Mathematics of Data: From Theory to Computation

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Lecture 8: From variance reduction to deep learning...

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An observation of GD vs. SGD step

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k \nabla f(\mathbf{x}^k) \quad \text{(GD)}$$

Lemma

Assume f is Lipschitz smooth with constant L. Then,

$$f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k) \leq \left(\frac{\gamma_k^2 L}{2} - \gamma_k \right) \|\nabla f(\mathbf{x}^k)\|^2.$$

An observation of GD vs. SGD step

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k G(\mathbf{x}^k, \theta_k) \quad \text{(SGD)}$$

Lemma

Assume f is Lipschitz smooth with constant L. Then,

$$\mathbb{E}[f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k)] \leq \left(\frac{\gamma_k^2 L}{2} - \gamma_k\right)\mathbb{E}[\|\nabla f(\mathbf{x}^k)\|^2] + \frac{L\gamma_k^2}{2}\mathbb{E}[\|G(\mathbf{x}^k, \theta_k) - \nabla f(\mathbf{x}^k)\|^2]$$

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Observations:
- ◦ The variance of gradient estimate dominates as $\nabla f(\mathbf{x}^k) \to 0$.
- ◦ To ensure convergence we need to control variance.

$$\gamma_k \to 0 \Longrightarrow \text{Slow convergence!}$$

Can we decrease the variance while using a constant step-size?

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Can we decrease the variance while using a constant step-size?

Choose a stochastic gradient, s.t. $\mathbb{E}\left[\|G(\mathbf{x}^k; \theta_k)\|^2\right] \to 0.$

A simple approach: Mini-batch SGD

◦ More samples imply a better estimate for full gradient.

SGD with mini batches

Let $G(\mathbf{x}, \theta)$ be an unbiased gradient estimate $(\mathbb{E}[G(\mathbf{x}, \theta)] = \nabla f(\mathbf{x}))$ and B_k be the batch size. Then, we have

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \frac{1}{B_k} \sum_{j=1}^{B_k} G(\mathbf{x}^k, \theta_{k,j}).$$

Theorem

Let $B_k > 0$ be the batch size and $G(\mathbf{x}, \theta)$ be an unbiased gradient estimate with bounded variance, i.e., $\mathbb{E}[\| G(\mathbf{x}, \theta) - \nabla f(\mathbf{x}) \|^2 \mid \mathbf{x}] \leq \sigma^2$. Then, the mini-batch estimate has the following properties:

$$\mathbb{E}\left[\frac{1}{B_k} \sum_{j=1}^{B_k} G(\mathbf{x}, \theta_{k,j})\right] = \nabla f(\mathbf{x}) \qquad \text{and} \qquad \mathbb{E}\left[\left\| \frac{1}{B_k} \sum_{j=1}^{B_k} G(\mathbf{x}, \theta_{k,j}) - \nabla f(\mathbf{x}) \right\|^2 \mid \mathbf{x}\right] \leq \frac{\sigma^2}{B_k}.$$

Remarks:

◦ We might need to increase the batch size over time to take variance to 0.

◦ We can come up with a “smarter” estimate for $\nabla f(\mathbf{x})$.

How to construct a new estimate $G(\mathbf{x}^k; \theta_k)$? [6]

Finite sum structure:	SGD update rule:
$f^\star := \min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{j=1}^n f_j(\mathbf{x}) \right\}$	$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma_k \nabla f_j(\mathbf{x}^k)$

- Let $X = \nabla f_j(\mathbf{x}^k)$ be a random variable (due to $j \sim \text{Uniform}(\{1, \cdots, n\})$).
- Let $Y = \nabla f_j(\tilde{\mathbf{x}})$ be another random variable, and $\tilde{\mathbf{x}}$ is a particularly selected point.

Remarks:
- We want X and Y to be correlated (we will see why!).
- Given Y, we should be able to estimate $\mathbb{E}[X]$ with more confidence.

Observations:
- Choice of $\tilde{\mathbf{x}}$ affects how correlated X and Y are.
- We can compute $\mathbb{E}[Y] = \frac{1}{n}\sum_{j=1}^n \nabla f_j(\tilde{\mathbf{x}}) = \nabla f(\tilde{\mathbf{x}})$.

Goal:
- Find a **good** estimate of $\mathbb{E}[X] = \frac{1}{n}\sum_{j=1}^n \nabla f_j(\mathbf{x}^k) = \nabla f(\mathbf{x}^k)$.

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◦ Let $X = \nabla f_j(\mathbf{x}^k)$ be a random variable (due to $j \sim$ Uniform$(\{1, \cdots, n\})$).

◦ Let $Y = \nabla f_j(\tilde{\mathbf{x}})$ be another random variable, and $\tilde{\mathbf{x}}$ is a particularly selected point.

