# On the tradeoff between computational complexity and sample complexity in learning

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Joint work with Sham Kakade, Ambuj Tewari, Ohad Shamir, Karthik Sridharan, Nati Srebro

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# PAC Learning

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- Prior knowledge:  $h^{\star} \in \mathcal{H}$

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# Complexity of Learning

• Sample complexity — How many examples are needed ?

• Vapnik: exactly  $\frac{VC(\mathcal{H}) \log(1/\delta)}{\epsilon}$ 

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- Sample complexity  $\arg\min\{m': \operatorname{err}(m', \infty) \leq \epsilon\}$
- Data laden  $\operatorname{err}(\infty, \tau)$

#### Main Question

How much time,  $\tau,$  is needed to achieve error  $\leq \epsilon$  as a function of sample size, m?



• 
$$\mathcal{X} = \{0,1\}^d$$



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  - Kearns & Vazirani: If RP $\neq$ NP, it is not possible to efficiently find  $h \in \mathcal{H}$  s.t.  $\operatorname{err}(h) \leq \epsilon$
- Claim: if  $m \geq d^3/\epsilon$  it is possible to find a predictor with error  $\leq \epsilon$  in polynomial time



#### How more data reduces time?

- Observation:  $T_1 \lor T_2 \lor T_3 = \land_{u \in T_1, v \in T_2, w \in T_3} (u \lor v \lor w)$
- Define:  $\psi : \mathcal{X} \to \{0,1\}^{2(2d)^3}$  s.t. for each triplet of literals u, v, w there are two variables indicating if  $u \lor v \lor w$  is true or false
- Observation: Exists Halfspace s.t.  $h^{\star}(\mathbf{x}) = \operatorname{sgn}(\langle \mathbf{w}, \psi(\mathbf{x}) \rangle + b)$
- Therefore, can solve ERM w.r.t. Halfspaces (linear programming)
- VC dimension of Halfspaces is the dimension
- Sample complexity is order  $d^3/\epsilon$



#### Trading samples for runtime

Algorithm	samples	runtime
3-DNF	$rac{d}{\epsilon}$	$2^d$
Halfspace	$\frac{d^3}{\epsilon}$	$\operatorname{poly}(d)$



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#### But,

- The lower bound on the computational complexity is only for *proper* learning there's no lower bound on the computational complexity of improper learning with  $d/\epsilon$  examples
- The lower bound on the sample complexity of Halfspaces is in the general case here we have a specific structure

#### The interesting questions:

- Is the curve really true ? Can one construct 'correct' lower bounds ?
- If the curve is true, one should be able to construct more algorithms on the curve. How?

For  $t = 1, 2, \ldots, m$ 

- Learner receives side information  $\mathbf{x}_t \in \mathbb{R}^d$
- Learner predicts  $\hat{y}_t \in [k]$
- Learner pay cost  $\mathbf{1}[\hat{y}_t \neq h^\star(\mathbf{x}_t)]$
- "Bandit setting" learner does not know  $h^{\star}(\mathbf{x}_t)$

Goal: Minimize error rate:

$$\mathsf{err} = \frac{1}{m} \sum_{t=1}^{m} \mathbf{1}[\hat{y}_t \neq h^{\star}(\mathbf{x}_t)] \; .$$

$$\mathcal{H} = \{ \mathbf{x} \mapsto \operatorname*{argmax}_r (W \, \mathbf{x})_r \; : \; W \in \mathbb{R}^{k,d}, \, \|W\|_F \leq 1 \}$$



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Assumption: Data is separable with margin  $\mu$ :

$$\forall t, \ \forall r \neq y_t, \ (W\mathbf{x}_t)_{y_t} - (W\mathbf{x}_t)_r \geq \mu$$



