k)}{\sigma^{(k)}(t_k)} - x^k \right| \to 0, \quad \text{as } h \to 0.$$

- for any $h > 0$, $(\sigma^{(k)}(t_k))^{-1} \Delta_h^k \sigma(t_k)$ can be realized by a shallow network with $k+1$ units
- $\rightsquigarrow$ build networks approximating the function $x \mapsto x^k$ arbitrarily well in sup-norm
- apply Weierstrass approximation theorem $\square$

some comments on the proof

- proof provides explicit construction of networks that closely resemble polynomials
- construction requires that some parameters are extremely small and others are very large
- uses only one point of the activation function to generate a specific power
- $\rightsquigarrow$ small perturbations of the activation function can lead to completely different properties
- networks can "zoom in" at local features of the activation function
- the universal approximation theorem can be extended to continuous activation functions using local smoothing

universal approximation via Fourier transform

- Fourier transform $\mathcal{F}f(\boldsymbol{\xi}) = \int e^{-i\boldsymbol{\xi}^\top \mathbf{x}} f(\mathbf{x})\, d\mathbf{x}$
- inverse Fourier transform $\mathcal{F}^{-1}f(\mathbf{x}) = (2\pi)^{-d} \int e^{i\mathbf{x}^\top \boldsymbol{\xi}} f(\boldsymbol{\xi})\, d\boldsymbol{\xi}$
- $f = \mathcal{F}^{-1}\mathcal{F}f$
- for any complex number z, $z = |z|e^{i\phi}$ for some real number $\phi = \phi(z)$
- $\rightsquigarrow$ there exists a real valued function $\phi(\mathbf{w})$ such that $\mathcal{F}f(\mathbf{w}) = e^{i\phi(\mathbf{w})}|\mathcal{F}f(\mathbf{w})|$
- Fourier inversion $\rightsquigarrow$

$$\begin{aligned} f(\mathbf{x}) &= \frac{1}{(2\pi)^d} \operatorname{Re} \int e^{i\mathbf{w}^\top \mathbf{x}} e^{i\phi(\mathbf{w})} |\mathcal{F}f(\mathbf{w})| d\mathbf{w} \\ &= \frac{1}{(2\pi)^d} \int \cos\left(\mathbf{w}^\top \mathbf{x} + \phi(\mathbf{w})\right) |\mathcal{F}f(\mathbf{w})| d\mathbf{w} \end{aligned}$$

- discretization of the integral on the right hand side gives the structure of a shallow network with activation function cos()
- $\rightsquigarrow$ will be used later for approximation rates

Approximation rates for shallow networks

How well can we approximate a function in dependence on smoothness etc. ?

- smooth activation functions
- approximation rates using multivariate polynomials
- Barron's class

approximation rates for smooth activation function

- Mhaskar '96
- smooth activation function
- β-smooth function (in L^2-Sobolev sense)
- rate of approximation over all shallow networks with m units is $m^{-\beta/d}$ with d the dimension
- proof first approximates polynomials of ridge functions and then continues with polynomial approximation

approximation rates for arbitrary activation function

- Petrushev '99
- good approximation rates can be obtained for functions that are smoother than the activation function

Theorem: if activation function is s-smooth (Sobolev), optimal approximation rates are obtained for $s + (d-1)/2$-smooth functions

- $\rightsquigarrow$ effect becomes better as input dimension increases
- **proof:** reduce to ridge functions + approximation of Radon inversion + polynomial eigenbasis
- proof is constructive $\rightsquigarrow$ several interesting conclusions

remarks

- proofs always relate shallow networks to polynomials
- we could start directly with polynomials and would obtain the same approximation rates
- does not help to identify problems where neural networks perform better than other methods
- **Next:** Barron's result

Barron's approximation theorem

- for any sigmoidal activation function
- any $m \geq 1$,
- any function f
- define $C_f := \int |\mathbf{w}|_1 \mathcal{F}(f)(\mathbf{w}) d\mathbf{w}$
- there exist shallow network such that

$$\left\| f(\cdot) - f(\mathbf{0}) - \sum_{j=1}^{m} c_j \sigma(\mathbf{w}_j^\top \cdot + v_j) \right\| \leq \frac{2C_f}{(2\pi)^d \sqrt{m}},$$

Remarks:

- rate $m^{-1/2}$ does not depend on the dimension d
- do neural networks avoid curse of dimensionality?