A generalized estimator: $R_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$

- $\mathbb{E}[R_\alpha] = \alpha\mathbb{E}[X] + (1-\alpha)\mathbb{E}[Y]$
- $\mathrm{Var}(R_\alpha) = \alpha^2(\mathrm{Var}(X) + \mathrm{Var}(Y) - 2\mathrm{Cov}(X, Y))$

Observations:
◦ When $\alpha = 1$, R_α becomes unbiased, i.e., $\mathbb{E}[R_\alpha] = \mathbb{E}[X]$.
◦ If $\mathrm{Cov}(X, Y)$ is large enough (X and Y are correlated enough), $\mathrm{Var}(R_\alpha) \le \mathrm{Var}(X)$.

How could we use this information to construct our estimate?

Variance reduction techniques: SVRG

- Select the stochastic gradient ∇f_{i_k}, and compute a gradient estimate

$$\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}).$$

- As $\tilde{\mathbf{x}} \to \mathbf{x}^\star$ and $\mathbf{x}^k \to \mathbf{x}^\star$, we have

$$\nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}) \to 0.$$

- As a result, we can ensure the following

$$\mathbb{E}\left[\|\nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\tilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}})\|^2\right] \to 0.$$

Remarks:

- Remember the generalized estimator: $R_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$.
- For SVRG, $\alpha = 1$, $X = \nabla f_{i_k}(\mathbf{x}^k)$ and $Y = \nabla f_{i_k}(\tilde{\mathbf{x}})$.
- We will see how $\tilde{\mathbf{x}}$ is computed!

Stochastic gradient algorithm with variance reduction

Stochastic gradient with variance reduction (SVRG) [11, 21]

1. Choose $\widetilde{\mathbf{x}}^0 \in \mathbb{R}^p$ as a starting point and $\gamma > 0$ and $q \in \mathbb{N}_+$.
2. For $s = 0, 1, 2 \cdots$, perform:
   - 2a. $\widetilde{\mathbf{x}} = \widetilde{\mathbf{x}}^s, \quad \widetilde{\mathbf{v}} = \nabla f(\widetilde{\mathbf{x}}), \quad \mathbf{x}^0 = \widetilde{\mathbf{x}}$.
   - 2b. For $k = 0, 1, \cdots q-1$, perform:

$$\begin{cases} \text{Pick } i_k \in \{1, \ldots, n\} \text{ uniformly at random} \\ \mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\widetilde{\mathbf{x}}) + \widetilde{\mathbf{v}} \\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \mathbf{r}_k, \end{cases} \qquad (1)$$

   - 2c. Update $\widetilde{\mathbf{x}}^{s+1} = \frac{1}{m} \sum_{j=0}^{q-1} \mathbf{x}^j$.

Features

- The SVRG method uses a multistage scheme to reduce the variance of the stochastic gradient $\mathbf{r}_k$.
- Learning rate γ does not necessarily tend to 0 while $\mathbf{x}^k$ and $\widetilde{\mathbf{x}}^s$ tend to $\mathbf{x}_\star$.
- Each stage, SVRG uses $n + 2q$ component gradient evaluations.
- n for the full gradient at the beginning of each stage, and $2q$ for each of the q stochastic gradient steps.

Convergence analysis

Assumption A5.

(i) f is μ-strongly convex

(ii) The learning rate $0 < \gamma < 1/(4L_{\max})$, where $L_{\max} = \max_{1\leq j\leq n} L_j$.

(iii) q is large enough such that

$$\kappa = \frac{1}{\mu\gamma(1-4\gamma L_{\max})q} + \frac{4\gamma L_{\max}(q+1)}{(1-4\gamma L_{\max})q} < 1.$$

Theorem

Assumptions:

- *The sequence $\{\widetilde{\mathbf{x}}^s\}_{k\geq 0}$ is generated by SVRG.*
- *Assumption A5 is satisfied.*

Conclusion: *Linear convergence is obtained:*

$$\mathbb{E}f(\widetilde{\mathbf{x}}^s) - f(\mathbf{x}^\star) \leq \kappa^s (f(\widetilde{\mathbf{x}}^0) - f(\mathbf{x}^\star)).$$

Choice of γ and q, and complexity

Chose γ and q such that $\kappa \in (0,1)$:

For example

$$\gamma = 0.1/L_{\max}, q = 100(L_{\max}/\mu) \Longrightarrow \kappa \approx 5/6.$$

Complexity

$$\mathbb{E}f(\widetilde{\mathbf{x}}^s) - f(\mathbf{x}^\star) \leq \varepsilon, \quad \text{when } s \geq \log((f(\widetilde{\mathbf{x}}^0) - f(\mathbf{x}^\star))/\epsilon)/\log(\kappa^{-1})$$

- Each stage needs $n + 2q$ component gradient evaluations
- With $q = \mathcal{O}(L_{\max}/\mu)$, we obtain an overall complexity of

$$\mathcal{O}\Big((n + L_{\max}/\mu)\log(1/\epsilon)\Big).$$

Comparison: GD vs. SGD vs. SVRG

- GD update:

$$\left\{\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \nabla f(\mathbf{x}^k),\right.$$

- SGD update:

$$\left\{\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \nabla f_{i_k}(\mathbf{x}^k),\right.$$

- SVRG update:

