The Sample-Computational Tradeoff

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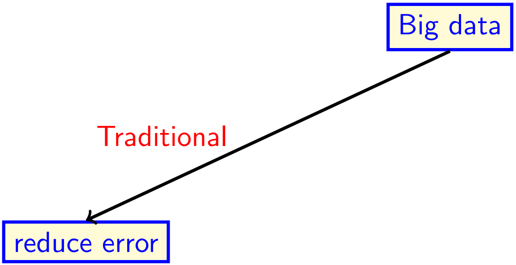
Collaborators:

- Nati Srebro
- Ohad Shamir and Eran Tromer (AISTATS'2012)
- Satyen Kale and Elad Hazan (COLT'2012)
- Aharon Birnbaum (NIPS'2012)
- Amit Daniely and Nati Linial (on arxiv)

What *else* can we do with more data?



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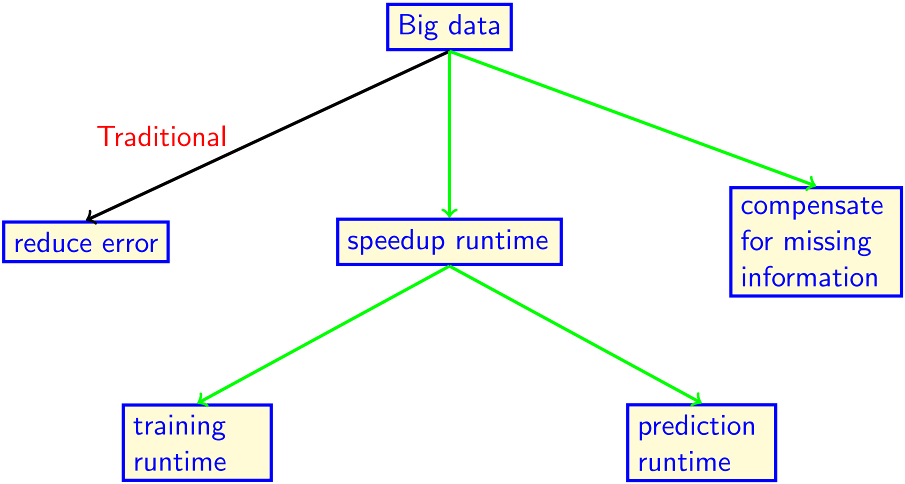

Agnostic PAC Learning

- Hypothesis class $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$
- Loss function: $\ell : \mathcal{H} \times (\mathcal{X} \times \mathcal{Y}) \to \mathbb{R}$
- $\mathcal{D}$ - unknown distribution over $\mathcal{X} \times \mathcal{Y}$
- True risk: $L_{\mathcal{D}}(h) = \mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(h,(x,y))]$
- Training set: $S = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m) \overset{\text{i.i.d.}}{\sim} \mathcal{D}^m$
- Goal: use S to find h_S s.t. with high probability,

$$L_{\mathcal{D}}(h_S) \le \min_{h\in\mathcal{H}} L_{\mathcal{D}}(h) + \epsilon$$

- ERM rule:

$$\mathrm{ERM}(S) \in \operatorname*{argmin}_{h\in\mathcal{H}} L_S(h) := \frac{1}{m}\sum_{i=1}^{m} \ell(h,(x_i,y_i))$$

Error Decomposition

$$h^\star = \operatorname*{argmin}_{h \in \mathcal{H}} L_{\mathcal{D}}(h) \quad ; \quad \mathrm{ERM}(S) = \operatorname*{argmin}_{h \in \mathcal{H}} L_S(h)$$

$$L_{\mathcal{D}}(h_S) = \underbrace{L_{\mathcal{D}}(h^\star)}_{\text{approximation}} + \underbrace{L_{\mathcal{D}}(\mathrm{ERM}(S)) - L_{\mathcal{D}}(h^\star)}_{\text{estimation}}$$

