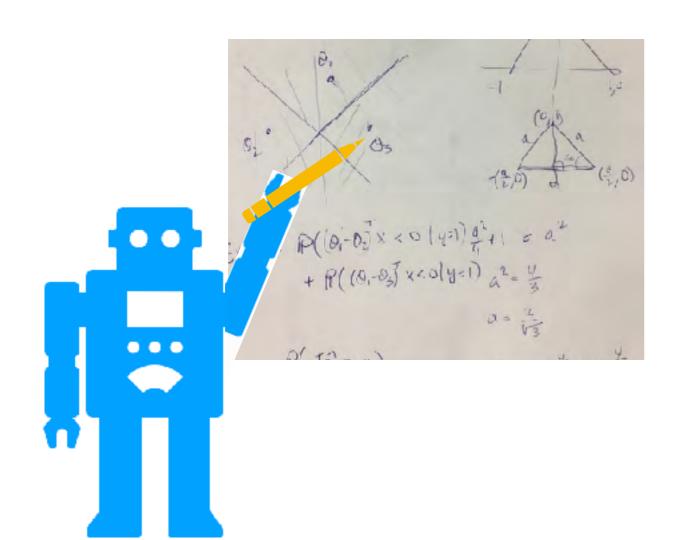
Active Learning from Theory to Practice



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ICML | 2019

Thirty-sixth International Conference on Machine Learning

Tutorial Outline



Part 1: Introduction to Active Learning (Rob)

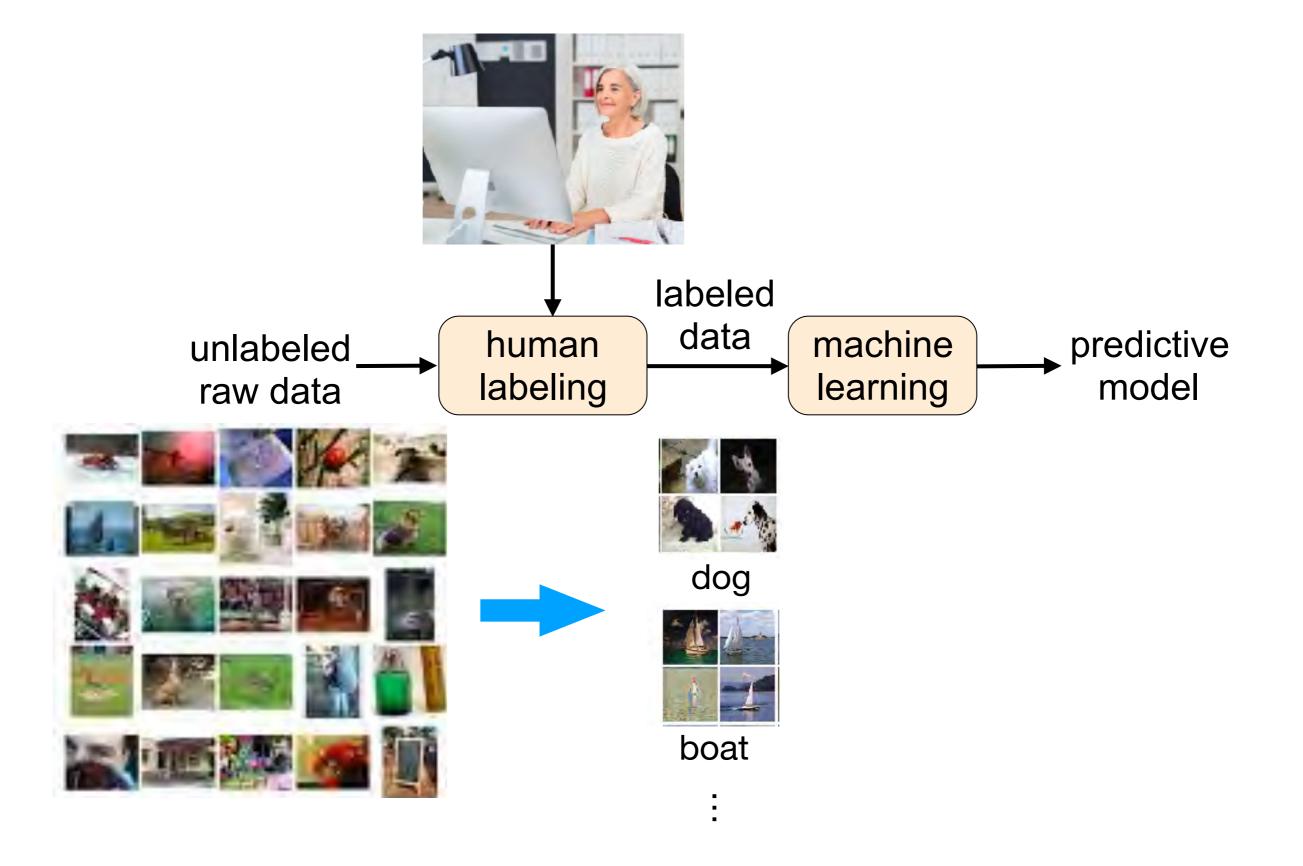
Part 2: Theory of Active Learning (Steve)

Part 3: Advanced Topics and Open Problems (Steve)

Part 4: Nonparametric Active Learning (Rob)

slides: http://nowak.ece.wisc.edu/ActiveML.html

Conventional (Passive) Machine Learning





theguardian

Computers now better than humans at recognising and sorting images

millions of labeled images 1000's of human hours

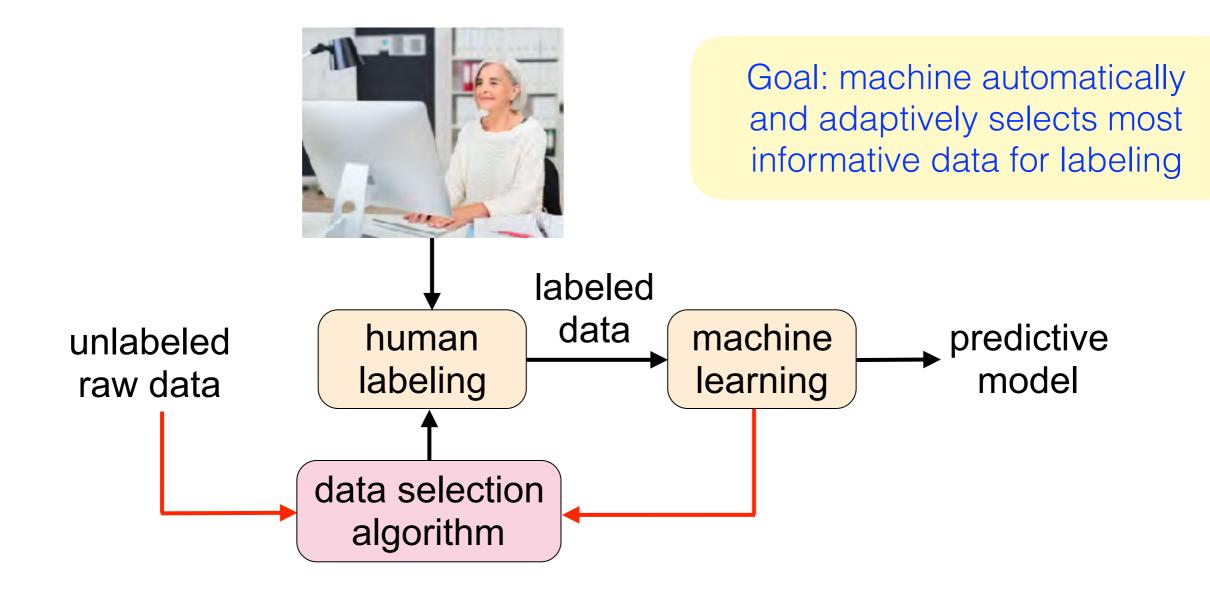
QUARTZ

Google says its new Al-powered translation tool scores nearly identically to human translators

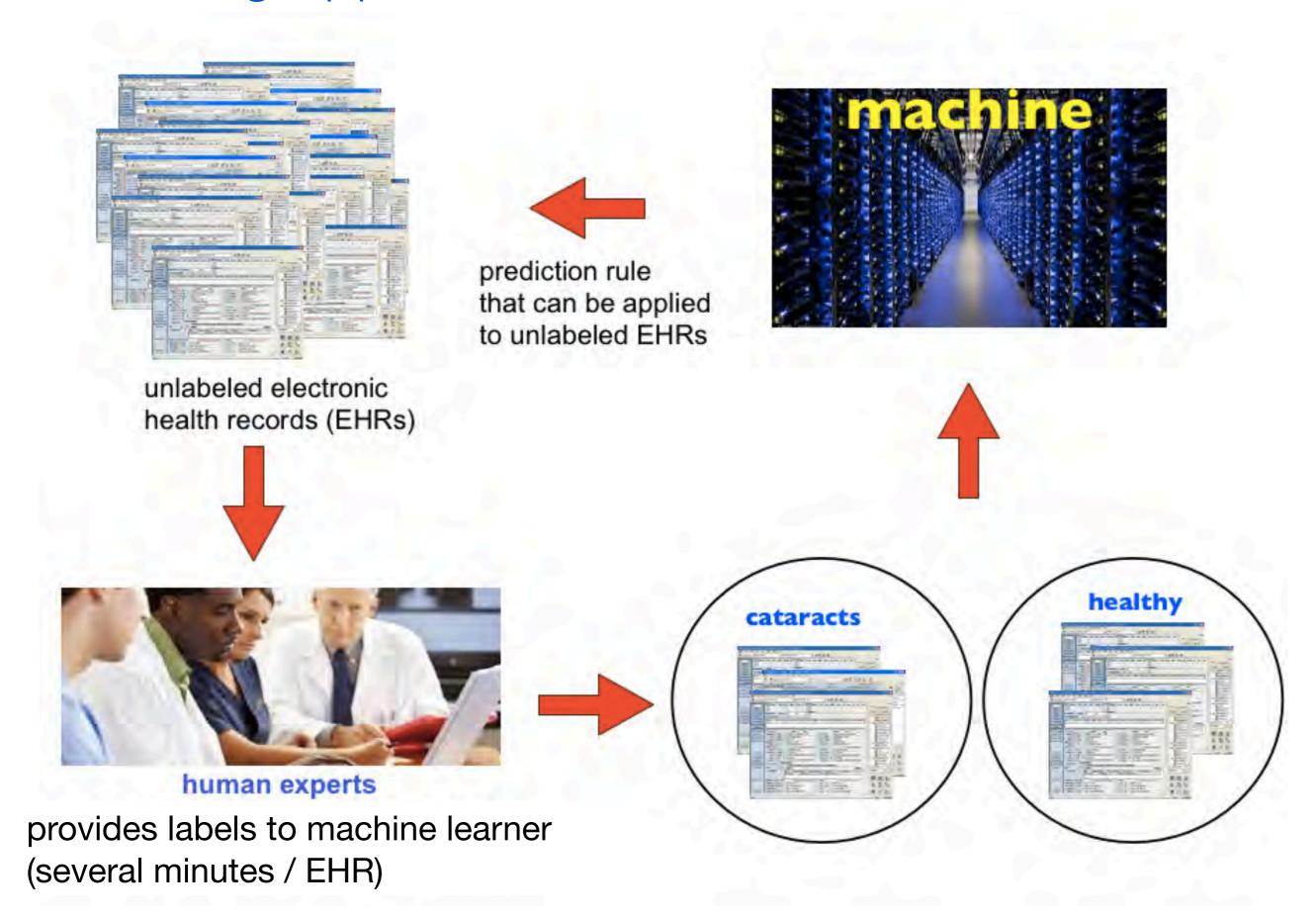
trained on more texts than a human could read in a lifetime

Can we train machines with less labeled data and less human supervision?

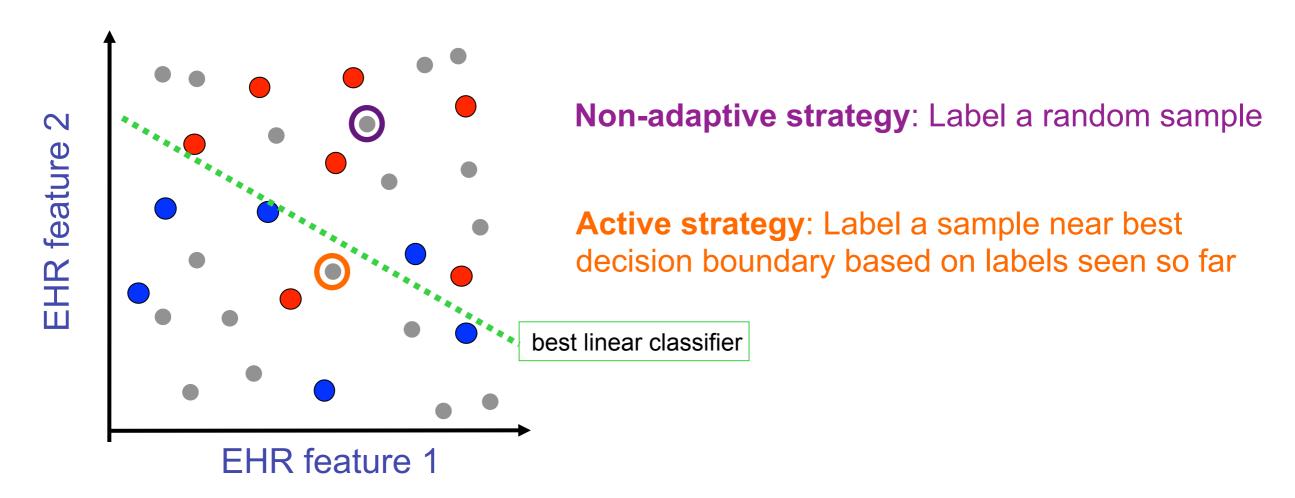
Active Machine Learning

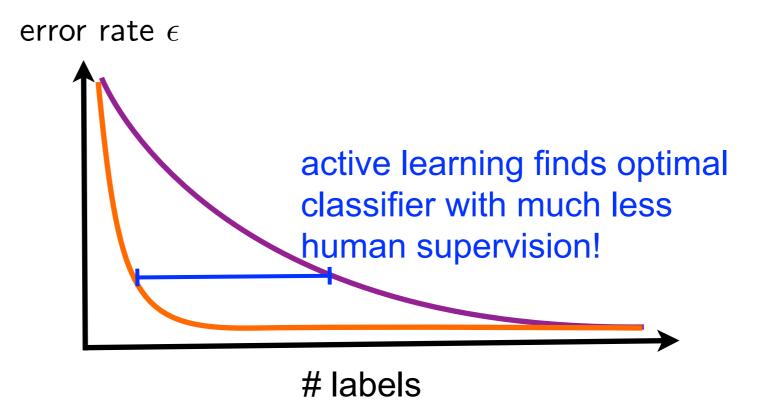


Motivating Application

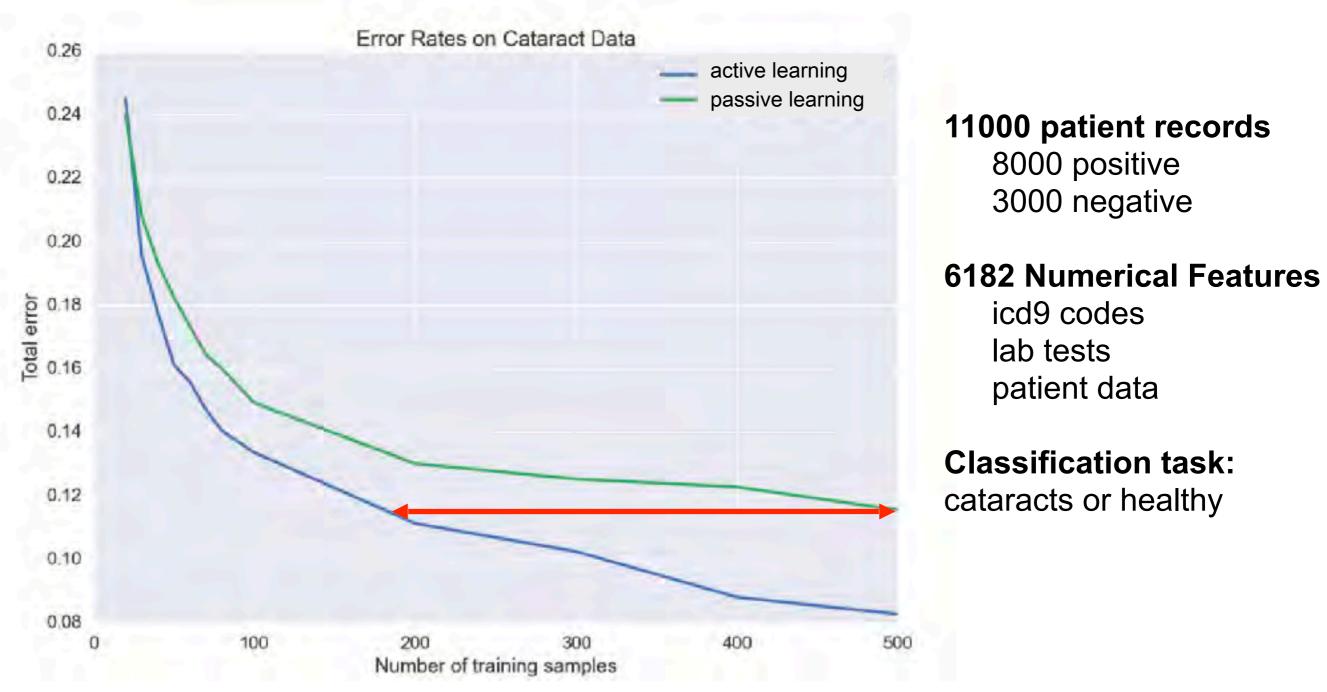


Active Learning





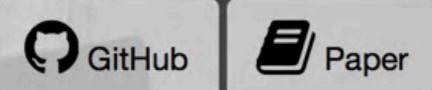
Active Logistic Regression



less than half as many labeled examples needed by active learning

NEXT

ASK BETTER QUESTIONS. GET BETTER RESULTS. FASTER. AUTOMATED.













Active learning to optimize crowdsourcing and rating in New Yorker Cartoon Caption Contest



digg



BY DOING THE EXACT OPPOSITE

How New Yorker Cartoons Could Teach Computers To Be Funny

3 diggs CNET Technology

With the help of computer scientists from the University of Wisconsin at Madison, The New Yorker for the first time is using crowdsourcing algorithms to uncover the best captions.









Actively learning user's beer preferences

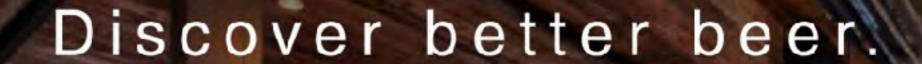


Home

Contact

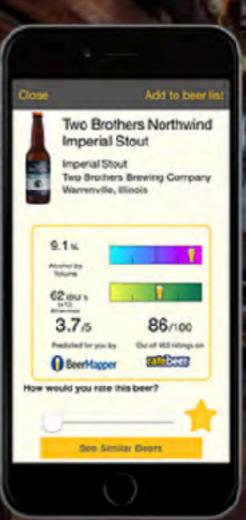
About

FAQs



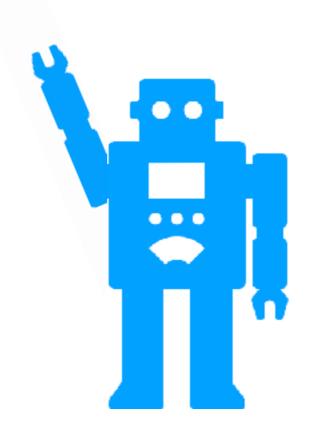






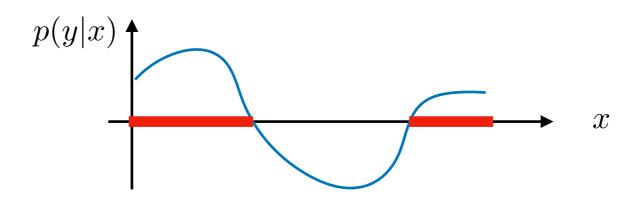
The most powerful beer app on the planet.

Principles of Active Learning



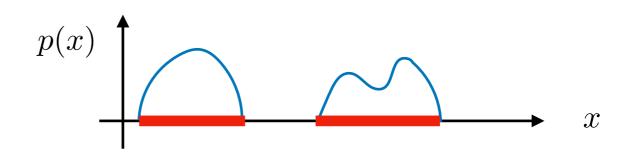
What and Where Information

Density estimation: What is p(y|x)? Classification: Where is p(y|x) > 0?



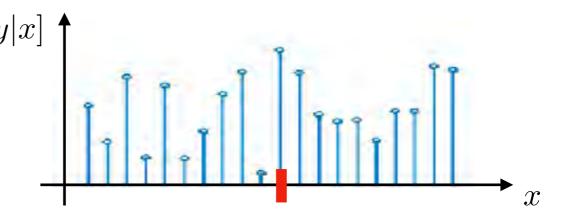
Density estimation: What is p(x)?

Clustering: Where is $p(x) > \epsilon$?



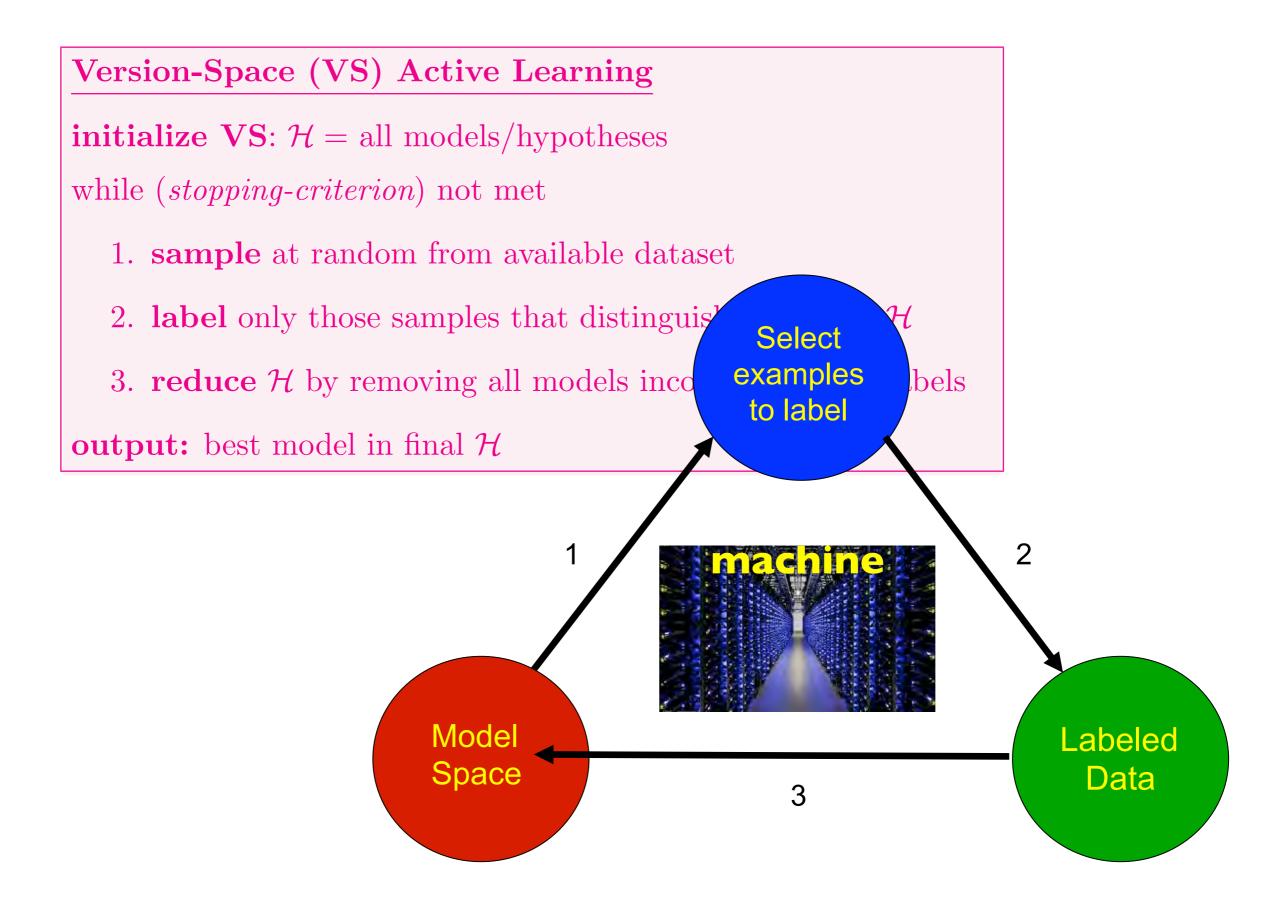
Function estimation: What is $\mathbb{E}[y|x]$?

Bandit optimization: Where is $\max_x \mathbb{E}[y|x]$?