On the rate

- **Recall:** $C_f = \int |\mathbf{w}|_1 |\mathcal{F}f(\mathbf{w})| d\mathbf{w}$
- indeed there is nothing special about neural networks here
- Candes '02 shows that truncated Fourier series achieves faster approximation rate
$$m^{-1/2-1/d}$$
for the same function class $\{f : C_f < \infty\}$
- gain is related to loss in Maurey's theorem

Up to now, no approximation problem has been found where shallow networks outperform Fourier series or polynomial approximation

statistical model

- combine approximation theory with statistical analysis
- given an i.i.d. sample $(\mathbf{X}_i, Y_i) \in \mathbb{R}^d \times \mathbb{R}$, $i = 1, \ldots, n$ with bounded responses $|Y_i| \leq 1$,
- want to recover the regression function

$$f(\mathbf{x}) = E\left[Y_i | \mathbf{X}_i = \mathbf{x}\right]$$

- covers binary classification
  $\rightsquigarrow Y_i \in \{0, 1\}$ and $f(\mathbf{x}) = P(Y_i | \mathbf{X}_i = x)$

oracle inequality

- $\widehat{f}$ be the empirical risk minimizer

$$\widehat{f} \in \operatorname{argmin}_{\boldsymbol{\theta}\in\Theta} \sum_{i=1}^{n} \big(Y_i - f_{\boldsymbol{\theta}}(\mathbf{X}_i)\big)^2.$$

- standard exponential inequalities
  $\rightsquigarrow$ if Θ is a discrete set with cardinality $|\Theta|$, then

$$E_f\left[\|\widehat{f} - f\|_2^2\right] \le C \inf_{\boldsymbol{\theta}\in\Theta} \|f - f_{\boldsymbol{\theta}}\|_2^2 + C\frac{\log|\Theta|}{n}$$

statistical bounds for shallow networks

- Barron '94
- discretizes network parameters
- study empirical risk minimizer
- $m(d+2)$ is the number of parameters
- $\log|\Theta| \lesssim m(d+2)\log n$
- oracle inequality + approximation theory $\rightsquigarrow$

$$E_f\left[\|\widehat{f}-f\|_2^2\right] \lesssim m^{-1} + \frac{m\log n}{n}.$$

if $C_f = \int |\mathbf{w}|_1 |\mathcal{F}f(\mathbf{w})| d\mathbf{w} < \infty.$

- bias variance trade-off $\rightsquigarrow$ $m = \sqrt{n/\log n}$
- yields the rate

$$\sqrt{\frac{\log n}{n}}$$

summary

shallow networks:

- universal approximation
- approximation rates
- estimation risk bounds

no gain in terms of rates with respect to series estimators

next lecture discusses advantages of additional layers

advantages of additional layers

- localization
- approximation of polynomials with deep networks
- Kolmogorov-Arnold representation theorem
- advantages of deep ReLU networks

localization with Heaviside activation function

- no localization for shallow networks in dimension $d > 1$ (?)
- for commonly used activation functions, taking two hidden layers allows us to localize in arbitrary dimensions
- Heaviside activation function $\sigma_0 = \mathbf{1}(\cdot \geq 0)$,

$$\mathbf{1}(\mathbf{x} \in [-1,1]^d) = \sigma_0\Big(\sum_{i=1}^{d} \sigma_0(x_i + 1) + \sigma_0(-x_i + 1) - 2d + \frac{1}{2}\Big)$$