- Bias-Complexity tradeoff: Larger $\mathcal{H}$ decreases approximation error but increases estimation error

3-term Error Decomposition (Bottou & Bousquet' 08)

$$h^\star = \operatorname*{argmin}_{h \in \mathcal{H}} L_{\mathcal{D}}(h) \quad ; \quad \mathrm{ERM}(S) = \operatorname*{argmin}_{h \in \mathcal{H}} L_S(h)$$

$$L_{\mathcal{D}}(h_S) = \underbrace{L_{\mathcal{D}}(h^\star)}_{\text{approximation}} + \underbrace{L_{\mathcal{D}}(\mathrm{ERM}(S)) - L_{\mathcal{D}}(h^\star)}_{\text{estimation}} + \underbrace{L_{\mathcal{D}}(h_S) - L_{\mathcal{D}}(\mathrm{ERM}(S))}_{\text{optimization}}$$

- Bias-Complexity tradeoff: Larger $\mathcal{H}$ decreases approximation error but increases estimation error
- What about optimization error ?
  - Two resources: samples and runtime
  - Sample-Computational complexity (Decatur, Goldreich, Ron '98)

Joint Time-Sample Complexity

Goal:

$$L_{\mathcal{D}}(h_S) \;\leq\; \min_{h \in \mathcal{H}} L_{\mathcal{D}}(h) \;+\; \epsilon$$

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- Sample complexity: How many examples are needed ?
- Time complexity: How much time is needed ?

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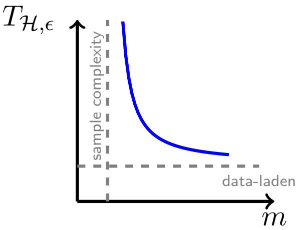
Time-sample complexity

$T_{\mathcal{H},\epsilon}(m) =$ how much time is needed when $|S| = m$?



Outline

The Sample-Computational tradeoff:

- Agnostic learning of preferences
- Learning margin-based halfspaces
- Formally establishing the tradeoff
- More data in partial information settings

Other things we can do with more data

- Missing information
- Testing time

Agnostic learning Preferences

The Learning Problem:

- $\mathcal{X} = [d] \times [d]$, $\mathcal{Y} = \{0, 1\}$
- Given $(i, j) \in \mathcal{X}$ predict if i is preferable over j
- $\mathcal{H}$ is all permutations over $[d]$
- Loss function $=$ zero-one loss

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Method I:

- $\mathrm{ERM}_{\mathcal{H}}$
- Sample complexity is $\frac{d}{\epsilon^2}$

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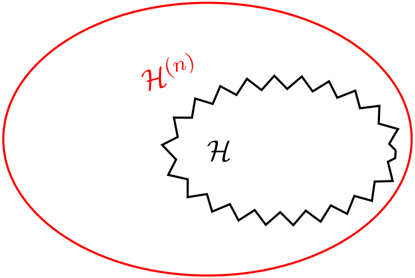
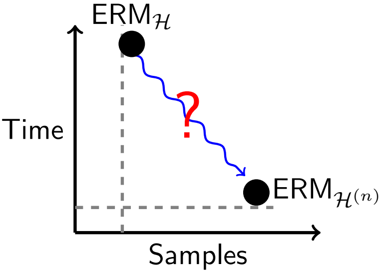
- Sample complexity is $\frac{d}{\epsilon^2}$
- Varun Kanade and Thomas Steinke (2011): If RP$\neq$NP, it is not possible to efficiently find an ϵ-accurate permutation
- Claim: If $m \geq d^2/\epsilon^2$ it is possible to find a predictor with error $\leq \epsilon$ in polynomial time

Agnostic learning Preferences

- Let $\mathcal{H}^{(n)}$ be the set of all functions from $\mathcal{X}$ to $\mathcal{Y}$
- $\text{ERM}_{\mathcal{H}^{(n)}}$ can be computed efficiently
- Sample complexity: $VC(\mathcal{H}^{(n)})/\epsilon^2 = d^2/\epsilon^2$
- Improper learning



Sample-Computational Tradeoff



	Samples	Time
$\text{ERM}_{\mathcal{H}}$	d	$d!$
$\text{ERM}_{\mathcal{H}^{(n)}}$	d^2	d^2

Is this the best we can do?

