Mathematics of Data: From Theory to Computation

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Lecture 7: A mathematical introduction to Deep Learning

Laboratory for Information and Inference Systems (LIONS)
École Polytechnique Fédérale de Lausanne (EPFL)

EE-556 (Fall 2021)

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Outline

- This class
  - Introduction to Deep Learning
  - The Deep Learning Paradigm
  - Challenges in Deep Learning Theory and Applications
  - Introduction to Generalization error bounds
    - Uniform Convergence and Rademacher Complexity
  - Generalization in Deep Learning (Part 1)
- Next class
  - Generalization in Deep Learning (Part 2)

Remark about notation

The Deep Learning literature might use a different notation:

	Our lectures	DL literature
data/sample	$\mathbf{a}$	$\mathbf{x}$
label	b	y
bias	μ	b
weight	$\mathbf{x}, \mathbf{X}$	$\mathbf{w}, \mathbf{W}$

Power of linear classifiers–I

Problem (Recall: Logistic regression)

Given a sample vector $\mathbf{a}_i \in \mathbb{R}^d$ *and a binary class label* $b_i \in \{-1,+1\}$ $(i = 1, \ldots, n)$, *we define the conditional probability of* b_i *given* $\mathbf{a}_i$ *as follows:*

$$\mathbb{P}(b_i|\mathbf{a}_i, \mathbf{x}) \propto 1/(1 + e^{-b_i\langle \mathbf{x}, \mathbf{a}_i\rangle}),$$

where $\mathbf{x} \in \mathbb{R}^d$ *is some weight vector.*

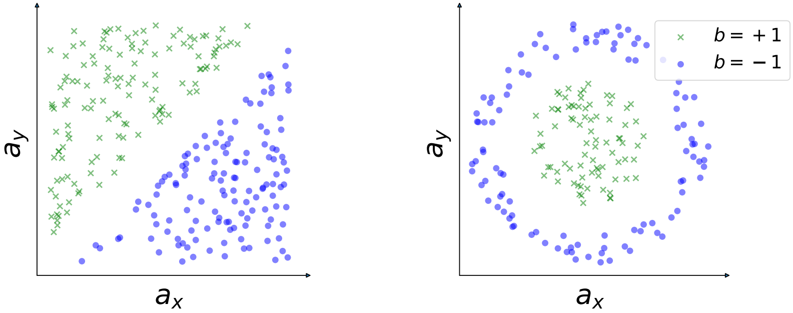

Figure: Linearly separable versus nonlinearly separable dataset

Power of linear classifiers–II

- Lifting dimensions to the rescue
  - Convex optimization objective
  - Side effect: The curse-of-dimensionality
  - Possible to avoid via kernel methods, such as SVMs

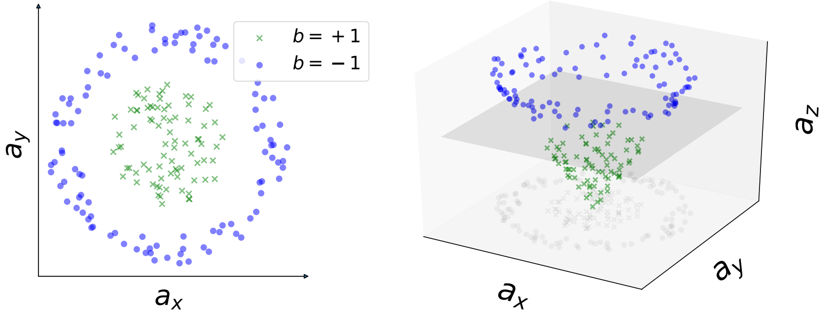

Figure: Non-linearly separable data (left). Linearly separable in $\mathbb{R}^3$ via $\mathbf{a}_z = \sqrt{\mathbf{a}_x^2 + \mathbf{a}_y^2}$ (right).

An important alternative for non-linearly separable data

1-hidden-layer neural network with m neurons (fully-connected architecture):

- Parameters: $\mathbf{X}_1 \in \mathbb{R}^{m\times d}$, $\mathbf{X}_2 \in \mathbb{R}^{c\times m}$ (weights), $\mu_1 \in \mathbb{R}^m, \mu_2 \in \mathbb{R}^c$ (biases)
- Activation function: $\sigma : \mathbb{R} \to \mathbb{R}$

$$h_{\mathbf{x}}(\mathbf{a}) := \qquad\qquad \overset{\substack{\text{input}\\ \downarrow}}{\begin{bmatrix} \\ \mathbf{a} \\ \\ \end{bmatrix}}$$

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recursively repeat activation + affine transformation to obtain “deeper” networks.

Why neural networks?: An approximation theoretic motivation

Theorem (Universal approximation [4])

Let $\sigma(\cdot)$ be a nonconstant, bounded, and increasing continuous function. Let $I_d = [0,1]^d$. The space of continuous functions on I_d is denoted by $\mathcal{C}(I_d)$.

Given $\epsilon > 0$ and $g \in \mathcal{C}(I_d)$ there exists a 1-hidden-layer network h with m neurons such that h is an ϵ-approximation of g, i.e.,

$$\sup_{\mathbf{a} \in I_d} |g(\mathbf{a}) - h(\mathbf{a})| \leq \epsilon$$

Caveat

The number of neurons m needed to approximate some function g can be arbitrarily large!

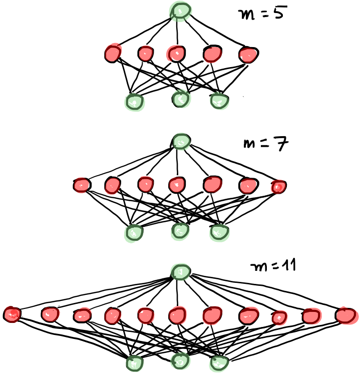

Figure: networks of increasing width

Why were NNs not popular before 2010?

