Neural Network Approximation Theory

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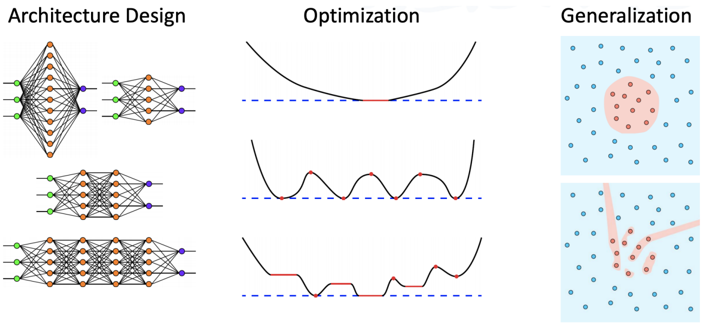
Three Problems in Deep Learning



from: *Mathematics of Deep Learning*, René Vidal, DeepMath Plenary Lecture, 2020

The Three Problems are Interrelated

↪ It is easier to optimize some architectures than others (Haeffele et al., 2017)

↪ Generalization is strongly affected by architecture (Zhang et al., 2017)

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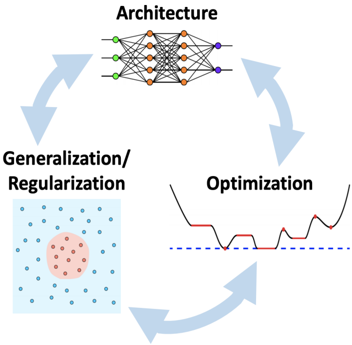

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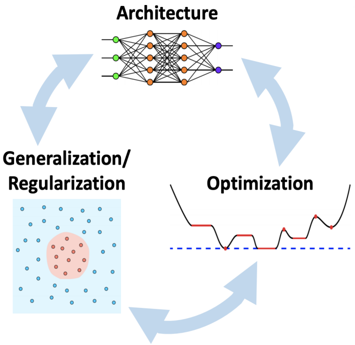

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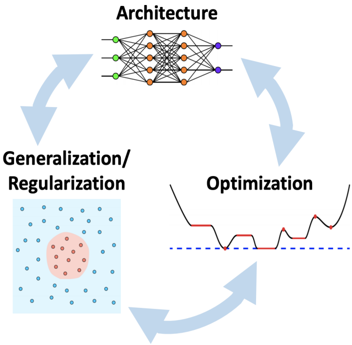

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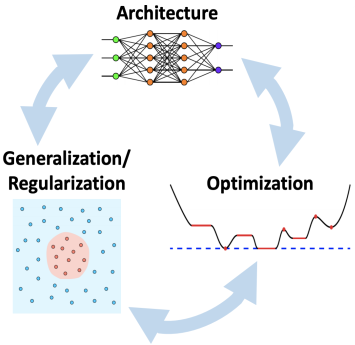

Error Decomposition

$$R(f) - R^* = \underbrace{(R(f) - R(\hat{f}))}_{\text{optimization error}} + \underbrace{(R(\hat{f}) - R_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{(R_{\mathcal{F}} - R^*)}_{\text{approximation error}}$$

for $R(f)$ the risk of a hypothesis f, $R^* = \inf_f R(f)$ the Bayes risk, $\hat{f}$ minimizer of the empirical risk $\hat{R}(f)$

Interplay of three areas

1. Learning
   ($\hookrightarrow$ Optimization, Optimal Control,...)
2. Generalization
   ($\hookrightarrow$ Statistics, Learning Theory, Stochastics,...)
3. Expressivity
   ($\hookrightarrow$ Approximation Theory, Applied Harmonic Analysis,...)