- $\rightsquigarrow$ outer neuron only gets activated **iff** all the inner neurons output one
- this is the case **iff** $-1 \leq x_i \leq 1$ for all $i = 1, \ldots, d$

localization by other activation functions

- for sigmoidal activation function

$$\sigma(\alpha x) \approx \sigma_0(x), \quad \text{for large } \alpha.$$

- for the ReLU $\sigma(x) = (x)_+$,

$$\sigma(\alpha x) - \sigma(\alpha x - 1) \approx \sigma_0(x), \quad \text{for large } \alpha.$$

- approximation quality depends on α
- $\leadsto$ results using neural networks with sigmoidal activation often have conditions on the speed at which $|\sigma(x)| \to 0$ for $x \to -\infty$, and $|1 - \sigma(x)| \to 0$ for $x \to +\infty$
- localization might be a useful property for approximation, being non-local might be helpful for the (stochastic) gradient descent

approximation of x^{2^k} with deep networks

- for a smooth activation function, the function $x \mapsto x^{2^k}$ lies in the closure of a shallow network with $2^k + 1$ units ($\nearrow$ previous lecture)
- stacking layers on top of each other, this can be reduced to $O(k)$ units in k layers
- rescaled finite second order differences

$$\frac{\sigma(t+2xh) - 2\sigma(t+xh) + \sigma(t)}{\sigma''(t)h^2} \approx x^2.$$

a graphical proof

$$\begin{tikzcd}
 & \approx x^{2^k} & \\
\approx \sigma(t+2x^{2^{k-1}}h) \arrow[ur] & \approx \sigma(t+x^{2^{k-1}}h) \arrow[u] & \sigma(t) \arrow[ul] \\
 & \approx x^{2^{k-1}} \arrow[ul] \arrow[u] & \\
\vdots & \vdots & \vdots \\
 & \approx x^4 & \\
\approx \sigma(t+2x^2h) \arrow[ur] & \approx \sigma(t+x^2h) \arrow[u] & \sigma(t) \arrow[ul] \\
 & \approx x^2 \arrow[ul] \arrow[u] & \\
\sigma(t+2xh) \arrow[ur] & \sigma(t+xh) \arrow[u] & \sigma(t) \arrow[ul] \\
 & x \arrow[ul] \arrow[u] &
\end{tikzcd}$$

$$\begin{tikzcd}
 & \approx x^{2^k} & \\
\approx \sigma(t+2x^{2^{k-1}}h) \arrow[ur] & \approx \sigma(t+x^{2^{k-1}}h) \arrow[u] & \sigma(t) \arrow[ul] \\
\approx \sigma(t+2x^{2^{k-2}}h) \arrow[u] \arrow[ur] & \approx \sigma(t+x^{2^{k-2}}h) \arrow[ul] \arrow[u] & \sigma(t) \arrow[ull] \arrow[ul] \\
\vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots \\
\approx \sigma(t+2x^2h) \arrow[u] \arrow[ur] & \approx \sigma(t+x^2h) \arrow[ul] \arrow[u] & \sigma(t) \arrow[ull] \arrow[ul] \\
\sigma(t+2xh) \arrow[u] \arrow[ur] & \sigma(t+xh) \arrow[ul] \arrow[u] & \sigma(t) \arrow[ull] \arrow[ul] \\
 & x \arrow[ul] \arrow[u] &
\end{tikzcd}$$

improved representation theorems

- Kolmogorov-Arnold approximation theorem shows that every continuous function can be represented by a specific two-layer network
- very different structure if compared with the universal approximation theorem for shallow networks
- indicates that additional layers can lead to new features of network functions