#### Halving for Bandit Multiclass categorization

Initialize:  $V_1 = \mathcal{H}$ For  $t = 1, 2, \ldots$ 

- Receive  $\mathbf{x}_t$
- For all  $r \in [k]$  let  $V_t(r) = \{h \in V_t : h(\mathbf{x}_t) = r\}$
- Predict  $\hat{y}_t \in \arg \max_r |V_t(r)|$
- If  $\mathbf{1}[\hat{y}_t \neq y_t]$  set  $V_{t+1} = V_t \setminus V_t(\hat{y}_t)$

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#### Analysis:

- Whenever we err  $|V_{t+1}| \leq \left(1-rac{1}{k}
  ight) |V_t| \leq \exp(-1/k) \left|V_t
  ight|$
- Therefore:  $\operatorname{err} \leq \frac{k \log(|\mathcal{H}|)}{m}$
- Equivalently, sample complexity is  $\frac{k \log(|\mathcal{H}|)}{\epsilon}$

- Step 1: Dimensionality reduction to  $d' = O(\frac{\ln(m+k)}{\mu^2})$
- Step 2: Discretize  ${\cal H}$  to  $(1/\mu)^{kd'}$  hypotheses
- Apply Halving on the resulting finite set of hypotheses

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Analysis:

- Sample complexity is order of  $\frac{k^2/\mu^2}{\epsilon}$
- But runtime grows like  $(1/\mu)^{kd'} = (m+k)^{ ilde{O}(k/\mu^2)}$

- $\bullet\,$  Halving is not efficient because it does not utilize the structure of  ${\cal H}$
- In the full information case: Halving can be made efficient because each version space  $V_t$  can be made convex !
- The Perceptron is a related approach which utilizes convexity and works in the full information case
- Next approach: Lets try to rely on the Perceptron

## The Mutliclass Perceptron

For t = 1, 2, ..., m

- Receive  $\mathbf{x}_t \in \mathbb{R}^d$
- Predict  $\hat{y}_t = \arg \max_r (W^t \mathbf{x}_t)_r$
- Receive  $y_t = h^*(\mathbf{x}_t)$
- If  $\hat{y}_t \neq y_t$  update:  $W^{t+1} = W^t + U^t$

# The Mutliclass Perceptron

For t = 1, 2, ..., m

• Receive 
$$\mathbf{x}_t \in \mathbb{R}^d$$

• Predict 
$$\hat{y}_t~=~$$
 arg max $_r(W^t\,\mathbf{x}_t)_r$ 



**Problem:** In the bandit case, we're blind to value of  $y_t$ 

- Explore: From time to time, instead of predicting  $\hat{y}_t$  guess some  $\tilde{y}_t$
- Suppose we get the feedback 'correct', i.e.  $\tilde{y}_t = y_t$
- Then, we have full information for Perceptron's update:  $(\mathbf{x}_t, \hat{y}_t, \tilde{y}_t = y_t)$

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- Exploration-Exploitation Tradeoff:
  - When exploring we may have  $\tilde{y}_t = y_t \neq \hat{y}_t$  and can learn from this
  - When exploring we may have  $\tilde{y}_t \neq y_t = \hat{y}_t$  and then we had the right answer in our hands but didn't exploit it

For  $t = 1, 2, \ldots, m$ 

- Receive  $\mathbf{x}_t \in \mathbb{R}^d$
- Set  $\hat{y}_t = \arg \max_r (W^t \mathbf{x}_t)_r$
- Define:  $P(r) = (1 \gamma)\mathbf{1}[r = \hat{y}_t] + \frac{\gamma}{k}$
- Randomly sample  $\tilde{y}_t$  according to P
- Predict  $\tilde{y}_t$
- Receive feedback  $\mathbf{1}[ ilde{y}_t = y_t]$
- Update:  $W^{t+1} = W^t + \tilde{U}^t$

For t = 1, 2, ..., m

• Define: 
$$P(r) = (1 - \gamma)\mathbf{1}[r = \hat{y}_t] + \frac{\gamma}{k}$$



#### Theorem

- Banditron's sample complexity is order of  $\frac{k/\mu^2}{\epsilon^2}$
- Banditron's runtime is  $O(k/\mu^2)$

