Mathematics of Data: From Theory to Computation

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Lecture 7: Deep learning I

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

EE-556 (Fall 2020)

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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:*

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

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

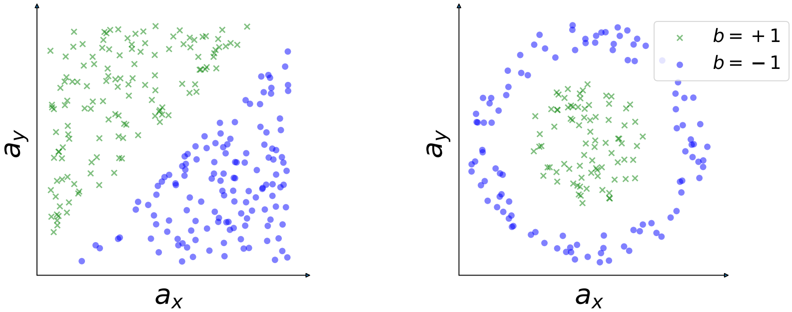

Figure: Linearly separable versus nonlinearly separable dataset

Power of linear classifiers–II

- Lifting dimensions to the rescue
  - Convex optimization objective
  - Might introduce the curse-of-dimensionality
  - Possible to avoid via kernel methods, such as SVMs

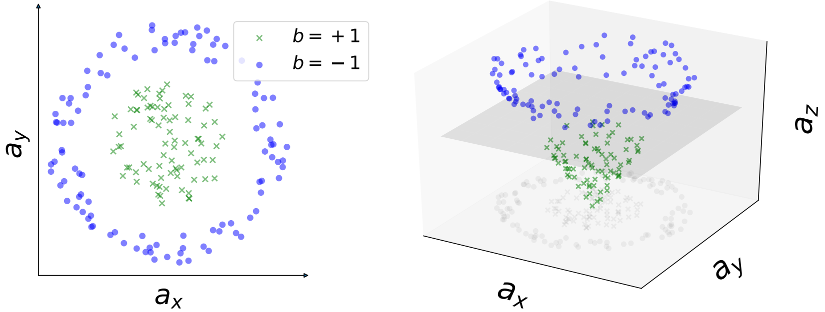

Figure: Non-linearly separable data (left). Linearly separable in $\mathbb{R}^3$ via $\mathbf{a}_z = \sqrt{\mathbf{a}_x^2 + \mathbf{a}_y^2}$ (right).

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: $\sigma : \mathbb{R} \to \mathbb{R}$

$$h_{\mathbf{x}}(\mathbf{a}) := \underset{\substack{\uparrow \\ \text{input}}}{\begin{bmatrix} \mathbf{a} \end{bmatrix}}$$

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recursively repeat activation + affine transformation to obtain "deeper" networks.

Why neural networks?: An approximation theoretic motivation

Theorem (Universal approximation [3])

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!

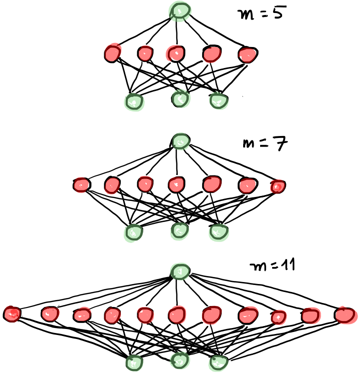

Figure: networks of increasing width

Why were NNs not popular before 2010?

- too big to optimize!
- did not have enough data
- could not find the optimum via algorithms

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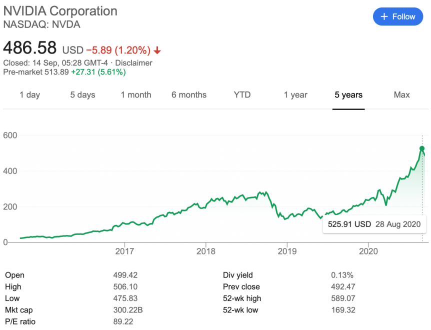
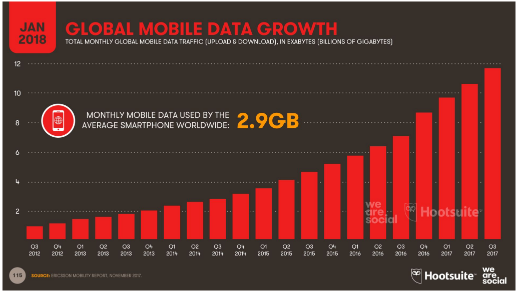