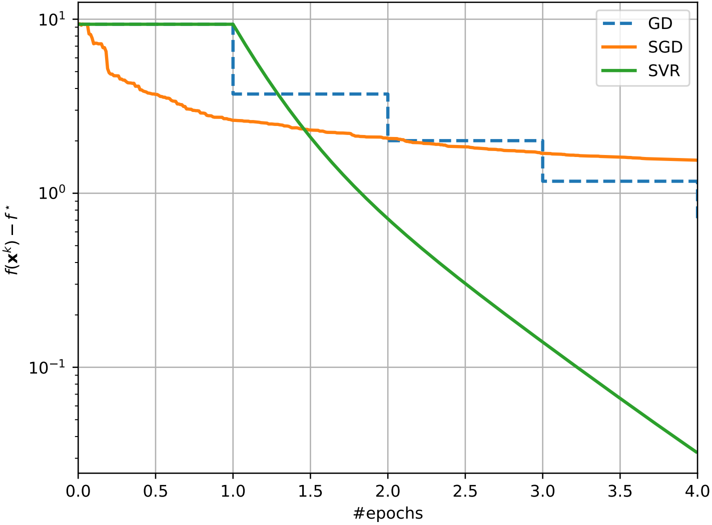
$$\begin{cases} \mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\widetilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}) \\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \mathbf{r}_k, \end{cases}$$

	SGD	SVRG	GD
Requires gradient storage?	no	no	no
Epoch-based	no	yes	no
Parameters	stepsize	stepsize & epoch length	stepsize
Gradient evaluations	1 per iteration	$n + 2q$ per epoch	n per iteration

Table: Comparisons of SGD, SVRG and GD [6]

- Recall that $q = \mathcal{O}(L_{\max}/\mu)$ is the epoch length for SVRG.

Example: ℓ_2-regularized least squares with synthetic data



Taxonomy of algorithms

$$f^\star := \min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{j=1}^{n} f_j(\mathbf{x}) \right\}.$$

- $f(\mathbf{x}) = \frac{1}{n}\sum_{j=1}^{n} f_j(\mathbf{x})$: μ-strongly convex with L-Lipschitz continuous gradient.

SVRG	GD	SGD
Linear	Linear	Sublinear

Table: Rate of convergence.

- $\kappa = L/\mu$.

SVRG	GD	SGD
$\mathcal{O}((n+\kappa)\log(1/\varepsilon))$	$\mathcal{O}((n\kappa)\log(1/\varepsilon))$	$1/\varepsilon$

Table: Complexity to obtain ε-solution.

The variance reduction zoo: convex

Setting	Algorithm	Lower bound	Complexity bound
L-smooth f_i's with bounded variance	Gradient descent	$L\Delta_0 \min\{\sigma/\epsilon^3, \sqrt{n}/\epsilon^2\}$ [10]	$nL\Delta_0/\epsilon^2$
	SVRG ($B_k = 1$) [16]		$nL\Delta_0/\epsilon^2$
	SVRG ($B_k = \Omega(n^{2/3})$) [16]		$n^{2/3}L\Delta_0/\epsilon^2$
	SAGA ($B_k = 1$) [16]		$nL\Delta_0/\epsilon^2$
	SAGA ($B_k = \Omega(n^{2/3})$) [16]		$n^{2/3}L\Delta_0/\epsilon^2$
	SpiderBoost [19]		$\sqrt{n}L\Delta_0/\epsilon^2$
	SpiderBoost-M [19]		$\sqrt{n}L\Delta_0/\epsilon^2$
	Spider [10]		$L\Delta_0 \min\{\sigma/\epsilon^3, \sqrt{n}/\epsilon^2\}$
	PAGE [15]		$L\Delta_0 \min\{\sigma/\epsilon^3, \sqrt{n}/\epsilon^2\}$
f is μ-SCVX and L-smooth f_i's are average L-smooth	KatyushaX [3]	$(n + n^{3/4}\sqrt{\frac{L}{\mu}}) \log \frac{\Delta_0}{\epsilon}$ [22]	$(n + n^{3/4}\sqrt{\frac{L}{\mu}}) \log \frac{\Delta_0}{\epsilon}$
f is CVX and L-smooth f_i's are average L-smooth	KatyushaX [3]	$n + n^{3/4}\sqrt{\frac{LD_0^2}{\epsilon}}$ [23]	$n + n^{3/4}\sqrt{\frac{LD_0^2}{\epsilon}}$

Remarks:
- ◦ Complexity ((S)CVX f): total number of stochastic first-order oracle calls to find $\mathbf{x}^\star_\epsilon$ with $\mathbb{E}[f(\mathbf{x}^\star_\epsilon) - f(\mathbf{x}^\star)] \leq \epsilon$.
- ◦ $\Delta_0 = f(\mathbf{x}^0) - f^\star$, $D_0 = \|\mathbf{x}^0 - \mathbf{x}^\star\|$.
- ◦ Bounded variance: $\mathbb{E}_i[\|\nabla f_i(\mathbf{x}) - \nabla f(\mathbf{x})\|^2] \leq \sigma^2 \quad \forall \mathbf{x}$.
- ◦ Average L-smooth: $\mathbb{E}_i[\|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{y})\|^2] \leq L^2\|\mathbf{x} - \mathbf{y}\|^2 \ \forall \mathbf{x}, \mathbf{y}$.