- Analysis is based on upper bounds
- Is it possible to (improperly) learn efficiently with $d \log(d)$ examples ? Posed as an open problem by:
  - Jake Abernathy (COLT'10)
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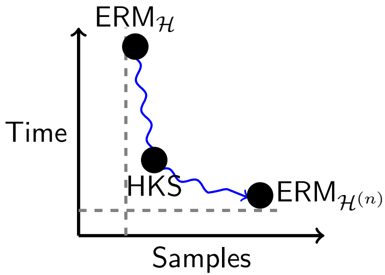
  - Kleinberg, Niculescu-Mizil, Sharma (Machine Learning 2010)
- Hazan, Kale, S. (COLT'12):
  - Can learn *efficiently* with $\frac{d\log^3(d)}{\epsilon^2}$ examples

Sample-Computational Tradeoff



	Samples	Time
$\mathrm{ERM}_{\mathcal{H}}$	d	$d!$
HKS	$d \log^3(d)$	$d^4 \log^3(d)$
$\mathrm{ERM}_{\mathcal{H}^{(n)}}$	d^2	d^2

HKS: Proof idea

- Each permutation π can be written as a matrix, s.t.,

$$W(i,j) = \begin{cases} 1 & \text{if } \pi(i) < \pi(j) \\ 0 & \text{o.w.} \end{cases}$$

- Definition: A matrix is (β, τ) decomposable if its symmetrization can be written as $P - N$ where P, N are PSD, have trace bounded by τ, and diagonal entries bounded by β
- Theorem: There's an efficient online algorithm with regret of $\sqrt{\tau\beta\log(d)T}$ for predicting the elements of (β, τ)-decomposable matrices
- Lemma: Permutation matrices are $(\log(d), d\log(d))$ decomposable.

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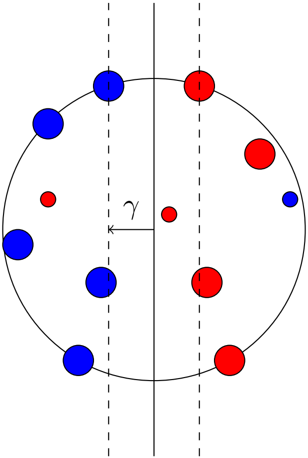
Learning Margin-Based Halfspaces

Prior assumption: $\min_{w:\|w\|=1} \mathbb{P}[y\langle w,x\rangle \le \gamma]$ is small.



Learning Margin-Based Halfspaces

- Goal: Find $h_S : \mathcal{X} \to \{\pm 1\}$ such that

$$\mathbb{P}[h_S(x) \neq y] \;\leq\; (1+\alpha) \min_{w:\|w\|=1} \mathbb{P}[y\langle w, x\rangle \leq \gamma] + \epsilon$$

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- Known results:

	α	Samples	Time
Ben-David and Simon	0	$\frac{1}{\gamma^2\,\epsilon^2}$	$\exp(1/\gamma^2)$
SVM (Hinge-loss)	$\frac{1}{\gamma}$	$\frac{1}{\gamma^2\,\epsilon^2}$	$\mathrm{poly}(1/\gamma)$

- Trading approximation factor for runtime
- What if $\alpha \in (0, 1/\gamma)$?