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#### The crux of difference between Halving and Banditron:

- Without having the full information, the version space is non-convex and therefore it is hard to utilize the structure of  $\mathcal H$
- Because we relied on the Perceptron we did utilize the structure of  ${\cal H}$  and got an efficient algorithm
- We managed to obtain 'full-information examples' by using exploration
- The price of exploration is a higher regret

### Trading samples for runtime

Algorithm	samples	runtime
Halving	$\frac{k^2/\mu^2}{\epsilon}$	$(m+k)^{\tilde{O}(k/\mu^2)}$
Banditron	$\frac{k/\mu^2}{\epsilon^2}$	$k/\mu^2$
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#### Agnostic PAC:

- ${\mathcal D}$  arbitrary distribution over  ${\mathcal X} \times {\mathcal Y}$
- Training set:  $S = (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)$
- Goal: use S to find  $h_S$  s.t. w.p.  $1 \delta$ ,

$$\operatorname{err}(h_S) \leq \min_{h \in \mathcal{H}} \operatorname{err}(h) + \epsilon$$

$$\mathcal{H} = \{ \mathbf{x} \mapsto \phi(\langle \mathbf{w}, \mathbf{x} \rangle) : \| \mathbf{w} \|_2 \le 1 \}, \quad \phi(z) = \frac{1}{1 + \exp(-z/\mu)}$$



- Probabilistic classifier:  $\mathbb{P}[h_{\mathbf{w}}(\mathbf{x}) = 1] = \phi(\langle \mathbf{w}, \mathbf{x} \rangle)$
- Loss function:  $\operatorname{err}(\mathbf{w}; (\mathbf{x}, y)) = \mathbb{P}[h_{\mathbf{w}}(\mathbf{x}) \neq y] = \left| \phi(\langle \mathbf{w}, \mathbf{x} \rangle) \frac{y+1}{2} \right|$
- Remark: Dimension can be infinite (kernel methods)

- Claim: exists  $1/(\epsilon\mu^2)$  examples from which we can efficiently learn w<sup>\*</sup> up to error of  $\epsilon$
- Proof idea:
  - $S' = \{(\mathbf{x}_i, y'_i) : y'_i = y_i \text{ if } y_i \langle \mathbf{w}^*, \mathbf{x}_i \rangle < -\mu \text{ and else } y'_i = -y_i\}$
  - Use surrogate convex loss  $\frac{1}{2}\max\{0,1-y\langle\mathbf{w},x\rangle/\gamma\}$
  - Minimizing surrogate loss on  $S' \Rightarrow$  minimizing original loss on S
  - Sample complexity w.r.t. surrogate loss is  $1/(\epsilon \mu^2)$

#### Analysis

• Sample complexity:  $1/(\epsilon\mu)^2$ 

• Time complexity: 
$$m^{1/(\epsilon\mu^2)} = \left(rac{1}{\epsilon\mu}
ight)^{1/(\epsilon\mu^2)}$$

# Second Approach – IDPK (S, Shamir, Sridharan)

Learning fuzzy halfspaces using Infinite-Dimensional-Polynomial-Kernel

• Original class:  $\mathcal{H} = \{\mathbf{x} \mapsto \phi(\langle \mathbf{w}, \mathbf{x} \rangle)\}$ 

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- Problem: Loss is non-convex w.r.t. w
- Main idea: Work with a larger hypothesis class for which the loss becomes convex