Active learning is more efficient than passive learning for localized "where" information

Meta-Algorithm for Active Learning



Learning a 1-D Classifier



binary search quickly finds decision boundary

passive : err $\sim n^{-1}$

 $\text{active}: \text{err} \, \sim \, \, 2^{-n}$

Vapnik-Chervonenkis (VC) Theory

Given training data $\{(x_j,y_j)\}_{j=1}^n$, learn a function f to predict y from x

Consider a possibly infinite set of hypotheses \mathcal{F} with *finite VC dimension* d and for each $f \in \mathcal{F}$ define the risk (error rate):

$$R(f) := \mathbb{P}(f(x) \neq y)$$

error rate on training data:
$$\widehat{R}(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1} \Big(f(x_i) \neq y_i \Big)$$
 "empirical risk"

VC bound:
$$\sup_{f\in\mathcal{F}}|R(f)-\widehat{R}(f)| \ \leq \ 6\sqrt{\frac{d\log(n/\delta)}{n}}$$
 w.p. $\geq \ 1-\delta$

Empirical Risk Minimization (ERM)

Goal: select hypothesis with true error rate within $\epsilon > 0$ of $\min_{f \in \mathcal{F}} R(f)$

$$f^* = \arg\min_{f \in \mathcal{F}} R(f)$$
 true risk minimizer

 \widehat{f} minimizes empirical risk:

$$\widehat{f} \quad = \quad \arg\min_{f \in \mathcal{F}} \widehat{R}(f) \quad \text{empirical risk minimizer}$$

$$\widehat{R}(\widehat{f}) \leq \widehat{R}(f^*)$$

$$R(\widehat{f}) \leq \widehat{R}(\widehat{f}) + 6\sqrt{\frac{d\log(n/\delta)}{n}}$$

$$R(f^*) \geq \widehat{R}(f^*) - 6\sqrt{\frac{d\log(n/\delta)}{n}}$$

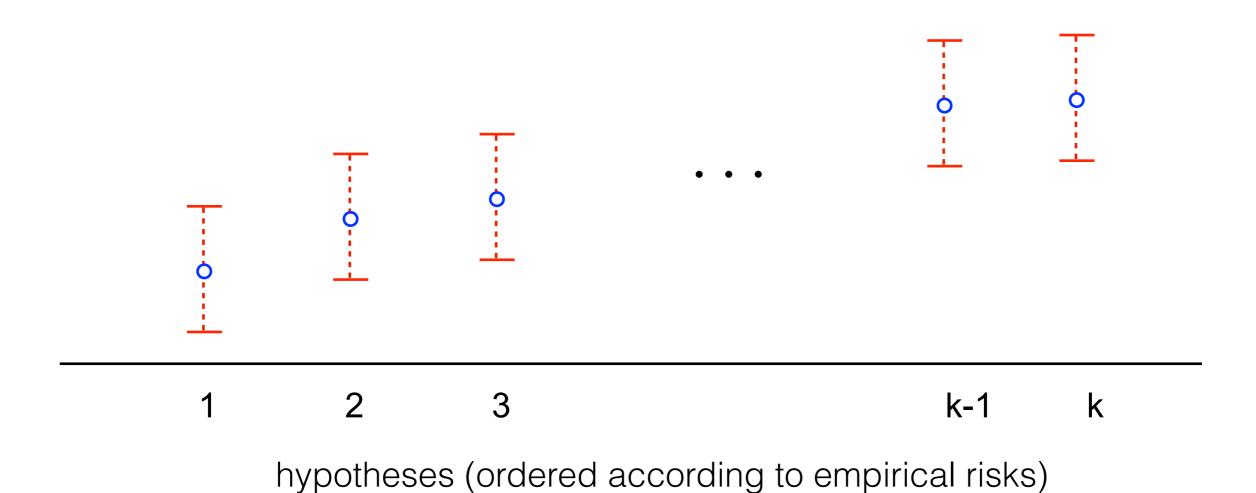
$$R(f^*) \geq \widehat{R}(f^*) - 6\sqrt{\frac{d\log(n/\delta)}{n}}$$

sufficient number of training examples:

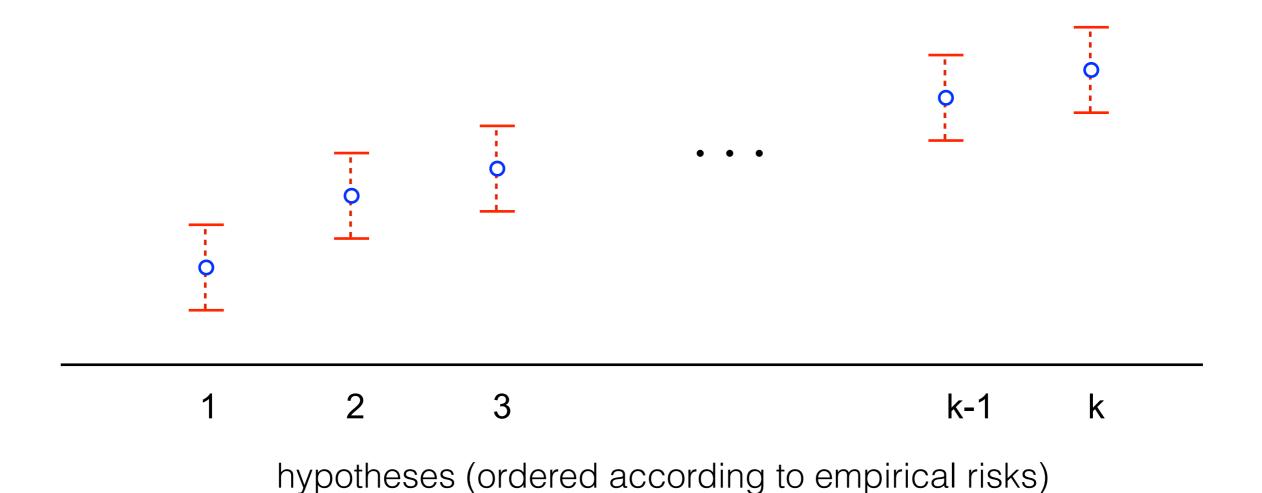
$$12\sqrt{\frac{d\log(n/\delta)}{n}} \le \epsilon \qquad \qquad n = \widetilde{O}\left(\frac{d\log(1/\delta)}{\epsilon^2}\right)$$

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Empirical Risks and Confidence Intervals

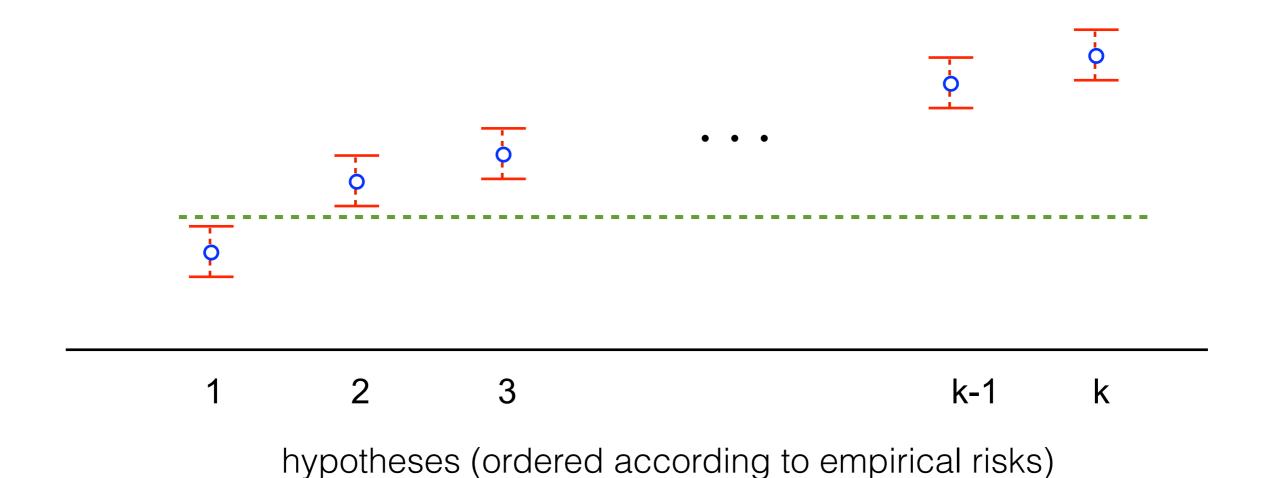


Empirical Risks and Confidence Intervals



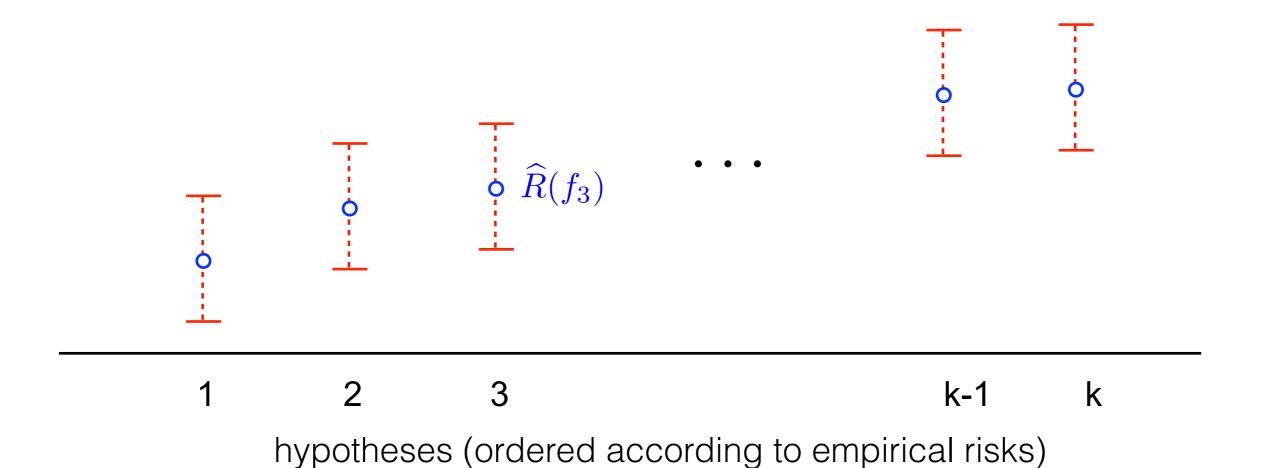
more training data ⇒ smaller confidence intervals

Empirical Risks and Confidence Intervals

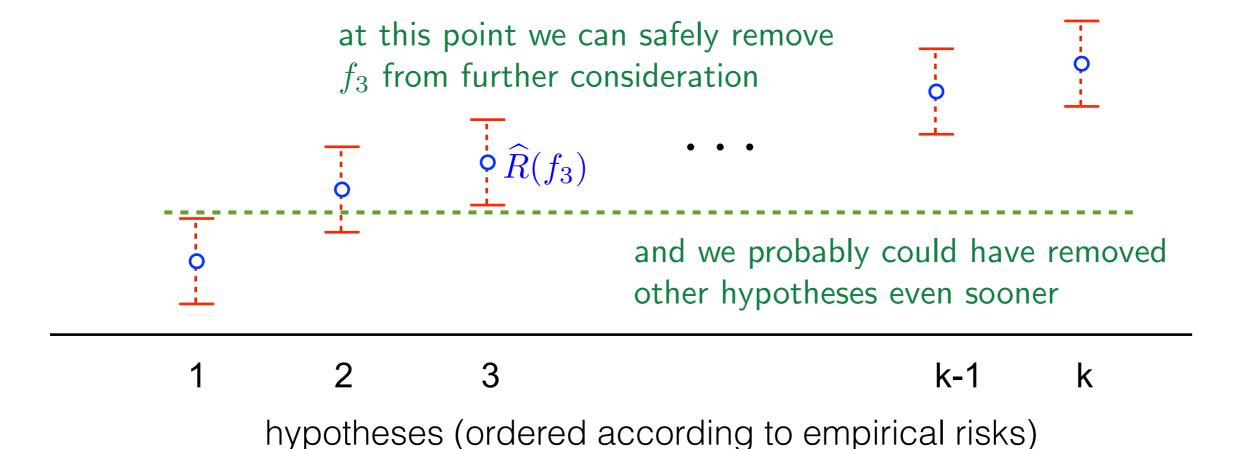


more training data ⇒ smaller confidence intervals

ERM is Wasting Labeled Examples



ERM is Wasting Labeled Examples

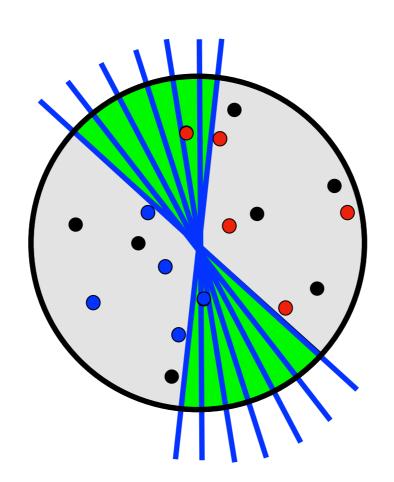


only require labels for examples that hypotheses 1 and 2 label differently (i.e., examples where they *disagree*)



Disagreement-Based Active Learning

consider points uniform on unit ball and linear classifiers passing through origin



only label points in the region of disagreement $\mathfrak D$

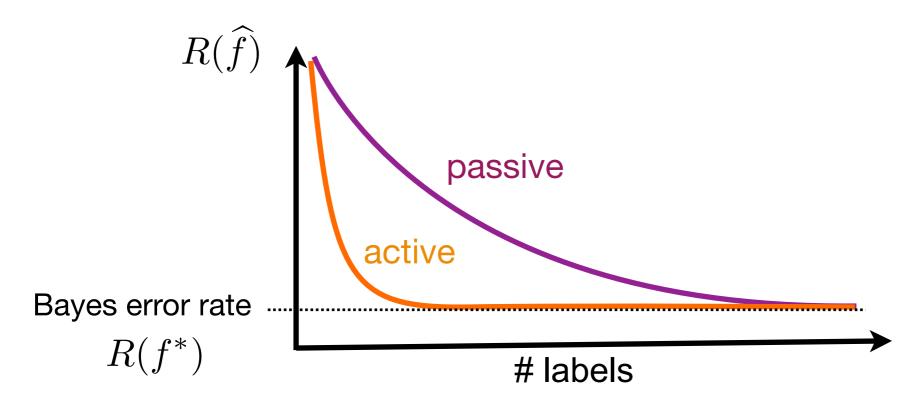
Active Binary Classification

Assuming optimal Bayes classifer f^* in VC class with dimension d and "nice" distributions (e.g., bounded label noise)

$$\epsilon = R(\widehat{f}) - R(f^*)$$

passive
$$\epsilon \sim \frac{d}{n}$$
 parametric rate

active
$$\epsilon \sim \exp\left(-c\frac{n}{d}\right)$$
 exponential speed-up



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Recommended Reading (Foundations of Active Learning)

Settles, Burr. "Active learning." *Synthesis Lectures on Artificial Intelligence and Machine Learning* 6.1 (2012): 1-114.

Dasgupta, Sanjoy. "Two faces of active learning." *Theoretical computer science* 412.19 (2011): 1767-1781.

Cohn, David, Les Atlas, and Richard Ladner. "Improving generalization with active learning." *Machine learning* 15.2 (1994): 201-221.

Castro, Rui M., and Robert D. Nowak. "Minimax bounds for active learning." *IEEE Transactions on Information Theory* 54, no. 5 (2008): 2339-2353.

Zhu, Xiaojin, John Lafferty, and Zoubin Ghahramani. "Combining active learning and semi-supervised learning using gaussian fields and harmonic functions." *ICML* 2003 workshop. Vol. 3. 2003.

Dasgupta, Sanjoy, Daniel J. Hsu, and Claire Monteleoni. "A general agnostic active learning algorithm." *Advances in neural information processing systems*. 2008.

Balcan, Maria-Florina, Alina Beygelzimer, and John Langford. "Agnostic active learning." *Journal of Computer and System Sciences* 75.1 (2009): 78-89.

Nowak, Robert D. "The geometry of generalized binary search." *IEEE Transactions on Information Theory* 57, no. 12 (2011): 7893-7906.

Hanneke, Steve. "Theory of active learning." *Foundations and Trends in Machine Learning* 7, no. 2-3 (2014).

Part 2: Theory of Active Learning General Case

- Disagreement-Based Agnostic Active Learning
- Disagreement Coefficient
- Sample Complexity Bounds

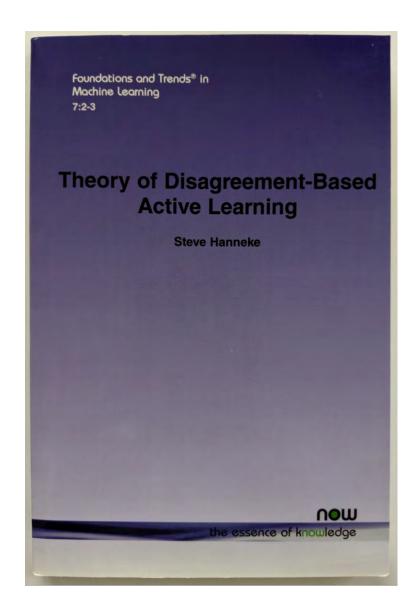
Tutorial on Active Learning: Theory to Practice

Steve Hanneke

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Robert Nowak

University of Wisconsin - Madison rdnowak@wisc.edu



Uniform Bernstein Inequality

Bernstein's inequality:

For m iid samples $\forall f, f', \text{ w.p. } 1 - \delta,$ $R(f) - R(f') \leq \hat{R}(f) - \hat{R}(f') + c\sqrt{\hat{P}(f \neq f') \frac{\log(1/\delta)}{m}} + \frac{\log(1/\delta)}{m}$

Uniform Bernstein inequality:

w.p.
$$1 - \delta$$
, $\forall f, f' \in \mathcal{H}$,

$$R(f) - R(f') \le \hat{R}(f) - \hat{R}(f') + c\sqrt{\hat{P}(f \ne f') \frac{d \log(m/\delta)}{m}} + \frac{d \log(m/\delta)}{m}$$

VC dimension

Roughly:

$$\forall f, f' \in \mathcal{H},$$

$$R(f) - R(f') \le \hat{R}(f) - \hat{R}(f') + \sqrt{\hat{P}(f \ne f') \frac{d}{m}}$$

Region of disagreement:

$$DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

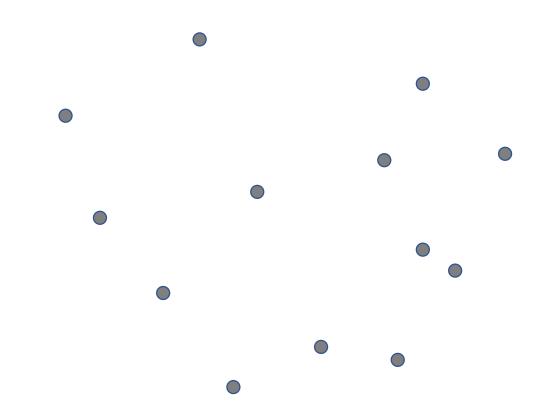
output final \hat{f}

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

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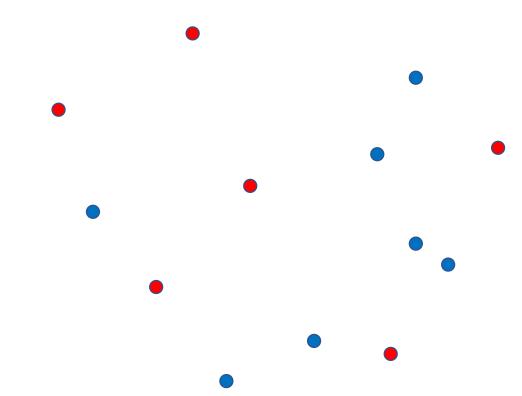
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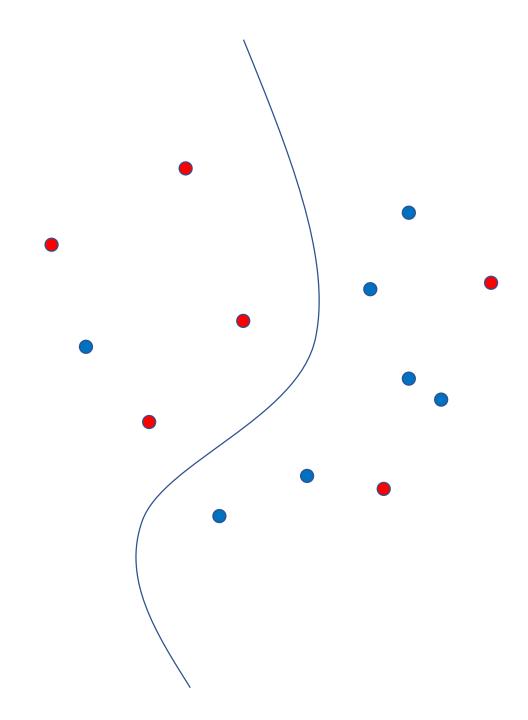


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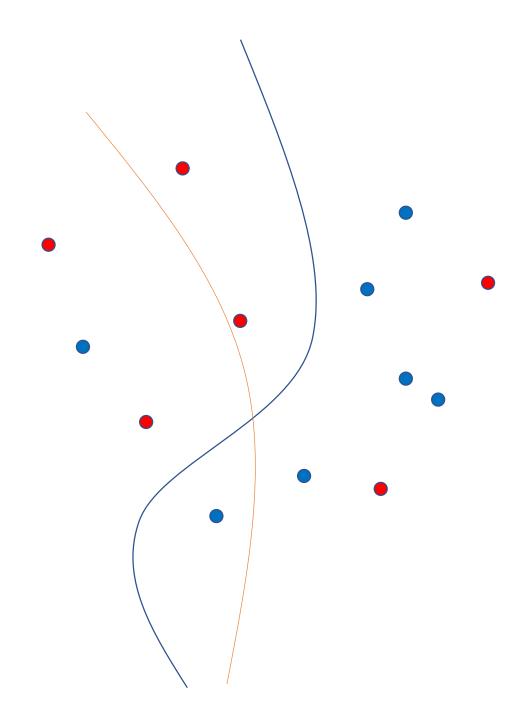


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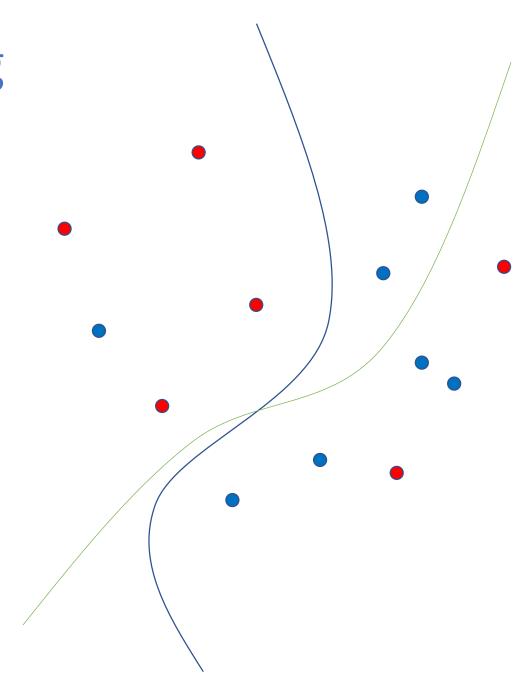


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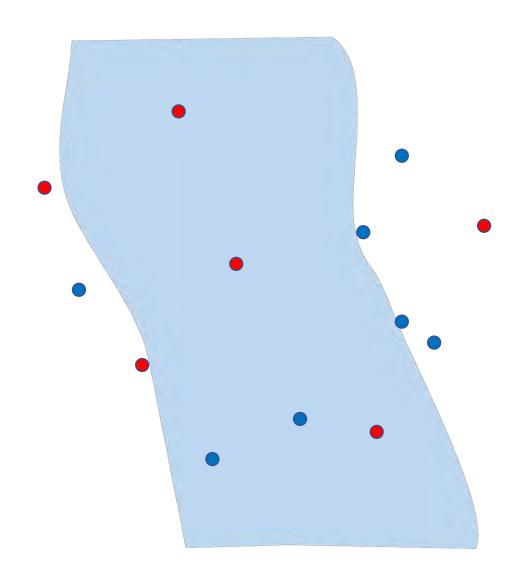


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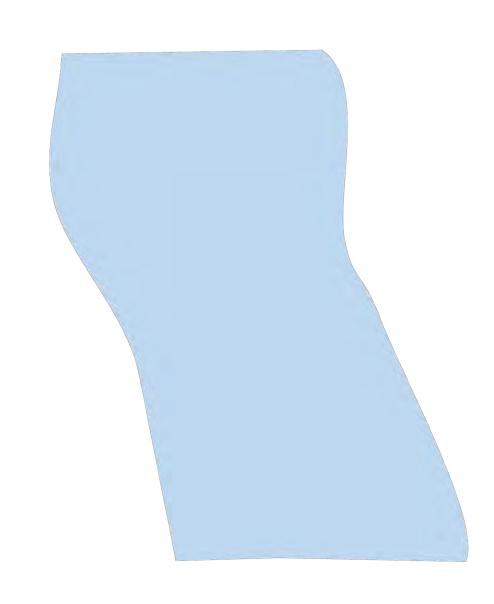