- too big to optimize!
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- could not find the optimum via algorithms

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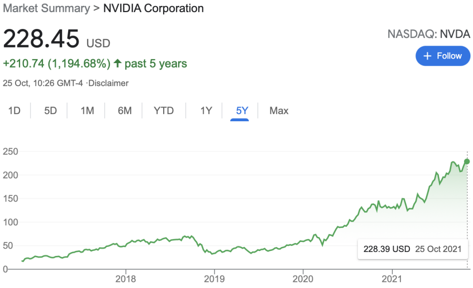


Market Summary > NVIDIA Corporation

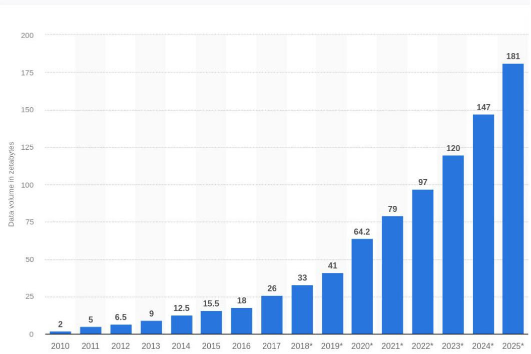
228.45 USD

+210.74 (1,194.68%) ↑ past 5 years

25 Oct, 10:26 GMT-4 ·Disclaimer

NASDAQ: NVDA

228.39 USD 25 Oct 2021



Supervised learning: Multi-class classification

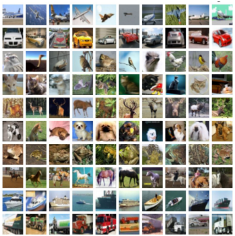


Figure: CIFAR10 dataset: 60000 32x32 color images (3 channels) from 10 classes

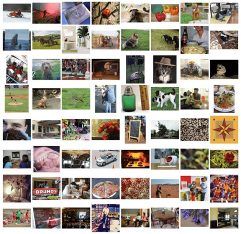


Figure: Imagenet dataset: 14 million color images (varying resolution, 3 channels) from 21K classes

Goal

Image-label pairs $(\mathbf{a}, b) \subseteq \mathbb{R}^d \times \{1, \ldots, c\}$ follow an unknown distibution $\mathbb{P}$. Find $h : \mathbb{R}^d \to \{1, \ldots, c\}$ with minimum *misclassification probability*

$$\min_{h \in \mathcal{H}} \mathbb{P}(h(\mathbf{a}) \neq b)$$

2010-today: Deep Learning becomes popular again

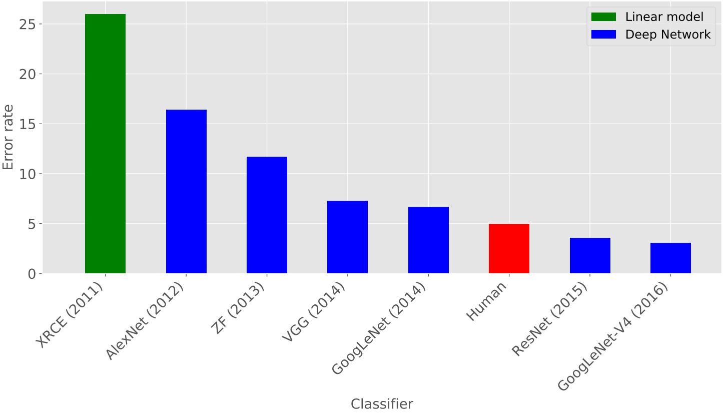


Figure: Error rate on the ImageNet challenge, for different network architectures.

2010-today: Deep Learning becomes popular again

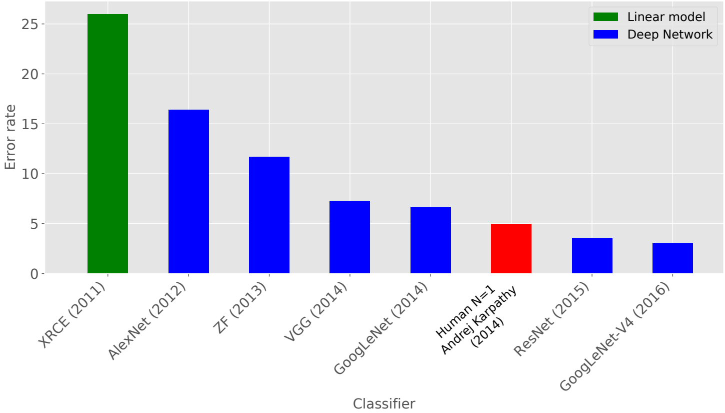


Figure: Error rate on the ImageNet challenge, for different network architectures.[**?**, **?**]

Convolutional architectures in Computer Vision tasks

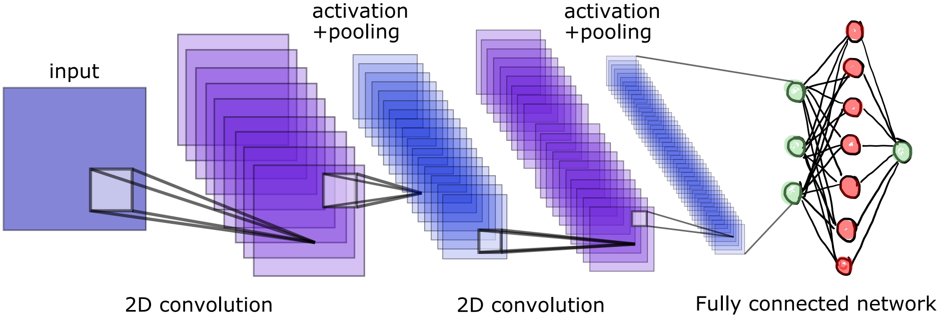
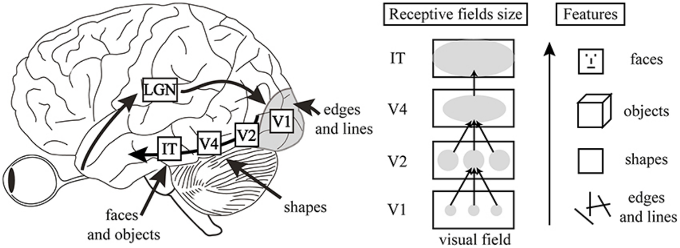
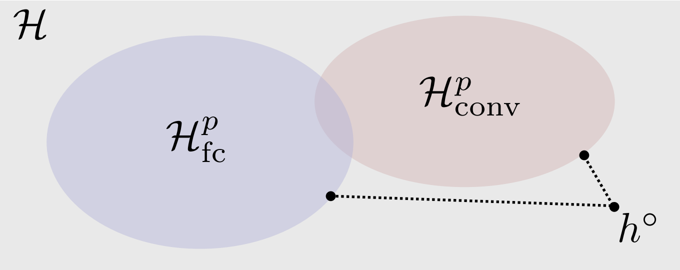


Figure: "Locality" Structure of a 2D deep convolutional neural network.