## Step 2 – Learning fuzzy halfspaces with IDPK

- Original class:  $\mathcal{H} = \{\mathbf{x} \mapsto \phi(\langle \mathbf{w}, \mathbf{x} \rangle) : \|\mathbf{w}\| \le 1\}$
- New class:  $\mathcal{H}' = \{\mathbf{x} \mapsto \langle \mathbf{v}, \psi(\mathbf{x}) \rangle : \|\mathbf{v}\| \le B\}$  where  $\psi : \mathcal{X} \to \mathbb{R}^{\mathbb{N}}$  s.t.  $\forall j, \forall (i_1, \ldots, i_j), \psi(\mathbf{x})_{(i_1, \ldots, i_j)} = 2^{j/2} x_{i_1} \cdots x_{i_j}$

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#### Lemma (S, Shamir, Sridharan 2009)

If  $B = \exp(\tilde{O}(1/\mu))$  then for all  $h \in \mathcal{H}$  exists  $h' \in \mathcal{H}'$  s.t. for all  $\mathbf{x}$ ,  $h(\mathbf{x}) \approx h'(\mathbf{x})$ .

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**Remark:** The above is a pessimistic choice of B. In practice, smaller B suffices. Is it tight? Even if it is, are there natural assumptions under which a better bound holds ? (e.g. Kalai, Klivans, Mansour, Servedio 2005)

# Proof idea

### • Polynomial approximation: $\phi(z) \approx \sum_{j=0}^{\infty} \beta_j z^j$

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# Proof idea

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• Therefore:

$$\begin{split} \phi(\langle \mathbf{w}, \mathbf{x} \rangle) &\approx \sum_{j=0}^{\infty} \beta_j (\langle \mathbf{w}, \mathbf{x} \rangle)^j \\ &= \sum_{j=0}^{\infty} \sum_{k_1, \dots, k_j} 2^{-j/2} \beta_j 2^{j/2} w_{k_1} \cdots w_{k_j} x_{k_1} \cdots x_{k_j} \\ &= \langle \mathbf{v}_{\mathbf{w}}, \psi(\mathbf{x}) \rangle \end{split}$$

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- Therefore:

$$\phi(\langle \mathbf{w}, \mathbf{x} \rangle) \approx \sum_{j=0}^{\infty} \beta_j (\langle \mathbf{w}, \mathbf{x} \rangle)^j$$
$$= \sum_{j=0}^{\infty} \sum_{k_1, \dots, k_j} 2^{-j/2} \beta_j 2^{j/2} w_{k_1} \cdots w_{k_j} x_{k_1} \cdots x_{k_j}$$
$$= \langle \mathbf{v}_{\mathbf{w}}, \psi(\mathbf{x}) \rangle$$

• To obtain a concrete bound we use Chebyshev approximation technique: Family of orthogonal polynomials w.r.t. inner product:

$$\langle f,g\rangle = \int_{x=-1}^{1} \frac{f(x)g(x)}{\sqrt{1-x^2}} dx$$

- Although the dimension is infinite, can be solved using the kernel trick
- The corresponding kernel (a.k.a. Vovk's infinite polynomial):

$$\langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle = K(\mathbf{x}, \mathbf{x}') = \frac{1}{1 - \frac{1}{2} \langle \mathbf{x}, \mathbf{x}' \rangle}$$

- Algorithm boils down to linear regression with the above kernel
- Convex! Can be solved efficiently
- Sample complexity:  $(B/\epsilon)^2 = 2^{\tilde{O}(1/\mu)}/\epsilon^2$
- Time complexity:  $m^2$

Algorithm	sample	time
Covering	$rac{1}{\epsilon^2\mu^2}$	$\left(rac{1}{\epsilon\mu} ight)^{1/(\epsilon\mu^2)}$
	∧	$\vee$
IDPK	$\left(rac{1}{\epsilon\mu} ight)^{1/\mu} rac{1}{\epsilon^2}$	$\left(rac{1}{\epsilon\mu} ight)^{2/\mu} rac{1}{\epsilon^4}$

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- Trading data for runtime (?)
- There are more examples of the phenomenon ....

Open questions:

- More points on the curve (new algorithms)
- Lower bounds ??? Can you help ?