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Density in $C(\mathbb{R}^n)$

Approximation-theoretic results for the single hidden layer

- Density associated with the single hidden layer perceptron model

$$\Sigma(\sigma) = \mathrm{span}\{\sigma(w \cdot x - \theta) : \theta \in \mathbb{R}, w \in \mathbb{R}^n\}$$

  $\sigma : \mathbb{R} \to \mathbb{R}$ activation function, weights $w \in \mathbb{R}^n$, bias $\theta \in \mathbb{R}$

- Find conditions under which $\Sigma(\sigma)$ is dense in $C(K)$ for any compact set $K \subset \mathbb{R}^n$
- Consider *sigmoidal* activation functions satisfying $\lim_{x\to-\infty} \sigma(x) = 0$ and $\lim_{x\to\infty} \sigma(x) = 1$
- Extend density to other function spaces (L^p spaces, the space of measurable functions $\mathcal{M}$)

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Density in $C(X)$ with continuous activation functions

Theorem (Cybenko, 1989)

If σ is continuous and sigmoidal, then $\Sigma(\sigma)$ is dense in $C(K)$.

- Density in $C(K)$ for any bounded, non-constant and monotonously increasing continuous activation function (Funahashi, 1989)
- Density in $C(K)$ for monotonic sigmoidal activation functions and potentially discontinuous at countably many points (Hornik et al., 1989)

$\hookrightarrow$ Density in $L^p(\mu)$ for finite μ and the measurable functions $\mathcal{M}$ for σ bounded and non-constant (Hornik, 1991)

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The universal approximation theorem for potentially discontinuous σ

Theorem (Leshno et al., 1993)

$\Sigma(\sigma)$ is dense in $C(\mathbb{R}^n)$ iff $\sigma \in L^\infty_{loc}(\mathbb{R})$ is not a polynomial (a.e.) and the closure of its points of discontinuity is of zero Lebesgue measure.

- Density in $C(\mathbb{R}^n)$ for any bounded and locally Riemann-integrable activation function (Pinkus, 1999)

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- A single hidden layer perceptron model can approximate arbitrarily well any continuous function of n variables on a compact domain

Questions:

↪ What is the complexity of the neural network needed to guarantee some specified error?

↪ Does the achievable error scale in favour of the input dimension?

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Order of Approximation (cont.)

- Consider perceptron model with at most r units in the hidden layer

$$\Sigma_r(\sigma) = \left\{ \sum_{i=1}^{r} a_i \sigma(w_i \cdot x - \theta_i) : a_i, \theta_i \in \mathbb{R}, w_i \in \mathbb{R}^n \right\}$$

Definition (Pinkus, 1999)

For function f in a normed linear space X define the order of approximation by

$$E(f; \Sigma_r(\sigma); X) = \inf_{g \in \Sigma_r(\sigma)} \|f - g\|_X .$$

Problem: target f is unknown!

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The Sobolev space

- Assume f is a member of the Sobolev space

$$\mathcal{W}_s^p(B^n) := \{f \in L^p(B^n) : \partial^\alpha f \in L^p(B^n), \forall |\alpha| \leq s\},$$

for $1 \leq p \leq \infty, s \in \mathbb{N}$, and B^n the unit ball in $\mathbb{R}^n$

- $\mathcal{W}_s^p(B^n)$ may be defined as the completion of $C^s(B^n)$ w.r.t. norm

$$\|f\|_{s,p,\mu} := \begin{cases} \left[\sum_{|\alpha| \leq s} \int_{\mathbb{R}^n} |\partial^\alpha f|^p d\mu \right]^{1/p}, & 1 \leq p < \infty \\ \max_{|\alpha| \leq s} \sup_{x \in K} |\partial^\alpha f(x)|, & p = \infty \end{cases}$$

for compact $K \subset \mathbb{R}^n$

- Consider norm one Sobolev classes

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Order of Approximation (cont.)

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- Since $\Sigma_r(\sigma) \subset \mathcal{R}_r$ for every $\sigma \in C(\mathbb{R})$

$$E(f; \Sigma_r(\sigma); X) = \inf_{g \in \Sigma_r(\sigma)} \|f - g\|_X \geq \inf_{g \in \mathcal{R}_r(\sigma)} \|f - g\|_X = E(f; \mathcal{R}_r(\sigma); X)$$

Theorem (Maiorov, 1999)

For each $n \geq 2$ and $s \geq 1$,

$$E(\mathcal{B}_2^s; \mathcal{R}_r; L_2) = \sup_{f \in \mathcal{B}_2^s} E(f; \mathcal{R}_r; L_2) \asymp r^{-s/(n-1)}$$

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$$E(\mathcal{B}_2^s; \mathcal{R}_r; L_2) = \sup_{f \in \mathcal{B}_2^s} E(f; \mathcal{R}_r; L_2) \asymp r^{-s/(n-1)}$$

Order of Approximation (cont.)