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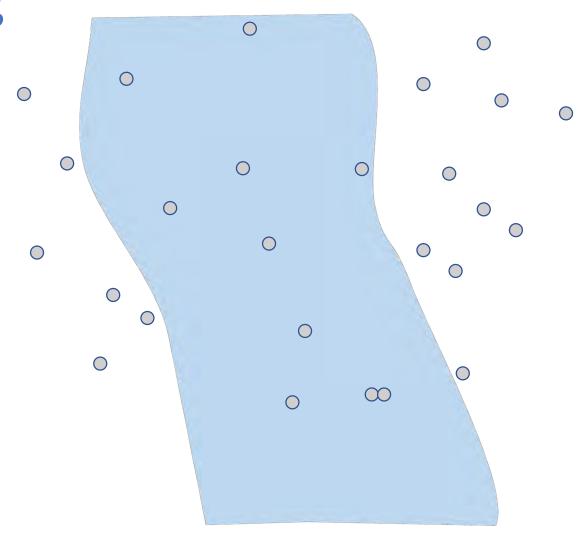


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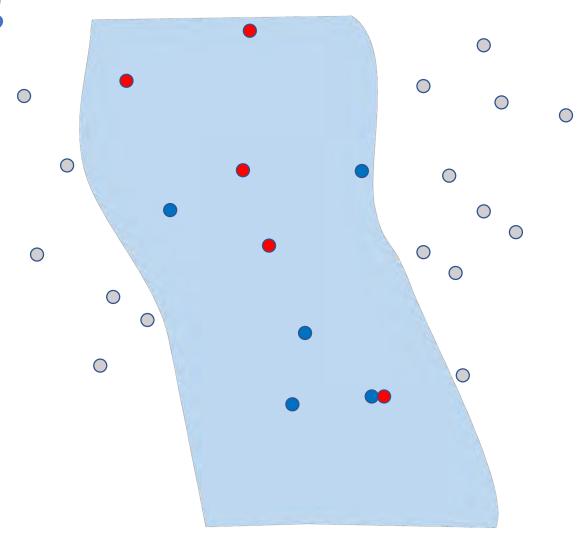


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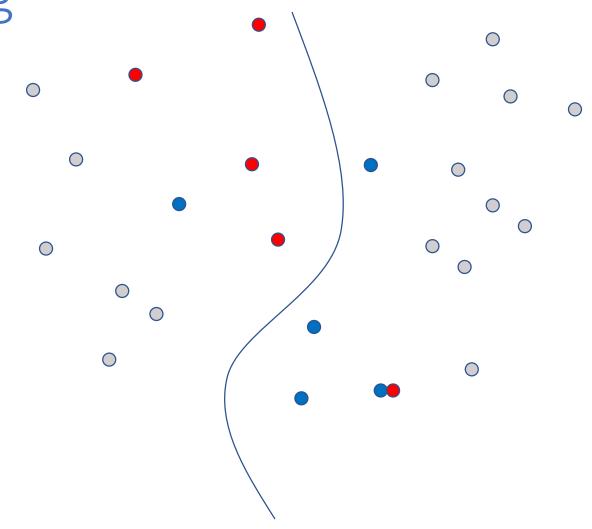
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 ${f output} \ {
m final} \ \hat{f}$



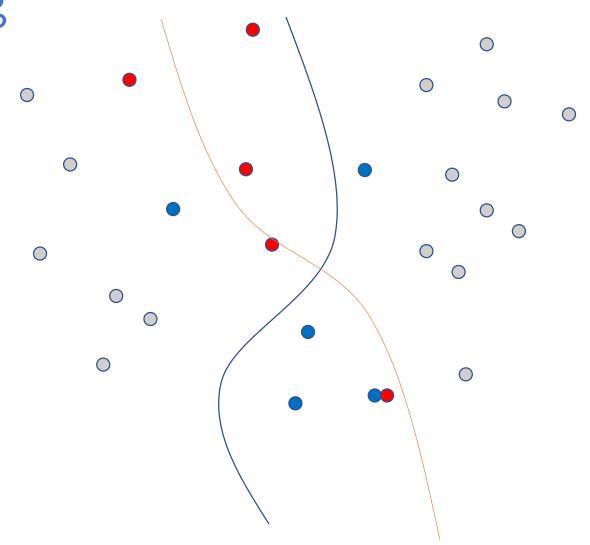
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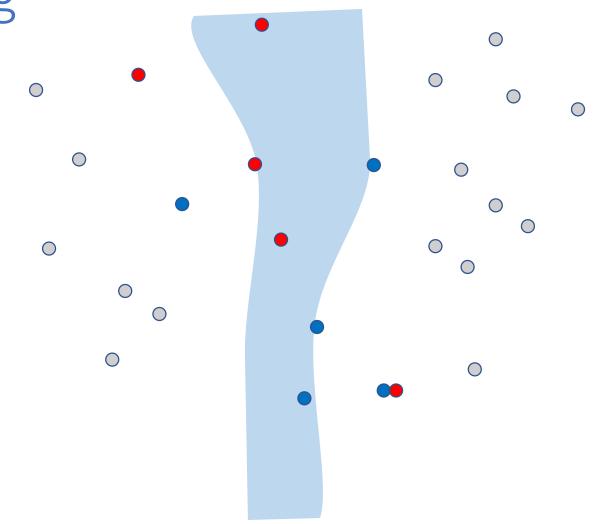
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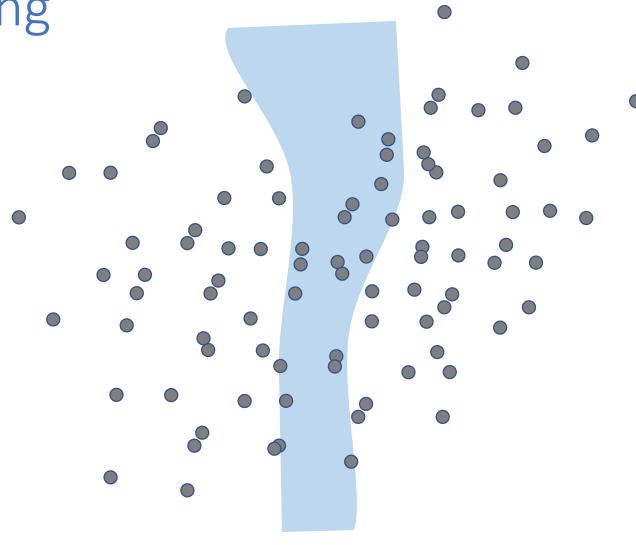


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```
for t = 1, 2, ... (til stopping\text{-}criterion)

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3. \mathbf{optimize}\ \hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}}\ \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}

output final \hat{f}
```

The point:

Any t with $f^* \in \mathcal{H}$ still, $R(f^*|\mathrm{DIS}(\mathcal{H}))$ still **minimal** in \mathcal{H}

$$\Rightarrow \hat{R}_{Q}(f^{*}) - \hat{R}_{Q}(\hat{f})$$

$$\leq R(f^{*}|\text{DIS}(\mathcal{H})) - R(\hat{f}|\text{DIS}(\mathcal{H})) + \sqrt{\hat{P}_{Q}(f^{*} \neq \hat{f})\frac{d}{|Q|}}$$

$$\leq \sqrt{\hat{P}_{Q}(f^{*} \neq \hat{f})\frac{d}{|Q|}}$$

 $\Rightarrow f^*$ never removed.

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping-criterion)

1. \mathbf{sample}\ 2^t unlabeled points S

2. \mathbf{label}\ points \ in \ Q = \mathrm{DIS}(\mathcal{H}) \cap S

3. \mathbf{optimize}\ \hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}}\ \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}

output final \hat{f}
```

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Any t with $f^* \in \mathcal{H}$ still, $R(f^*|\mathrm{DIS}(\mathcal{H}))$ still **minimal** in \mathcal{H}

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 $\Rightarrow f^*$ never removed.

Next: How many labels does it use?

Hanneke (2007,...)

Ball:
$$B(f^*, r) := \{ f \in \mathcal{H} : P_X(f \neq f^*) \leq r \}$$

$$DIS(B(f^*, r)) := \{x \in \mathcal{X} : \exists f, f' \in B(f^*, r), f(x) \neq f'(x)\}$$

Disagreement coefficient:

$$\theta = \sup_{r > \epsilon} \frac{P_X(\mathrm{DIS}(\mathrm{B}(f^*, r)))}{r}$$

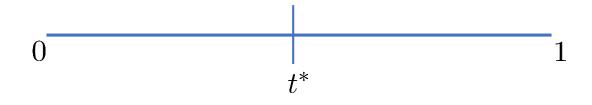
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Example: **Thresholds**, P_X Uniform(0,1) $f(x) = \mathbb{I}[x \ge t]$



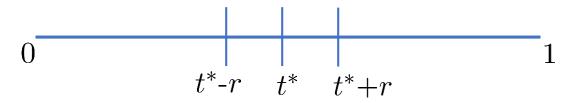
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Example: **Thresholds**, P_X Uniform(0, 1) $f(x) = \mathbb{I}[x \ge t]$



$$DIS(B(f^*, r)) = [t^* - r, t^* + r)$$

$$P_X(DIS(B(f^*, r))) = 2r$$

$$\theta = 2$$

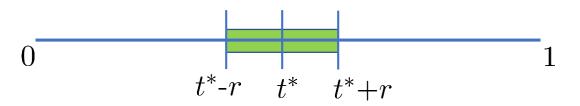
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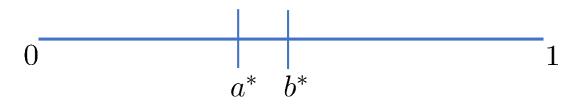
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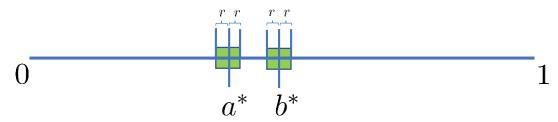


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Disagreement coefficient:

$$\theta = \sup_{r > \epsilon} \frac{P_X(\text{DIS}(B(f^*, r)))}{r}$$



$$w^* := b^* - a^*$$

If
$$r < w^*$$
,

$$DIS(B(f^*, r)) = [a^* - r, a^* + r) \cup (b^* - r, b^* + r]$$

$$P_X(DIS(B(f^*,r))) = 4r$$

Ball:
$$B(f^*, r) := \{ f \in \mathcal{H} : P_X(f \neq f^*) \leq r \}$$

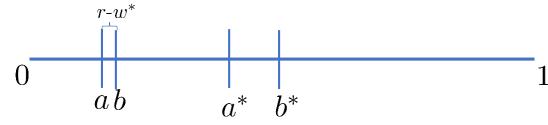
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Disagreement coefficient:

$$\theta = \sup_{r > \epsilon} \frac{P_X(\mathrm{DIS}(\mathrm{B}(f^*, r)))}{r}$$

Example: Intervals, P_X Uniform(0,1)

$$f(x) = \mathbb{I}[a \le x \le b]$$



$$w^* := b^* - a^*$$

If
$$r > w^*$$
,

$$DIS(B(f^*, r)) = \mathcal{X}$$

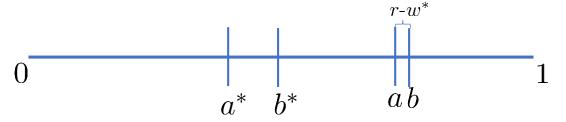
$$P_X(\mathrm{DIS}(\mathrm{B}(f^*,r)))=1$$

Ball:
$$B(f^*, r) := \{ f \in \mathcal{H} : P_X(f \neq f^*) \le r \}$$

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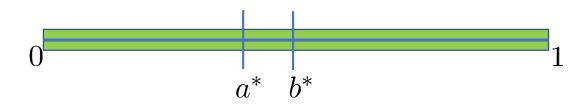
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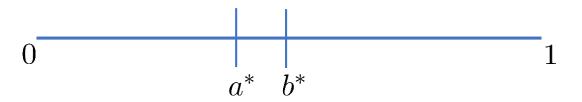
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Disagreement coefficient:

$$\theta = \sup_{r > \epsilon} \frac{P_X(\text{DIS}(B(f^*, r)))}{r}$$



$$w^* := b^* - a^*$$

If
$$\mathbf{r} < \mathbf{w}^*$$
, $P_X(\mathrm{DIS}(\mathrm{B}(f^*, r))) = 4r$

If
$$r > w^*$$
, $P_X(DIS(B(f^*, r))) = 1$

$$\Rightarrow \theta \leq \max\{4, \frac{1}{w^*}\}$$

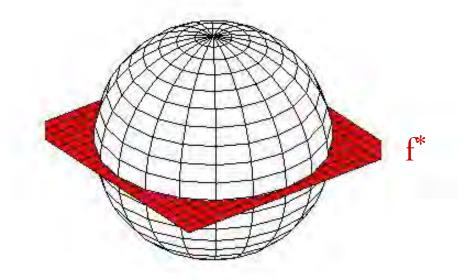
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Disagreement coefficient:

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Example: homog. linear separators (bias 0), n dimensions, uniform P_X on sphere.



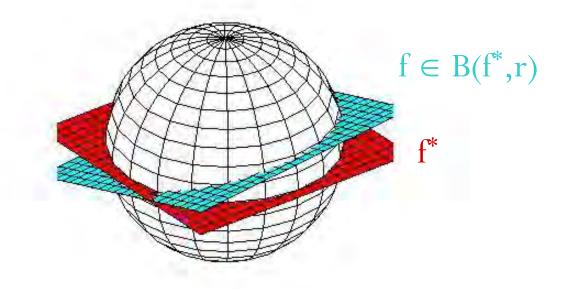
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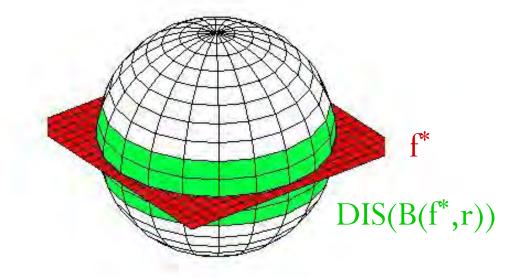
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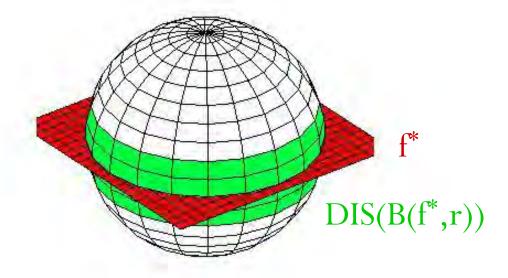
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Example: homog. linear separators (bias 0), n dimensions, uniform P_X on sphere.



Some geometry \Rightarrow for small r,

$$P_X(DIS(B(f^*,r))) \propto \sqrt{n}r.$$

$$\Rightarrow$$
 $heta \propto \sqrt{n}$.

Bounded Noise assumption: (aka Massart noise)

$$\exists \beta < 1/2 \text{ s.t. } P(Y \neq f^*(X)|X) \leq \beta \text{ everywhere}$$

	Sample Complexity: $R(\hat{f}) \leq R(f^*) + \epsilon$	Excess Error: n labels
Passive	$rac{d}{\epsilon}$	$\frac{d}{n}$
Active	$d\theta \log(\frac{1}{\epsilon})$	$e^{-n/d\theta}$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping\text{-}criterion)

1. \mathbf{sample}\ 2^t unlabeled points S

2. \mathbf{label}\ points in Q = \mathrm{DIS}(\mathcal{H}) \cap S

3. \mathbf{optimize}\ \hat{f} \leftarrow \operatorname*{argmin} \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}

output final \hat{f}
```

Theorem: $P(Y \neq f^*(X)|X) \leq \beta$. $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels $\approx d\theta \log(\frac{1}{\epsilon})$.

Proof Sketch:

Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

Roughly, that means Step 4 only keeps f with $R(f) - R(f^*) \lesssim \sqrt{P_X(f \neq f^*) \frac{d}{2^t}}$

 \Rightarrow surviving f after round t have $R(f) - R(f^*) \lesssim \frac{d}{2^t}$ $\Rightarrow t \gtrsim \log(\frac{d}{\epsilon})$ suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B(f^*, d/2^{t-1})$

$$\Rightarrow |Q| \lesssim P_X(\mathrm{DIS}(\mathrm{B}(f^*,d/2^{t-1})))|S| \leq \theta \tfrac{d}{2^{t-1}}|S| = \theta d2$$

$$\sum_{t=1}^{\log(d/\epsilon)} \theta d = \theta d \log(\frac{d}{\epsilon})$$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. **optimize** $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$

output final \hat{f}

Bounded noise:

$$R(f) - R(f^*) = \int_{f \neq f^*} (P(Y = f^*(X)|X) - P(Y \neq f^*(X)|X)) dP_X$$

$$\geq (1 - 2\beta)P_X(f \neq f^*)$$

Theorem: $P(Y \neq f^*(X)|X) \leq \beta$. $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels $\approx d\theta \log(\frac{1}{\epsilon})$.

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Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

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Agnostic Learning: (no assumptions)

Denote $\beta = R(f^*)$

	Sample Complexity: $R(\hat{f}) \leq R(f^*) + \epsilon$	Excess Error: n labels
Passive	$drac{eta}{\epsilon^2}$	$\sqrt{rac{deta}{n}}$
Active	$d heta rac{eta^2}{\epsilon^2}$	$\sqrt{rac{deta^2 heta}{n}}$

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A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. **optimize** $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

output final \hat{f}

Theorem:
$$\beta = R(f^*)$$
. $R(\hat{f}) \leq R(f^*) + \epsilon$ with

labels
$$\approx d\theta \frac{\beta^2}{\epsilon^2}$$
.

Proof Sketch:

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Roughly, that means Step 4 only keeps f with

$$R(f) - R(f^*) \lesssim \sqrt{P_X(f \neq f^*) \frac{d}{2^t}}$$

 \Rightarrow surviving f after round t have $R(f) - R(f^*) \lesssim \sqrt{\beta \frac{d}{2^t}} + \frac{d}{2^t}$

(Roughly)
$$\sqrt{\beta \frac{d}{2^t}}$$

$$\Rightarrow t \gtrsim \log(d\frac{\beta}{\epsilon^2})$$
 suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B\left(f^*, 2\beta + \sqrt{\beta \frac{d}{2^{t-1}}}\right) \subseteq B(f^*, 3\beta)$ (for large t)

$$\Rightarrow |Q| \lesssim P_X(\mathrm{DIS}(\mathrm{B}(f^*, 3\beta)))|S| \lesssim \theta\beta|S| = \theta\beta 2^t$$

$$\sum_{t=1}^{\log(d\beta/\epsilon^2)} \theta \beta 2^t \sim \theta d \frac{\beta^2}{\epsilon^2}$$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. **optimize** $\hat{f} \leftarrow \operatorname*{argmin}_{f \in \mathcal{H}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$

output final \hat{f}

$$P_X(f \neq f^*) \le R(f) + R(f^*) = 2\beta + R(f) - R(f^*)$$

Theorem:
$$\beta = R(f^*)$$
. $R(\hat{f}) \leq R(f^*) + \epsilon$ with

labels
$$\approx d\theta \frac{\beta^2}{\epsilon^2}$$
.

Proof Sketch:

Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

Roughly, that means Step 4 only keeps f with

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 \Rightarrow surviving f after round t have $R(f) - R(f^*) \lesssim \sqrt{\beta \frac{d}{2^t}} + \frac{d}{2^t}$ (Roughly) $\sqrt{\beta \frac{d}{2^t}}$

$$\Rightarrow t \gtrsim \log(d\frac{\beta}{\epsilon^2})$$
 suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B\left(f^*, 2\beta + \sqrt{\beta \frac{d}{2^{t-1}}}\right) \subseteq B(f^*, 3\beta)$ (for large t)

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When is θ small?

- Linear separators, P_X has a density, f^* boundary intersects interior of support $\Rightarrow \theta$ bounded
- Linear separators, P_X has a density $\Rightarrow \theta \ll \frac{1}{\epsilon}$
- \mathcal{H} smoothly-parametrized model, P_X "regular" density w/ compact support, other technical conditions on \mathcal{H} $\Rightarrow \theta \propto \#$ parameters for \mathcal{H}

• • • •

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- \mathcal{H} smoothly-parametrized model, P_X "regular" density w/ compact support, other technical conditions on \mathcal{H} $\Rightarrow \theta \propto \#$ parameters for \mathcal{H}
- . . .

Lots more



Stopping Criterion

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping\text{-}criterion)

1. \mathbf{sample}\ 2^t unlabeled points S

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3. \mathbf{optimize}\ \hat{f} \leftarrow \operatorname*{argmin}\ \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}.

\mathbf{output}\ \text{final}\ \hat{f}
```

Stopping criteria:

- Any-time
- Label budget
- Run out of unlabeled data
- Check $\max_{f \in \mathcal{H}} \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}} < \epsilon$

Simpler Agnostic Active Learning

Hsu (2010,...)

```
Q \leftarrow \{\}
for m = 1, 2, \dots (til stopping-criterion)
      1. sample a random point x
      2. optimize \forall y, \hat{f}_y \leftarrow \underset{f \in \mathcal{H}: f(x)=y}{\operatorname{argmin}} \hat{R}_Q(f)
      3. if |\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_- \ne \hat{f}_+) \frac{d}{|Q|}}
           then label x, add it to Q
output \hat{f} = \operatorname{argmin} \hat{R}_{\mathcal{O}}(f)
```

- Roughly same sample complexity as A^2 .
- Can implement as a **reduction** to ERM.
- In practice, replace ERM with any passive learner.

Surrogate Loss

```
Q \leftarrow \{\}
for m = 1, 2, \dots (til stopping-criterion)
       1. sample a random point x
      2. optimize \forall y, \hat{f}_y \leftarrow \underset{f \in \mathcal{H}: f(x) = y}{\operatorname{argmin}} \hat{R}_Q^{\ell}(f)
      3. if |\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_- \ne \hat{f}_+) \frac{d}{|Q|}}
            then label x, add it to Q
output \hat{f} = \operatorname{argmin} \hat{R}_{\mathcal{O}}(f)
```

- Roughly same sample complexity as A^2 .
- Can implement as a **reduction** to ERM.
- In practice, replace ERM with any passive learner.

Consider learner that minimizes a **surrogate loss** $\ell : \mathbb{R} \times \{-1, +1\} \to \mathbb{R}_+$ (e.g., hinge loss, squared loss, exponential loss, ...)

Now \mathcal{H} is **real-valued** functions

$$\hat{R}_Q^{\ell}(f) = \frac{1}{|Q|} \sum_{(x,y)\in Q} \ell(f(x), y)$$

Theorem: Bounded noise, plus strong assumptions on \mathcal{H}, ℓ, P still get $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels

$$\approx \theta d \log(\frac{1}{\epsilon})$$

Importance-Weighted Active Learning

Beygelzimer, Dasgupta, Langford (2009)

```
Q \leftarrow \{\} for m=1,2,\ldots (til stopping	ext{-}criterion)
```

- 1. sample a random point x
- 2. **set** sampling probability p_x
- 3. flip coin with prob p_x of heads
- 4. if heads, label x, add to Q with weight $1/p_x$

output
$$\hat{f} = \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$$
 (weighted loss)

Use importance weights to stay **unbiased**: $\mathbb{E}[\hat{R}_Q(f)] = R(f)$

Now Q set of triples (x, y, w)

$$\hat{R}_Q(f) = \frac{1}{|Q|} \sum_{(x,y,w)\in Q} w \mathbb{I}[f(x) \neq y]$$

- Any choice of Step 2 (setting p_x) is fine (just p_x not too small, else high variance)
- Can set p_x in a way to recover A^2 sample complexity $p_x = \mathbb{I}\left[|\hat{R}_Q(\hat{f}_+) \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_+ \ne \hat{f}_-) \frac{d}{|Q|}} \right]$

Importance-Weighted Active Learning

Beygelzimer, Dasgupta, Langford (2009)

```
Q \leftarrow \{\} for m=1,2,\ldots (til stopping-criterion)
```

- 1. sample a random point x
- 2. **set** sampling probability p_x
- 3. **flip** coin with prob p_x of heads
- 4. if heads, label x, add to Q with weight $1/p_x$

output
$$\hat{f} = \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$$
 (weighted loss)

Use importance weights to stay **unbiased**: $\mathbb{E}[\hat{R}_Q(f)] = R(f)$

Now Q set of triples (x, y, w)

$$\hat{R}_Q(f) = \frac{1}{|Q|} \sum_{(x,y,w)\in Q} w \mathbb{I}[f(x) \neq y]$$

- Any choice of Step 2 (setting p_x) is fine (just p_x not too small, else high variance)
- Can set p_x in a way to recover A^2 sample complexity $p_x = \mathbb{I}\left[|\hat{R}_Q(\hat{f}_+) \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_+ \ne \hat{f}_-) \frac{d}{|Q|}} \right]$
- In practice, replace ERM with any passive learner (e.g., ERM with a surrogate loss)
- (approx) implementation in **Vowpal Wabbit** library

Questions?