Supervised learning: Multi-class classification

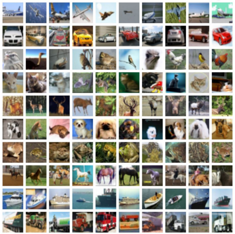


Figure: CIFAR10 dataset: 60000 32x32 color images (3 channels) from 10 classes

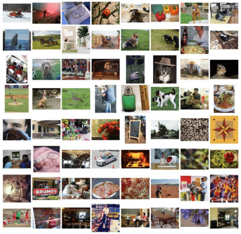


Figure: Imagenet dataset: 14 million color images (varying resolution, 3 channels) from 21K classes

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

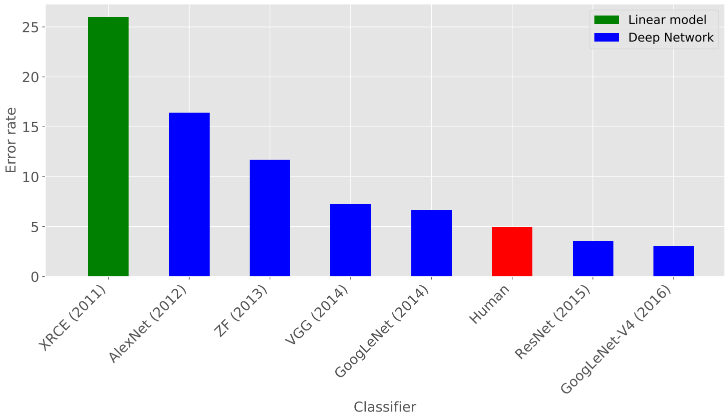


Figure: Error rate on the ImageNet challenge, for different network architectures.

Convolutional architectures in Computer Vision tasks

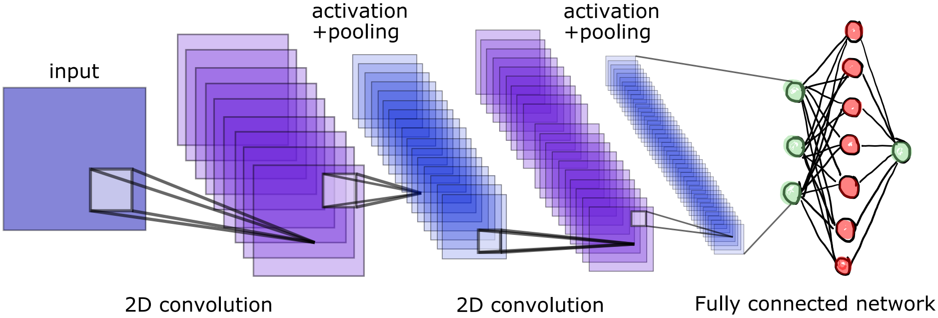
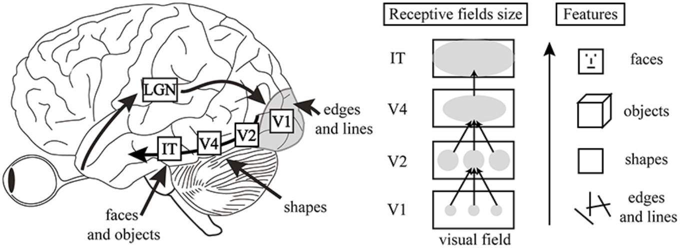
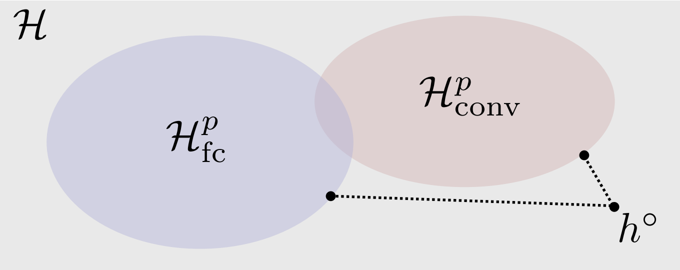


Figure: "Locality" Structure of a 2D deep convolutional neural network.

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!