- The upper bound $r^{-s/(n-1)}$ valid for $E(\mathcal{B}_p^s; \Sigma_r(\sigma); L_p)$ for a $\sigma \in C^\infty$, sigmoidal and strictly increasing (Pinkus, 1999)

1. Denote H_k the linear space of homogeneous polynomials of degree k (in $\mathbb{R}^n$) and $P_k = \cup_{s=0}^k H_s$ the linear space of polynomials of degree at most k
2. Set $\dim H_k = r = \binom{n-1+k}{k} \asymp k^{n-1}$
3. But $E(\mathcal{B}_p^s; P_k; L_p) \le Ck^{-s} \le Cr^{-s/(n-1)}$

Question:

$\hookrightarrow$ Why is it worth using neural networks?

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Continuous Methods of Approximation

- The approximation error in practice does not depend only on the order of approximation, but also on other factors (i.e., the method of approximation)
- Consider networks with parameters which depend continuously on the target function

Theorem (Maiorov, 1999)

Let $Q_r : L_p \to \Sigma_r(\sigma)$ be an approximating method where the network parameters c_i, θ_i and w_i are continuously dependent on the target function $f \in L_p$. Then

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Curse of Dimensionality

- Relax the continuity assumption on the approximation procedure for specific σ (e.g. logistic sigmoid) (Maiorov et al., 2000)

Theorem (Petrushev, 1998)

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Circumventing the Curse of Dimensionality
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Deep Neural Networks

Deep Neural Networks

- Deep neural networks - generalisation of shallow neural networks
- Theoretical accuracy achievable with deep or shallow networks is the same

Questions:

↪ Why are deep neural networks so widespread, even though it is harder to train them due to their depth?

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- (Poggio et al., 2017) succeed in beating the curse of dimensionality by assuming the target function is *compositional*

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$\mathcal{G} - function$

Definition (Poggio et al., 2017)

Let $\mathcal{G}$ be a directed acyclic graph (DAG) with the set of nodes V. Define a $\mathcal{G}-$function $f : \mathbb{R}^n \to \mathbb{R}$ with an architecture corresponding to $\mathcal{G}$, where each of the n source nodes of $\mathcal{G}$ represents a one dimensional input of f. Inner nodes of $\mathcal{G}$ represent constituent functions which get one real one-dimensional input from every incoming edge and the outgoing edges feed the one dimensional function value to the next node. There is only one sink node, whose output is the $\mathcal{G}$-function.

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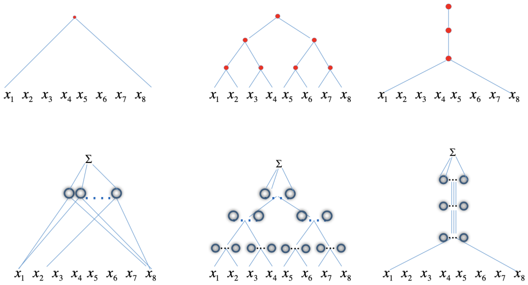
Compositional Functions



Graphs in the top row represent $\mathcal{G}$-functions of 8 variables. Each graph on the bottom row shows the optimal network architecture approximating the function above.