Further reading:

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Part 3: Beyond Disagreement-Based Active Learning – Current Directions

- Subregion-Based Active Learning
- Margin-Based Active Learning: Linear Separators
- Shattering-Based Active Learning
- Distribution-Free Analysis, Optimality
- TicToc: Adapting to Heterogeneous Noise
- Tsybakov Noise

Tutorial on Active Learning: Theory to Practice

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University of Wisconsin - Madison rdnowak@wisc.edu

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping-criterion)

1. \mathbf{sample}\ 2^t unlabeled points S

2. \mathbf{label}\ points in Q = \mathrm{DIS}(\mathcal{H}) \cap S

3. \mathbf{optimize}\ \hat{f} \leftarrow \operatorname*{argmin} \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}

output final \hat{f}
```

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

Subregion-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = \mathcal{R}_{\epsilon'_{t}}(\mathcal{H}) \cap S$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$

 ${f output}$ final \hat{f}

Instead, pick **region** $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t. $\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$

Pick ϵ' carefully each round, $R(\hat{f}) - R(f^*) \le \epsilon$ at end

e.g., Bounded noise: $\epsilon' \propto d2^{-t}$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

Subregion-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. **label** points in $Q = \mathcal{R}_{\epsilon'_{+}}(\mathcal{H}) \cap S$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

 $\mathbf{output} \ \mathrm{final} \ \hat{f}$

Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

$$\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$$

$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

$$\approx \varphi_c d \log(\frac{1}{\epsilon})$$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

Subregion-based Active Learning

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$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

Theorem: with Bounded noise,

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

$$\approx \varphi_c d \log(\frac{1}{\epsilon})$$

Agnostic case:
$$\varphi'_c := \sup_{r>\epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,2\beta+r)))}{2\beta+r}$$

Theorem:

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

 $\approx \varphi'_c d \frac{\beta^2}{\epsilon^2}$

How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

- $\mathcal{R}_{\epsilon'}(\mathcal{H}) = \mathrm{DIS}(\mathcal{H})$ works
- Empirically (Zhang & Chaudhuri, 2014)
- Nice structure: e.g., Linear separators

Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

$$\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$$

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 Margin-based Active Learning
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$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

$$R(\hat{f}) \le R(f^*) + \epsilon$$
 using # labels

$$\approx \varphi_c d \log(\frac{1}{\epsilon})$$

How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

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(Dasgupta, Kalai, Monteleoni, 2005; Balcan, Broder, Zhang, 2007; ...) Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

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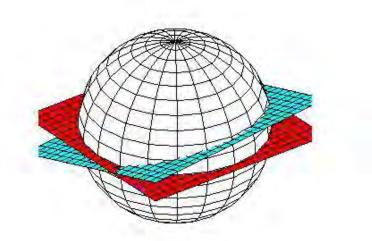
Margin-based Active Learning

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$$\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$$

Uniform P_X on d-dim sphere

For
$$w \in B(w^*, r)$$
, **project** to $Span(w, w^*)$



How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

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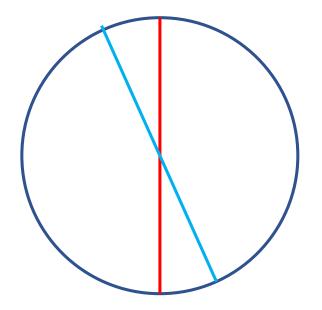
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Most projected prob mass toward middle



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Margin-based Active Learning

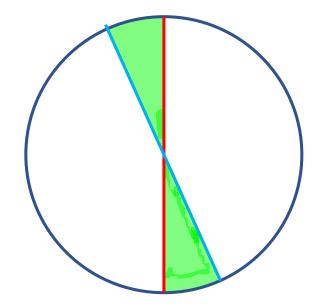
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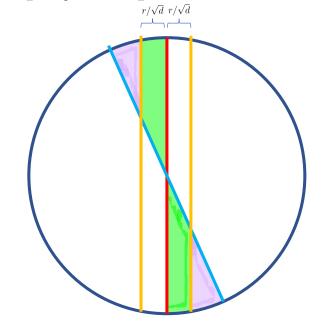
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For
$$w \in B(w^*, r)$$
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Most projected prob mass toward middle



 $DIS(\{w, w^*\})$ in slab of width $\approx r$

Most of its prob in slab of width $\approx r/\sqrt{d}$

How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

• Nice structure: e.g., **Linear separators**

Margin-based Active Learning

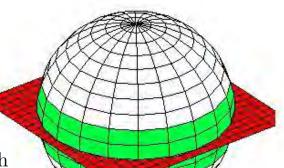
(Dasgupta, Kalai, Monteleoni, 2005; Balcan, Broder, Zhang, 2007; ...)

 $DIS(B(f^*, r)) =$ slab of width $\approx r$

Take $\mathcal{R}_{r/c}(\mathbf{B}(f^*, r)) =$ slab of width $\approx r/\sqrt{d}$

Prob in slab $\approx \sqrt{d} \times \text{width}$

 $\Rightarrow \varphi_c \leq \text{constant}$



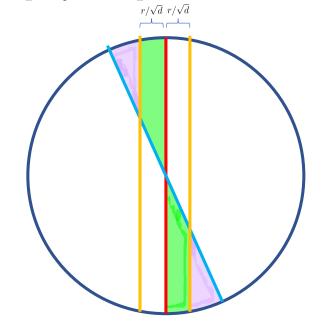
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Uniform P_X on d-dim sphere

For
$$w \in B(w^*, r)$$
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Margin-based Active Learning

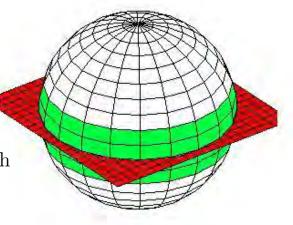
(Dasgupta, Kalai, Monteleoni, 2005; Balcan

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$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

Theorem: with Bounded noise,

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

 $\approx \varphi_c d \log(\frac{1}{\epsilon})$

$$\Rightarrow$$
 # labels $\approx d \log(\frac{1}{\epsilon})$ suffice

Recall: Passive $\approx \frac{d}{\epsilon}$

Comparison:

Recall
$$\theta \approx \sqrt{d}$$

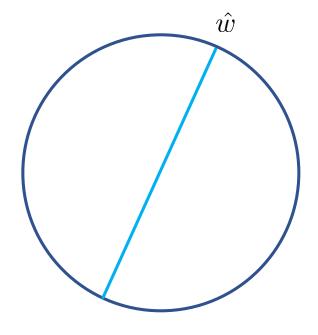
 $\Rightarrow A^2 \# \text{ labels } \approx d^{3/2} \log(\frac{1}{\epsilon})$

Margin-based Active Learning

Initialize \hat{w}

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample $d2^t$ unlabeled points S
- 2. label points in $Q = \text{all } x \in S \text{ s.t. } \langle \hat{w}, x \rangle \leq c2^{-t}/\sqrt{d}$
- 3. optimize $\hat{w} \leftarrow \underset{w:||w-\hat{w}|| \leq c'2^{-t}}{\operatorname{argmin}} \hat{R}_Q(w)$



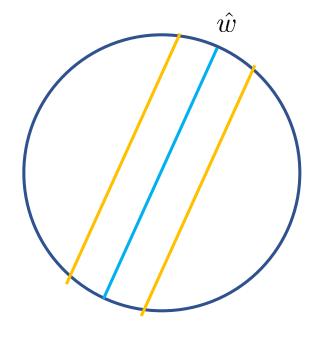
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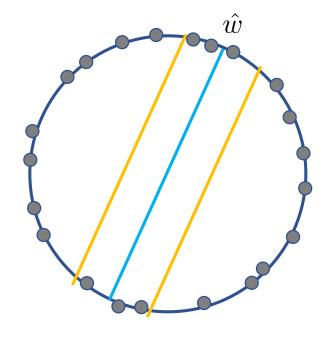
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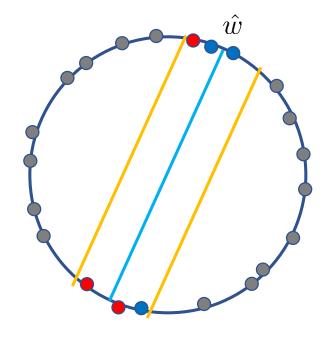
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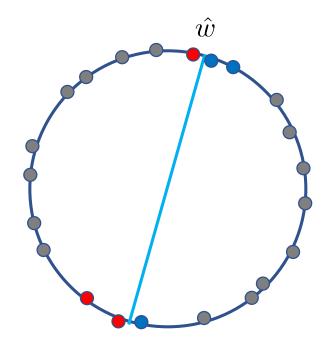
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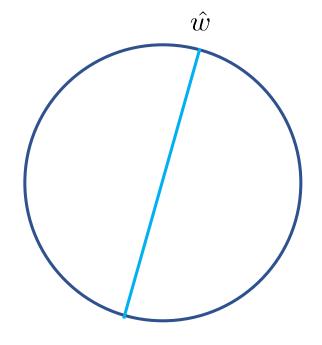
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output final \hat{w}



Uniform P_X on d-dim sphere

Theorem: with Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels $\approx d \log(\frac{1}{\epsilon})$

(also works for isotropic log-concave distributions)

(Awasthi, Balcan, Long, 2014,...)

Computational Efficiency

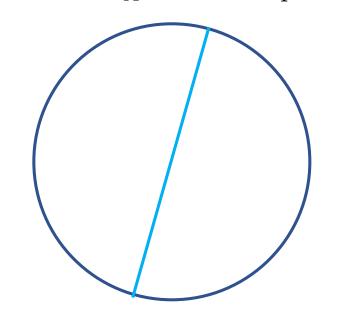
Efficient Alg Initialize \hat{w} for $t=1,2,\ldots$ (til stopping-criterion) 1. $\mathbf{sample}\ d2^t$ unlabeled points S2. $\mathbf{label}\ points$ in $Q=\text{all}\ x\in S\ \text{s.t.}\ <\hat{w},x>\ \le\ c2^{-t}/\sqrt{d}$ 3. $\mathbf{optimize}\ \hat{w}\leftarrow \underset{w:\|w-\hat{w}\|\le c'2^{-t}}{\operatorname{argmin}} \hat{R}_Q^{\ell_t}(w)$ output final \hat{w}

Surrogate loss

$$\ell_t(< w, x>, y) \approx \max\{1 - 2^t \sqrt{d}(y < w, x>), 0\}$$

Hinge loss slope changes each round

Uniform P_X on d-dim sphere



(Awasthi, Balcan, Long, 2014,...)

Computational Efficiency

```
Efficient Alg

Initialize \hat{w}

for t = 1, 2, ... (til stopping\text{-}criterion)

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Theorem: with Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels $\approx d \log \left(\frac{1}{\epsilon}\right)$ and running in polynomial time

Computational Efficiency

Efficient Alg

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Hinge loss slope changes each round

Uniform P_X on d-dim sphere

Theorem: with Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels $\approx d \log \left(\frac{1}{\epsilon}\right)$ and running in polynomial time

Theorem: with Agnostic case, $R(\hat{f}) \leq CR(f^*)$ in polynomial time

(was first alg. known to achieve these; even passively)

(also works for isotropic log-concave distributions)

Up Next: Shattering-Based Active Learning

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

 $DIS(\mathcal{H})$ checks for shattering 1 point.

Idea: Generalize to shattering ≥ 1 points.

(Hanneke, 2009, 2012)

Shattering-Based Active Learning

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

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4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}.

\mathbf{output}\ final\ \hat{f}
```

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(Hanneke, 2009, 2012)

Shattering-Based Active Learning

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

Shattering-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. **label** points in $Q = \text{all } x \in S \text{ s.t.}$ $P_X^k(A \in \mathcal{X}^k : \mathcal{H} \text{ shatters } A \cup \{x\} | \mathcal{H} \text{ shatters } A) \ge \frac{1}{2}$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
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output final \hat{f}

 $DIS(\mathcal{H})$ checks for shattering 1 point.

Idea: Generalize to shattering ≥ 1 points.

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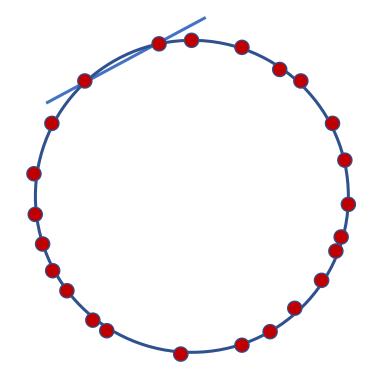
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Example: Linear separators, Uniform P_X on circle Suppose true labels are all -1

$$DIS(\mathcal{H}) = \mathbf{entire} \ \mathbf{circle}$$



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$$Try \ k = 1$$

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$$Rand \ x' \text{ probably not close}$$

$$Can't \text{ shatter } \{x, x'\}$$

$$without a lot of points wrong$$

$$So \text{ won't query } x$$

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So won't query x

$$DIS(\mathcal{H}_{x,-1})$$
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$$\theta^{(k)} := \sup_{r > \epsilon} \frac{P_X^k(A \in \mathcal{X}^k : B(f^*, r) \text{ shatters } A)}{r}$$

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Theorem: For Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels

$$\approx C\tilde{\theta}d\log(\frac{1}{\epsilon})$$

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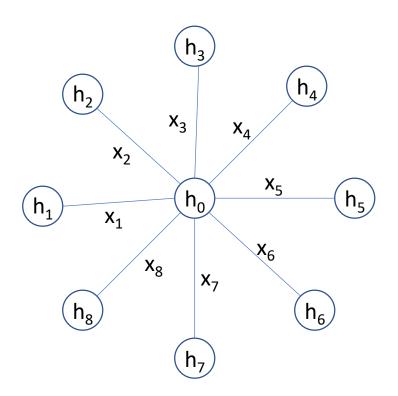
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Up Next:
Distribution-free Analysis

 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

Can we do sample complexity analysis **without** distribution-dependence?

<u>Definition:</u> The **star number** \mathfrak{s} is the largest k s.t. $\exists h_0, h_1, \ldots, h_k \in \mathcal{H}$, $\exists x_1, \ldots, x_k \in \mathcal{X}$ s.t. $\forall i \in \{1, \ldots, k\}, \{x_j : h_i(x_j) \neq h_0(x_j)\} = \{x_i\}.$



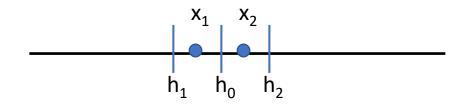
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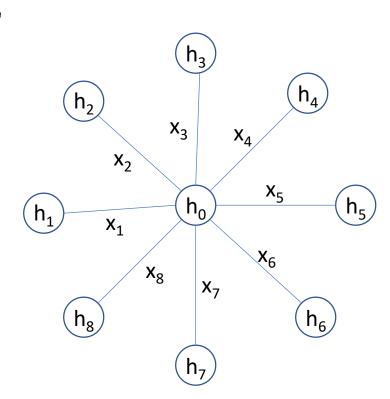
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Example: Thresholds: $f(x) = \mathbb{I}[x \ge t]$.

$$\mathfrak{s}=2.$$



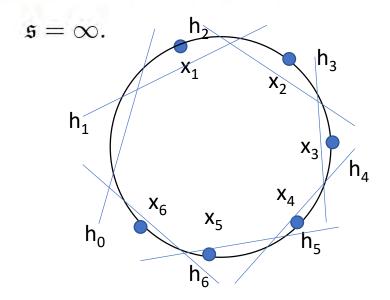


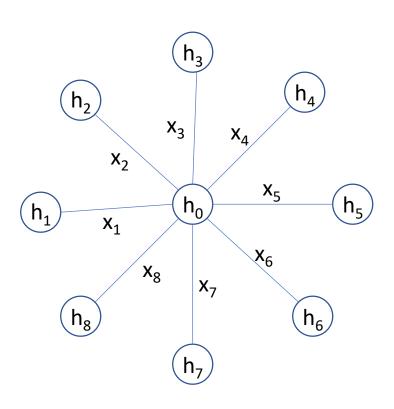
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Example: Linear Separators in \mathbb{R}^n , $n \geq 2$:





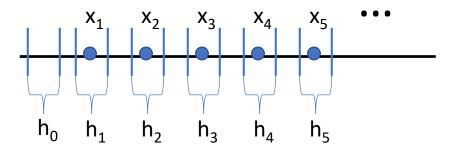
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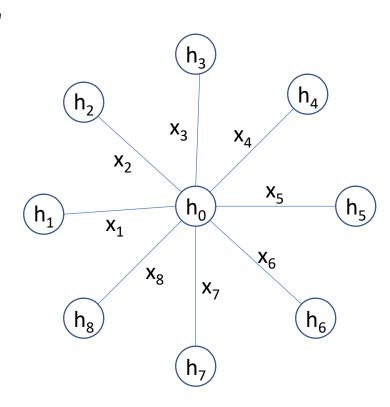
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Example: Intervals: $x \mapsto \mathbb{I}[a \le x \le b]$

$$\mathfrak{s}=\infty$$
.



Intervals of width w (b-a=w>0) on $\mathcal{X}=[0,1]$: $\mathfrak{s}\approx \lfloor \frac{1}{w} \rfloor$.



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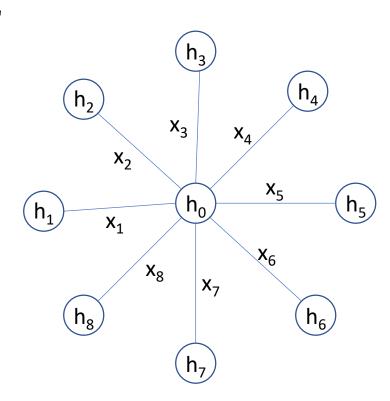
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Corollary:

Bounded noise # labels $\approx \mathfrak{s}_{\epsilon} d \log(\frac{1}{\epsilon})$ Agnostic $(\beta = R(f^*))$ # labels $\approx \mathfrak{s}_{\beta} d \frac{\beta^2}{\epsilon^2}$

Achieved by A^2



(Hanneke & Yang, 2015; Hanneke, 2016)

Distribution-Free Analysis

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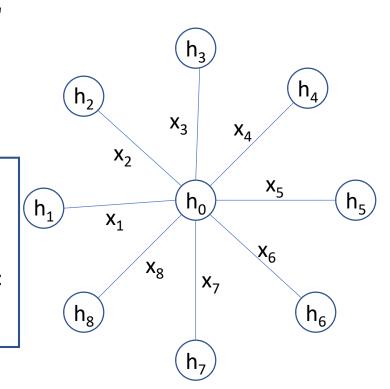
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Different alg., Bounded noise # labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

Near-matching lower bound: $\mathfrak{s}_{\epsilon} + d \log(\frac{1}{\epsilon})$



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Different alg., Bounded noise # labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

Near-matching lower bound: $\mathfrak{s}_{\epsilon} + d \log(\frac{1}{\epsilon})$

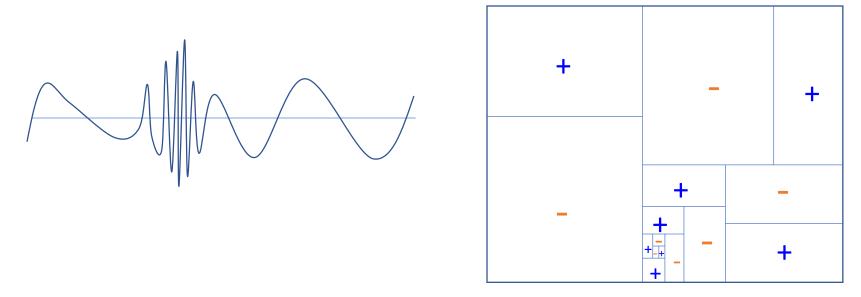
Open Question:

Agnostic $(\beta = R(f^*))$ # labels $\approx d \frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$?

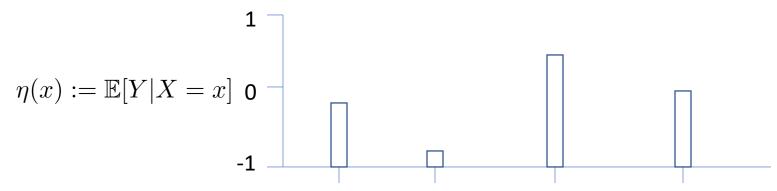
lower bound:
$$d\frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon} + d\log(\frac{1}{\epsilon})$$

Adapting to Heterogeneous Noise

So far: Active learning for spatial heterogeneity of opt function:



Also consider: Spatial heterogeneity of **noise**:



(Hanneke & Yang, 2015)

Active Learning with TicToc

```
Algorithm: \mathbb{A}(n)
Input: Label budget n
Output: Classifier \hat{f}_n.

1. \mathbb{L} \leftarrow \{\}
2. For m = 1, 2, ...
3. X_{s_m} \leftarrow \text{GetSeed}(\mathbb{L}, m) \leftarrow
4. \mathcal{L}_m \leftarrow \text{TicToc}(X_{s_m}, m) \leftarrow
5. if \mathcal{L}_m exists, \mathbb{L} \leftarrow \mathbb{L} \cup \{(s_m, \mathcal{L}_m)\}
6. If we've made n queries
7. Return \hat{f}_n \leftarrow \text{Learn}(\mathbb{L}) \leftarrow
An active learning alg.

(e.g. A^2)

Main new part

A passive learning alg.
```

Active Learning with TicToc

```
Algorithm: \mathbb{A}(n)
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1. \mathbb{L} \leftarrow \{\}
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6. If we've made n queries
7. Return \hat{f}_n \leftarrow \text{Learn}(\mathbb{L})
```

```
Denote \eta(x) = \mathbb{E}[Y|X=x]
Suppose f^* is the global optimal function: f^*(x) = \text{sign}(\eta(x))
```

```
TICTOC(X, m):
Query X (or nearby) to try to guess f^*(X)
If can figure it out, return that label
If can't figure it out by \tau_m queries give up (don't return a label)
```

Focus queries on less-noisy points.

Double advantage:

• Focusing on the points we actually care about:

$$R(f|x) - R(f^*|x) = |\eta(x)|\mathbb{I}[f(x) \neq f^*(x)]$$

(small $|\eta(x)| \Rightarrow$ not much effect on $R(f|x)$ if $f(x) = f^*(x)$ or not).

• And those points require fewer queries to determine $f^*(X_i)!$

$$\sim \frac{1}{\eta(X_i)^2}$$
 queries to determine $f^*(X_i)$.

Active Learning with TicToc

```
Algorithm: \mathbb{A}(n)

Input: Label budget n

Output: Classifier \hat{f}_n.