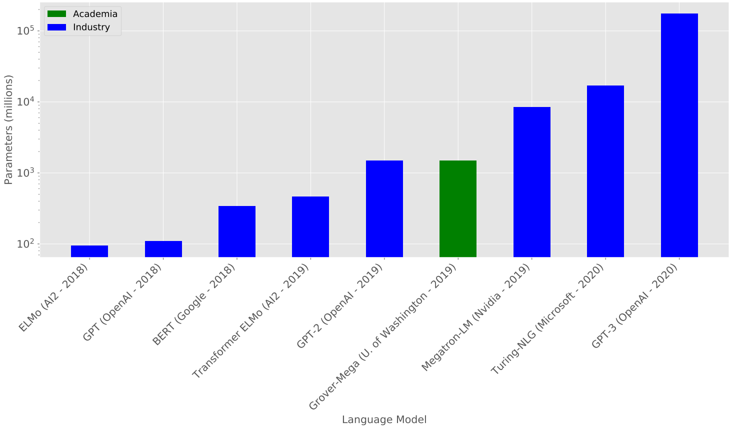


Figure: Number of parameters in Language models based on Deep Learning.

The 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

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

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

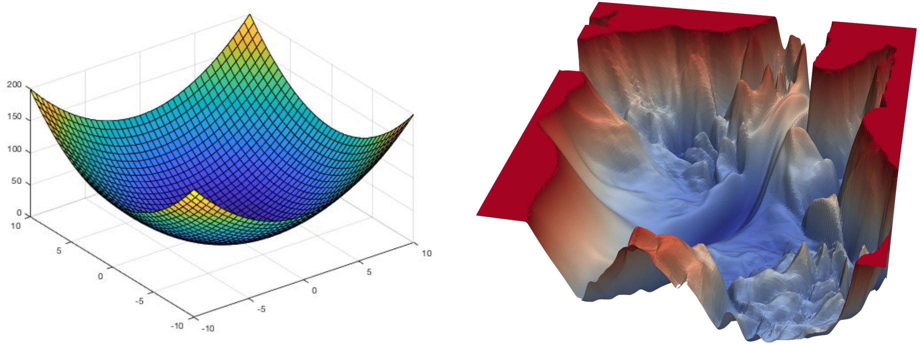
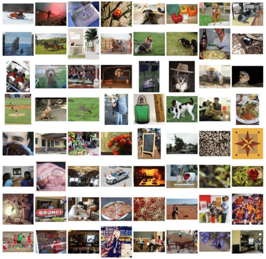


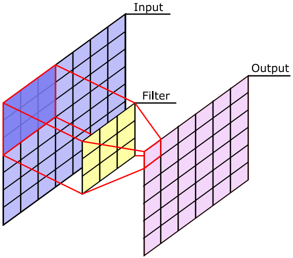
Figure: convex (left) vs non-convex (right) optimization landscape

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

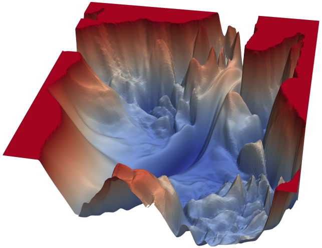
The Deep Learning Paradigm



(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

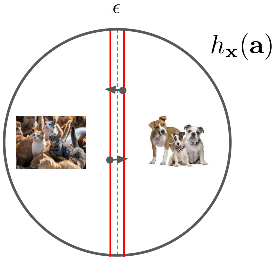
Challenges in DL/ML applications: Robustness (I)

(a) Turtle classified as rifle. Athalye et al. 2018.

(b) Stop sign classified as 45 mph sign. Eykholt et al. 2018

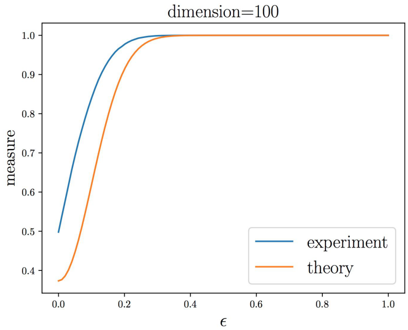
Figure: Natural or human-crafted modifications that trick neural networks used in computer vision tasks

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



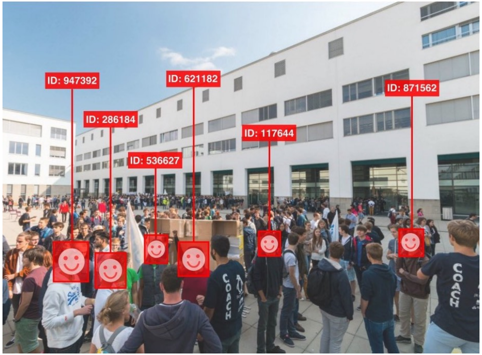
(b) Concentration of measure phenomenon on high dimensions

Figure: Understanding the robustness of a classifier in high-dimensional spaces. Shafahi et al. 2019.

