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Based on joint work with: Roi Livni and Ohad Shamir, Amit Daniely and Nati Linial, Tong Zhang Goal (informal): Learn an accurate mapping $h : \mathcal{X} \to \mathcal{Y}$ based on examples $((x_1, y_1), \dots, (x_n, y_n)) \in (\mathcal{X} \times \mathcal{Y})^n$

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PAC learning: Given $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$, probably approximately solve

$$\min_{h \in \mathcal{H}} \left[\mathbb{P}_{(x,y) \sim \mathcal{D}}[h(x) \neq y] \right] ,$$

where \mathcal{D} is unknown but the learner can sample $(x,y) \sim \mathcal{D}$

$$\min_{h \in \mathcal{H}} \left[\mathbb{P}_{(x,y) \sim \mathcal{D}}[h(x) \neq y] \right]$$

Expressiveness

 $\mathsf{Larger}\ \mathcal{H}\ \Rightarrow\ \mathsf{smaller}\ \mathsf{minimum}$

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What should be ${\cal H}$?

$$\min_{h \in \mathcal{H}} \left[\mathbb{P}_{(x,y) \sim \mathcal{D}}[h(x) \neq y] \right]$$

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Larger $\mathcal{H} \Rightarrow$ smaller minimum

Sample complexity

How many samples are needed to be ϵ -accurate?

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Prior Knowledge:

We must choose smaller ${\mathcal H}$ based on prior knowledge on ${\mathcal D}$

Prior Knowledge

- SVM and AdaBoost learn a halfspace on top of features, and most of the practical work is on finding good features
- Very strong prior knowledge



• Let \mathcal{H}_T be all functions from $\{0,1\}^p \to \{0,1\}$ that can be implemented by a Turing machine using at most T operations.

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Theorem

- \mathcal{H}_T is contained in the class of neural networks of depth O(T) and size $O(T^2)$
- The sample complexity of this class is $O(T^2)$

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The ultimate hypothesis class



• A single neuron with activation function $\sigma:\mathbb{R}\to\mathbb{R}$



• E.g., σ is a sigmoidal function



• A multilayer neural network of depth 3 and size 6



- Neural networks were popular in the 70's and 80's
- Then, suppressed by SVM and Adaboost on the 90's
- In 2006, several deep architectures with unsupervised pre-training have been proposed
- In 2012, Krizhevsky, Sutskever, and Hinton significantly improved state-of-the-art without unsupervised pre-training
- Since 2012, state-of-the-art in vision, speech, and more

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- Empirical Risk Minimization (ERM): Sample $S = ((x_1, y_1), \dots, (x_n, y_n)) \sim \mathcal{D}^n$ and approximately solve

$$\min_{w \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n \ell_i(w)$$

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- Realizable sample: $\exists w^* \text{ s.t. } \forall i, h_{w^*}(x_i) = y_i$
- Blum and Rivest 1992: Distinguishing between realizable and unrealizable S is NP hard even for depth 2 networks with 3 hidden neurons (reduction to k coloring)
 Hence, solving the ERM problem is NP hard even under realizability

The argument of Pitt and Valiant (1988)

If it is NP-hard to distinguish realizable from un-realizable samples, then properly learning ${\cal H}$ is hard (unless RP=NP)

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Proof: Run the learning algorithm on the empirical distribution over the sample to get $h \in \mathcal{H}$ with empirical error < 1/n:

- If $\forall i, h(x_i) = y_i$, return "realizable"
- Otherwise, return "unrealizable"

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Improper Learning



• Allow the learner to output $h \notin \mathcal{H}$

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- The argument of Pitt and Valiant fails because the algorithm may return consistent h even though S is unrealizable by ${\cal H}$
- Is deep learning still hard in the improper model ?

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Hope ...

- Generated examples in \mathbb{R}^{150} and passed them through a random depth-2 network that contains 60 hidden neurons with the ReLU activation function.
- Tried to fit a new network to this data with over-specification factors of 1,2,4,8



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Key Observation

- If a learning algorithm is computationally efficient its output must come from a class of "small" VC dimension
- Hence, it cannot perform well on "very random" samples

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Key Observation

- If a learning algorithm is computationally efficient its output must come from a class of "small" VC dimension
- Hence, it cannot perform well on "very random" samples

Using the above observation we conclude:

Hardness of distinguishing realizable form "random" samples implies hardness of improper learning of ${\cal H}$

Using the new technique and under a natural hardness assumption we can show:

- It is hard to improperly learn intersections of $\omega(1)$ halfspaces
- It is hard to improperly learn depth ≥ 2 networks with $\omega(1)$ neurons, with the threshold or ReLU or sigmoid activation functions

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- Network implements polynomials, where the depth correlative to degree
- Is this class still very expressive ?