Theorem (Braun '09): Fix $d \geq 2$. There are real numbers a, b_p, c_q and a continuous and monotone function $\psi : \mathbb{R} \to \mathbb{R}$, such that for any continuous function $f : [0,1]^d \to \mathbb{R}$, there exists a continuous function $g : \mathbb{R} \to \mathbb{R}$ with

$$f(x_1, \dots, x_d) = \sum_{q=0}^{2d} g\Big(\sum_{p=1}^{d} b_p \psi(x_p + qa) + c_q \Big).$$

remarks

$$f(x_1,\dots,x_d) = \sum_{q=0}^{2d} g\Big(\sum_{p=1}^{d} b_p \psi(x_p + qa) + c_q\Big).$$

- one inner function ψ and one outer function g
- inner function is independent of f
- q-dependence in the first layer comes through the shifts qa.
- right hand side can be realized by a network with two hidden layers, architecture $\mathbf{p} = (d, d, 2d+1, 1)$, and ψ being the activation function in the first layer.

link to pre-training

- inner function in the Kolmogorov-Arnold representation theorem is independent of the represented function f
- in deep learning it has been observed that the first layers build function systems which can be used for other classification problems
- exploited in pre-training where a trained deep network from a possibly completely different classification problem is taken and only the last layer is learned by the new dataset
- fact that pre-training works shows that deep networks build generic function systems in the first layers.

deep ReLU networks

we discuss several advantages of deep ReLU networks

- representation of identity
- growth of number of linear pieces
- approximation by ReLU networks with small parameters

deep ReLU networks can learn skip connections

$$\sigma(x) = \max(x, 0)$$

- projection property

$$\sigma \circ \sigma = \sigma$$

- $\rightsquigarrow$ pass a signal without change through several layers in the network
- $\rightsquigarrow$ network synchronization by adding hidden layers
- related to skip connections and ResNets
- for other activation functions it is much harder to approximate the identity

number of linear pieces of deep ReLU networks

- deep ReLU networks are piecewise linear functions of the input
- adding layers $\rightsquigarrow$ highly oscillating functions with few parameters
- consider ReLU network with two hidden layers and width vector $(1, m, 1, 1)$ of the form

$$\Big(\sum_{j=1}^{m} c_j (w_j x + v_j)_+\Big)_+$$

- $\rightsquigarrow$ number of added pieces by outer ReLU is proportional to number of zero crossings of inner function
- any ReLU network with width vector $(1, p_1, \ldots, p_L, 1)$ has at most

$$\Big(\frac{3}{2}\Big)^L \prod_{j=1}^{L} (p_j + 1)$$

pieces

example of a highly oscillating function

Functions:

- let $T : [0, 1] \to [1]$,

$$T(x) := (2x) \wedge (1 - 2x) = (2x)_+ - (4x - 2)_+$$

- can be realized by shallow network with two units
- $R^k : [0, 1] \to [0, 1]$,

$$R^k := \underbrace{T \circ T \circ \dots T}_{k \text{ times}}$$

network representation

$$\begin{tikzcd}
 & T^k(x) & \\
(2T^{k-1}(x))_+ \arrow[ur, "1"] & & (4T^{k-1}(x)-2)_+ \arrow[ul, "-1"'] \\
 & T^{k-1}(x) \arrow[ul, "2"] \arrow[ur, "4"'] & \\
\vdots \arrow[ur, dash] & & \vdots \arrow[ul, dash] \\
\vdots & & \vdots \\
 & T^2(x) \arrow[ul] \arrow[ur] & \\
(2T(x))_+ \arrow[ur, "1"] & & (4T(x)-2)_+ \arrow[ul, "-1"'] \\
 & T(x) \arrow[ul, "2"] \arrow[ur, "4"'] & \\
(2x)_+ \arrow[ur, "1"] & & (4x-2)_+ \arrow[ul, "-1"'] \\
 & x \arrow[ul, "2"] \arrow[ur, "4"'] &
\end{tikzcd}$$