Challenges in DL/ML applications: Robustness (References)

1. Madry, Aleksander and Makelov, Aleksandar and Schmidt, Ludwig and Tsipras, Dimitris and Vladu, Adrian. *Towards Deep Learning Models Resistant to Adversarial Attacks*. ICLR 2018.
2. Raghunathan, A., Steinhardt, J., and Liang, P. S. *Semidefinite relaxations for certifying robustness to adversarial examples*. Neurips 2018.
3. Wong, E. and Kolter, Z. (2018). *Provable defenses against adversarial examples via the convex outer adversarial polytope*. ICML 2018.
4. Huang, X., Kwiatkowska, M., Wang, S., and Wu, M. *Safety verification of deep neural networks*. Computer Aided Verification 2017.
5. Athalye, A., et al. *Synthesizing robust adversarial examples*. International conference on machine learning. PMLR, 2018.
6. Eykholt, K., Evtimov, I., Fernandes, E., Li, B., Rahmati, A., Xiao, C., and Song, D. *Robust physical-world attacks on deep learning visual classification*. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (pp. 1625-1634). 2018.
7. Shafahi A., Ronny Huang, W., Studer, C., Feizi, S. and Goldstein, T. *Are adversarial examples inevitable?*. International Conference on Learning Representations. 2019.

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



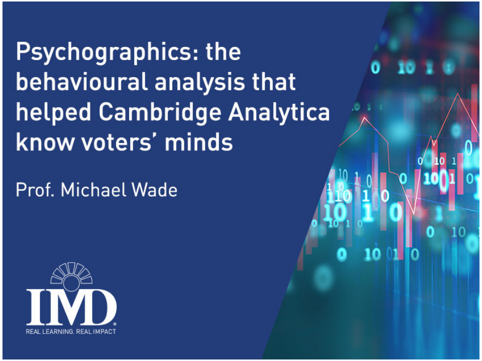
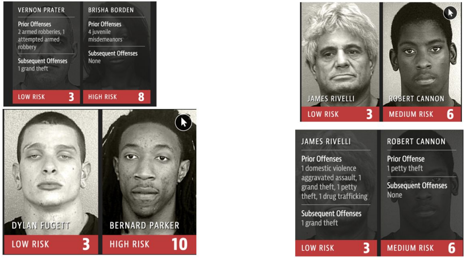


Figure: Political and societal concerns about some DL/ML applications

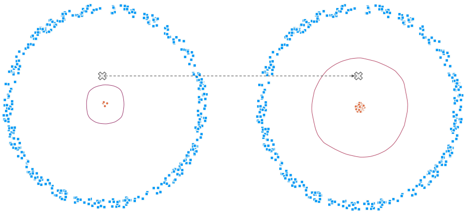
Challenges in DL/ML applications: Surveillance/Privacy/Manipulation (References)

1. Dwork, C., and Roth, A. *The Algorithmic Foundations of Differential Privacy*. Foundations and Trends in Theoretical Computer Science, 9, 2013.
2. Abadi, M., Chu, A., Goodfellow, I., McMahan, H. B., Mironov, I., Talwar, K., and Zhang, L. *Deep learning with differential privacy*. In Proceedings of the 2016 ACM SIGSAC Conference on Computer and Communications Security (pp. 308-318). 2016.
3. Sreenu, G., Saleem Durai, M.A. *Intelligent video surveillance: a review through deep learning techniques for crowd analysis*. J Big Data 6, 48. 2019.
4. O'Neil, C., *Weapons of Math Destruction: How Big Data Increases Inequality and Threatens Democracy* Broadway Books, (2016);
5. Wade, M. *Psychographics: the behavioural analysis that helped Cambridge Analytica know voters' minds*. `https://theconversation.com/psychographics-the-behavioural-analysis-that-helped-cambridge-analytica-know-voters-minds-93675` 2018.