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Expressiveness of polynomial networks

Recall the definition of \mathcal{H}_T (functions that can be implemented by T operations of a turing machine). Then, \mathcal{H}_T is contained in the class of polynomial networks of depth $O(T \log(T))$ and size $O(T^2 \log^2(T))$



• Proper learning is still hard even for depth $2\,$

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- \bullet Proper learning is still hard even for depth 2
- But, for constant depth, improper learning works
 - $\bullet\,$ Replace original class with a linear classifier over all degree $2^{depth-1}$ monomials
- Size of the network is very large. Can we do better?

Forward Greedy Selection for Polynomial Networks

- Consider depth 2 polynomial networks
- Let ${\mathcal S}$ be the Euclidean sphere of ${\mathbb R}^d$
- Observation: Two layer polynomial networks equivalent to mappings from ${\cal S}$ to ${\mathbb R}$ with sparse support
- Apply forward greedy selection for learning the sparse mapping
- Main caveat: at each greedy iteration we need to find \boldsymbol{v} that approximately solve

$$\operatorname*{argmax}_{v \in \mathcal{S}} |\nabla_v R(w)|$$

• Luckily, this is an eigenvalue problem

$$\nabla_v R(w) = v^\top \left(\underset{(x,y)}{\mathbb{E}} \ell' \left(\sum_{u \in \text{supp}(w)} w_u \langle u, x \rangle^2, y \right) x x^\top \right) v$$

- Let $\mathcal{H}_{t,n,L,\text{sig}}$ be the class of sigmoidal networks with depth t, size n, and bound L on the ℓ_1 norm of the input weights of each neuron
- Let $\mathcal{H}_{t,n,\mathrm{poly}}$ be defined similarly for polynomial networks

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Theorem

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Corollary

• Constant depth sigmoidal networks with L = O(1) are efficiently learnable !

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Corollary

- Constant depth sigmoidal networks with L = O(1) are efficiently learnable !
- It is hard to learn polynomial networks of depth $\Omega(\log(d))$ and size $\Omega(d)$

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How to circumvent hardness?

- Change the problem ...
- Add more assumptions
- Depart from worst-case analysis When does SGD work ? Can we make it better ?

SGD for Deep Learning

• Advantages:

- Works well in practice
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SGD for Deep Learning

• Advantages:

- Works well in practice
- ${\ensuremath{\, \bullet }}$ Per iteration cost independent of n
- Disadvantage: slow convergence



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Variance Reduction

- SAG, SDCA, SVRG
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SelfieBoost:

- AdaBoost, with SGD as weak learner, **converges exponentially faster** than vanilla SGD
- But yields an ensemble of networks very expensive at prediction time
- A new boosting algorithm that boost the performance of the same network
- Faster convergence under some "SGD success" assumption

Deep Networks are Non-Convex

- A 2-dim slice of a network with hidden layers $\{10, 10, 10, 10\}$, on MNIST, with the clamped ReLU activation function and logistic loss.
- The slice is defined by finding a global minimum (using SGD) and creating two random permutations of the first hidden layer.



But Deep Networks Seem Convex Near a Miminum

• Now the slice is based on 2 random points at distance 1 around a global minimum



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SDCA for Deep Learning

$$\min_{w \in \mathbb{R}^d} P(w) := \frac{1}{n} \sum_{i=1}^n \phi_i(w) + \frac{\lambda}{2} \|w\|^2$$

• SDCA is motivated by duality, which is meaningless for non-convex functions, but yields an algorithm we can run without duality:

"Dual" update:
$$\alpha_i^{(t)} = \alpha_i^{(t-1)} - \eta \lambda n \left(\nabla \phi_i(w^{(t-1)}) + \alpha_i^{(t-1)} \right)$$

"Primal dual" relationship: $w^{(t-1)} = \frac{1}{\lambda n} \sum_{i=1}^n \alpha_i^{(t-1)}$
Primal update: $w^{(t)} = w^{(t-1)} - \eta \left(\nabla \phi_i(w^{(t-1)}) + \alpha_i^{(t-1)} \right)$

• Converges rate (for convex and smooth): $\left(n + \frac{1}{\lambda}\right)\log\left(\frac{1}{\epsilon}\right)$

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• Recall that SDCA primal update rule is

$$w^{(t)} = w^{(t-1)} - \eta \underbrace{\left(\nabla \phi_i(w^{(t-1)}) + \alpha_i^{(t-1)} \right)}_{v^{(t)}}$$

and that $w^{(t-1)} = \frac{1}{\lambda n} \sum_{i=1}^{n} \alpha_i^{(t-1)}$.