Inductive Bias: Why convolution works so well in Computer Vision tasks?



h°	true unknown function
$\mathcal{H}$	space of all functions
$\mathcal{H}^p_{\text{fc}}$	fully-connected networks with p parameters
$\mathcal{H}^p_{\text{conv}}$	convolutional networks with p parameters



2010-today: Size of neural networks grows exponentially!

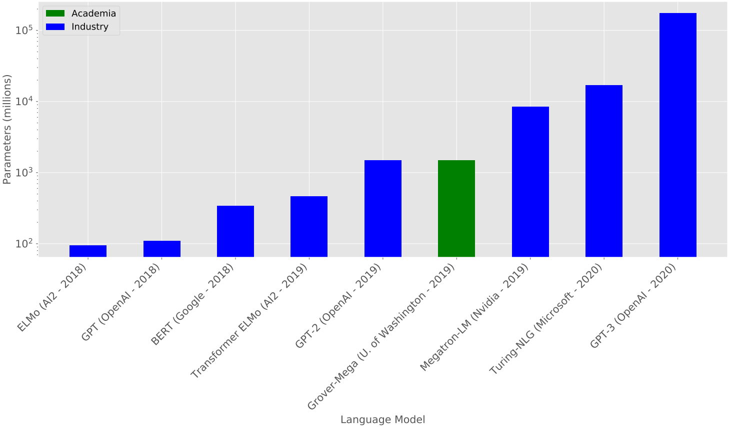


Figure: Number of parameters in Language models based on Deep Learning.

The era of model scaling

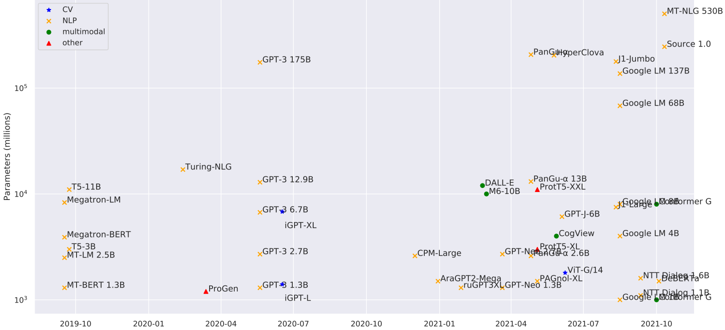


Figure: Scale of most recent SotA models across modalities.
Data from `https://lair.lighton.ai/akronomicon/`:

The Landscape of ERM with multilayer networks

Recall: Empirical risk minimization (ERM)

Let $h_{\mathbf{x}} : \mathbb{R}^n \to \mathbb{R}$ be network and let $\{(\mathbf{a}_i, b_i)\}_{i=1}^n$ be a sample with $b_i \in \{-1, 1\}$ and $\mathbf{a}_i \in \mathbb{R}^n$. The *empirical risk minimization* (ERM) is defined as follows

$$\min_{\mathbf{x}} \left\{ R_n(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} L(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \right\} \tag{1}$$

where $L(h_{\mathbf{x}}(\mathbf{a}_i), b_i)$ is the loss on the sample $(\mathbf{a}_i, b_i)$ and $\mathbf{x}$ are the parameters of the network.

Some frequently used loss functions

- $L(h_{\mathbf{x}}(\mathbf{a}), b) = \log(1 + \exp(-b \cdot h_{\mathbf{x}}(\mathbf{a})))$ (logistic loss)
- $L(h_{\mathbf{x}}(\mathbf{a}), b) = (b - h_{\mathbf{x}}(\mathbf{a}))^2$ (squared error)
- $L(h_{\mathbf{x}}(\mathbf{a}), b) = \max(0, 1 - b \cdot h_{\mathbf{x}}(\mathbf{a}))$ (hinge loss)

The Landscape of ERM with multilayer networks

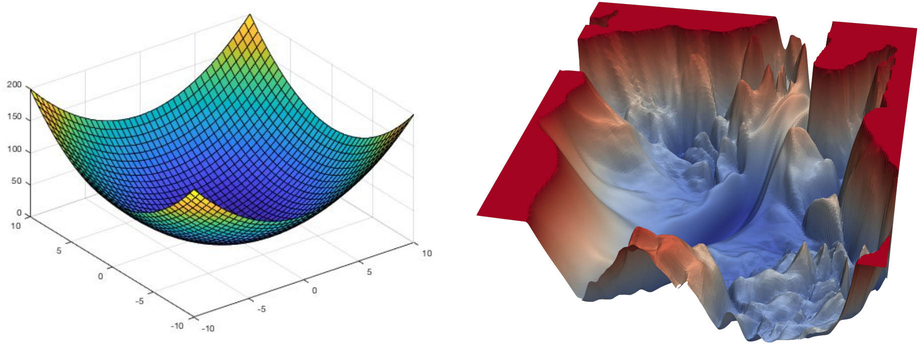
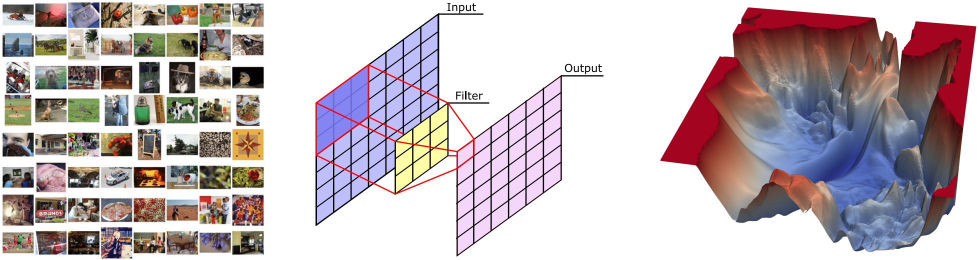