1. \mathbb{L} \leftarrow \{\}

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

3. X_{s_m} \leftarrow \text{GETSEED}(\mathbb{L}, m)

4. \mathcal{L}_m \leftarrow \text{TICTOC}(X_{s_m}, m)

5. if \mathcal{L}_m exists, \mathbb{L} \leftarrow \mathbb{L} \cup \{(s_m, \mathcal{L}_m)\}

6. If we've made n queries

7. Return \hat{f}_n \leftarrow \text{LEARN}(\mathbb{L})
```

Theorem: Bounded noise: # labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

Denote $\eta(x) = \mathbb{E}[Y|X=x]$ Suppose f^* is the **global** optimal function: $f^*(x) = \text{sign}(\eta(x))$

TICTOC(X, m):
Query X (or nearby) to try to guess $f^*(X)$ If can figure it out, return that label
If can't figure it out by τ_m queries give up (don't return a label)

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 queries to determine $f^*(X_i)$.

Active Learning with TicToc

Algorithm: $\mathbb{A}(n)$

Input: Label budget n

Output: Classifier f_n .

- $|1. \mathbb{L} \leftarrow \{\}|$
- $|2. \text{ For } m = 1, 2, \dots$
- 3. $X_{s_m} \leftarrow \text{GetSeed}(\mathbb{L}, m)$
- 4. $\mathcal{L}_m \leftarrow \text{TicToc}(X_{s_m}, m)$
- 5. if \mathcal{L}_m exists, $\mathbb{L} \leftarrow \mathbb{L} \cup \{(s_m, \mathcal{L}_m)\}$
- If we've made n queries
- Return $\hat{f}_n \leftarrow \text{Learn}(\mathbb{L})$

Theorem: Agnostic $(\beta = R(f^*))$

and suppose $f^* = \text{global best}$:

labels

$$\approx d \frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$$

Confirms agnostic sample complexity conjecture but with extra assumption $f^* = \text{global opt.}$

Near-match lower bound: $d\frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon} + d\log(\frac{1}{\epsilon})$

Denote $\eta(x) = \mathbb{E}[Y|X=x]$

Suppose f^* is the **global** optimal function: $f^*(x) = \text{sign}(\eta(x))$

 $\mathrm{TicToc}(X,m)$:

Query X (or nearby) to try to guess $f^*(X)$

If can figure it out, return that label

If can't figure it out by τ_m queries give up (don't return a label)

Focus queries on less-noisy points.

Double advantage:

• Focusing on the points we actually care about:

$$R(f|x) - R(f^{\star}|x) = |\eta(x)|\mathbb{I}[f(x) \neq f^{\star}(x)]$$

(small $|\eta(x)| \Rightarrow$ not much effect on R(f|x) if $f(x) = f^*(x)$ or not).

• And those points require fewer queries to determine $f^*(X_i)!$

$$\sim \frac{1}{\eta(X_i)^2}$$
 queries to determine $f^*(X_i)$.

Principles of Active Learning

- 1. Query in dense regions where \hat{f} could disagree a lot with f^*
- 2. Query in regions with low noise

The alg. adapts to heterogeneity in the noise.

Let's try it with a model that explicitly describes heterogeneous noise:

Tsybakov Noise

Denote $\eta(x) = \mathbb{E}[Y|X=x]$

Definition: (Tsybakov noise) $f^{\star}(x) = \operatorname{sign}(\eta(x))$ and $\exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$ $P_X(x: |\eta(x)| \leq \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$

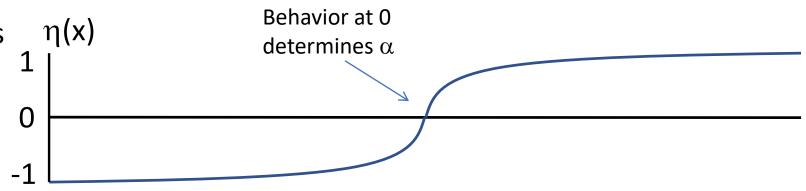
(Tsybakov, 2004; Mammen & Tsybakov 1999)

Denote
$$\eta(x) = \mathbb{E}[Y|X=x]$$

Definition: (Tsybakov noise) $f^{\star}(x) = \operatorname{sign}(\eta(x))$ and $\exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$ $P_X(x: |\eta(x)| \leq \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$

Example:

Thresholds



(unif. distrib)

Denote $\eta(x) = \mathbb{E}[Y|X=x]$

Definition: (Tsybakov noise)

$$f^{\star}(x) = \operatorname{sign}(\eta(x)) \text{ and } \exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$$

$$P_X(x : |\eta(x)| \le \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$$

Passive OPT: $\tilde{\Theta}\left(\frac{d}{\epsilon^{2-\alpha}}\right)$.

Active OPT:
$$\begin{cases} \frac{d}{\epsilon^{2-2\alpha}} & \text{if } 0 < \alpha \le 1/2\\ \min\left\{\frac{d}{\epsilon^{2-2\alpha}} \left(\frac{\mathfrak{s}}{d}\right)^{2\alpha-1}, \frac{d}{\epsilon}\right\} & \text{if } 1/2 < \alpha < 1 \end{cases}.$$

$$\sim \begin{cases} rac{1}{arepsilon^{2-2lpha}}, & ext{if } \mathfrak{s} < \infty \ rac{1}{arepsilon}, & ext{if } \mathfrak{s} = \infty \end{cases}.$$

Active Opt \ll Passive Opt. (always)

(Massart & Nédélec, 2006)

(Hanneke & Yang, 2015)

Conclusions

- Many proposals for going beyond Disagreement-based Active Learning
- Each exhibits improvements in certain cases
- We still don't know the optimal agnostic active learning algorithm

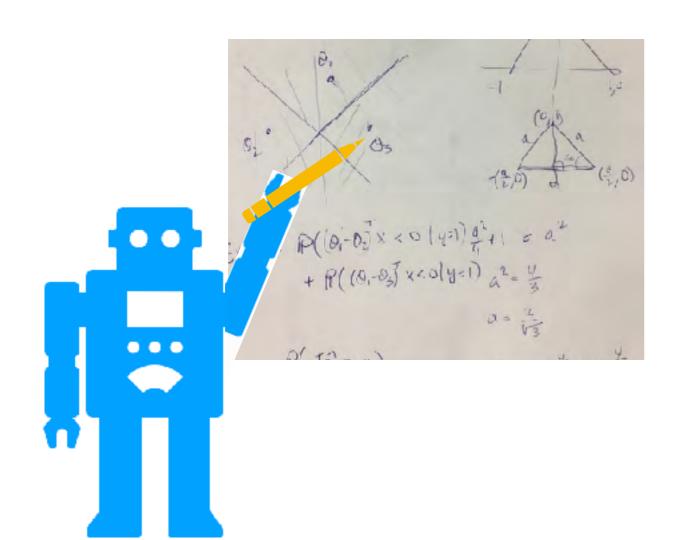
$$d\frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d}\log(\frac{1}{\epsilon})$$

Questions?

Further reading:

- S. Dasgupta, A. Kalai, C. Monteleoni. Analysis of perceptron-based active learning. COLT 2005.
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- S. Hanneke, L. Yang. Minimax analysis of active learning. Journal of Machine Learning Research, 2015.
- S. Hanneke. Refined error bounds for several learning algorithms. Journal of Machine Learning Research, 2016.
- M. F. Balcan, S. Hanneke, J. Wortman Vaughan. The true sample complexity of active learning. *Machine Learning*, 2010.

Active Learning from Theory to Practice



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ICML | 2019

Thirty-sixth International Conference on Machine Learning

Tutorial Outline



Part 1: Introduction to Active Learning (Rob)

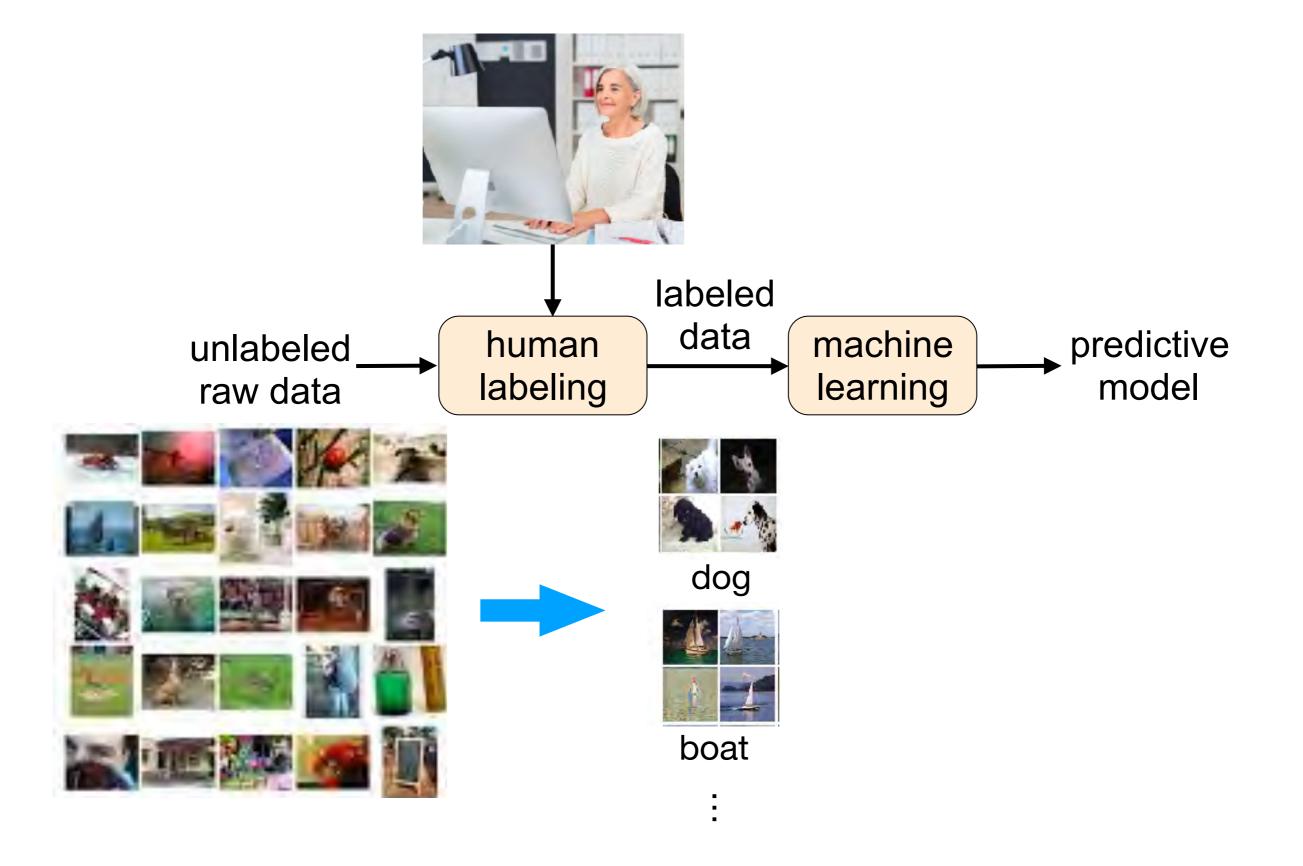
Part 2: Theory of Active Learning (Steve)

Part 3: Advanced Topics and Open Problems (Steve)

Part 4: Nonparametric Active Learning (Rob)

slides: http://nowak.ece.wisc.edu/ActiveML.html

Conventional (Passive) Machine Learning





theguardian

Computers now better than humans at recognising and sorting images

millions of labeled images 1000's of human hours

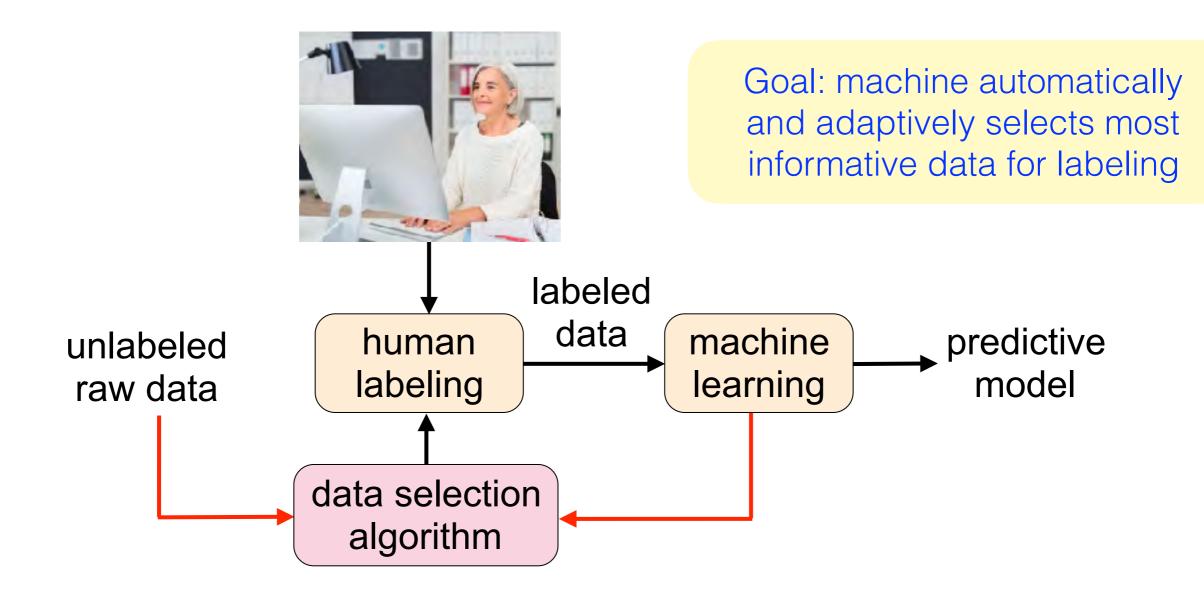
QUARTZ

Google says its new Al-powered translation tool scores nearly identically to human translators

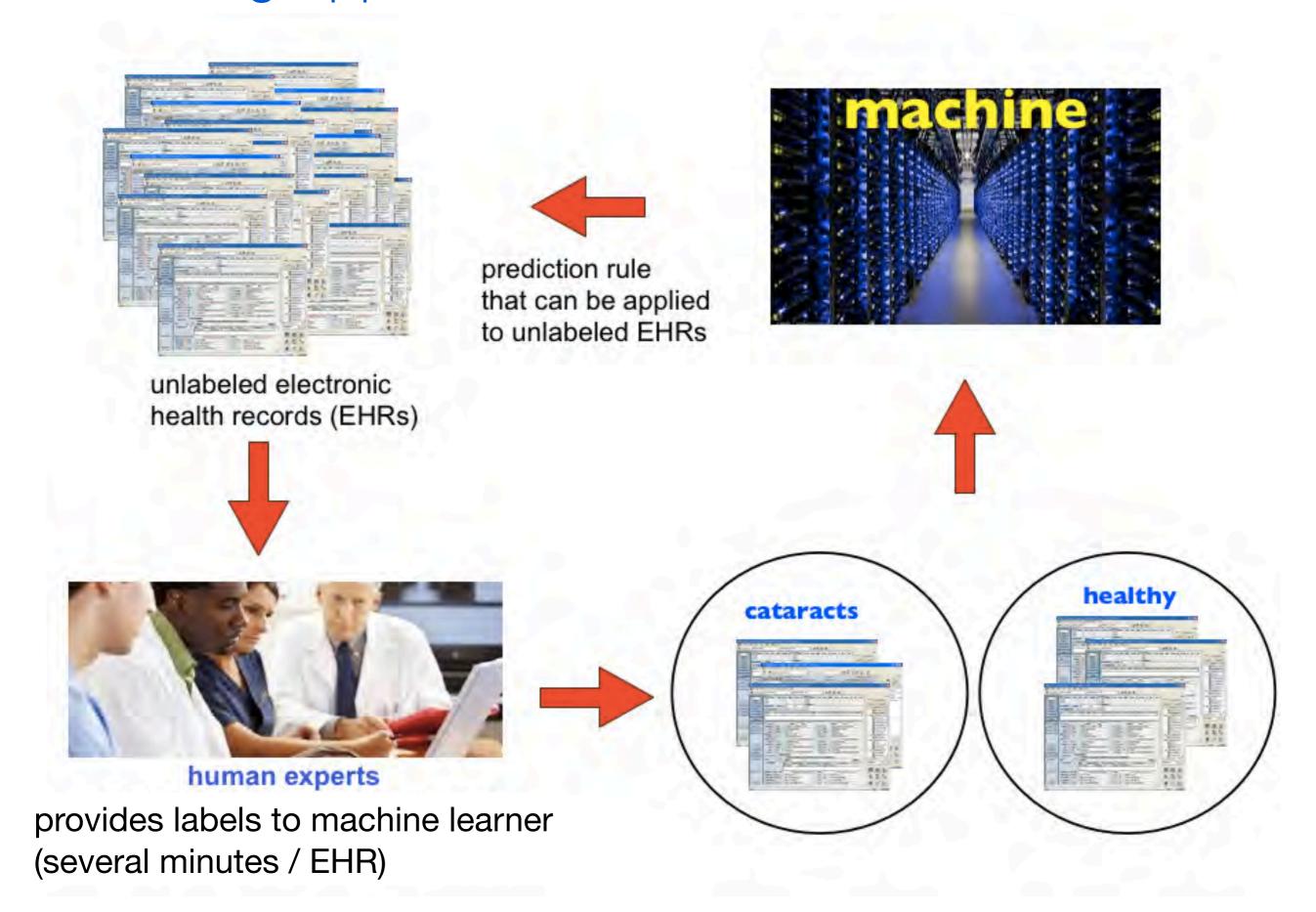
trained on more texts than a human could read in a lifetime

Can we train machines with less labeled data and less human supervision?

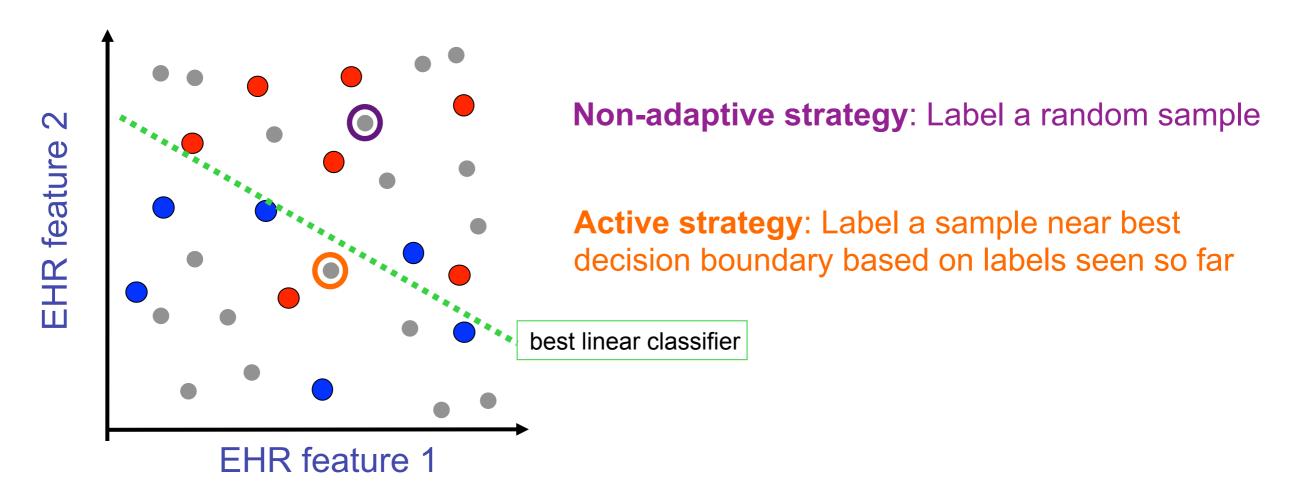
Active Machine Learning

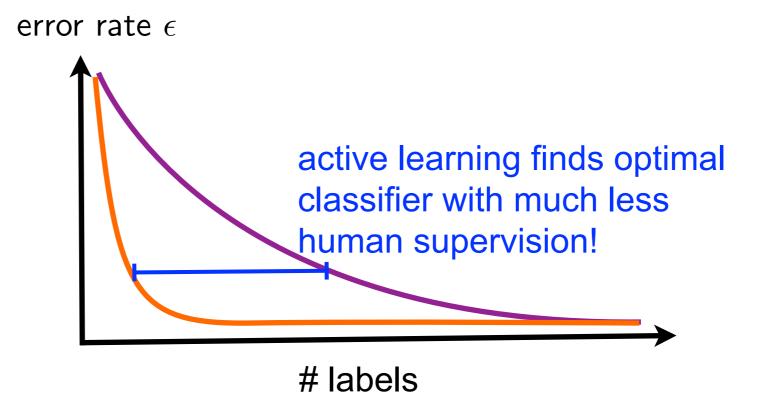


Motivating Application

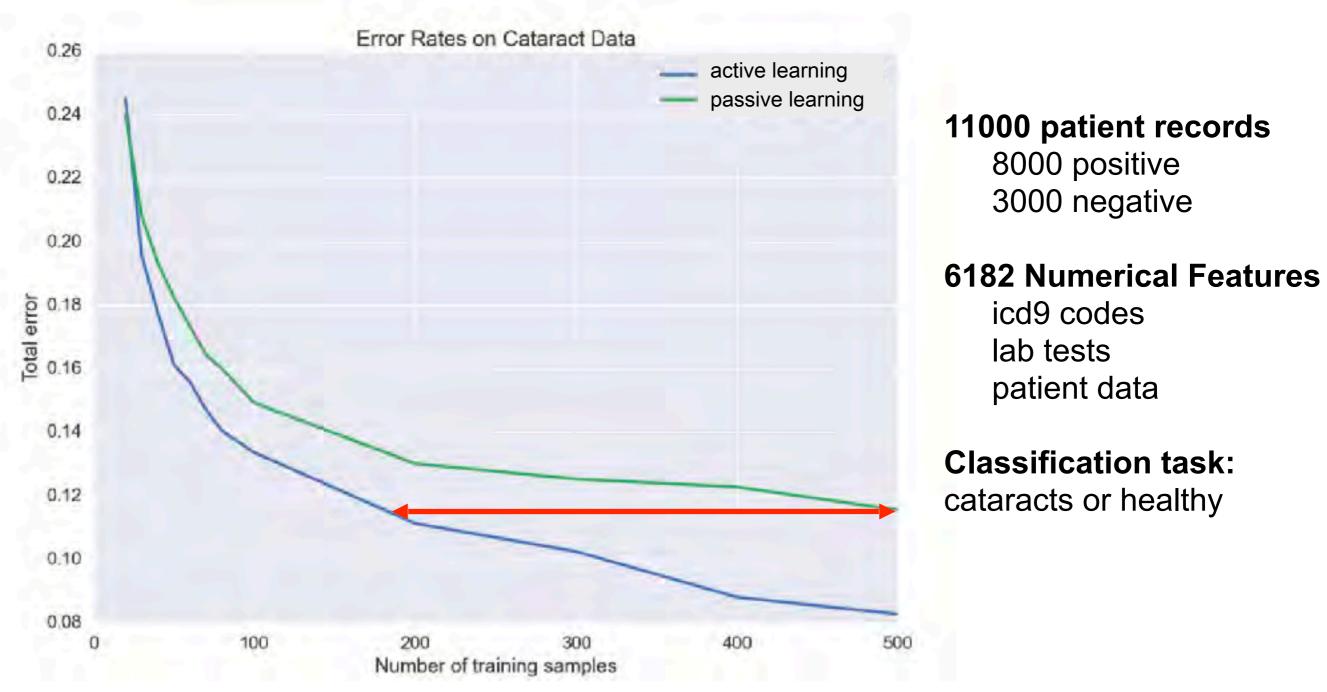


Active Learning





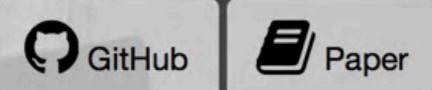
Active Logistic Regression



less than half as many labeled examples needed by active learning

NEXT

ASK BETTER QUESTIONS. GET BETTER RESULTS. FASTER. AUTOMATED.













Active learning to optimize crowdsourcing and rating in New Yorker Cartoon Caption Contest



digg



BY DOING THE EXACT OPPOSITE

How New Yorker Cartoons Could Teach Computers To Be Funny

3 diggs CNET Technology

With the help of computer scientists from the University of Wisconsin at Madison, The New Yorker for the first time is using crowdsourcing algorithms to uncover the best captions.









Actively learning user's beer preferences

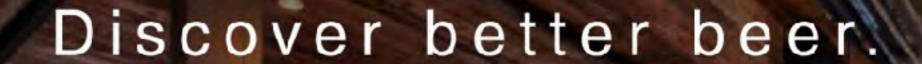


Home

Contact

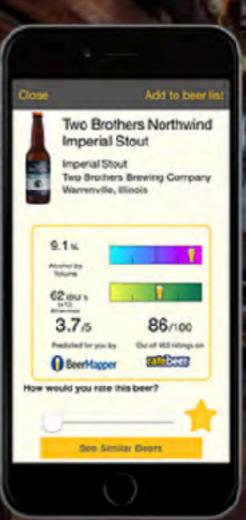
About

FAQs



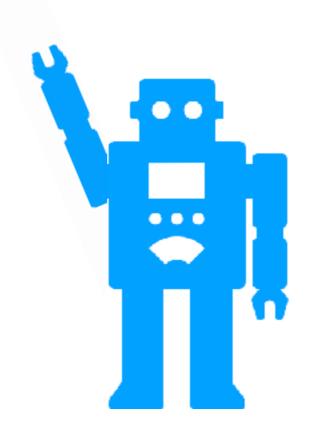






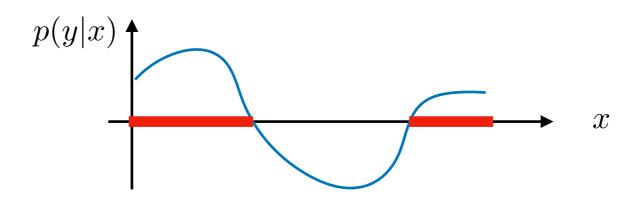
The most powerful beer app on the planet.

Principles of Active Learning



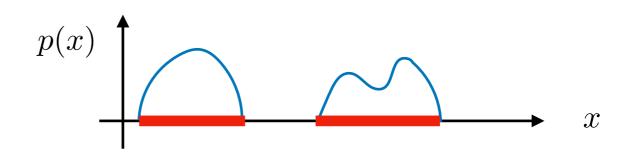
What and Where Information

Density estimation: What is p(y|x)? Classification: Where is p(y|x) > 0?



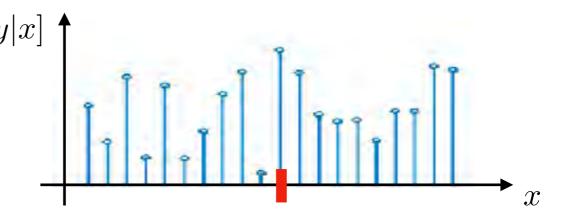
Density estimation: What is p(x)?

Clustering: Where is $p(x) > \epsilon$?



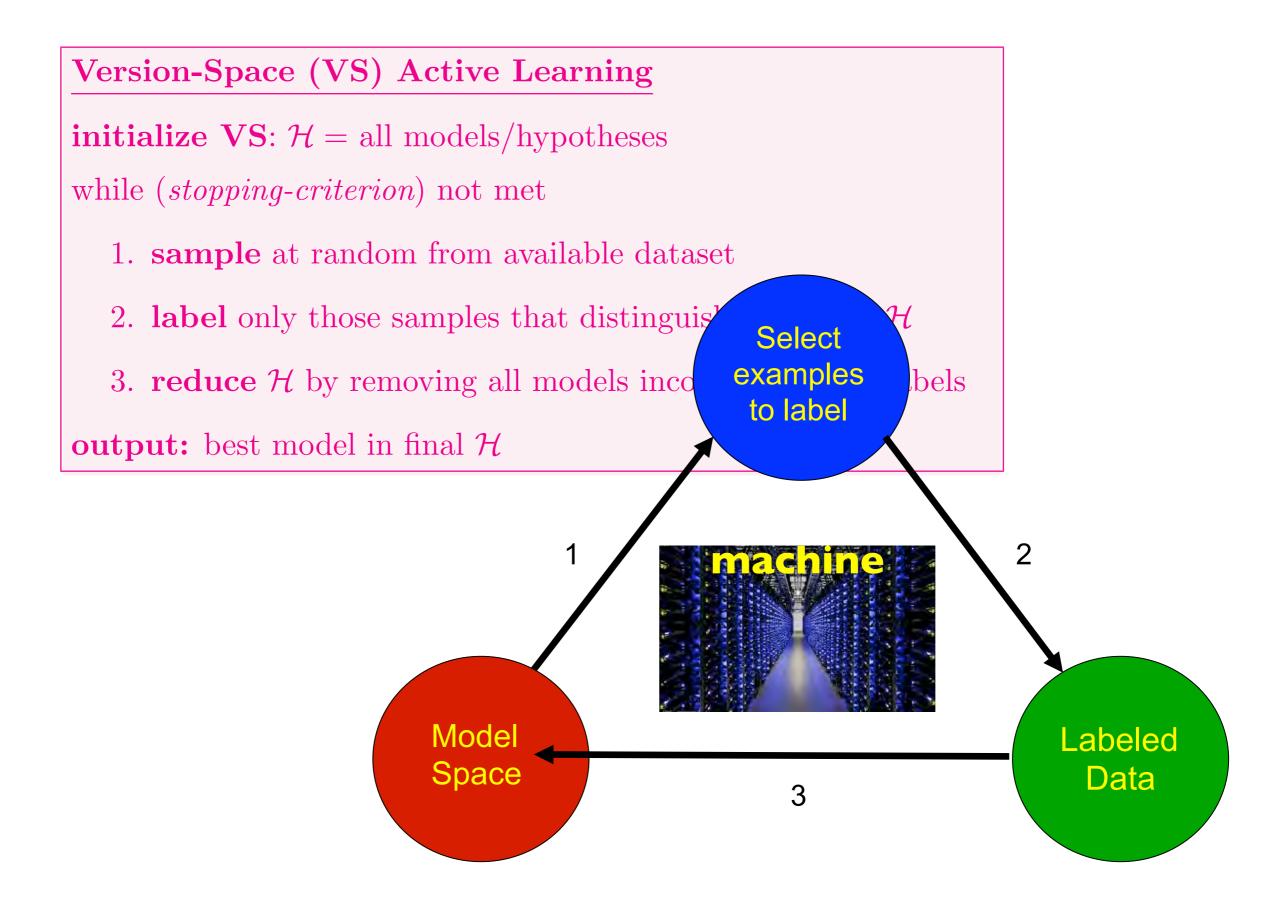
Function estimation: What is $\mathbb{E}[y|x]$?

Bandit optimization: Where is $\max_x \mathbb{E}[y|x]$?



Active learning is more efficient than passive learning for localized "where" information

Meta-Algorithm for Active Learning



Learning a 1-D Classifier



binary search quickly finds decision boundary

passive : err $\sim n^{-1}$

 $\text{active}: \text{err} \, \sim \, \, 2^{-n}$

Vapnik-Chervonenkis (VC) Theory

Given training data $\{(x_j,y_j)\}_{j=1}^n$, learn a function f to predict y from x

Consider a possibly infinite set of hypotheses \mathcal{F} with *finite VC dimension* d and for each $f \in \mathcal{F}$ define the risk (error rate):

$$R(f) := \mathbb{P}(f(x) \neq y)$$

error rate on training data:
$$\widehat{R}(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1} \Big(f(x_i) \neq y_i \Big)$$
 "empirical risk"

VC bound:
$$\sup_{f\in\mathcal{F}}|R(f)-\widehat{R}(f)| \ \leq \ 6\sqrt{\frac{d\log(n/\delta)}{n}}$$
 w.p. $\geq \ 1-\delta$

Empirical Risk Minimization (ERM)

Goal: select hypothesis with true error rate within $\epsilon > 0$ of $\min_{f \in \mathcal{F}} R(f)$

$$f^* = \arg\min_{f \in \mathcal{F}} R(f)$$
 true risk minimizer

 \widehat{f} minimizes empirical risk:

$$\widehat{f} \quad = \quad \arg\min_{f \in \mathcal{F}} \widehat{R}(f) \quad \text{empirical risk minimizer}$$

$$\widehat{R}(\widehat{f}) \leq \widehat{R}(f^*)$$

$$R(\widehat{f}) \leq \widehat{R}(\widehat{f}) + 6\sqrt{\frac{d\log(n/\delta)}{n}}$$