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• Observe: $v^{(t)}$ is unbiased estimate of the gradient:

$$\mathbb{E}[v^{(t)}|w^{(t-1)}] = \frac{1}{n} \sum_{i=1}^{n} \left(\nabla \phi_i(w^{(t-1)}) + \alpha_i^{(t-1)} \right)$$

= $\nabla P(w^{(t-1)}) - \lambda w^{(t-1)} + \lambda w^{(t-1)}$
= $\nabla P(w^{(t-1)})$

• The update step of both SGD and SDCA is $w^{(t)} = w^{(t-1)} - \eta v^{(t)}$ where

$$v^{(t)} = \begin{cases} \nabla \phi_i(w^{(t-1)}) + \lambda w^{(t-1)} & \text{for SGD} \\ \nabla \phi_i(w^{(t-1)}) + \alpha_i^{(t-1)} & \text{for SDCA} \end{cases}$$

- In both cases $\mathbb{E}[v^{(t)}|w^{(t-1)}] = \nabla P(w^{(t)})$
- What about the variance?
- For SGD, even if $w^{(t-1)} = w^*$, the variance of $v^{(t)}$ is still constant
- \bullet For SDCA, it can be shown that the variance of $v^{(t)}$ goes to zero as $w^{(t-1)} \to w^*$

How to improve SGD?



Why SGD is slow at the end?

- High variance, even close to the optimum
- Rare mistakes: Suppose all but 1% of the examples are correctly classified. SGD will now waste 99% of its time on examples that are already correct by the model

- For simplicity, consider a binary classification problem in the realizable case
- For a fixed ϵ_0 (not too small), few SGD iterations find an $\epsilon_0\text{-accurate}$ solution
- However, for a small ϵ , SGD requires many iterations
- Smells like we need to use boosting

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First idea: learn an ensemble using AdaBoost

- Fix ϵ_0 (say 0.05), and assume SGD can find a solution with error $< \epsilon_0$ quite fast
- Lets apply AdaBoost with the SGD learner as a weak learner:
 - At iteration t, we sub-sample a training set based on a distribution D_t over $\left[n\right]$
 - ${\ensuremath{\, \bullet }}$ We feed the sub-sample to a SGD learner and gets a weak classifier h_t
 - Update D_{t+1} based on the predictions of h_t
 - The output of AdaBoost is an ensemble with prediction $\sum_{t=1}^{T} \alpha_t h_t(x)$
- The celebrated Freund & Schapire theorem states that if $T=O(\log(1/\epsilon))$ then the error of the ensemble classifier is at most ϵ
- Observe that each boosting iteration involves calling SGD on a relatively small data, and updating the distribution on the entire big data. The latter step can be performed in parallel
- Disadvantage of learning an ensemble: at prediction time, we need to apply many networks

- Can we obtain "boosting-like" convergence, while learning a single network?
- The SelfieBoost Algorithm:
 - Start with an initial network f_1
 - At iteration t, define weights over the n examples according to $D_i \propto e^{-y_i f_t(x_i)}$
 - $\bullet\,$ Sub-sample a training set $S\sim D$
 - Use SGD for approximately solving the problem

$$f_{t+1} \approx \underset{g}{\operatorname{argmin}} \sum_{i \in S} y_i (f_t(x_i) - g(x_i)) + \frac{1}{2} \sum_{i \in S} (g(x_i) - f_t(x_i))^2$$

- Lemma: At each iteration, with high probability over the choice of S, there exists a network g with objective value of at most -1/4
- Theorem: If at each iteration, the SGD algorithm finds a solution with objective value of at most $-\rho$, then after

$$\frac{\log(1/\epsilon)}{\rho}$$

SelfieBoost iterations the error of f_t will be at most ϵ

• To summarize: we have obtained $\log(1/\epsilon)$ convergence assuming that the SGD algorithm can solve each sub-problem to a fixed accuracy (which seems to hold in practice)

SelfieBoost vs. SGD

• On MNIST dataset, depth 5 network



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- Why deep networks: Deep networks are the ultimate hypothesis class from the statistical perspective
- Why not: Deep networks are a horrible class from the computational point of view
- This work: Deep networks with bounded depth and ℓ_1 norm are not hard to learn
- Provably correct theoretical algorithms are in general not practical.
- Why SGD works ???
- How can we make it better ?