Learning Margin-Based Halfspaces

Theorem (Birnbaum and S., NIPS'12)

Can achieve α-approximation using time and sample complexity of

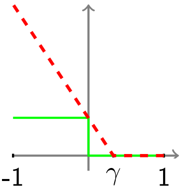
$$\mathrm{poly}(1/\gamma) \cdot \exp\left(\frac{4}{(\gamma\,\alpha)^2}\right)$$

Corollary

Can achieve $\alpha = \frac{1}{\gamma\sqrt{\log(1/\gamma)}}$ in polynomial time

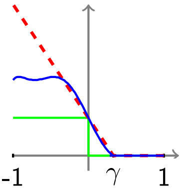
Proof Idea

- SVM relies on the hinge-loss as a convex surrogate:
  $\ell(w,(x,y)) = \left[1 - y\frac{\langle w,x\rangle}{\gamma}\right]_+$



Proof Idea

- SVM relies on the hinge-loss as a convex surrogate: $\ell(w,(x,y)) = \left[1 - y\frac{\langle w,x\rangle}{\gamma}\right]_+$
- Compose the hinge-loss over a polynomial $[1 - yp(\langle w,x\rangle)]_+$



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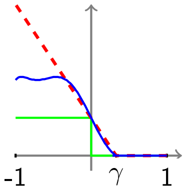
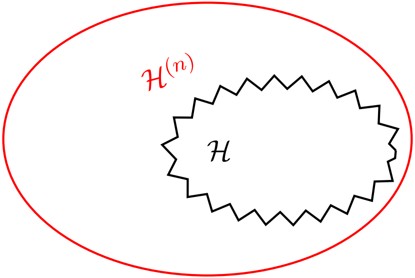


- But now the loss function is non convex ...

Proof Idea (Cont.)

- Let $p(x) = \sum_j \beta_j x^j$ be the polynomial
- Original class: $\mathcal{H} = \{x \mapsto p(\langle w, x \rangle) : \|w\| = 1\}$
- Define kernel: $k(x, x') = \sum_j |\beta_j| (\langle x, x' \rangle)^j$
- New class: $\mathcal{H}^{(n)} = \{x \mapsto \langle v, \Psi(x) \rangle : \|v\| \leq B\}$ where Ψ is the mapping corresponds to the kernel
- $\mathrm{ERM}_{\mathcal{H}^{(n)}}$ can be computed efficiently (due to convexity)
- Sample complexity: B^2/ϵ^2



Can we do better ?

Theorem (Daniely, Lineal, S. 2012)

For every kernel, SVM cannot obtain $\alpha < \frac{1}{\gamma \,\mathrm{poly}(\log(\gamma))}$ *with* $\mathrm{poly}(1/\gamma)$ *samples. A similar lower bound holds for any feature-based mapping (not necessarily kernel-based).*

- Open problem: lower bounds for other techniques / any technique ?

Proof ideas

- A one dimensional problem: $\mathcal{D} = (1-\lambda)\mathcal{D}_1 + \lambda\mathcal{D}_2$

- Every low degree polynomial with hinge-loss smaller than 1 must have $p(\gamma) \approx p(-\gamma)$.
- Pull back the distribution to high dimension
- Use a characterization of Hilbert spaces corresponding to symmetric kernels, from which we can write f using Legendre polynomials and reduce to the 1-dim case
- By averaging the kernel over the group of linear isometries of $\mathbb{R}^d$, we relax the assumption that the kernel is symmetric

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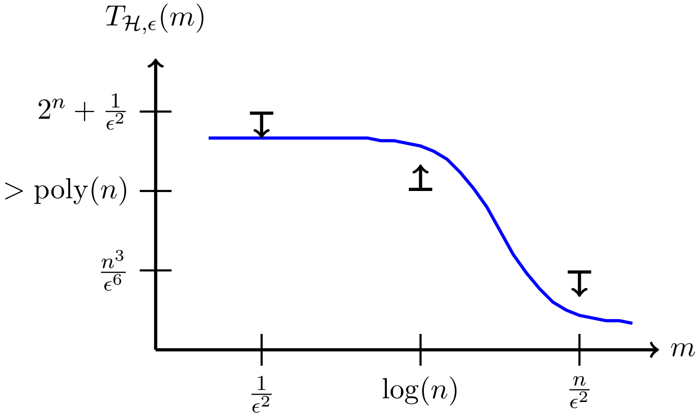
Formal Derivation of Gaps