Figure: convex (left) vs non-convex (right) optimization landscape

Conventional wisdom in ML until 2010:
Simple models + simple errors

The deep learning paradigm



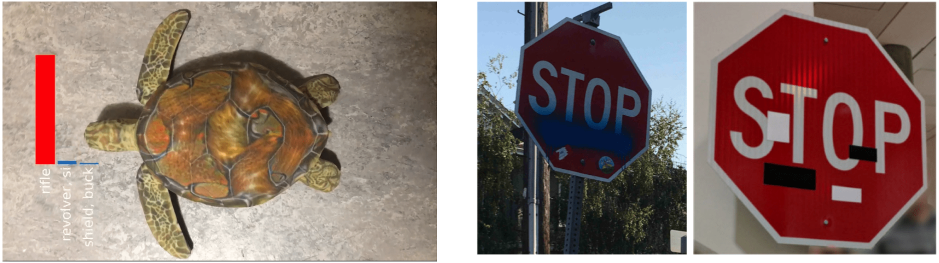
(a) Massive datasets

(b) Inductive bias from large and complex architectures

(c) ERM using stochastic non-convex first-order optimization algorithms (SGD)

Figure: Most common components in a Deep Learning Pipeline

Challenges in DL/ML applications: Robustness (I)

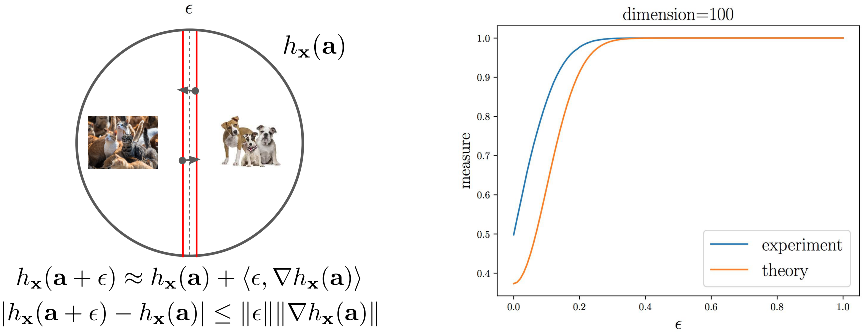


(a) Turtle classified as rifle [1].

(b) Stop sign classified as 45 mph sign [6].

Figure: Natural or human-crafted modifications that trick neural networks used in computer vision tasks

Challenges in DL/ML applications: Robustness (II)



$$h_{\mathbf{x}}(\mathbf{a}+\epsilon) \approx h_{\mathbf{x}}(\mathbf{a}) + \langle \epsilon, \nabla h_{\mathbf{x}}(\mathbf{a}) \rangle$$

$$|h_{\mathbf{x}}(\mathbf{a}+\epsilon) - h_{\mathbf{x}}(\mathbf{a})| \leq \|\epsilon\| \|\nabla h_{\mathbf{x}}(\mathbf{a})\|$$

(a) Linear classifier on data distributed on a sphere

(b) Concentration of measure phenomenon on high dimensions

Figure: Understanding the robustness of a classifier in high-dimensional spaces [12]

Challenges in DL/ML applications: Robustness (References I)

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Challenges in DL/ML applications: Robustness (References II)

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Challenges in DL/ML applications: Robustness (References III)

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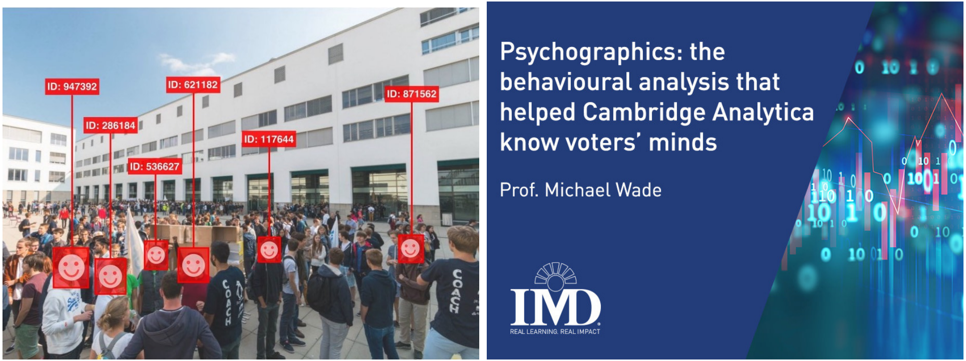
Challenges in DL/ML applications: Surveillance/Privacy/Manipulation



Psychographics: the behavioural analysis that helped Cambridge Analytica know voters' minds

Prof. Michael Wade

IMD
REAL LEARNING. REAL IMPACT

Figure: Political and societal concerns about some DL/ML applications

Challenges in DL/ML applications: Surveillance/Privacy/Manipulation (References)

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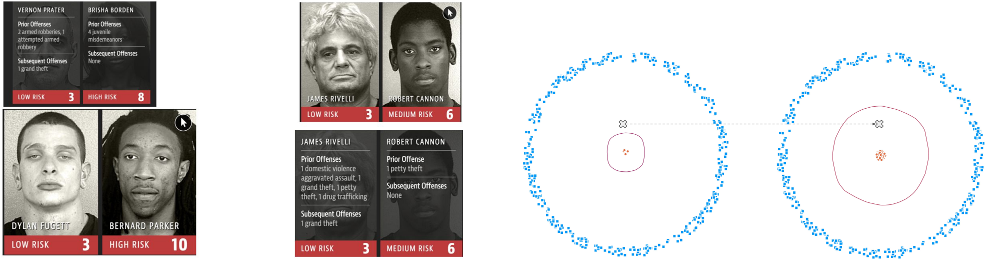
Challenges in DL/ML applications: Fairness



VERNON PRATER

Prior Offenses
2 armed robberies, 1 attempted armed robbery

Subsequent Offenses
1 grand theft

LOW RISK 3

BRISHA BORDEN

Prior Offenses
4 juvenile misdemeanors

Subsequent Offenses
None

HIGH RISK 8

DYLAN FUGETT
LOW RISK 3

BERNARD PARKER
HIGH RISK 10

JAMES RIVELLI
LOW RISK 3

ROBERT CANNON
MEDIUM RISK 6

JAMES RIVELLI

Prior Offenses
1 domestic violence aggravated assault, 1 grand theft, 1 petty theft, 1 drug trafficking

Subsequent Offenses
1 grand theft

LOW RISK 3

ROBERT CANNON

Prior Offense
1 petty theft

Subsequent Offenses
None

MEDIUM RISK 6

(a) Racist classifier

(b) Effect of unbalanced data

Figure: Unfair classifiers due to biased or unbalanced datasets/algorithms

Challenges in DL/ML applications: Fairness (References)

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Challenges in DL/ML applications: Interpretability