$$\begin{tikzcd}
 & T^k(x) & \\
(2T^{k-1}(x))_+ \arrow[ur, "1"] & & (4T^{k-1}(x)-2)_+ \arrow[ul, "-1"'] \\
(2T^{k-2}(x))_+ \arrow[u, "2"] \arrow[urr, "4"] & & (4T^{k-2}(x)-2)_+ \arrow[u, "-4"'] \arrow[ull, "-2"] \\
\vdots \arrow[u] \arrow[urr] & & \vdots \arrow[u] \arrow[ull] \\
\vdots & & \vdots \\
(2T^2(x))_+ \arrow[u] \arrow[urr] & & (4T^2(x)-2)_+ \arrow[u] \arrow[ull] \\
(2T(x))_+ \arrow[u, "2"] \arrow[urr, "4"] & & (4T(x)-2)_+ \arrow[u, "-4"'] \arrow[ull, "-2"] \\
(2x)_+ \arrow[u, "2"] \arrow[urr, "4"] & & (4x-2)_+ \arrow[u, "-4"'] \arrow[ull, "-2"] \\
 & x \arrow[ul, "2"] \arrow[ur, "4"'] &
\end{tikzcd}$$

multiplication

how can we (approximately) multiply two inputs with a network?

- crucial problem for approximation theory
- for deep networks this can be reduced to approximation of square function $x \mapsto x^2$ via

$$xy = \left(\frac{x+y}{2}\right)^2 - \left(\frac{x-y}{2}\right)^2$$

- has a surprising answer for ReLU networks

approach from Lecture 2

network approximation of the function $x \mapsto x^2$ is very important!

- for twice differentiable activation function, we used

$$\frac{\sigma(t+2xh) - 2\sigma(t+xh) + \sigma(xh)}{h^2\sigma''(t)} \to x^2 \text{ for } h \to 0$$

- $\rightsquigarrow$ network parameters become large
- for deep ReLU networks we use a different construction

ReLU approximation of the square function

Functions:

- let $T^k : [0, 2^{2-2k}] \to [0, 2^{-2k}]$,

$$T^k(x) := (x/2) \wedge (2^{1-2k} - x/2) = (x/2)_+ - (x - 2^{1-2k})_+$$

- $R^k : [0, 1] \to [0, 2^{-2k}]$,

$$R^k := T^k \circ T^{k-1} \circ \ldots T^1.$$

Lemma (Telgarsky '16, Yarotski '18, SH '17):

$$\left| x(1-x) - \sum_{k=1}^{m} R^k(x) \right| \leq 2^{-m}.$$

rewriting approximation as network

$$\left| x(1-x) - \sum_{k=1}^{m} R^k(x) \right| \leq 2^{-m}.$$

deep ReLU approximation:

- m hidden layers
- $O(m)$ network parameters
- bounded parameters
- approximation 2^{-m}

shallow ReLU network

- for $x(1-x)$ a shallow ReLU network needs at least $O(2^{m/2})$ parameters to achieve approximation error 2^{-m}

multiplication with deep ReLU networks

Lemma: There exists a network Mult_m with $m+4$ hidden layers, width vector $(2, 6, 6, \ldots, 6, 1)$ and all network parameters bounded by one, such that

$$\left|\mathrm{Mult}_m(x,y) - xy\right| \leq 2^{-m}, \quad \text{for all } x, y \in [0,1].$$

Proof:

- use polarization identity

$$xy = \left(\frac{x+y}{2}\right)^2 - \left(\frac{x-y}{2}\right)^2$$

- separation of positive and negative part
- compute $(x+y)/2$ and $(x-y)/2$ in first layer (non-negativity!)
- square network has to be incorporated twice (inefficient)