Challenges in DL/ML applications: Fairness



(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)

1. Barocas, S. Hardt, M. Narayanan, Arvind. *Fairness in Machine Learning Limitations and Opportunities*. `https://fairmlbook.org/pdf/fairmlbook.pdf` 2020.
2. Hardt, M. *How Big Data Is Unfair*. `https://medium.com/@mrtz/how-big-data-is-unfair-9aa544d739de` 2014.
3. Munoz, C., Smith, M., and Patil, D. *Big Data: A Report on Algorithmic Systems, Opportunity, and Civil Rights*. Executive Office of the President. The White House, 2016.
4. Campolo, A., Sanfilippo, M., Whittaker, M., Crawford, K. *AI Now 2017 Report*. AI Now Institute at New York University, 2017.
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7. Noble, S.U. *Algorithms of Oppression: How Search Engines Reinforce Racism*. NYU Press. 2018.

Challenges in DL/ML applications: Interpretability

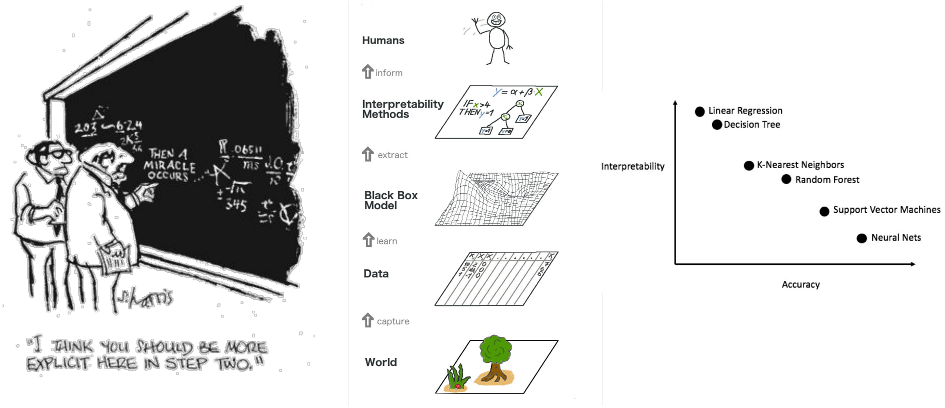

Figure: Performance vs Interpretability trade-offs in DL/ML

Challenges in DL/ML applications: Interpretability (References)

1. Baehrens, David and Schroeter, Timon and Harmeling, Stefan and Kawanabe, Motoaki and Hansen, Katja and Mueller, Klaus-Robert. Simonyan, Karen and Vedaldi, Andrea and Zisserman, Andrew. How to Explain Individual Classification Decisions. JMLR 2010.
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3. Ribeiro, Marco and Singh, Sameer and Guestrin, Carlos. "Why Should I Trust You?": Explaining the Predictions of Any Classifier. KDD 2016.
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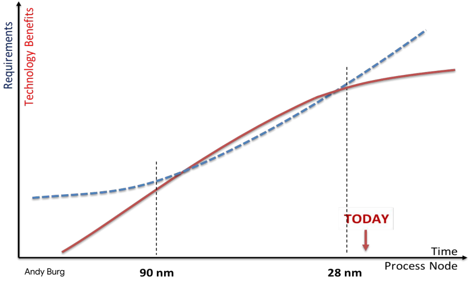
5. Shrikumar, Avanti and Greenside, Peyton and Kundaje, Anshul. Learning Important Features Through Propagating Activation Differences. ICML 2017.

Challenges in DL/ML applications: Energy efficiency and cost



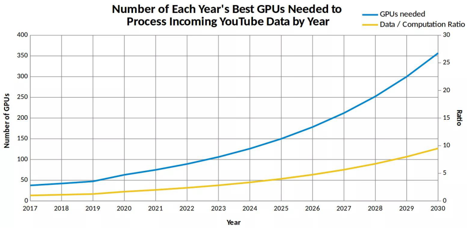


Figure: Efficiency and Scalability concerns in DL/ML

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

1. García-Marín, E., Rodrigues, C. F., Riley, G., and Grahn, H. *Estimation of energy consumption in machine learning*. Journal of Parallel and Distributed Computing, 134, 75-88. 2019.
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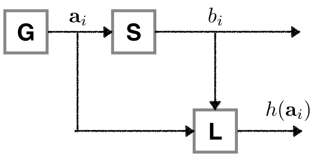
What theoretical challenges in Deep Learning will we study?



Models

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

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

Practical performance in Deep Learning

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

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. $\Rightarrow$ lecture 9
2. We expect large generalization error. It does not happen in practice. $\Rightarrow$ lecture 7 (this one) and 8
3. Large architectures + inductive bias might lead to small model error.

Generalization error bounds

The value of $|R(\mathbf{x}) - R_n(\mathbf{x})|$ is called the *generalization error* of the parameter $\mathbf{x}$.