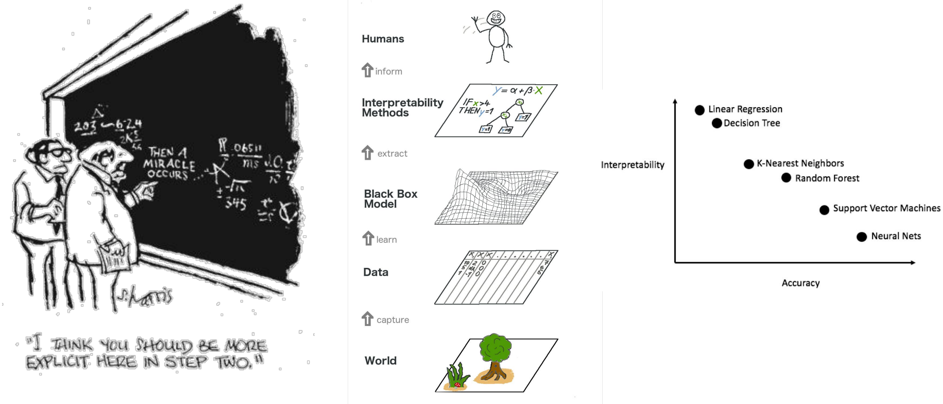

Figure: Performance vs Interpretability trade-offs in DL/ML

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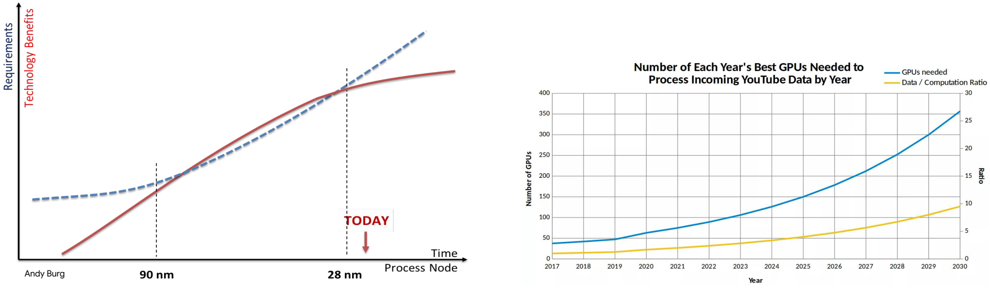
Challenges in DL/ML applications: Energy efficiency and cost



(a)

(b)

Figure: Efficiency and Scalability concerns in DL/ML

Challenges in DL/ML applications: Energy efficiency and cost (References)

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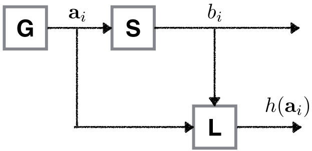
Peeling the onion



Models

Let $d(\cdot,\cdot) : \mathcal{H}^\circ \times \mathcal{H}^\circ \to \mathbb{R}^+$ be a metric in an extended function space $\mathcal{H}^\circ$ that includes $\mathcal{H}$; i.e., $\mathcal{H} \subseteq \mathcal{H}^\circ$. Let

1. $h^\circ \in \mathcal{H}^\circ$ be the true, expected risk minimizing model
2. $h^\natural \in \mathcal{H}$ be the solution under the assumed function class $\mathcal{H} \subseteq \mathcal{H}^\circ$
3. $h^\star \in \mathcal{H}$ be the estimator solution
4. $h^t \in \mathcal{H}$ be the numerical approximation of the algorithm at time t

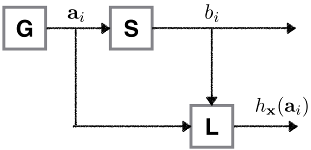
Practical performance

$$\underbrace{d(h^t, h^\circ)}_{\bar{\varepsilon}(t,n)} \leq \underbrace{d(h^t, h^\star)}_{\text{optimization error}} + \underbrace{d(h^\star, h^\natural)}_{\text{statistical error}} + \underbrace{d(h^\natural, h^\circ)}_{\text{model error}},$$

where $\bar{\varepsilon}(t,n)$ denotes the total error of the Learning Machine. We can try to

1. reduce the optimization error with computation
2. reduce the statistical error with more data samples, with better estimators, and with prior information
3. reduce the model error with flexible or universal representations

Estimation of parameters vs estimation of risk



Recall the general setting

Let $R(h_{\mathbf{x}}) = \mathbb{E}L(h_{\mathbf{x}}(\mathbf{a}), b)$ be the risk function and $R_n(h_{\mathbf{x}}) = \frac{1}{n}\sum_{i=1}^{n} L(h_{\mathbf{x}}(\mathbf{a}_i), b_i)$ be the empirical estimate. Let $\mathcal{X} \subseteq \mathcal{X}^{\circ}$ be parameter domains, where $\mathcal{X}$ is known. Define

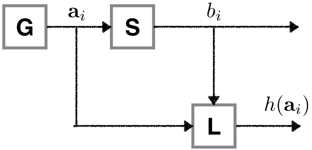
1. $\mathbf{x}^{\circ} \in \arg\min_{\mathbf{x}\in\mathcal{X}^{\circ}} R(h_{\mathbf{x}})$: true minimum risk model
2. $\mathbf{x}^{\natural} \in \arg\min_{\mathbf{x}\in\mathcal{X}} R(h_{\mathbf{x}})$: assumed minimum risk model
3. $\mathbf{x}^{\star} \in \arg\min_{\mathbf{x}\in\mathcal{X}} R_n(h_{\mathbf{x}})$: ERM solution
4. $\mathbf{x}^{t}$: numerical approximation of $\mathbf{x}^{\star}$ at time t

Nomenclature

$R_n(\cdot)$	training error
$R(\cdot)$	test error
$R(\mathbf{x}^{\natural}) - R(\mathbf{x}^{\circ})$	modeling error
$R(\mathbf{x}^{\star}) - R(\mathbf{x}^{\natural})$	excess risk
$\sup_{\mathbf{x}\in\mathcal{X}} \lvert R(\mathbf{x}) - R_n(\mathbf{x})\rvert$	generalization error
$R_n(\mathbf{x}^{t}) - R_n(\mathbf{x}^{\star})$	optimization error

	$\mathcal{X} \to \mathcal{X}^{\circ}$	$n \uparrow$	$p \uparrow$
Training error	$\searrow$	$\nearrow$	$\searrow$
Excess risk	$\nearrow$	$\searrow$	$\nearrow$
Generalization error	$\nearrow$	$\searrow$	$\nearrow$
Modeling error	$\searrow$	$=$	$\leftrightsquigarrow$
Time	$\nearrow$	$\nearrow$	$\nearrow$

What theoretical challenges in Deep Learning will we study?