a step in the proof

$$\begin{tikzcd}
 & \sum_{k=1}^{m+1} R^k(u) + h(u) & \\
T_+(R^m(u)) \arrow[ur] & \sum_{k=1}^{m} R^k(u) + h(u) \arrow[u] & T_-^{m+1}(R^m(u)) \arrow[ul] \\
\vdots \arrow[u] \arrow[ur] \arrow[urr] & \vdots \arrow[u] & \vdots \arrow[u] \arrow[ul] \arrow[ull] \\
\vdots & \vdots & \vdots \\
T_+(R^1(u)) \arrow[u] \arrow[ur] \arrow[urr] & R^1(u) + h(u) \arrow[u] & T_-^2(R^1(u)) \arrow[u] \arrow[ul] \arrow[ull] \\
T_+(u) \arrow[u] \arrow[ur] \arrow[urr] & h(u) \arrow[u] & T_-^1(u) \arrow[u] \arrow[ul] \arrow[ull]
\end{tikzcd}$$

localization and approximation

- we have seen that with two hidden layers we can localize
- how can this be done for ReLU networks?
- goes back to Yarotsky '18
- define $\mathbf{D}(M)$ as all grid points on the grid

$$\left\{(\ell_j/M)_{j=1,\dots,r} : \boldsymbol{\ell} = (\ell_1, \dots, \ell_r) \in \{0, 1, \dots, M\}^r\right\}$$

- partition of unity on unit cube

$$\sum_{\mathbf{x}_{\boldsymbol{\ell}} \in \mathbf{D}(M)} \underbrace{\prod_{j=1}^{r} (1 - M|x_j - x_j^{\boldsymbol{\ell}}|)_+}_{\text{localized functions}} = \prod_{j=1}^{r} \sum_{\ell=0}^{M} (1 - M|x_j - \ell/M|)_+ = 1,$$

local Taylor approximation

- on each localized bit ($\mathbf{a} \in \mathbf{D}(M)$) do a Taylor approximation

$$f(\mathbf{x}) \approx P_{\mathbf{a}}^{\beta} f(\mathbf{x}) := \sum_{0 \le |\boldsymbol{\alpha}| < \beta} (\partial^{\boldsymbol{\alpha}} f)(\mathbf{a}) \frac{(\mathbf{x} - \mathbf{a})^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} = \sum_{0 \le |\boldsymbol{\gamma}| < \beta} \mathbf{x}^{\boldsymbol{\gamma}} c_{\boldsymbol{\gamma}}$$

- this can be approximately realized by a deep ReLU network
- many technicalities occur (see the article SH '17)

approximation rate

Theorem: For any β-smooth function $f : [0,1]^r \to \mathbb{R}$ and any integers $m, N \geq 1$, there exists a ReLU network with

- depth $L \asymp m$
- width in each layer bounded by $\lesssim N$
- number of non-zero network parameters $s \lesssim Nm$

such that

$$\|\widetilde{f} - f\|_{L^\infty([0,1]^r)} \lesssim \underbrace{N2^{-m}}_{\text{small for deep networks}} + \underbrace{N^{-\frac{\beta}{r}}}_{\text{approx. rate}} .$$

remarks

$$\|\widetilde{f} - f\|_{L^\infty([0,1]^r)} \lesssim \underbrace{N2^{-m}}_{\text{small for deep networks}} + \underbrace{N^{-\frac{\beta}{r}}}_{\text{approx. rate}} .$$

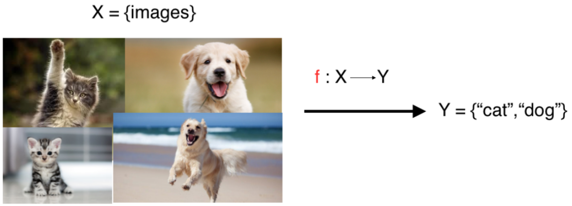
- for deep networks first term is of smaller order
- second term becomes suboptimal for large depth
- trade-off
- sparse networks

risk bounds for deep ReLU networks

Framework:

- we now study a statistical problem
- requires that we first need to specify a statistical model
- we study nonparametric regression

mathematical problem



The data are used to fit a network, i.e. estimate the network parameters.