$$R(f^*) \geq \widehat{R}(f^*) - 6\sqrt{\frac{d\log(n/\delta)}{n}}$$

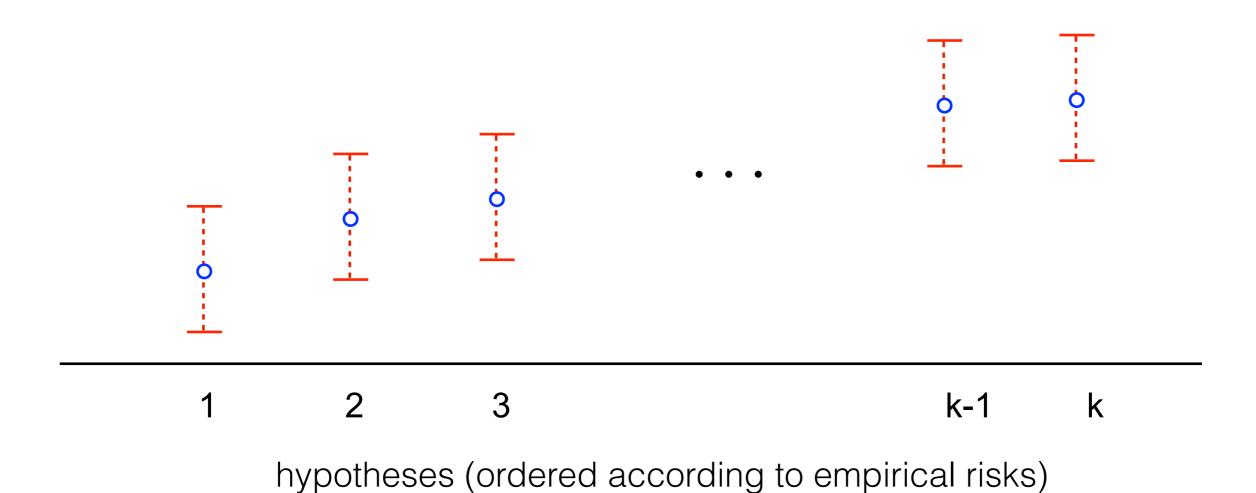
$$R(f^*) \geq \widehat{R}(f^*) - 6\sqrt{\frac{d\log(n/\delta)}{n}}$$

sufficient number of training examples:

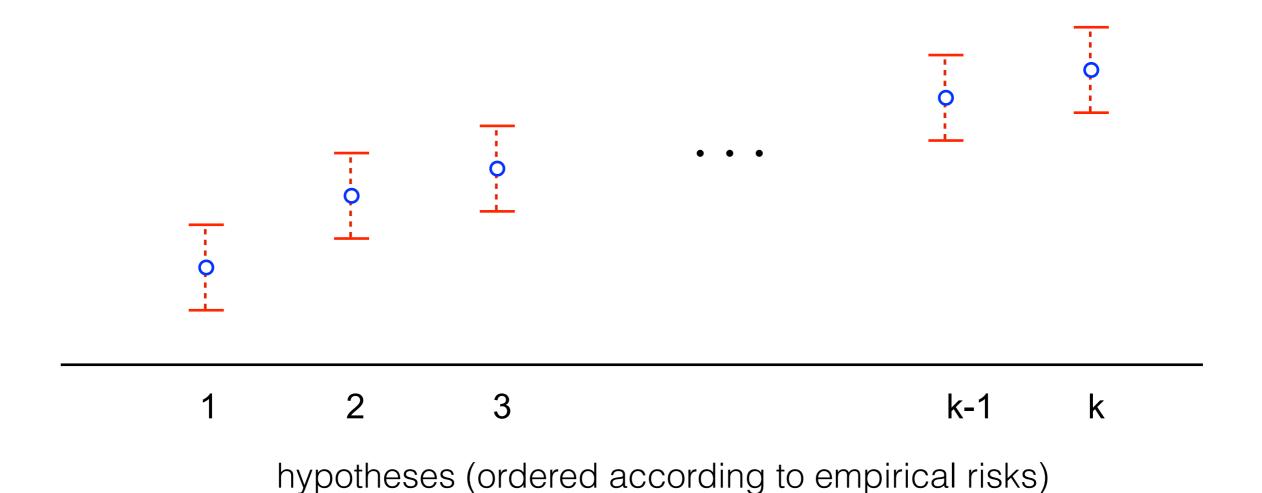
$$12\sqrt{\frac{d\log(n/\delta)}{n}} \le \epsilon \qquad \qquad n = \widetilde{O}\left(\frac{d\log(1/\delta)}{\epsilon^2}\right)$$

$$n = \widetilde{O}\left(\frac{d\log(1/\delta)}{\epsilon^2}\right)$$

Empirical Risks and Confidence Intervals

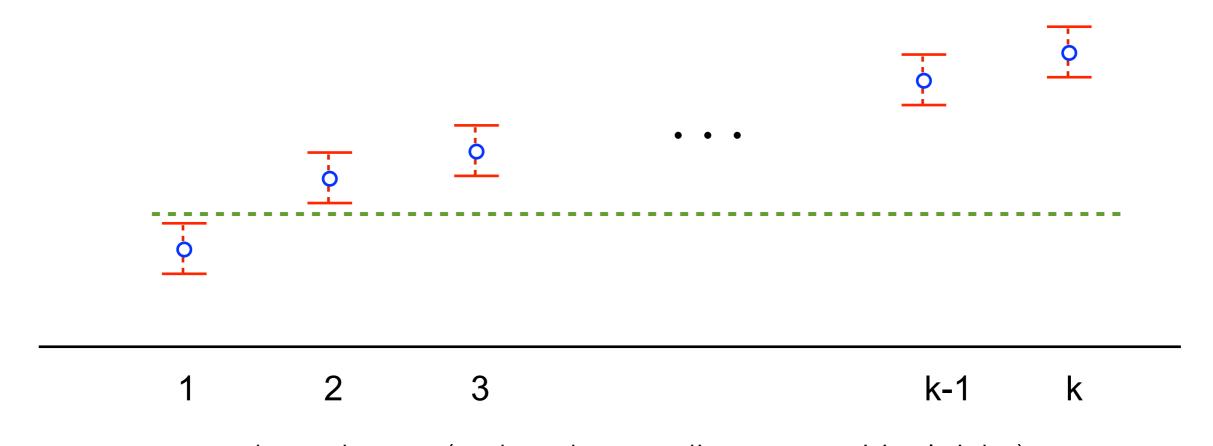


Empirical Risks and Confidence Intervals



more training data ⇒ smaller confidence intervals

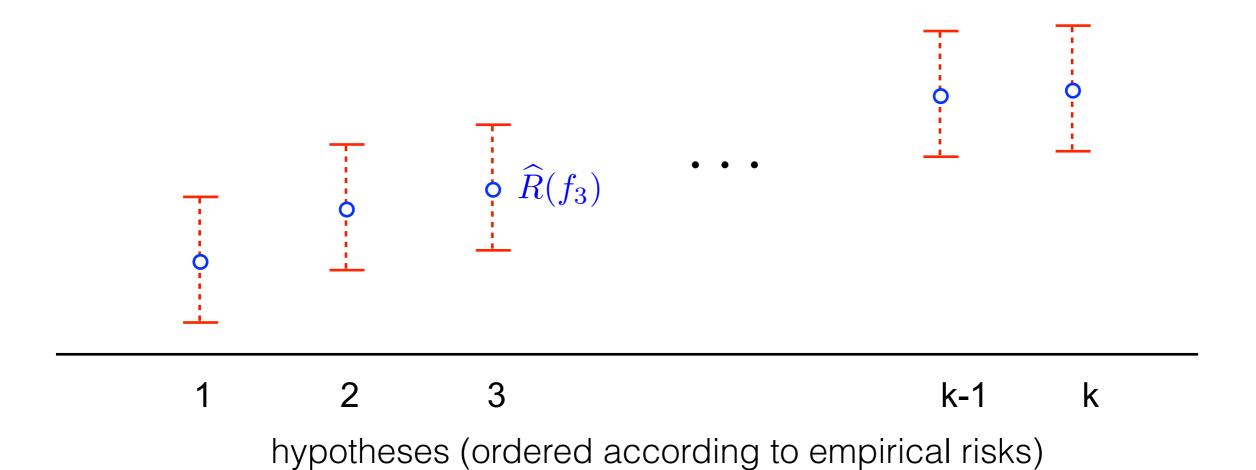
Empirical Risks and Confidence Intervals



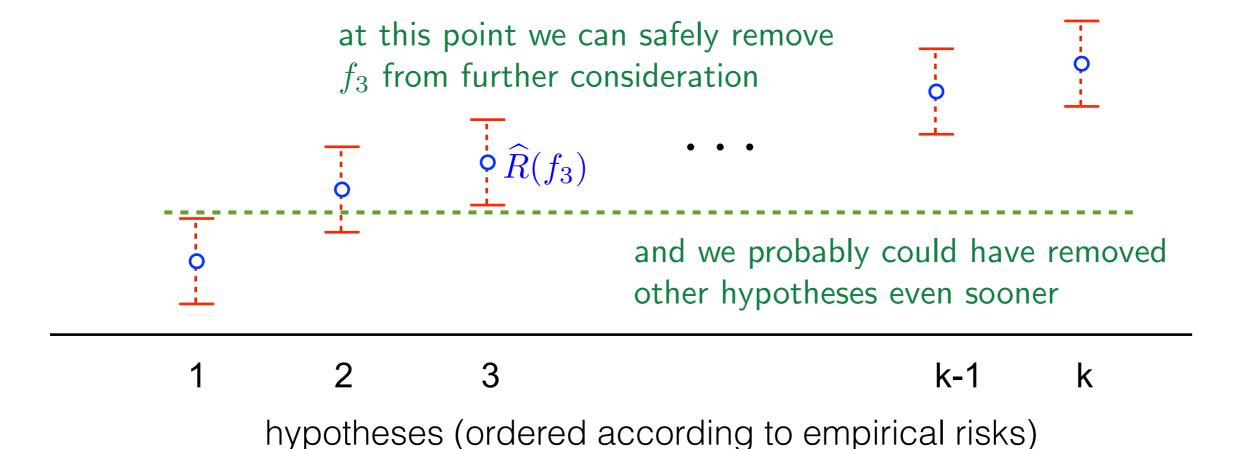
hypotheses (ordered according to empirical risks)

more training data ⇒ smaller confidence intervals

ERM is Wasting Labeled Examples



ERM is Wasting Labeled Examples

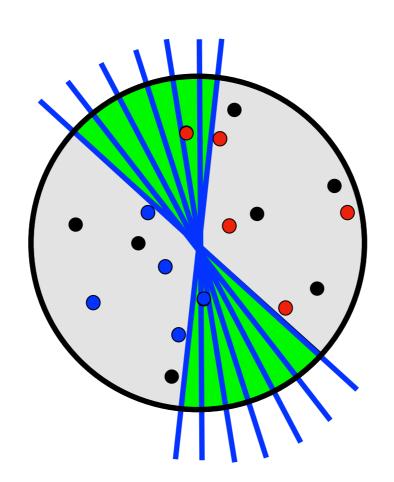


only require labels for examples that hypotheses 1 and 2 label differently (i.e., examples where they *disagree*)



Disagreement-Based Active Learning

consider points uniform on unit ball and linear classifiers passing through origin



only label points in the region of disagreement $\mathfrak D$

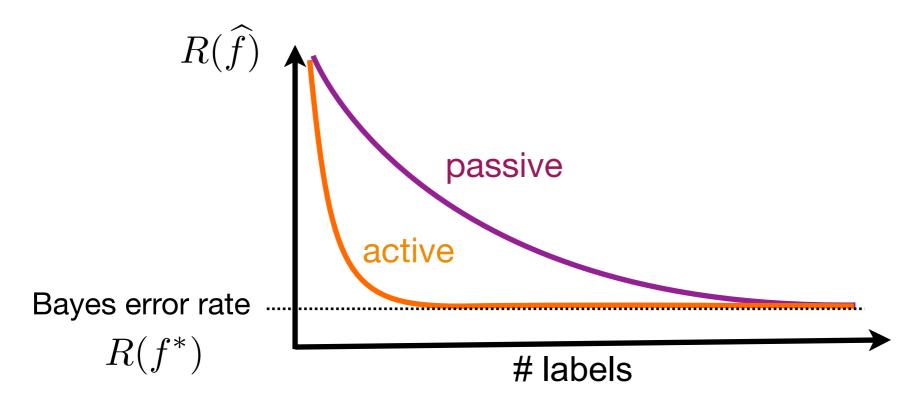
Active Binary Classification

Assuming optimal Bayes classifer f^* in VC class with dimension d and "nice" distributions (e.g., bounded label noise)

$$\epsilon = R(\widehat{f}) - R(f^*)$$

passive
$$\epsilon \sim \frac{d}{n}$$
 parametric rate

active
$$\epsilon \sim \exp\left(-c\frac{n}{d}\right)$$
 exponential speed-up



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slides: http://nowak.ece.wisc.edu/ActiveML.html

Recommended Reading (Foundations of Active Learning)

Settles, Burr. "Active learning." *Synthesis Lectures on Artificial Intelligence and Machine Learning* 6.1 (2012): 1-114.

Dasgupta, Sanjoy. "Two faces of active learning." *Theoretical computer science* 412.19 (2011): 1767-1781.

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Hanneke, Steve. "Theory of active learning." *Foundations and Trends in Machine Learning* 7, no. 2-3 (2014).

Part 2: Theory of Active Learning General Case

- Disagreement-Based Agnostic Active Learning
- Disagreement Coefficient
- Sample Complexity Bounds

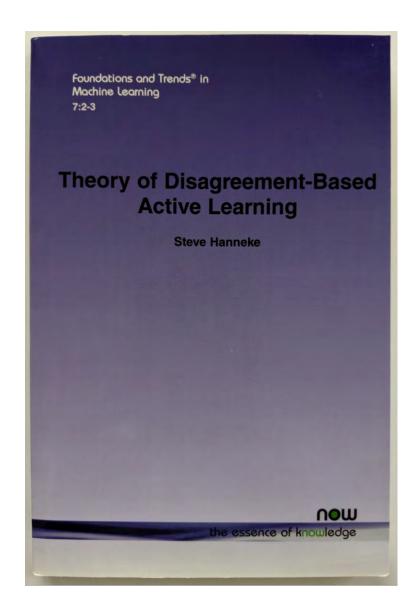
Tutorial on Active Learning: Theory to Practice

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Robert Nowak

University of Wisconsin - Madison rdnowak@wisc.edu



Uniform Bernstein Inequality

Bernstein's inequality:

For m iid samples $\forall f, f', \text{ w.p. } 1 - \delta,$ $R(f) - R(f') \leq \hat{R}(f) - \hat{R}(f') + c\sqrt{\hat{P}(f \neq f') \frac{\log(1/\delta)}{m}} + \frac{\log(1/\delta)}{m}$

Uniform Bernstein inequality:

w.p.
$$1 - \delta$$
, $\forall f, f' \in \mathcal{H}$,

$$R(f) - R(f') \le \hat{R}(f) - \hat{R}(f') + c\sqrt{\hat{P}(f \ne f') \frac{d \log(m/\delta)}{m}} + \frac{d \log(m/\delta)}{m}$$

VC dimension

Roughly:

$$\forall f, f' \in \mathcal{H},$$

$$R(f) - R(f') \le \hat{R}(f) - \hat{R}(f') + \sqrt{\hat{P}(f \ne f') \frac{d}{m}}$$

Region of disagreement:

$$DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

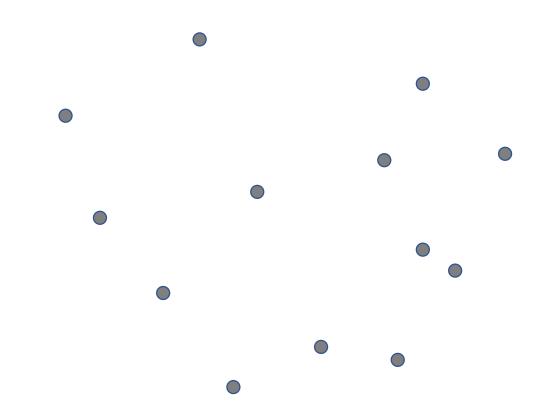
output final \hat{f}

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

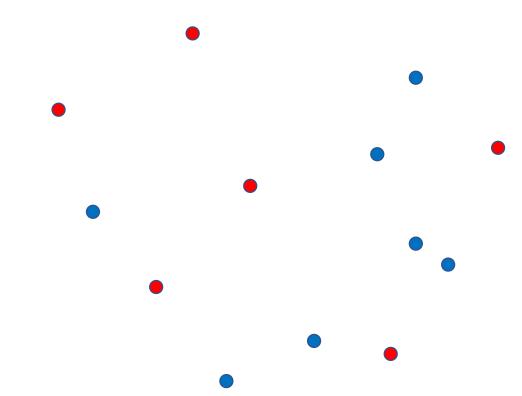
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- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

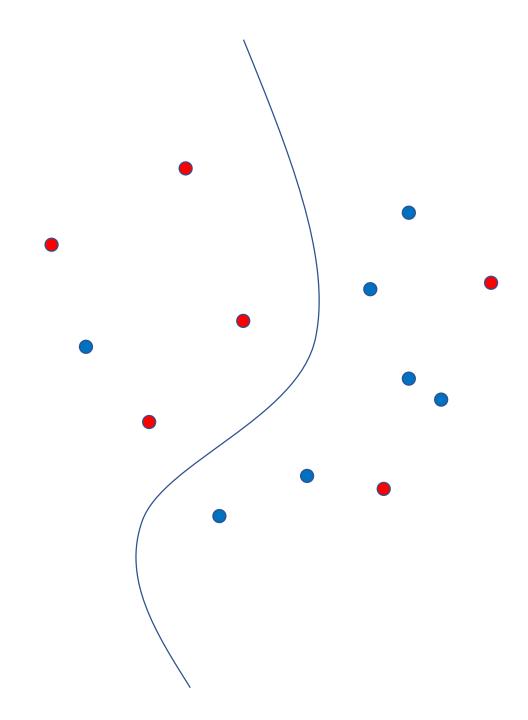


 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

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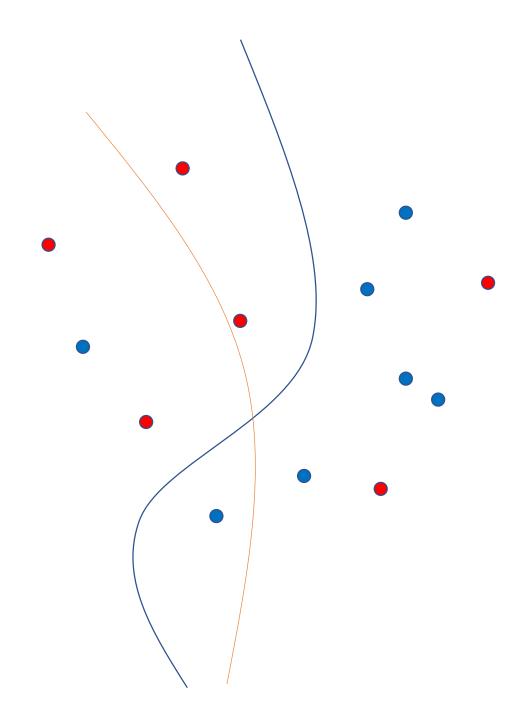


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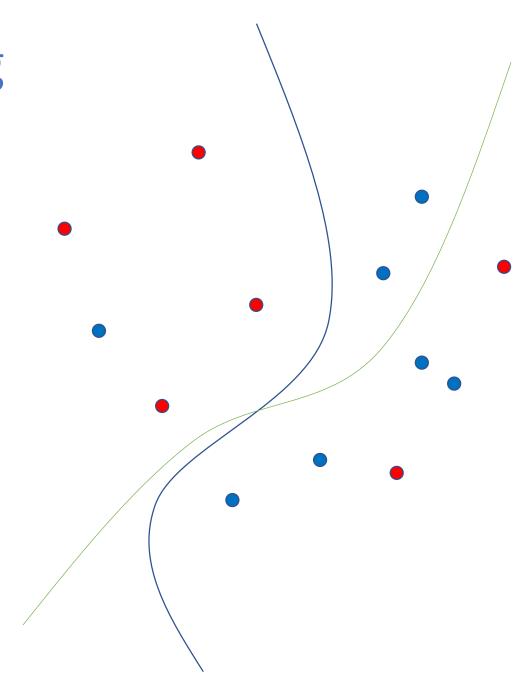


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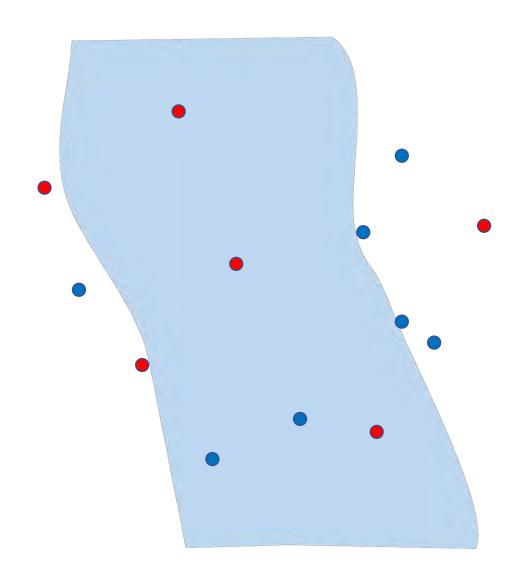
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 ${f output} \ {
m final} \ \hat{f}$



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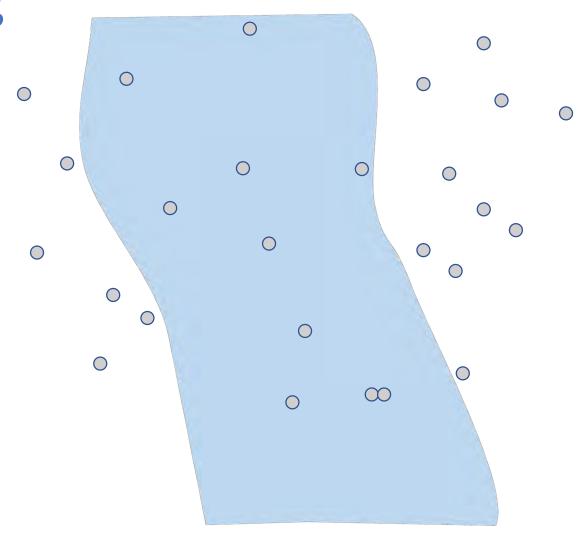


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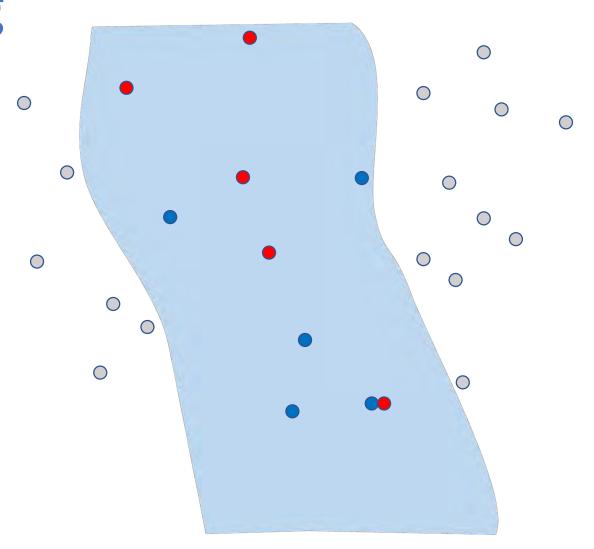


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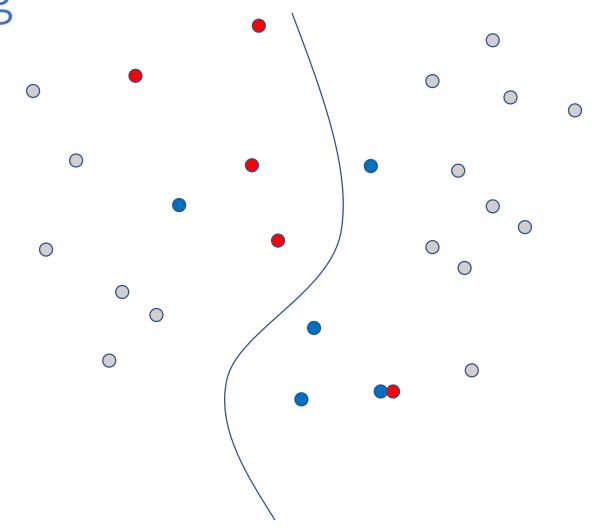


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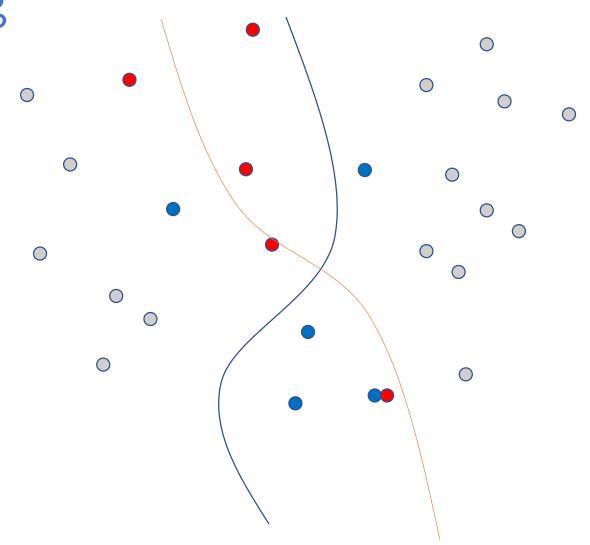
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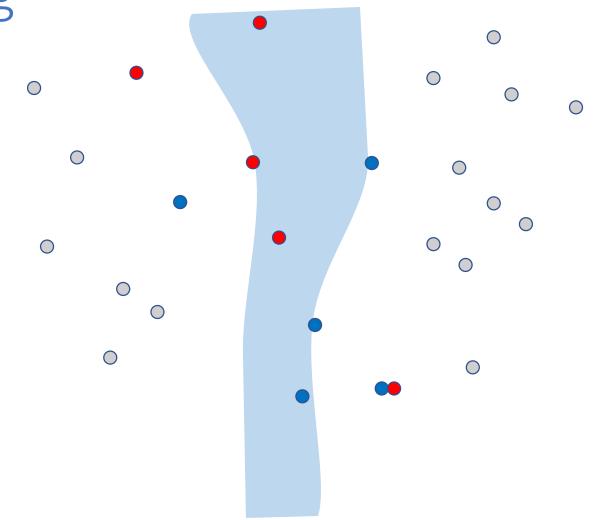
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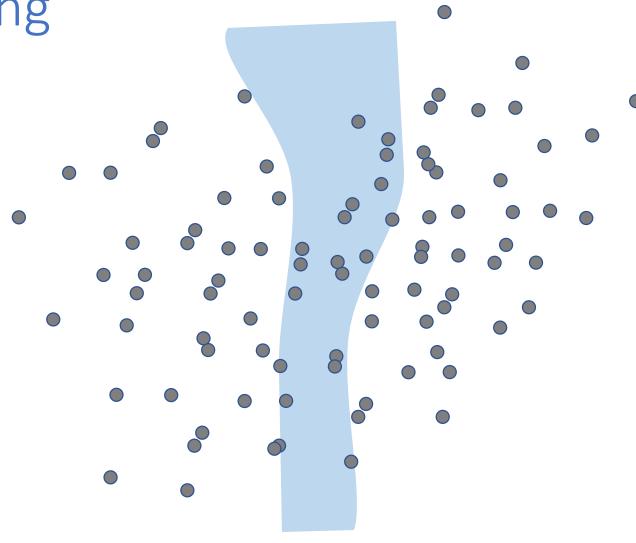


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for t = 1, 2, ... (til stopping-criterion) 1. $\mathbf{sample}\ 2^t$ unlabeled points S2. $\mathbf{label}\ points\ in\ Q = \mathrm{DIS}(\mathcal{H}) \cap S$ 3. $\mathbf{optimize}\ \hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}}\ \hat{R}_Q(f)$ 4. $\mathbf{reduce}\ \mathcal{H}$: remove all f with $\hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$ output final \hat{f}

The point:

Any t with $f^* \in \mathcal{H}$ still, $R(f^*|\mathrm{DIS}(\mathcal{H}))$ still **minimal** in \mathcal{H}

$$\Rightarrow \hat{R}_{Q}(f^{*}) - \hat{R}_{Q}(\hat{f})$$

$$\leq R(f^{*}|\mathrm{DIS}(\mathcal{H})) - R(\hat{f}|\mathrm{DIS}(\mathcal{H})) + \sqrt{\hat{P}_{Q}(f^{*} \neq \hat{f})\frac{d}{|Q|}}$$

$$\leq \sqrt{\hat{P}_{Q}(f^{*} \neq \hat{f})\frac{d}{|Q|}}$$

 $\Rightarrow f^*$ never removed.

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping-criterion)

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Next: How many labels does it use?

Hanneke (2007,...)

Ball:
$$B(f^*, r) := \{ f \in \mathcal{H} : P_X(f \neq f^*) \le r \}$$

$$DIS(B(f^*, r)) := \{x \in \mathcal{X} : \exists f, f' \in B(f^*, r), f(x) \neq f'(x)\}$$

Disagreement coefficient:

$$\theta = \sup_{r > \epsilon} \frac{P_X(\mathrm{DIS}(\mathrm{B}(f^*, r)))}{r}$$

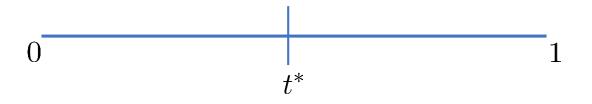
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Example: **Thresholds**, P_X Uniform(0,1) $f(x) = \mathbb{I}[x \ge t]$



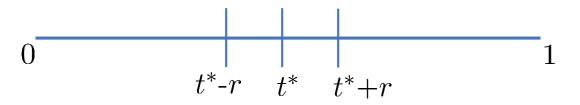
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Example: **Thresholds**, P_X Uniform(0,1) $f(x) = \mathbb{I}[x \ge t]$



$$DIS(B(f^*, r)) = [t^* - r, t^* + r)$$

$$P_X(DIS(B(f^*,r))) = 2r$$

$$\theta = 2$$

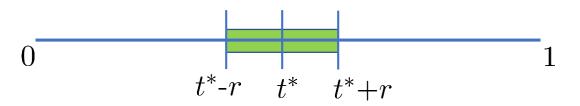
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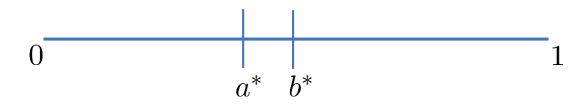
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Example: **Intervals**, P_X Uniform(0,1) $f(x) = \mathbb{I}[a \le x \le b]$

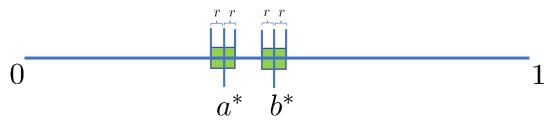


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Disagreement coefficient:

$$\theta = \sup_{r > \epsilon} \frac{P_X(\text{DIS}(B(f^*, r)))}{r}$$



$$w^* := b^* - a^*$$

If
$$r < w^*$$
,

$$DIS(B(f^*, r)) = [a^* - r, a^* + r) \cup (b^* - r, b^* + r]$$

$$P_X(DIS(B(f^*,r))) = 4r$$

Ball:
$$B(f^*, r) := \{ f \in \mathcal{H} : P_X(f \neq f^*) \le r \}$$

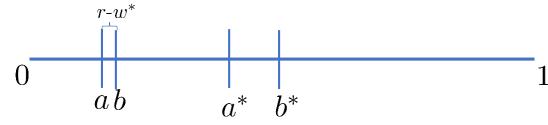
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Example: Intervals, P_X Uniform(0,1)

$$f(x) = \mathbb{I}[a \le x \le b]$$



$$w^* := b^* - a^*$$

If
$$r > w^*$$
,

$$DIS(B(f^*, r)) = \mathcal{X}$$

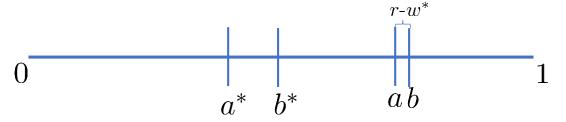
$$P_X(\mathrm{DIS}(\mathrm{B}(f^*,r)))=1$$

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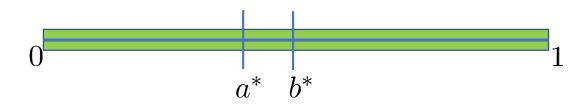
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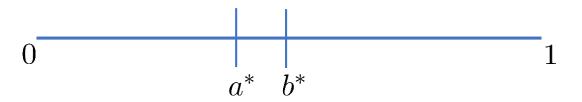
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$$w^* := b^* - a^*$$

If
$$\mathbf{r} < \mathbf{w}^*$$
, $P_X(\mathrm{DIS}(\mathrm{B}(f^*, r))) = 4r$

If
$$r > w^*$$
, $P_X(DIS(B(f^*, r))) = 1$

$$\Rightarrow \theta \leq \max\{4, \frac{1}{w^*}\}$$

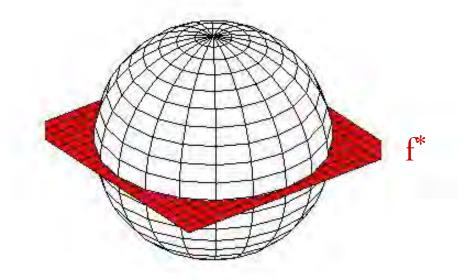
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Example: homog. linear separators (bias 0), n dimensions, uniform P_X on sphere.



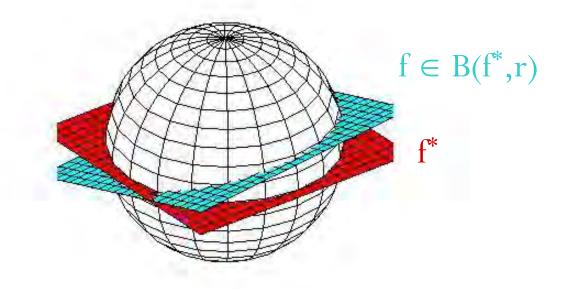
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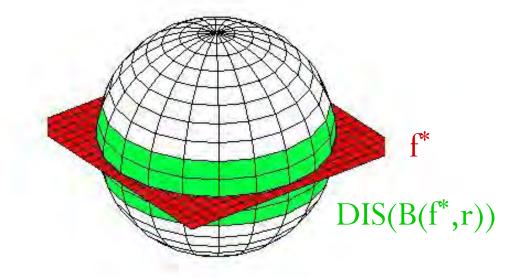
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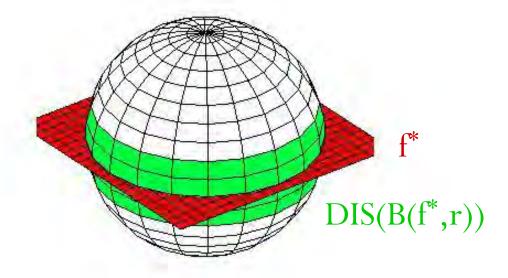
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Example: homog. linear separators (bias 0), n dimensions, uniform P_X on sphere.



Some geometry \Rightarrow for small r,

$$P_X(DIS(B(f^*,r))) \propto \sqrt{n}r.$$

$$\Rightarrow$$
 $heta \propto \sqrt{n}$.

Bounded Noise assumption: (aka Massart noise)

$$\exists \beta < 1/2 \text{ s.t. } P(Y \neq f^*(X)|X) \leq \beta \text{ everywhere}$$

	Sample Complexity: $R(\hat{f}) \leq R(f^*) + \epsilon$	Excess Error: n labels
Passive	$rac{d}{\epsilon}$	$\frac{d}{n}$
Active	$d\theta \log(\frac{1}{\epsilon})$	$e^{-n/d\theta}$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping\text{-}criterion)

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output final \hat{f}
```