- Compositional function with a binary tree architecture

$$f(x_1, x_2.x_3, x_4) = h(h_1(x_1, x_2), h_2(x_3, x_4)) \tag{1}$$

- Dimensionality of constituent functions $\ll$ overall input dimension

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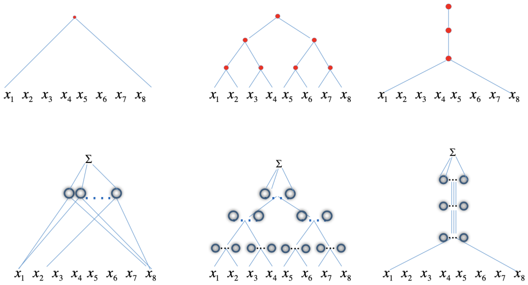

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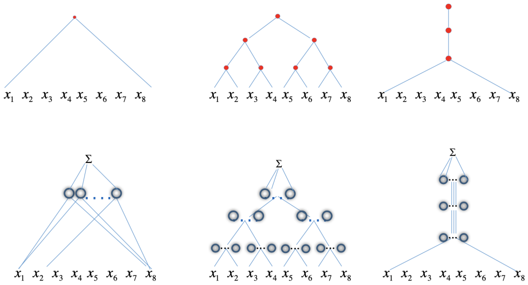

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Effective dimension

Definition (Poggio et al., 2017)

The effective dimension of a function class X is said to be the smallest positive integer k if for every $\epsilon > 0$, any function in X can be approximated up to accuracy ϵ by a neural network of ϵ^{-k} parameters.

- $\mathcal{B}_p^s(\mathbb{R}^n)$ has effective dimension $\frac{n}{s}$

Theorem (Poggio et al., 2017)

For $f \in \mathcal{B}_2^{s,2}$ consider a deep network with the same compositional architecture and $\sigma \in C^\infty$ which is not a polynomial. The complexity of the network to achieve accuracy at least ϵ in the supremum norm is

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Breaking the Curse of Dimensionality with DNNs

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Let $f : \mathbb{R}^n \to \mathbb{R}$ be a compositional $\mathcal{G}-$function corresponding to a DAG $\mathcal{G}$ with nodes V where each constituent function represented by node $v \in V$ is in $\mathcal{B}_p^{s_v}(\mathbb{R}^{n_v})$ for n_v the number of incoming edges of v. Then for $\sigma \in C^\infty$, the complexity of the shallow network to achieve accuracy at least ϵ in the supremum norm is

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- If the effective dimensionality of constituent functions is smaller than the effective dimensionality of the shallow network $\frac{n}{\min_{v \in V} s_v}$, then deep networks avoid the curse of dimensionality
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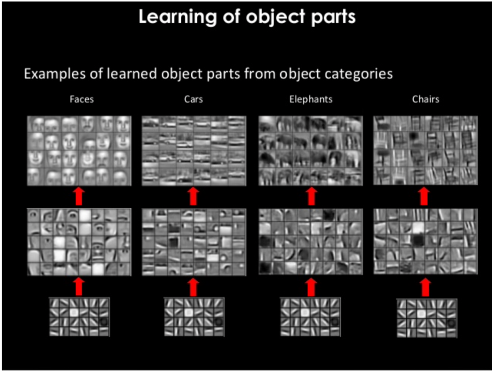
- Deep networks learn 'features' of 'features' - better generalization
- A shallow network tends to memorize the data



from: *Understanding and Improving Deep Learning Algorithms*, Yoshua Bengio, ML Google Distinguished Lecture, 2010

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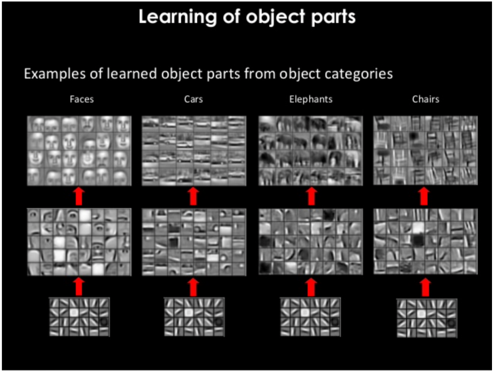

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Related work

- The number of linear regions that can be synthesized by a deep network with ReLU nonlinearities is much larger than by a shallow network (Bengio et al., 2014)
- Examples of specific functions that cannot be represented efficiently by shallow networks (Telgarsky, 2015, Shamir et al., 2016)
- Approximation with sparsely connected deep networks (Bölcskei et al., 2019)