Models

Let $\mathcal{X} \subseteq \mathcal{X}^\circ$ be parameter domains, where $\mathcal{X}$ is known. Define

1. $\mathbf{x}^\circ \in \arg\min_{\mathbf{x}\in\mathcal{X}^\circ} R(h_{\mathbf{x}})$: true minimum risk model
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3. $\mathbf{x}^\star \in \arg\min_{\mathbf{x}\in\mathcal{X}} R_n(h_{\mathbf{x}})$: ERM solution
4. $\mathbf{x}^t$: numerical approximation of $\mathbf{x}^\star$ at time t

Practical performance in Deep Learning

$$\underbrace{R(\mathbf{x}^t) - R(\mathbf{x}^\circ)}_{\bar{\varepsilon}(t,n)} \leq \underbrace{R_n(\mathbf{x}^t) - R_n(\mathbf{x}^\star)}_{\text{optimization error}} + \underbrace{2\sup_{\mathbf{x}\in\mathcal{X}} |R(\mathbf{x}) - R_n(\mathbf{x})|}_{\text{generalization error}} + \underbrace{R(\mathbf{x}^\natural) - R(\mathbf{x}^\circ)}_{\text{model error}}$$

where $\bar{\varepsilon}(t,n)$ denotes the total error of the Learning Machine. In Deep Learning applications

1. Optimization error is almost zero, in spite of non-convexity. ⇒ lecture 9
2. Generalization error is usually small, but theory is lacking. ⇒ lecture 7 (this one) and lecture 8
3. Large architectures + inductive bias might lead to small model error.

Generalization error bounds

Goal: Obtain generalization bounds for multi-layer, fully-connected neural networks

- We want to find high-probability upper bounds for the quantity

$$\sup_{\mathbf{x}\in\mathcal{X}} |R(\mathbf{x}) - R_n(\mathbf{x})|$$

- Main tool: concentration inequalities!
  - Measure of how far is an empirical average from the true mean

Theorem (Hoeffding's Inequality [9])

Let $Y_1, \dots, Y_n$ be i.i.d. random variables with Y_i taking values in the interval $[a_i, b_i] \subseteq \mathbb{R}$ for all $i = 1, \dots, n$. Let $S_n := \frac{1}{n}\sum_{i=1}^n Y_i$. It holds that

$$\mathbb{P}\left(|S_n - \mathbb{E}[S_n]| > t\right) \leq 2\exp\left(-\frac{2n^2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right)$$

Warmup: Generalization bound for a singleton

Lemma

For $i = 1, \dots, n$, let $(\mathbf{a}_i, b_i) \in \mathbb{R}^p \times \{-1, 1\}$ be independent random variables and $h_{\mathbf{x}} : \mathbb{R}^p \to \mathbb{R}$ be a function parametrized by $\mathbf{x} \in \mathcal{X}$. Let $\mathcal{X} = \{\mathbf{x}_0\}$ and $L(h_{\mathbf{x}}(\mathbf{a}), b) = \{sign(h_{\mathbf{x}}(\mathbf{a})) \neq b\}$ be the 0-1 loss.
With probability at least $1 - \delta$, we have that

$$\sup_{\mathbf{x} \in \mathcal{X}} |R(\mathbf{x}) - R_n(\mathbf{x})| = |R(\mathbf{x}_0) - R_n(\mathbf{x}_0)| \leq \sqrt{\frac{\ln(2/\delta)}{2n}}.$$

Proof.

Note that $\mathbb{E}[\frac{1}{n} \sum_{i=1}^n L(h_{\mathbf{x}_0}(\mathbf{a}_i), b_i)] = R(\mathbf{x}_0)$, the expected risk of the parameter $\mathbf{x}_0$. Moreover $L(h_{\mathbf{x}_0}(\mathbf{a}_i), b_i) \in [0, 1]$. We can use Hoeffding's inequality and obtain

$$\mathbb{P}(|R_n(\mathbf{x}_0) - R(\mathbf{x}_0)| > t) = \mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^n L_i(h_{\mathbf{x}_0}(\mathbf{a}_i), b_i) - R(\mathbf{x}_0)\right| > t\right) \leq 2\exp\left(-2nt^2\right)$$

Setting $\delta := 2\exp\left(-2nt^2\right)$ we have that $t = \sqrt{\frac{\ln 2/\delta}{2n}}$, thus obtaining the result. □

Generalization bound for finite sets

Lemma

For $i = 1, \ldots, n$, let $(\mathbf{a}_i, b_i) \in \mathbb{R}^p \times \{-1, 1\}$ be independent random variables and $h_{\mathbf{x}} : \mathbb{R}^p \to \mathbb{R}$ be a function parametrized by $\mathbf{x} \in \mathcal{X}$. Let $\mathcal{X}$ be a finite set and $L(h_{\mathbf{x}}(\mathbf{a}), b) = \{\text{sign}(h_{\mathbf{x}}(\mathbf{a})) \neq b\}$ be the 0-1 loss.
With probability at least $1 - \delta$, we have that

$$\sup_{\mathbf{x} \in \mathcal{X}} |R(\mathbf{x}) - R_n(\mathbf{x})| \leq \sqrt{\frac{\ln |\mathcal{X}| + \ln(2/\delta)}{2n}}.$$

Proof.

Let $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_{|\mathcal{X}|}\}$. We can use a union bound and the analysis of the singleton case to obtain:

$$\mathbb{P}(\exists j : |R_n(\mathbf{x}_j) - R(\mathbf{x}_j)| > t) \leq \sum_{j=1}^{|\mathcal{X}|} \mathbb{P}(|R_n(\mathbf{x}_j) - R(\mathbf{x}_j)| > t) = 2|\mathcal{X}| \exp\Big(- 2nt^2 \Big)$$

Setting $\delta := 2|\mathcal{X}| \exp\left(-2nt^2\right)$, we have that $t = \sqrt{\frac{\ln |\mathcal{X}| + \ln \frac{2}{\delta}}{2n}}$, thus obtaining the result. □

Generalization bounds for infinite classes - The Rademacher complexity

However, in most applications in ML/DL we optimize over an infinite parameter space $\mathcal{X}$!