Variance-reduction for non-convex problems

SVRG estimator vs. a recursive estimator

◦ SVRG update:

$$\begin{cases} \mathbf{r}_1 = \nabla f(\tilde{\mathbf{x}}) \\ \mathbf{r}_k := \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\widetilde{\mathbf{x}}) + \nabla f(\tilde{\mathbf{x}}) \\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \mathbf{r}_k, \end{cases}$$

◦ Spider [10] update:

$$\begin{cases} \mathbf{r}_1 = \nabla f(\tilde{\mathbf{x}}) \\ \mathbf{r}_k := \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\widetilde{\mathbf{x}}) + \mathbf{r}_{k-1} \\ \mathbf{x}^{k+1} := \mathbf{x}^k - \gamma \mathbf{r}_k, \end{cases}$$

Spider [10]

1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point and $\gamma = \epsilon / L$.
2. For $k = 0, 1, 2, \ldots,$ perform:
   - 2a. If $k \bmod n = 0$, do:
     $\mathbf{r}_k = \nabla f(\mathbf{x}^k)$
     else:
     Pick $i_k \in \{1, \ldots, n\}$ uniformly at random
     $\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\mathbf{x}^{k-1}) + \mathbf{r}_{k-1}$
   - 2b. Update $\mathbf{x}^{k+1} := \mathbf{x}^k - \frac{\gamma}{\| \mathbf{r}_k \|} \mathbf{r}_k$
3. Return $\mathbf{x}^k$

Remarks:

◦ Sample complexity: $O\left(n + \sqrt{n}\frac{\Delta L}{\epsilon^2}\right)$.

◦ Sets the final accuracy apriori.

◦ Step-size depends on ϵ and L.

Adaptive variance-reduction for non-convex problems

AdaSpider [13]
1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$ as a starting point.
2. For $k = 0, 1, 2 \cdots$, perform:
2a. If k mod $n = 0$, do:
$\mathbf{r}_k = \nabla f(\mathbf{x}^k)$
else:
Pick $i_k \in \{1, \ldots, n\}$ uniformly at random
$\mathbf{r}_k = \nabla f_{i_k}(\mathbf{x}^k) - \nabla f_{i_k}(\mathbf{x}^{k-1}) + \mathbf{r}_{k-1}$
2b. Compute $\gamma_k := 1/\left(n^{1/4}\sqrt{n^{1/2} + \sum_{i=0}^{k} \Vert\mathbf{r}_i\Vert^2}\right)$
2c. Update $\mathbf{x}^{k+1} := \mathbf{x}^k - \gamma_k \mathbf{r}_k$
3. Return $\mathbf{x}^k$

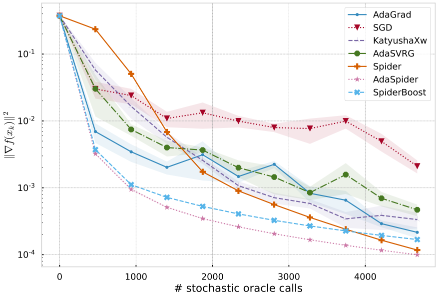
Theorem

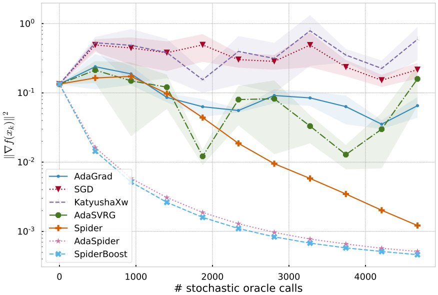
Let $\Delta_0 = f(\mathbf{x}^0) - \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x})$. The sequence $\mathbf{x}^0, \cdots, \mathbf{x}^k$ generated by AdaSpider satisfies:

$$\frac{1}{k}\sum_{i=0}^{k-1} \mathbb{E}[\Vert\nabla f(\mathbf{x}^i)\Vert] \leq O\left(n^{1/4}\frac{\Delta_0 + L^2}{\sqrt{k}}\log(k)\right), \quad \textit{with sample complexity } \tilde{O}\left(n + \sqrt{n}\frac{\Delta_0^2 + L^4}{\varepsilon^2}\right).$$

Performance of AdaSpider

- Image classification with neural networks (spoiler alert!) trained with cross entropy loss.
- AdaGrad [8], KatyushaXw [2], AdaSVRG[7], Spider [10], SpiderBoost [20].