Theorem (Shamir, S., Tromer 2012): Assume one-way permutations exist, there exists an agnostic learning problem such that:



Proof: One Way Permutations

$P : \{0,1\}^n \rightarrow \{0,1\}^n$ is one-way permutation if it's one-to-one and

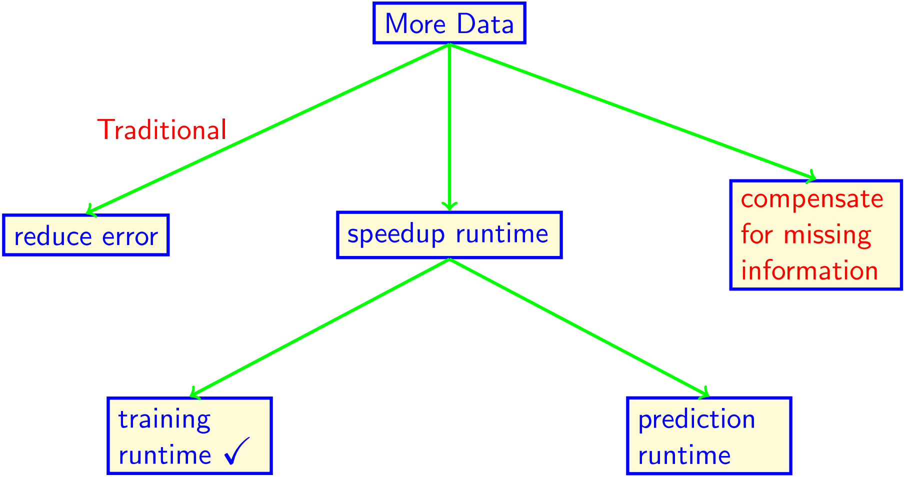
- It is easy to compute $\mathbf{w} = P(\mathbf{s})$
- It is hard to compute $\mathbf{s} = P^{-1}(\mathbf{w})$

Goldreich-Levin Theorem: If P is one way, then for any algorithm A,

$$\exists \mathbf{w} \text{ s.t. } \mathop{\mathbb{P}}_{\mathbf{r}}[A(\mathbf{r}, P(\mathbf{w})) = \langle \mathbf{r}, \mathbf{w} \rangle] < \frac{1}{2} + \frac{1}{\text{poly}(n)}$$

Proof: One Way Permutations

What *else* can we do with more data?



Online Bandit Multiclass Prediction

- A hypothesis class $\mathcal{H}$
- For $t = 1, 2, \ldots, T$
  - Receive $\mathbf{x}_t \in \mathbb{R}^d$
  - Predict $\hat{y}_t \in \{1, \ldots, k\}$
  - Pay $\mathbf{1}[\hat{y}_t \neq h^*(\mathbf{x}_t)]$

Goal: Minimize number of mistakes

Online Bandit Multiclass Prediction

- Consider $\mathcal{H}$ to be linear predictors with large margin
- In the full information setting (i.e. learner observes $h^*(\mathbf{x}_t)$), Perceptron achieves error rate of $O(1/T)$
- In the bandit case:
  - Error rate of $O(1/T)$ is achievable in exponential time
  - Error rate of $O(1/\sqrt{T})$ is achievable in linear time
  - Main idea: Exploration— Guess the label randomly with probability $\Theta(1/\sqrt{T})$.