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

We want to find high-probability upper bounds for the worst case generalization error over a class $\mathcal{X}$:

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

Main tool: concentration inequalities!

- Measure of how far is an empirical average from the true mean

Theorem (Hoeffding's Inequality [6])

Let $Y_1, \ldots, Y_n$ be i.i.d. random variables with Y_i taking values in the interval $[a_i, b_i] \subseteq \mathbb{R}$ for all $i = 1, \ldots, n$. 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* $L(h_{\mathbf{x}}(\mathbf{a}), b) = \{\textit{sign}(h_{\mathbf{x}}(\mathbf{a})) \neq b\}$ *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 $i = 1, \dots, n$ 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 $\mathcal{X}$ 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 $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_{|\mathcal{X}|}\}$. 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. $\square$

Generalization bounds for infinite classes - The Rademacher complexity

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

◦ A useful notion of *complexity* to derive generalization bounds for infinite classes of functions:

Definition (Rademacher Complexity [2])

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 follows:

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

◦ $\mathcal{R}_A(\mathcal{H})$ 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

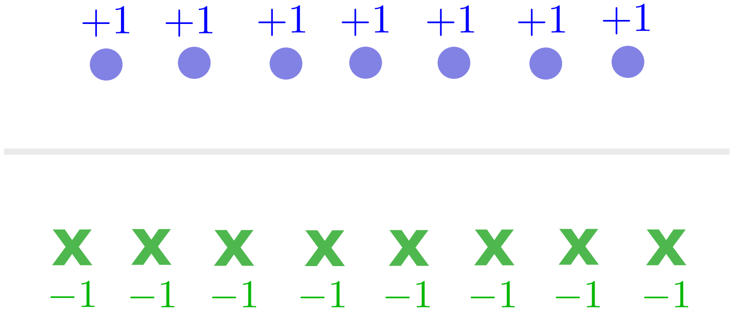
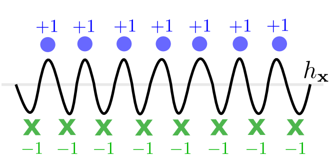
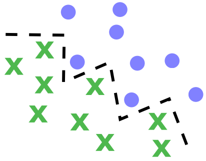


Figure: Rademacher complexity measures correlation with random signs

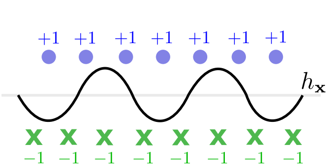
Visualizing Rademacher complexity



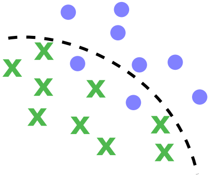
(a) High Rademacher Complexity



(b) Large Generalization error (memorization)



(c) Low Rademacher Complexity



(d) Low Generalization error

Figure: Rademacher complexity and Generalization error

A fundamental theorem about the Rademacher Complexity

Theorem (See Theorem 3.3 and 5.8 in [6])

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:*

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

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

The assumption is satisfied 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 for 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 [1])

For positive integers $p_0, p_1, \ldots, p_d = 1$*, and positive reals* $\lambda_1, \ldots, \lambda_d$ $\nu_1, \ldots, \nu_d$ *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 [7]	$\sum_{i=1}^{d} \|\mathbf{X}_i - \mathbf{X}_i^0\|_F^2$	-0.263
Spectral complexity[2] [1]	$\prod_{i=1}^{d} \|\mathbf{X}_i\| \left(\sum_{i=1}^{d} \frac{\|\mathbf{X}_i\|_{2,1}^{3/2}}{\|\mathbf{X}_i\|^{3/2}} \right)^{2/3}$	$\mathbf{-0.537}$
Parameter Frobenius norm	$\sum_{i=1}^{d} \|\mathbf{X}_i\|_F^2$	0.073
Fisher-Rao [5]	$\frac{(d+1)^2}{n} \sum_{i=1}^{n} \langle \mathbf{x}, \nabla_{\mathbf{x}} \ell(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \rangle$	0.078
Path-norm [8]	$\sum_{(i_0,\ldots,i_d)} \prod_{j=1}^{d} \left(\mathbf{X}_{i_j, i_{j-1}}\right)^2$	$\mathbf{0.373}$

Table: Complexity measures compared in the empirical study [4], and their correlation with generalization

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

[1] Kendall's rank correlation coefficient.

[2] The definition in [4] differs slightly.

Wrap up!

- Deep learning recitation on Friday!

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