The variance reduction zoo: non-convex

Setting	Algorithm	Lower bound	Complexity bound
f is α-weakly CVX and L-smooth f_i's are average L-smooth	Spider [10]	$\frac{\Delta_0}{\epsilon^2} \min\{n^{3/4}\sqrt{\alpha L}, \sqrt{n}L\}$ [23]	$\frac{\Delta_0}{\epsilon^2} \min\{n^{3/4}\sqrt{\alpha L}, \sqrt{n}L\}$
f_i's are α-weakly CVX and L-smooth	Natasha [1]	$\frac{\Delta_0}{\epsilon^2} \min\{\sqrt{n\alpha L}, L\}$ [23]	$\frac{\Delta_0}{\epsilon^2} \min\{\sqrt{n\alpha L}, \sqrt{n}L\}$
f is non-CVX f_i's are non-CVX and L-smooth	AdaSpider [13]	$\frac{\Delta_0 L}{\epsilon^2}\sqrt{n}$ [23, 10]	$\tilde{O}\left(n + \frac{\Delta_0^2 + L^4}{\epsilon^2}\sqrt{n}\right)$

Remarks:
- Complexity (nonCVX f): total number of stochastic first-order oracle calls to find $\mathbf{x}^\star_\epsilon$ with $\mathbb{E}[\|\nabla f(\mathbf{x}^\star_\epsilon)\|^2] \leq \epsilon^2$.
- $\Delta_0 = f(\mathbf{x}^0) - f^\star$, $D_0 = \|\mathbf{x}^0 - \mathbf{x}^\star\|$.
- Bounded variance: $\mathbb{E}_i[\|\nabla f_i(\mathbf{x}) - \nabla f(\mathbf{x})\|^2] \leq \sigma^2 \quad \forall \mathbf{x}$.
- L-smooth: $\|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \; \forall \mathbf{x}, \mathbf{y}$.
- $f(\mathbf{x})$ is α-weakly convex if $f(\mathbf{x}) + \frac{\alpha}{2}\|\mathbf{x}\|^2$ is convex $\forall \mathbf{x}$.

Deep learning outline

- In the sequel,
  - Introduction to deep learning
  - The deep learning paradigm
  - Challenges in deep learning theory and applications
- Next class
  - Generalization in deep learning

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.*

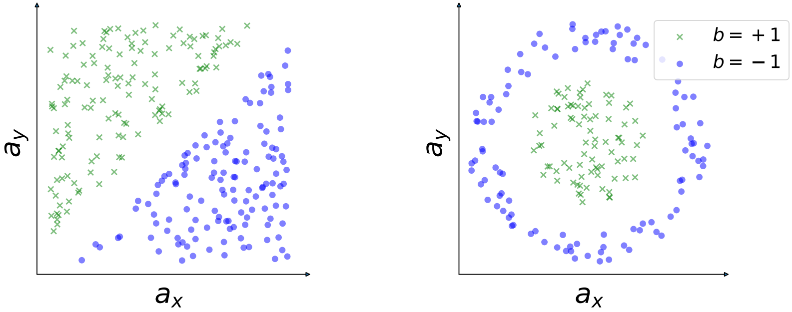


Figure: Linearly separable versus nonlinearly separable dataset

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

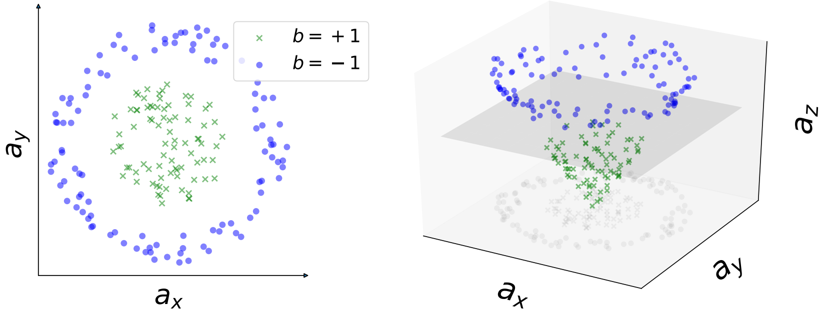


Figure: Non-linearly separable data (left). Linearly separable in $\mathbb{R}^3$ via $\mathbf{a}_z = \sqrt{\mathbf{a}_x^2 + \mathbf{a}_y^2}$ (right).

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

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

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$$h_{\mathbf{x}}(\mathbf{a}) := \underset{\text{weight}}{\underset{\downarrow}{\begin{bmatrix} \mathbf{X}_1 \end{bmatrix}}} \underset{\text{input}}{\underset{\downarrow}{\begin{bmatrix} \mathbf{a} \end{bmatrix}}}$$

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

$$h_{\mathbf{x}}(\mathbf{a}) := \underbrace{\overset{\text{activation}}{\overset{\downarrow}{\color{red}\sigma}} \color{red}{\Bigg(} \color{black} \overset{\text{weight}}{\overset{\downarrow}{\Big[\ \mathbf{X}_1\ \Big]}} \overset{\text{input}}{\overset{\downarrow}{\color{green}\big[\mathbf{a}\big]}} + \overset{\text{bias}}{\overset{\downarrow}{\color{blue}\big[\mu_1\big]}} \color{red}{\Bigg)}}_{\text{hidden layer = learned features}}$$

An important alternative for non-linearly separable data

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

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

Why neural networks?: An approximation theoretic motivation

Theorem (Universal approximation [5])

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!