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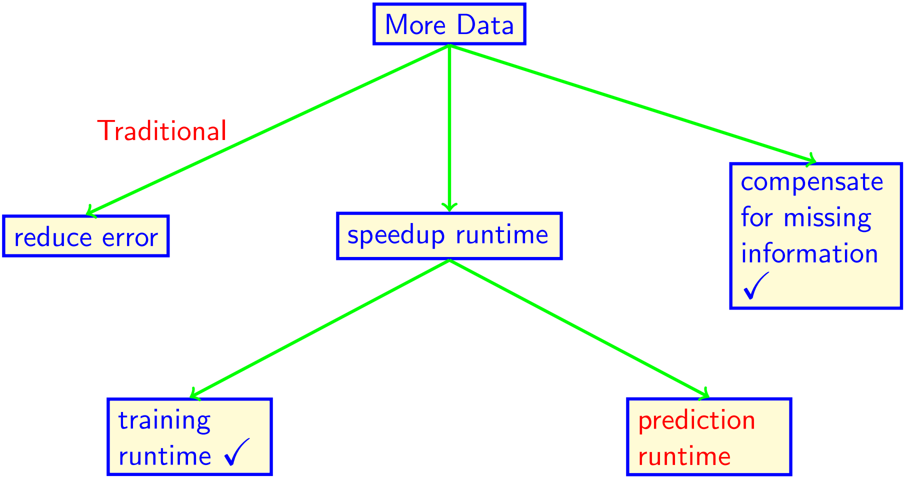

More data can speedup prediction time

- Semi-Supervised Learning: Many unlabeled examples, few labeled examples
- Most previous work: how unlabeled data can improve accuracy ?
- Our goal: how unlabeled data can help constructing *faster* classifiers
- Modeling: *Proper*-Semi-Supervised-Learning — we must output a classifier from a predefined class $\mathcal{H}$ (of fast predictors)

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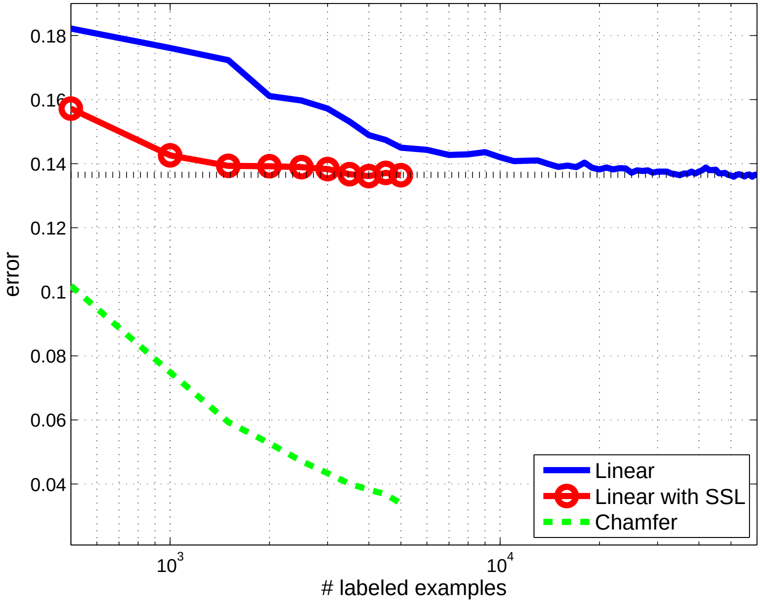
A simple two phase procedure:

- Use labeled examples to learn an arbitrary classifier (which is as accurate as possible)
- Apply the learned classifier to label the unlabeled examples
- Feed the now-labeled examples to a *proper* supervised learning for $\mathcal{H}$
- Analysis is based on the simple inequality:

$$P[h(x) \neq f(x)] \leq P[h(x) \neq g(x)] + P[g(x) \neq f(x)]$$

Demonstration



Summary

- The Bias-Variance tradeoff is well understood
- We study the Sample-Computational tradeoff
- More data can reduce runtime (both training and testing)
- More data can compensate for missing information

Open Questions

- Other techniques to control the tradeoff
- Stronger lower bounds for real-world problems