Theorem: $P(Y \neq f^*(X)|X) \leq \beta$. $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels $\approx d\theta \log(\frac{1}{\epsilon})$.

Proof Sketch:

Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

Roughly, that means Step 4 only keeps f with $R(f) - R(f^*) \lesssim \sqrt{P_X(f \neq f^*) \frac{d}{2^t}}$

 \Rightarrow surviving f after round t have $R(f) - R(f^*) \lesssim \frac{d}{2^t}$ $\Rightarrow t \gtrsim \log(\frac{d}{\epsilon})$ suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B(f^*, d/2^{t-1})$

$$\Rightarrow |Q| \lesssim P_X(\mathrm{DIS}(\mathrm{B}(f^*,d/2^{t-1})))|S| \leq \theta \tfrac{d}{2^{t-1}}|S| = \theta d2$$

$$\sum_{t=1}^{\log(d/\epsilon)} \theta d = \theta d \log(\frac{d}{\epsilon})$$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. **optimize** $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$

output final \hat{f}

Bounded noise:

$$R(f) - R(f^*) = \int_{f \neq f^*} (P(Y = f^*(X)|X) - P(Y \neq f^*(X)|X)) dP_X$$

$$\geq (1 - 2\beta)P_X(f \neq f^*)$$

Theorem: $P(Y \neq f^*(X)|X) \leq \beta$. $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels $\approx d\theta \log(\frac{1}{\epsilon})$.

Proof Sketch:

Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

Roughly, that means Step 4 only keeps f with $R(f) - R(f^*) \lesssim \sqrt{P_X(f \neq f^*) \frac{d}{2^t}}$

 \Rightarrow surviving f after round t have $R(f) - R(f^*) \lesssim \frac{d}{2^t}$ $\Rightarrow t \gtrsim \log(\frac{d}{\epsilon})$ suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B(f^*, d/2^{t-1})$

$$\Rightarrow |Q| \lesssim P_X(\mathrm{DIS}(\mathrm{B}(f^*,d/2^{t-1})))|S| \leq \theta \frac{d}{2^{t-1}}|S| = \theta d2$$

$$\sum_{t=1}^{\log(d/\epsilon)} \theta d = \theta d \log(\frac{d}{\epsilon})$$

Agnostic Learning: (no assumptions)

Denote $\beta = R(f^*)$

	Sample Complexity: $R(\hat{f}) \leq R(f^*) + \epsilon$	Excess Error: n labels
Passive	$drac{eta}{\epsilon^2}$	$\sqrt{rac{deta}{n}}$
Active	$d heta rac{eta^2}{\epsilon^2}$	$\sqrt{rac{deta^2 heta}{n}}$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

A^2 (Agnostic Active)

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = DIS(\mathcal{H}) \cap S$
- 3. **optimize** $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

output final \hat{f}

Theorem:
$$\beta = R(f^*)$$
. $R(\hat{f}) \leq R(f^*) + \epsilon$ with

labels
$$\approx d\theta \frac{\beta^2}{\epsilon^2}$$
.

Proof Sketch:

Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

Roughly, that means Step 4 only keeps f with

$$R(f) - R(f^*) \lesssim \sqrt{P_X(f \neq f^*) \frac{d}{2^t}}$$

 \Rightarrow surviving f after round t have $R(f) - R(f^*) \lesssim \sqrt{\beta \frac{d}{2^t}} + \frac{d}{2^t}$

(Roughly)
$$\sqrt{\beta \frac{d}{2^t}}$$

$$\Rightarrow t \gtrsim \log(d\frac{\beta}{\epsilon^2})$$
 suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B\left(f^*, 2\beta + \sqrt{\beta \frac{d}{2^{t-1}}}\right) \subseteq B(f^*, 3\beta)$ (for large t)

$$\Rightarrow |Q| \lesssim P_X(\mathrm{DIS}(\mathrm{B}(f^*, 3\beta)))|S| \lesssim \theta\beta|S| = \theta\beta 2^t$$

$$\sum_{t=1}^{\log(d\beta/\epsilon^2)} \theta \beta 2^t \sim \theta d \frac{\beta^2}{\epsilon^2}$$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

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for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
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- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$

output final \hat{f}

$$P_X(f \neq f^*) \le R(f) + R(f^*) = 2\beta + R(f) - R(f^*)$$

Theorem:
$$\beta = R(f^*)$$
. $R(\hat{f}) \leq R(f^*) + \epsilon$ with

labels
$$\approx d\theta \frac{\beta^2}{\epsilon^2}$$
.

Proof Sketch:

Round t, all $f \in \mathcal{H}$ agree on pts in $S \setminus Q$

Roughly, that means Step 4 only keeps f with

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$$\Rightarrow t \gtrsim \log(d\frac{\beta}{\epsilon^2})$$
 suffices

Also \Rightarrow after round t-1, $\mathcal{H} \subseteq B\left(f^*, 2\beta + \sqrt{\beta \frac{d}{2^{t-1}}}\right) \subseteq B(f^*, 3\beta)$ (for large t)

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When is θ small?

- Linear separators, P_X has a density, f^* boundary intersects interior of support $\Rightarrow \theta$ bounded
- Linear separators, P_X has a density $\Rightarrow \theta \ll \frac{1}{\epsilon}$
- \mathcal{H} smoothly-parametrized model, P_X "regular" density w/ compact support, other technical conditions on \mathcal{H} $\Rightarrow \theta \propto \#$ parameters for \mathcal{H}

• • • •

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- \mathcal{H} smoothly-parametrized model, P_X "regular" density w/ compact support, other technical conditions on \mathcal{H} $\Rightarrow \theta \propto \#$ parameters for \mathcal{H}
- . . .

Lots more



Stopping Criterion

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping\text{-}criterion)

1. \mathbf{sample}\ 2^t unlabeled points S

2. \mathbf{label}\ points\ in\ Q = \mathrm{DIS}(\mathcal{H}) \cap S

3. \mathbf{optimize}\ \hat{f} \leftarrow \operatorname*{argmin}\ \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}.

\mathbf{output}\ \text{final}\ \hat{f}
```

Stopping criteria:

- Any-time
- Label budget
- Run out of unlabeled data
- Check $\max_{f \in \mathcal{H}} \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}} < \epsilon$

Simpler Agnostic Active Learning

Hsu (2010,...)

```
Q \leftarrow \{\}
for m = 1, 2, \dots (til stopping-criterion)
      1. sample a random point x
      2. optimize \forall y, \hat{f}_y \leftarrow \underset{f \in \mathcal{H}: f(x)=y}{\operatorname{argmin}} \hat{R}_Q(f)
      3. if |\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_- \ne \hat{f}_+) \frac{d}{|Q|}}
           then label x, add it to Q
output \hat{f} = \operatorname{argmin} \hat{R}_{\mathcal{O}}(f)
```

- Roughly same sample complexity as A^2 .
- Can implement as a **reduction** to ERM.
- In practice, replace ERM with any passive learner.

Surrogate Loss

```
Q \leftarrow \{\}
for m = 1, 2, \dots (til stopping-criterion)
       1. sample a random point x
      2. optimize \forall y, \hat{f}_y \leftarrow \underset{f \in \mathcal{H}: f(x) = y}{\operatorname{argmin}} \hat{R}_Q^{\ell}(f)
      3. if |\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_- \ne \hat{f}_+) \frac{d}{|Q|}}
            then label x, add it to Q
output \hat{f} = \operatorname{argmin} \hat{R}_{\mathcal{O}}(f)
```

- Roughly same sample complexity as A^2 .
- Can implement as a **reduction** to ERM.
- In practice, replace ERM with any passive learner.

Consider learner that minimizes a **surrogate loss** $\ell : \mathbb{R} \times \{-1, +1\} \to \mathbb{R}_+$ (e.g., hinge loss, squared loss, exponential loss, ...)

Now \mathcal{H} is **real-valued** functions

$$\hat{R}_Q^{\ell}(f) = \frac{1}{|Q|} \sum_{(x,y)\in Q} \ell(f(x), y)$$

Theorem: Bounded noise, plus strong assumptions on \mathcal{H}, ℓ, P still get $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels

$$\approx \theta d \log(\frac{1}{\epsilon})$$

Importance-Weighted Active Learning

Beygelzimer, Dasgupta, Langford (2009)

```
Q \leftarrow \{\} for m=1,2,\ldots (til stopping	ext{-}criterion)
```

- 1. sample a random point x
- 2. **set** sampling probability p_x
- 3. flip coin with prob p_x of heads
- 4. if heads, label x, add to Q with weight $1/p_x$

output
$$\hat{f} = \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$$
 (weighted loss)

Use importance weights to stay **unbiased**: $\mathbb{E}[\hat{R}_Q(f)] = R(f)$

Now Q set of triples (x, y, w)

$$\hat{R}_Q(f) = \frac{1}{|Q|} \sum_{(x,y,w)\in Q} w \mathbb{I}[f(x) \neq y]$$

- Any choice of Step 2 (setting p_x) is fine (just p_x not too small, else high variance)
- Can set p_x in a way to recover A^2 sample complexity $p_x = \mathbb{I}\left[|\hat{R}_Q(\hat{f}_+) \hat{R}_Q(\hat{f}_-)| \le \sqrt{\hat{P}_Q(\hat{f}_+ \ne \hat{f}_-) \frac{d}{|Q|}} \right]$

Importance-Weighted Active Learning

Beygelzimer, Dasgupta, Langford (2009)

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Q \leftarrow \{\} for m=1,2,\ldots (til stopping-criterion)
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- 1. sample a random point x
- 2. **set** sampling probability p_x
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- In practice, replace ERM with any passive learner (e.g., ERM with a surrogate loss)
- (approx) implementation in **Vowpal Wabbit** library

Questions?

Further reading:

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- S. Hanneke, L. Yang. Surrogate losses in passive and active learning. arXiv:1207.3772.

Part 3: Beyond Disagreement-Based Active Learning – Current Directions

- Subregion-Based Active Learning
- Margin-Based Active Learning: Linear Separators
- Shattering-Based Active Learning
- Distribution-Free Analysis, Optimality
- TicToc: Adapting to Heterogeneous Noise
- Tsybakov Noise

Tutorial on Active Learning: Theory to Practice

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Robert Nowak

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 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

```
for t = 1, 2, ... (til stopping-criterion)