◦ Need a notion of *complexity* to derive generalization bounds for infinite classes of functions

Definition (Rademacher Complexity [3])

Let $S = \{\mathbf{a}_1, \ldots, \mathbf{a}_n\} \subseteq \mathbb{R}^p$ and let $\{\sigma_i : i = 1, \ldots, n\}$ be independent Rademacher random variables i.e., taking values uniformly in $\{-1, +1\}$ (coin flip). Let $\mathcal{H}$ be a class of functions of the form $h : \mathbb{R}^p \to \mathbb{R}$. The Rademacher complexity of $\mathcal{H}$ with respect to A is defined as:

$$\mathcal{R}_A(\mathcal{H}) := \mathbb{E} \sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i h(\mathbf{a}_i).$$

$\mathcal{R}_A(\mathcal{H})$ measures how well can we fit random signs (± 1) with the output of an element of $\mathcal{H}$ on the set A.

Visualizing Rademacher complexity

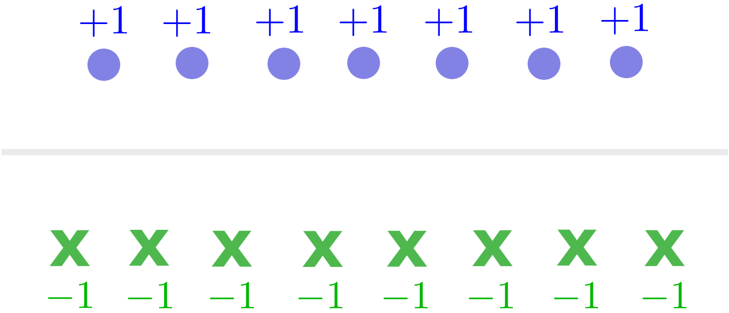
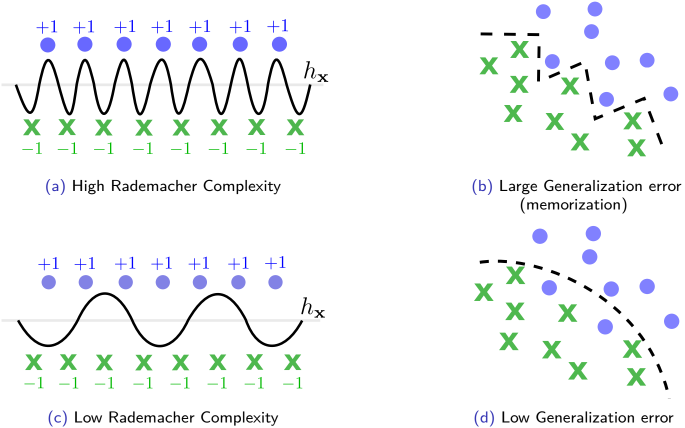


Figure: Rademacher complexity measures correlation with random signs

Visualizing Rademacher complexity



(a) High Rademacher Complexity

(b) Large Generalization error (memorization)

(c) Low Rademacher Complexity

(d) Low Generalization error

Figure: Rademacher complexity and Generalization error

Fundamental theorem about the Rademacher Complexity

Theorem (See Theorem 3.3 and 5.8 in [9])

Suppose that the loss function has the form $L(h_{\mathbf{x}}(\mathbf{a}), b) = \phi(b \cdot h_{\mathbf{x}}(\mathbf{a}))$ *for a* 1*-Lipschitz function* $\phi : \mathbb{R} \to \mathbb{R}$.

Let $\mathcal{H}_{\mathcal{X}} := \{h_{\mathbf{x}} : \mathbf{x} \in \mathcal{X}\}$ *be a class of parametric functions* $h_{\mathbf{x}} : \mathbb{R}^p \to \mathbb{R}$. *For any* $\delta > 0$, *with probability at least* $1 - \delta$ *over the draw of an i.i.d. sample* $\{(\mathbf{a}_i, b_i)\}_{i=1}^n$, *letting* $A = (\mathbf{a}_1, \ldots, \mathbf{a}_n)$, *the following holds:*

$$\sup_{\mathbf{x} \in \mathcal{X}} |R_n(\mathbf{x}) - R(\mathbf{x})| \leq 2\mathbb{E}_A \mathcal{R}_A(\mathcal{H}_{\mathcal{X}}) + \sqrt{\frac{\ln(2/\delta)}{2n}}$$

$$\sup_{\mathbf{x} \in \mathcal{X}} |R_n(\mathbf{x}) - R(\mathbf{x})| \leq 2\mathcal{R}_A(\mathcal{H}_{\mathcal{X}}) + 3\sqrt{\frac{\ln(4/\delta)}{2n}}$$

Assumption is true for common losses

- $L(h_{\mathbf{x}}(\mathbf{a}), b) = \log(1 + \exp(-b \cdot h_{\mathbf{x}}(\mathbf{a}))) \Rightarrow \phi(z) := \log(1 + \exp(z))$ (logistic loss)
- $L(h_{\mathbf{x}}(\mathbf{a}), b) = \max(0, 1 - b \cdot h_{\mathbf{x}}(\mathbf{a})) \Rightarrow \phi(z) := \max(0, 1 - z)$ (hinge loss)

Computing the Rademacher complexity of linear functions

Theorem

Let $\mathcal{X} := \{\mathbf{x} \in \mathbb{R}^p : \|\mathbf{x}\|_2 \leq \lambda\}$ *and let* $\mathcal{H}_{\mathcal{X}}$ *be the class of functions of the form* $h_{\mathbf{x}} : \mathbb{R}^p \to \mathbb{R}, h_{\mathbf{x}}(\mathbf{a}) = \langle \mathbf{x}, \mathbf{a} \rangle$, *for some* $\mathbf{x} \in \mathcal{X}\}$*. Let* $A = \{\mathbf{a}_1, \ldots, \mathbf{a}_n\} \subseteq \mathbb{R}^p$ *such that* $\max_{i=1,\ldots,n} \|\mathbf{a}_i\| \leq M$*. It holds that* $\mathcal{R}_A(\mathcal{H}_{\mathcal{X}}) \leq \lambda M / \sqrt{n}$*.*

Proof.