How fast does the estimated network converge to the truth f as sample size increases?

statistical analysis

- we observe n i.i.d. copies $(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_n, Y_n)$,

$$Y_i = f(\mathbf{X}_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, 1)$$

  - $\mathbf{X}_i \in \mathbb{R}^d, \; Y_i \in \mathbb{R}$,
  - goal is to reconstruct the function $f : \mathbb{R}^d \to \mathbb{R}$
- has been studied extensively
  (kernel smoothing, wavelets, splines, . . .)

the estimator

- choose network architecture $(L, \mathbf{p})$ and sparsity s
- denote by $\mathcal{F}(L, \mathbf{p}, s)$ the class of all networks with
    - architecture $(L, \mathbf{p})$
    - number of active (e.g. non-zero) parameters is s
- our theory applies to any estimator $\widehat{f}_n$ taking values in $\mathcal{F}(L, \mathbf{p}, s)$
- prediction error

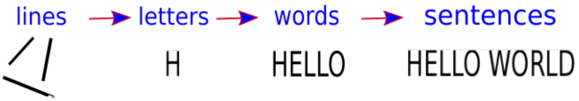
$$R(\widehat{f}_n, f) := E_f\Big[\big(\widehat{f}_n(\mathbf{X}) - f(\mathbf{X})\big)^2\Big],$$

  with $\mathbf{X} \overset{\mathcal{D}}{=} \mathbf{X}_1$ being independent of the sample
- study the dependence of n on $R(\widehat{f}_n, f)$

function class

- classical idea: assume that regression function is β-smooth
- optimal nonparametric estimation rate is $n^{-2\beta/(2\beta+d)}$
- suffers from curse of dimensionality
- to understand deep learning this setting is therefore useless
- $\rightsquigarrow$ make a good structural assumption on f

hierarchical structure



- Important: Only few objects are combined on deeper abstraction level
  - few letters in one word
  - few words in one sentence

function class

- We assume that

$$f = g_q \circ \ldots \circ g_0$$

with

  - $g_i : \mathbb{R}^{d_i} \to \mathbb{R}^{d_{i+1}}$.
  - each of the d_{i+1} components of g_i is β_i-smooth and depends only on t_i variables
  - t_i can be much smaller than d_i
  - effective smoothness

$$\beta_i^* := \beta_i \prod_{\ell=i+1}^{q} (\beta_\ell \wedge 1).$$

  - we show that **the rate depends on the pairs**

$$(t_i, \beta_i^*), \quad i = 0, \ldots, q.$$

  - similar conditions have been proposed by Horowitz & Mammen (2007), Kohler & Kryzak (2017), Bauer & Kohler (2017), Kohler & Langer (2018)

example

$$f_0(x_1, x_2, x_3) = g_{11}\Big(g_{01}(x_3), g_{02}(x_2)\Big)$$

- $f_0 = g_1 \circ g_0$
- $d_0 = 3,\ t_0 = 1,\ d_1 = t_1 = 2,\ d_2 = 1$

main result

Theorem: If

(i) depth $\asymp \log n$

(ii) width $\geq$ network sparsity $\asymp \max_{i=0,\ldots,q} n^{\frac{t_i}{2\beta_i^*+t_i}} \log n$

Then, for any network reconstruction method $\widehat{f}_n$,

$$\text{prediction error} \asymp \phi_n + \Delta_n$$

(up to $\log n$-factors) with

$$\Delta_n := E\Big[\frac{1}{n}\sum_{i=1}^{n}(Y_i - \widehat{f}_n(\mathbf{X}_i))^2 - \inf_{f\in\mathcal{F}(L,\mathbf{p},s)} \frac{1}{n}\sum_{i=1}^{n}(Y_i - f(\mathbf{X}_i))^2\Big]$$

and

$$\phi_n := \max_{i=0,\ldots,q} n^{-\frac{2\beta_i^*}{2\beta_i^*+t_i}}.$$