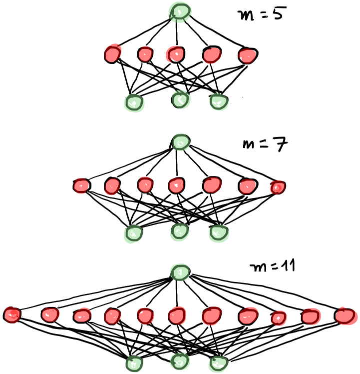

Figure: networks of increasing width

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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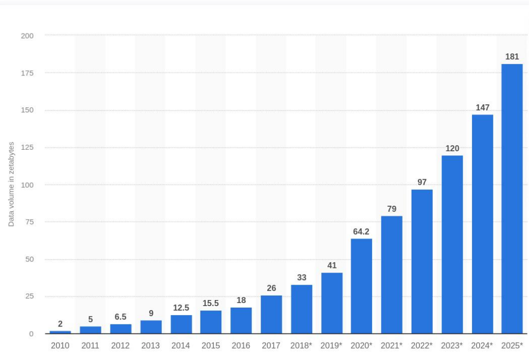


Supervised learning: Multi-class classification

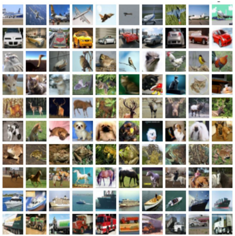


Figure: CIFAR10 dataset: 60000 32x32 color images (3 channels) from 10 classes

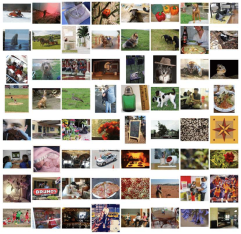


Figure: Imagenet dataset: 14 million color images (varying resolution, 3 channels) from 21K classes

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

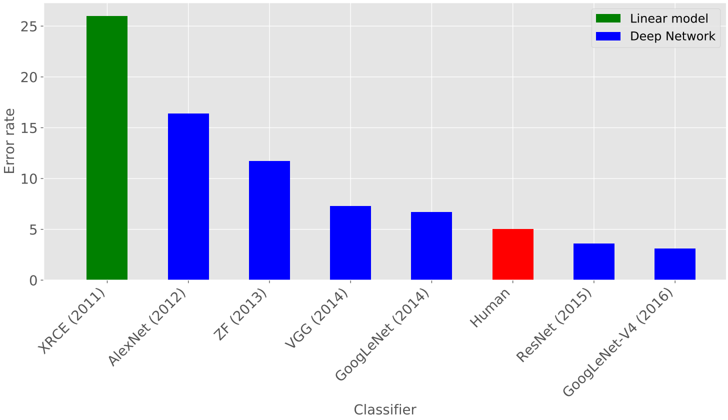


Figure: Error rate on the ImageNet challenge, for different network architectures.

2010-today: Deep Learning becomes popular again

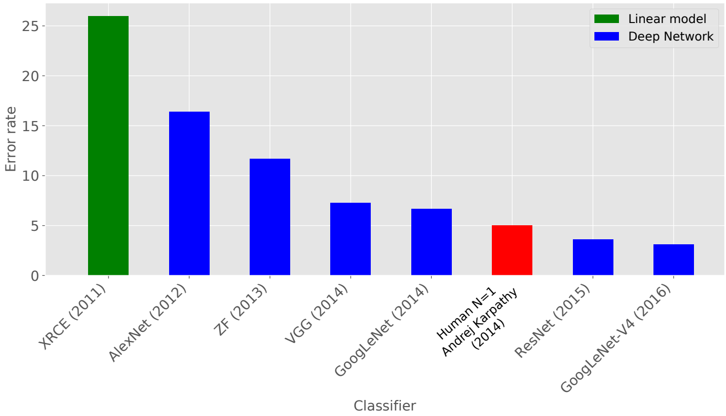


Figure: Error rate on the ImageNet challenge, for different network architectures [17, 12].