$$
\begin{aligned}
\mathcal{R}_A(\mathcal{H}_{\mathcal{X}}) &= \mathbb{E} \sup_{\|\mathbf{x}\|_2 \leq \lambda} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \langle \mathbf{x}, \mathbf{a} \rangle \\
&= \mathbb{E} \sup_{\|\mathbf{x}\|_2 \leq \lambda} \frac{1}{n} \left\langle \mathbf{x}, \sum_{i=1}^{n} \sigma_i \mathbf{a} \right\rangle \\
&\leq \frac{1}{n} \lambda \mathbb{E} \left\| \sum_{i=1}^{n} \sigma_i \mathbf{a}_i \right\|_2 \qquad \text{(C-S)}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \mathcal{R}_A(\mathcal{H}_{\mathcal{X}}) &\leq \frac{1}{n} \lambda \left(\mathbb{E} \sum_{i=1}^{n} \|\sigma_i \mathbf{a}_i\|_2^2 \right)^{1/2} \qquad \text{(Jensen)} \\
&\leq \frac{1}{n} \lambda \left(\sum_{i=1}^{n} \|\mathbf{a}_i\|_2^2 \right)^{1/2} \\
&\leq \lambda M / \sqrt{n}
\end{aligned}
$$

□

Rademacher complexity estimates of fully connected Neural Networks

Notation

For a matrix $\mathbf{X} \in \mathbb{R}^{n,m}$, $\|\mathbf{X}\|$ denotes its spectral norm. Let $\mathbf{X}_{:,k}$ be the k-th column of $\mathbf{X}$. We define

$$\|\mathbf{X}\|_{2,1} = \|(\|\mathbf{X}_{:,1}\|_2, \ldots, \|\mathbf{X}_{:,m}\|_2)\|_1. \tag{2}$$

Theorem (Spectral bound [2])

For positive integers $p_0, p_1, \ldots, p_d = 1$, and positive reals $\lambda_1, \ldots, \lambda_d$ and $\nu_1, \ldots, \nu_d$, define the set

$$\mathcal{X} := \{(\mathbf{X}_1, \ldots, \mathbf{X}_d) : \mathbf{X}_i \in \mathbb{R}^{p_i \times p_{i-1}}, \|\mathbf{X}_i\| \leq \lambda_i, \|\mathbf{X}_i^T\|_{2,1} \leq \nu_i\}$$

Let $H_{\mathcal{X}}$ be the class of neural networks $h_{\mathbf{x}} : \mathbb{R}^p \to \mathbb{R}$, $h_{\mathbf{x}} = \mathbf{X}_d \circ \sigma \circ \ldots \circ \sigma \circ \mathbf{X}_1$ where $\mathbf{x} = (\mathbf{X}_1, \ldots, \mathbf{X}_d) \in \mathcal{X}$. Suppose that σ is 1-Lipschitz. Let $A = \{\mathbf{a}_1, \ldots, \mathbf{a}_n\} \subseteq \mathbb{R}^p$, $M := \max_{i=1,\ldots,n} \|\mathbf{a}_i\|$ and
$W := \max\{p_i : i = 0, \ldots, d\}$.

The Rademacher complexity of $\mathcal{H}_{\mathcal{X}}$ with respect to A is bounded as

$$\mathcal{R}_A(\mathcal{H}_{\mathcal{X}}) = \mathcal{O}\left(\frac{\log(W)M}{\sqrt{n}} \prod_{i=1}^{d} \lambda_i \left(\sum_{j=1}^{d} \frac{\nu_j^{2/3}}{\lambda_j^{2/3}} \right)^{3/2} \right). \tag{3}$$

How well do complexity measures correlate with generalization?

name	definition	correlation[1]
Frobenius distance to initialization [10]	$\sum_{i=1}^{d} \|\mathbf{X}_i - \mathbf{X}_i^0\|_F^2$	-0.263
Spectral complexity[2] [2]	$\prod_{i=1}^{d} \|\mathbf{X}_i\| \left(\sum_{i=1}^{d} \frac{\|\mathbf{X}_i\|_{2,1}^{3/2}}{\|\mathbf{X}_i\|^{3/2}} \right)^{2/3}$	$\mathbf{-0.537}$
Parameter Frobenius norm	$\sum_{i=1}^{d} \|\mathbf{X}_i\|_F^2$	0.073
Fisher-Rao [8]	$\frac{(d+1)^2}{n} \sum_{i=1}^{n} \langle \mathbf{x}, \nabla_{\mathbf{x}} \ell(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \rangle$	0.078
Path-norm [11]	$\sum_{(i_0,\dots,i_d)} \prod_{j=1}^{d} \left(\mathbf{X}_{i_j, i_{j-1}} \right)^2$	$\mathbf{0.373}$

Table: Complexity measures compared in the empirical study [7], and their correlation with generalization

Complexity measures are still far from explaining generalization in Deep Learning!

A more recent evaluation of many complexity measures is available [5].

[1] Kendall's rank correlation coefficient

[2] The definition in [7] differs slightly

Wrap up!

- Deep learning tricks-of-the-trade recitation on Friday!

*Peeling the onion (risk minimization setting) - Decomposition details

$$R(\mathbf{x}^t) - R(\mathbf{x}^\natural) = R(\mathbf{x}^t) - R_n(\mathbf{x}^t) + R_n(\mathbf{x}^t) - R_n(\mathbf{x}^\star) + \underbrace{R_n(\mathbf{x}^\star) - R_n(\mathbf{x}^\natural)}_{\leq 0} + R_n(\mathbf{x}^\natural) - R(\mathbf{x}^\natural)$$

$$\leq R_n(\mathbf{x}^t) - R_n(\mathbf{x}^\star) + \underbrace{R(\mathbf{x}^t) - R_n(\mathbf{x}^t) + R_n(\mathbf{x}^\natural) - R(\mathbf{x}^\natural)}_{2\sup_{\mathbf{x}\in\mathcal{X}} |R_n(\mathbf{x}) - R(\mathbf{x})|}$$

$$\begin{aligned} R(\mathbf{x}^t) - R(\mathbf{x}^\circ) &= R(\mathbf{x}^t) - R(\mathbf{x}^\natural) + R(\mathbf{x}^\natural) - R(\mathbf{x}^\circ) \\ &\leq R_n(\mathbf{x}^t) - R_n(\mathbf{x}^\star) + 2\sup_{\mathbf{x}\in\mathcal{X}} |R_n(\mathbf{x}) - R(\mathbf{x})| + R(\mathbf{x}^\natural) - R(\mathbf{x}^\circ) \end{aligned}$$

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