Convolutional architectures in Computer Vision tasks

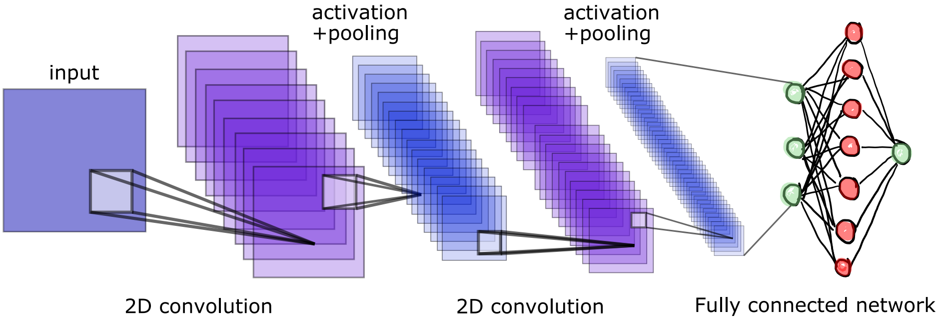
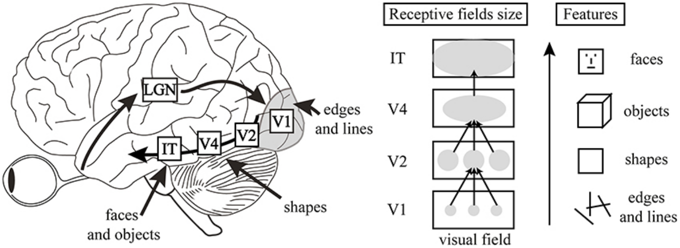
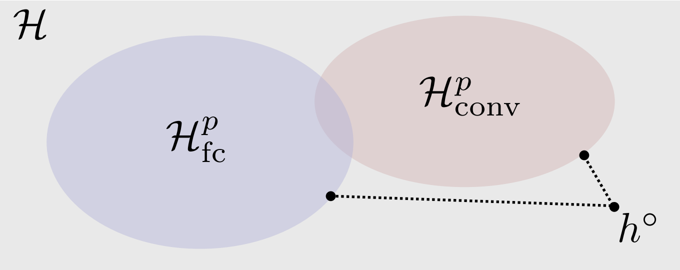


Figure: "Locality" structure of a 2D deep convolutional neural network.

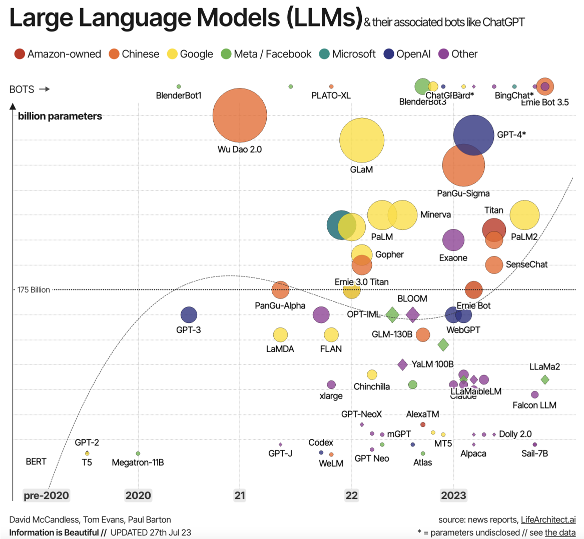
Inductive Bias: Why convolution works so well in Computer Vision tasks?



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



The era of model scaling



From: `https://informationisbeautiful.net/visualizations/the-rise-of-generative-ai-large-language-models-llms-like-chatgpt/`

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

$$\min_{\mathbf{x}} \left\{ R_n(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} L(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \right\} \tag{2}$$

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

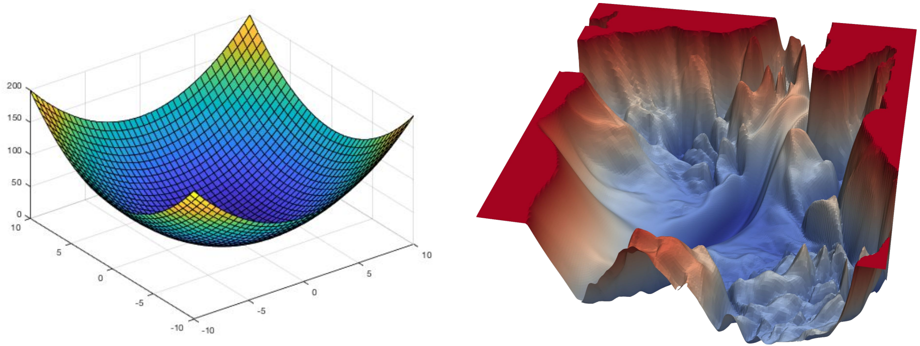


Figure: convex (left) vs non-convex (right) optimization landscape [14]

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

The landscape of ERM with multilayer networks

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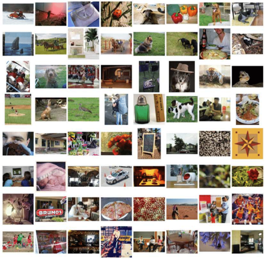
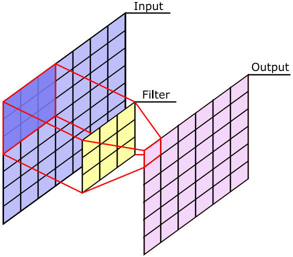
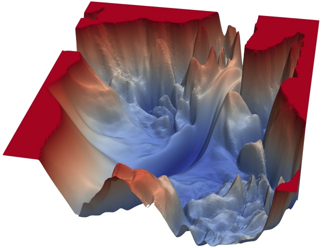
The deep learning paradigm



(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

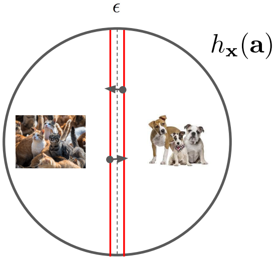
Challenges in DL/ML applications: Robustness (I)

(a) Turtle classified as rifle [4].

(b) Stop sign classified as 45 mph sign [9].

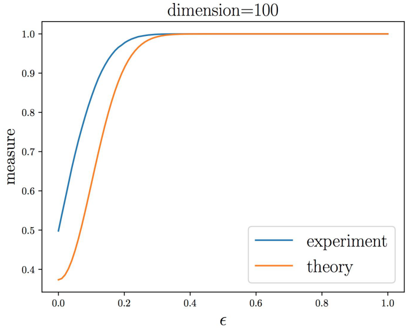
Figure: Natural or human-crafted modifications that trick neural networks used in computer vision tasks

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 [18]

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

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

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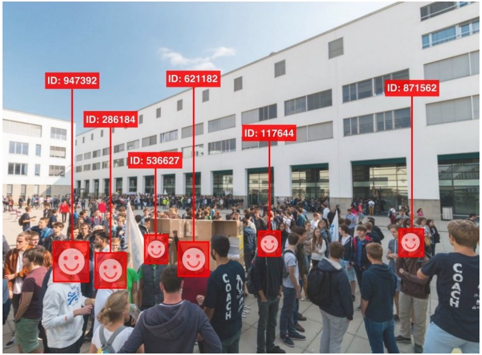
Challenges in DL/ML applications: Surveillance/Privacy/Manipulation



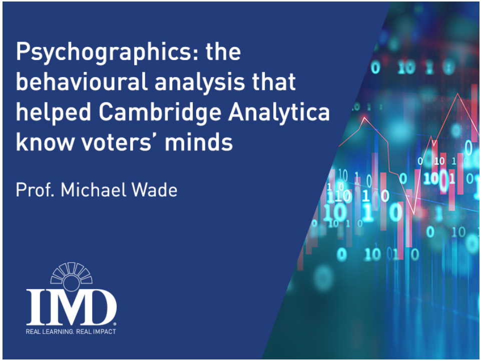


Figure: Political and societal concerns about some DL/ML applications

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

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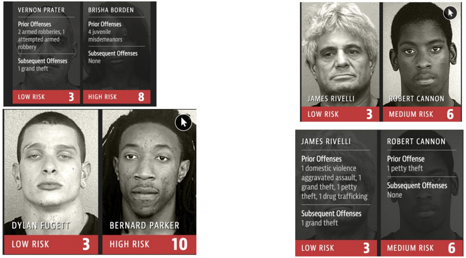
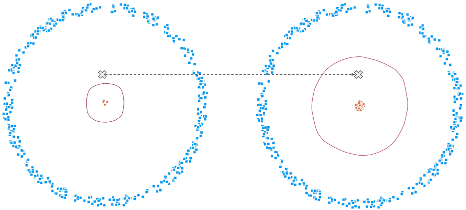
Challenges in DL/ML applications: Fairness



(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 I)

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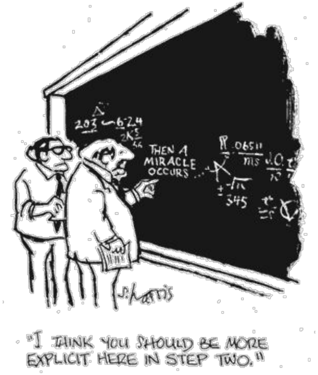
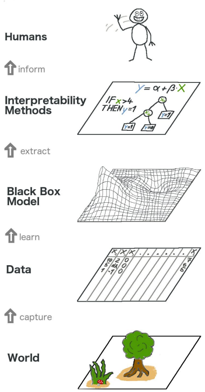
Challenges in DL/ML applications: Interpretability





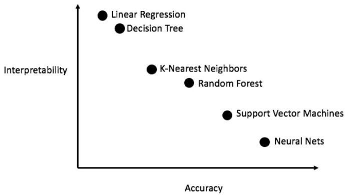


Figure: Performance vs Interpretability trade-offs in DL/ML

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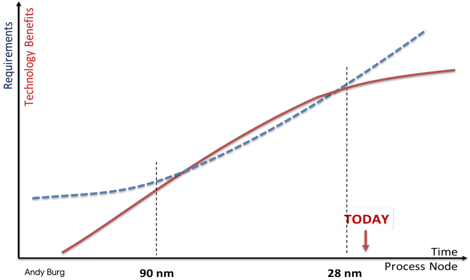
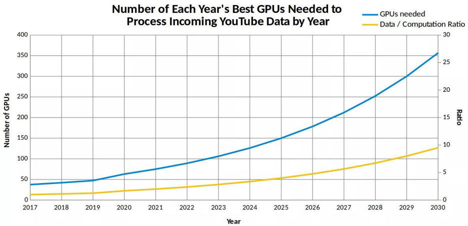
Challenges in DL/ML applications: Energy efficiency and cost



(a)



(b)

Figure: Efficiency and Scalability concerns in DL/ML

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Wrap up!

- Learning deep continues!

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