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output final \hat{f}
```

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

Subregion-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. label points in $Q = \mathcal{R}_{\epsilon'_t}(\mathcal{H}) \cap S$
- 3. optimize $\hat{f} \leftarrow \operatorname*{argmin}_{f \in \mathcal{H}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}$

 ${f output}$ final \hat{f}

Instead, pick **region** $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t. $\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$

Pick ϵ' carefully each round, $R(\hat{f}) - R(f^*) \le \epsilon$ at end

e.g., Bounded noise: $\epsilon' \propto d2^{-t}$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

Subregion-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. **label** points in $Q = \mathcal{R}_{\epsilon'_{+}}(\mathcal{H}) \cap S$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. reduce \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

 $\mathbf{output} \ \mathrm{final} \ \hat{f}$

Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

$$\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$$

$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

$$\approx \varphi_c d \log(\frac{1}{\epsilon})$$

 $DIS(\mathcal{H}) := \{ x \in \mathcal{X} : \exists f, f' \in \mathcal{H}, f(x) \neq f'(x) \}$

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$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

Theorem: with Bounded noise,

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

$$\approx \varphi_c d \log(\frac{1}{\epsilon})$$

Agnostic case:
$$\varphi'_c := \sup_{r>\epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,2\beta+r)))}{2\beta+r}$$

Theorem:

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

 $\approx \varphi'_c d \frac{\beta^2}{\epsilon^2}$

How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

- $\mathcal{R}_{\epsilon'}(\mathcal{H}) = \mathrm{DIS}(\mathcal{H})$ works
- Empirically (Zhang & Chaudhuri, 2014)
- Nice structure: e.g., Linear separators

Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

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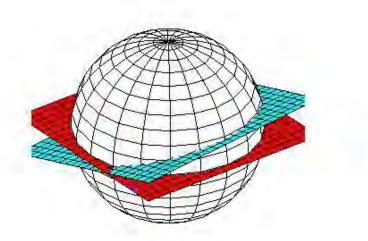
Margin-based Active Learning

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Uniform P_X on d-dim sphere

For
$$w \in B(w^*, r)$$
, **project** to $Span(w, w^*)$



How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

• Nice structure: e.g., **Linear separators**

Margin-based Active Learning

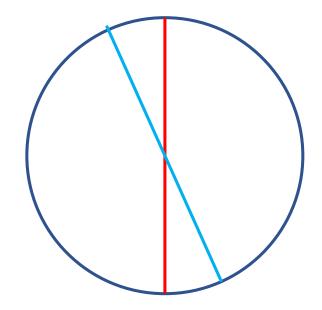
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Uniform P_X on d-dim sphere

For
$$w \in B(w^*, r)$$
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Most projected prob mass toward middle



How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

• Nice structure: e.g., **Linear separators**

Margin-based Active Learning

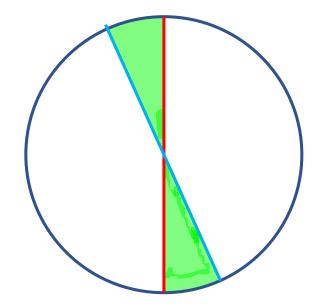
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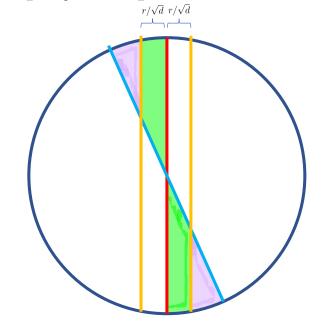
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Uniform P_X on d-dim sphere

For
$$w \in B(w^*, r)$$
, **project** to $Span(w, w^*)$

Most projected prob mass toward middle



 $DIS(\{w, w^*\})$ in slab of width $\approx r$

Most of its prob in slab of width $\approx r/\sqrt{d}$

How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

• Nice structure: e.g., **Linear separators**

Margin-based Active Learning

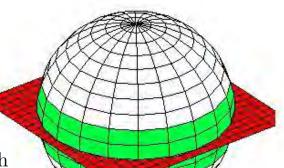
(Dasgupta, Kalai, Monteleoni, 2005; Balcan, Broder, Zhang, 2007; ...)

 $DIS(B(f^*, r)) =$ slab of width $\approx r$

Take $\mathcal{R}_{r/c}(\mathbf{B}(f^*, r)) =$ slab of width $\approx r/\sqrt{d}$

Prob in slab $\approx \sqrt{d} \times \text{width}$

 $\Rightarrow \varphi_c \leq \text{constant}$



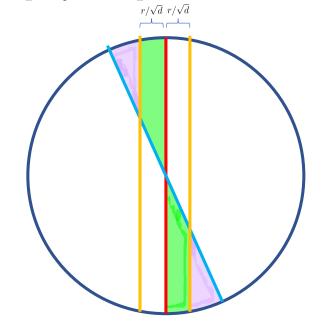
Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

$$\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$$

Uniform P_X on d-dim sphere

For
$$w \in B(w^*, r)$$
, **project** to $Span(w, w^*)$

Most projected prob mass toward middle



 $DIS(\{w, w^*\})$ in slab of width $\approx r$

Most of its prob in slab of width $\approx r/\sqrt{d}$

Subregion-Based Active Learning

How to find such an $\mathcal{R}_{\epsilon'}(\mathcal{H})$?

• Nice structure: e.g., **Linear separators**

Margin-based Active Learning

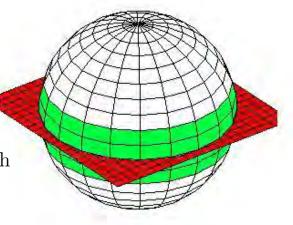
(Dasgupta, Kalai, Monteleoni, 2005; Balcan

$$DIS(B(f^*, r)) =$$
slab of width $\approx r$

Take $\mathcal{R}_{r/c}(\mathbf{B}(f^*, r)) =$ slab of width $\approx r/\sqrt{d}$

Prob in slab $\approx \sqrt{d} \times \text{width}$

 $\Rightarrow \varphi_c \leq \text{constant}$



Pick region $\mathcal{R}_{\epsilon'}(\mathcal{H})$ s.t.

$$\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$$

$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(B(f^*,r)))}{r}$$

Theorem: with Bounded noise,

$$R(\hat{f}) \le R(f^*) + \epsilon \text{ using } \# \text{ labels}$$

 $\approx \varphi_c d \log(\frac{1}{\epsilon})$

$$\Rightarrow$$
 # labels $\approx d \log(\frac{1}{\epsilon})$ suffice

Recall: Passive $\approx \frac{d}{\epsilon}$

Comparison:

Recall
$$\theta \approx \sqrt{d}$$

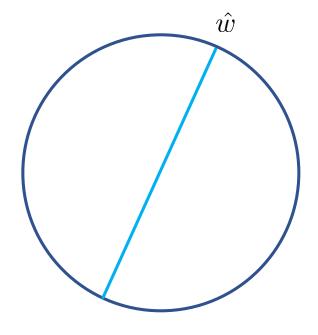
 $\Rightarrow A^2 \# \text{ labels } \approx d^{3/2} \log(\frac{1}{\epsilon})$

Margin-based Active Learning

Initialize \hat{w}

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample $d2^t$ unlabeled points S
- 2. label points in $Q = \text{all } x \in S \text{ s.t. } \langle \hat{w}, x \rangle \leq c2^{-t}/\sqrt{d}$
- 3. optimize $\hat{w} \leftarrow \underset{w:||w-\hat{w}|| \leq c'2^{-t}}{\operatorname{argmin}} \hat{R}_Q(w)$



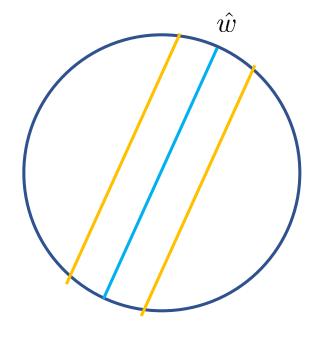
Uniform P_X on d-dim sphere

Margin-based Active Learning

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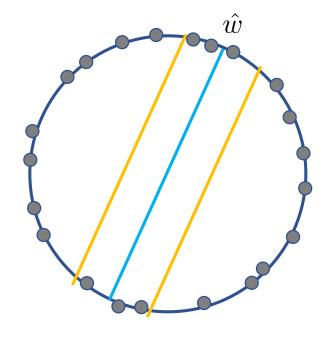
Uniform P_X on d-dim sphere

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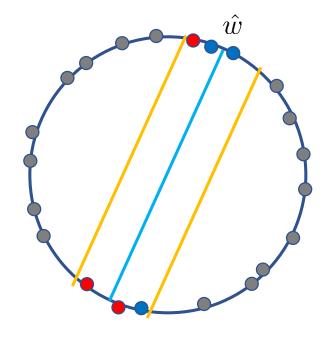
Uniform P_X on d-dim sphere

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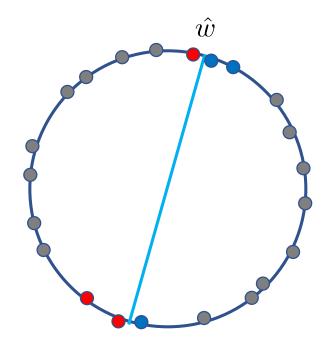
Uniform P_X on d-dim sphere

Margin-based Active Learning

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Uniform P_X on d-dim sphere

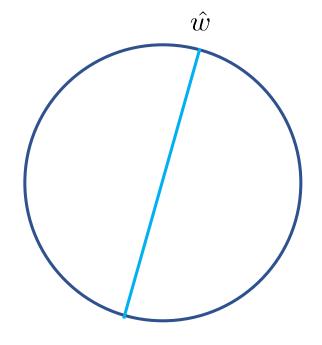
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- 3. optimize $\hat{w} \leftarrow \underset{w:||w-\hat{w}|| \le c'2^{-t}}{\operatorname{argmin}} \hat{R}_Q(w)$

output final \hat{w}



Uniform P_X on d-dim sphere

Theorem: with Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels $\approx d \log(\frac{1}{\epsilon})$

(also works for isotropic log-concave distributions)

(Awasthi, Balcan, Long, 2014,...)

Computational Efficiency

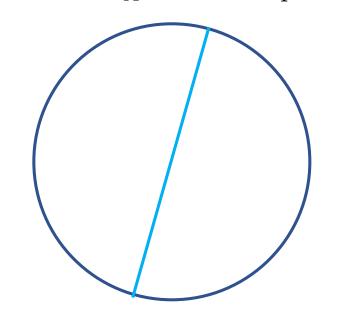
Efficient Alg Initialize \hat{w} for $t=1,2,\ldots$ (til stopping-criterion) 1. $\mathbf{sample}\ d2^t$ unlabeled points S2. $\mathbf{label}\ points$ in $Q=\text{all}\ x\in S\ \text{s.t.}\ <\hat{w},x>\ \le\ c2^{-t}/\sqrt{d}$ 3. $\mathbf{optimize}\ \hat{w}\leftarrow \underset{w:\|w-\hat{w}\|\le c'2^{-t}}{\operatorname{argmin}} \hat{R}_Q^{\ell_t}(w)$ output final \hat{w}

Surrogate loss

$$\ell_t(< w, x>, y) \approx \max\{1 - 2^t \sqrt{d}(y < w, x>), 0\}$$

Hinge loss slope changes each round

Uniform P_X on d-dim sphere



(Awasthi, Balcan, Long, 2014,...)

Computational Efficiency

```
Efficient Alg

Initialize \hat{w}

for t = 1, 2, ... (til stopping\text{-}criterion)

1. \mathbf{sample}\ d2^t unlabeled points S

2. \mathbf{label}\ points in Q = \text{all}\ x \in S \text{ s.t. } <\hat{w}, x> \leq c2^{-t}/\sqrt{d}

3. \mathbf{optimize}\ \hat{w} \leftarrow \underset{w:||w-\hat{w}|| \leq c'2^{-t}}{\operatorname{argmin}} \hat{R}_Q^{\ell_t}(w)

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Theorem: with Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels $\approx d \log \left(\frac{1}{\epsilon}\right)$ and running in polynomial time

Computational Efficiency

Efficient Alg

Initialize \hat{w}

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample $d2^t$ unlabeled points S
- 2. label points in $Q = \text{all } x \in S \text{ s.t. } \langle \hat{w}, x \rangle \leq c2^{-t}/\sqrt{d}$
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Surrogate loss

$$\ell_t(< w, x>, y) \approx \max\{1 - 2^t \sqrt{d}(y < w, x>), 0\}$$

Hinge loss slope changes each round

Uniform P_X on d-dim sphere

Theorem: with Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels $\approx d \log \left(\frac{1}{\epsilon}\right)$ and running in polynomial time

Theorem: with Agnostic case, $R(\hat{f}) \leq CR(f^*)$ in polynomial time

(was first alg. known to achieve these; even passively)

(also works for isotropic log-concave distributions)

Up Next: Shattering-Based Active Learning

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

 $DIS(\mathcal{H})$ checks for shattering 1 point.

Idea: Generalize to shattering ≥ 1 points.

(Hanneke, 2009, 2012)

Shattering-Based Active Learning

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

```
for t = 1, 2, ... (til stopping\text{-}criterion)

1. \mathbf{sample}\ 2^t unlabeled points S

2. \mathbf{label}\ points\ in\ Q = \mathrm{DIS}(\mathcal{H}) \cap S

3. \mathbf{optimize}\ \hat{f} \leftarrow \operatorname*{argmin}\ \hat{R}_Q(f)

4. \mathbf{reduce}\ \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}.

\mathbf{output}\ final\ \hat{f}
```

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Shattering-Based Active Learning

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

Shattering-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
- 2. **label** points in $Q = \text{all } x \in S \text{ s.t.}$ $P_X^k(A \in \mathcal{X}^k : \mathcal{H} \text{ shatters } A \cup \{x\} | \mathcal{H} \text{ shatters } A) \ge \frac{1}{2}$
- 3. optimize $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
- 4. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$.

output final \hat{f}

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Shattering-based Active Learning
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- 3. add the remaining points $x \in S$ to Q with label $\hat{y}_x := \underset{y}{\operatorname{argmax}} P_X^k (A \in \mathcal{X}^k : \mathcal{H}_{x,y} \text{ shatters } A | \mathcal{H} \text{ shatters } A)$
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 ${f output}$ final \hat{f}

 $DIS(\mathcal{H})$ checks for shattering 1 point.

Idea: Generalize to shattering ≥ 1 points.

Denote $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

Shattering-based Active Learning

for $t = 1, 2, \dots$ (til stopping-criterion)

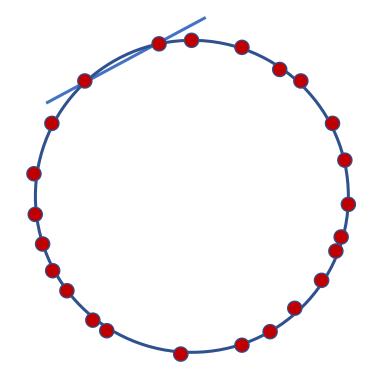
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 ${f output}$ final \hat{f}

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Example: Linear separators, Uniform P_X on circle Suppose true labels are all -1

$$DIS(\mathcal{H}) = \mathbf{entire} \ \mathbf{circle}$$



Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

```
Shattering-based Active Learning
for t = 1, 2, \dots (til stopping-criterion)
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     3. add the remaining points x \in S to Q with label
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     5. reduce \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}
output final \hat{f}
```

Example: Linear separators, Uniform P_X on circle Suppose true labels are all -1

$$DIS(\mathcal{H}) = \textbf{entire circle}$$

$$Try \ k = 1$$

$$Given sample \ x$$

$$Rand \ x' \text{ probably not close}$$

$$Can't \text{ shatter } \{x, x'\}$$

$$without a lot of points wrong$$

$$So \text{ won't query } x$$

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

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Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Example: Linear separators, Uniform P_X on circle Suppose true labels are all -1

So won't query x

$$DIS(\mathcal{H}_{x,-1})$$
 still entire circle (minus x)
 $DIS(\mathcal{H}_{x,+1})$ small region
 $\Rightarrow \hat{y}_x = -1$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

```
Shattering-based Active Learning
for t = 1, 2, \dots (til stopping-criterion)
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output final \hat{f}
```

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Example: Linear separators, Uniform P_X on circle Suppose true labels are all -1

DIS(
$$\mathcal{H}$$
) = entire circle

Try $k = 1$

Given sample x

Rand x' probably not close

Can't shatter $\{x, x'\}$

without a lot of points wrong

So won't query x

So won't query x

$$DIS(\mathcal{H}_{x,-1})$$
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Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Example: Linear separators, Uniform P_X on circle Suppose true labels are all -1

$$\operatorname{DIS}(\mathcal{H}) = \operatorname{\mathbf{entire\ circle}}$$
 $\operatorname{Try} k = 1$
 $\operatorname{Given\ sample\ } x$
 $\operatorname{Rand\ } x' \operatorname{probably\ not\ close}$
 $\operatorname{Can't\ shatter\ } \{x,x'\}$

without a lot of points wrong

 $\operatorname{Sample\ } x$
 $\operatorname{Sample\ point\ } x$

So won't query x

$$DIS(\mathcal{H}_{x,-1})$$
 still entire circle (minus x)
 $DIS(\mathcal{H}_{x,+1})$ small region
 $\Rightarrow \hat{y}_x = -1$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

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```

Generally, need to try various k and pick one (See the papers)

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

```
Shattering-based Active Learning
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 $oldsymbol{ ext{output}}$ final \hat{f}

Generally, need to try various k and pick one (See the papers)

$$\theta^{(k)} := \sup_{r > \epsilon} \frac{P_X^k(A \in \mathcal{X}^k : B(f^*, r) \text{ shatters } A)}{r}$$

$$\tilde{d} := \min \left\{ k : P_X^k (A \in \mathcal{X}^k : \mathcal{B}(f^*, r) \text{ shatters } A) \xrightarrow[r \to 0]{} 0 \right\}$$

$$\tilde{\theta} := \theta^{(\tilde{d})}$$

Theorem: For Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels

$$\approx C\tilde{\theta}d\log(\frac{1}{\epsilon})$$

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Note: $\tilde{\theta} \ll \frac{1}{\epsilon}$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

```
Shattering-based Active Learning
```

for $t = 1, 2, \dots$ (til stopping-criterion)

- 1. sample 2^t unlabeled points S
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- 3. add the remaining points $x \in S$ to Q with label $\hat{y}_x := \underset{y}{\operatorname{argmax}} P_X^k (A \in \mathcal{X}^k : \mathcal{H}_{x,y} \text{ shatters } A | \mathcal{H} \text{ shatters } A)$
- 4. optimize $\hat{f} \leftarrow \operatorname*{argmin}_{f \in \mathcal{H}} \hat{R}_Q(f)$
- 5. **reduce** \mathcal{H} : remove all f with $\hat{R}_Q(f) \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{|Q|}}$

 $oldsymbol{ ext{output}}$ final \hat{f}

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

Generally, need to try various k and pick one (See the papers)

$$\theta^{(k)} := \sup_{r > \epsilon} \frac{P_X^k(A \in \mathcal{X}^k : B(f^*, r) \text{ shatters } A)}{r}$$

$$\tilde{d} := \min \Big\{ k : P_X^k (A \in \mathcal{X}^k : \mathcal{B}(f^*, r) \text{ shatters } A) \xrightarrow[r \to 0]{} 0 \Big\}$$

$$\tilde{\theta} := \theta^{(\tilde{d})}$$

Theorem: For Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels

$$\approx C\tilde{\theta}d\log(\frac{1}{\epsilon})$$

Note: $\tilde{\theta} \ll \frac{1}{\epsilon}$

In the example: $\tilde{\theta} = 2$, $\theta = \frac{1}{\epsilon}$

Recall: \mathcal{H} shatters x_1, \ldots, x_k if all 2^k classifications realized by \mathcal{H}

```
Shattering-based Active Learning

for t = 1, 2, ... (til stopping-criterion)

1. sample 2^t unlabeled points S

2. label points in Q = \text{all } x \in S s.t.
P_X^k(A \in \mathcal{X}^k : \mathcal{H} \text{ shatters } A \cup \{x\} | \mathcal{H} \text{ shatters } A) \geq \frac{1}{2}

3. add the remaining points x \in S to Q with label
\hat{y}_x := \underset{y}{\operatorname{argmax}} P_X^k(A \in \mathcal{X}^k : \mathcal{H}_{x,y} \text{ shatters } A | \mathcal{H} \text{ shatters } A)

4. optimize \hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)
5. reduce \mathcal{H}: remove all f with \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|}.
```

Denoting $\mathcal{H}_{x,y} := \{ h \in \mathcal{H} : h(x) = y \}$

output final \hat{f}

Generally, need to try various k and pick one (See the papers)

$$\theta^{(k)} := \sup_{r > \epsilon} \frac{P_X^k(A \in \mathcal{X}^k : B(f^*, r) \text{ shatters } A)}{r}$$

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$$\tilde{\theta} := \theta^{(\tilde{d})}$$

Theorem: For Bounded noise, $R(\hat{f}) \leq R(f^*) + \epsilon$ with # labels

$$pprox C ilde{ heta}d\log\left(rac{1}{\epsilon}
ight)$$

Note: $\tilde{\theta} \ll \frac{1}{\epsilon}$ (may depend on f^* , P_X)

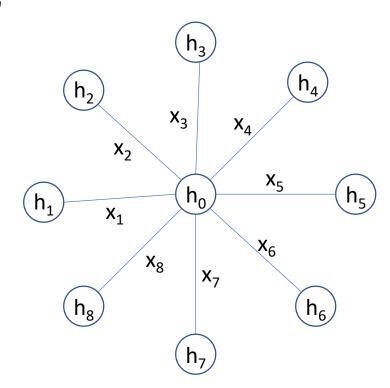
In the example: $\tilde{\theta} = 2$, $\theta = \frac{1}{\epsilon}$

Up Next:
Distribution-free Analysis

 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

Can we do sample complexity analysis **without** distribution-dependence?

<u>Definition:</u> The **star number** \mathfrak{s} is the largest k s.t. $\exists h_0, h_1, \ldots, h_k \in \mathcal{H}$, $\exists x_1, \ldots, x_k \in \mathcal{X}$ s.t. $\forall i \in \{1, \ldots, k\}, \{x_j : h_i(x_j) \neq h_0(x_j)\} = \{x_i\}.$



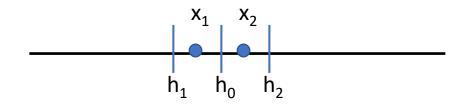
 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

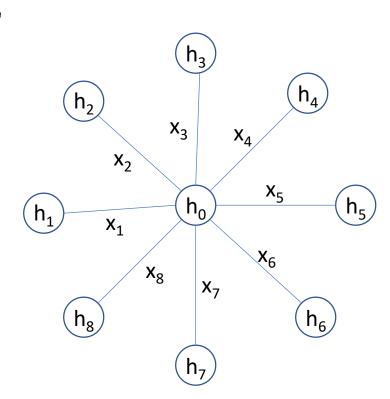
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Example: Thresholds: $f(x) = \mathbb{I}[x \ge t]$.

$$\mathfrak{s}=2.$$



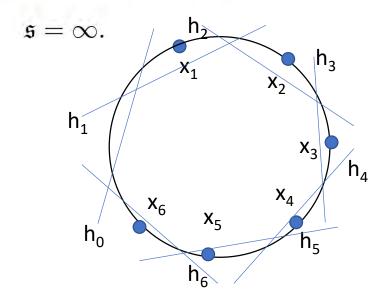


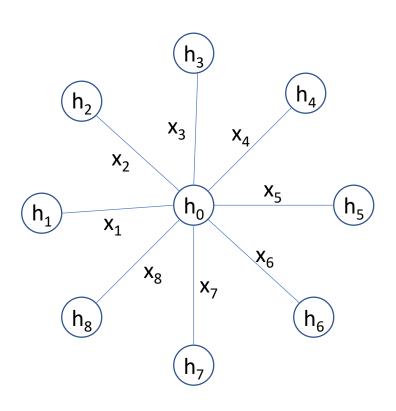
 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

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Example: Linear Separators in \mathbb{R}^n , $n \geq 2$:





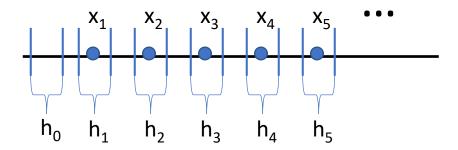
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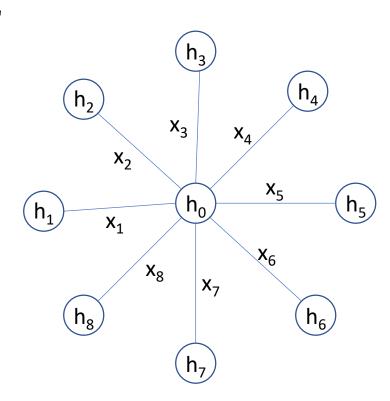
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Example: Intervals: $x \mapsto \mathbb{I}[a \le x \le b]$

$$\mathfrak{s}=\infty$$
.



Intervals of width w (b-a=w>0) on $\mathcal{X}=[0,1]$: $\mathfrak{s}\approx \lfloor \frac{1}{w} \rfloor$.



 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

Can we do sample complexity analysis **without** distribution-dependence?

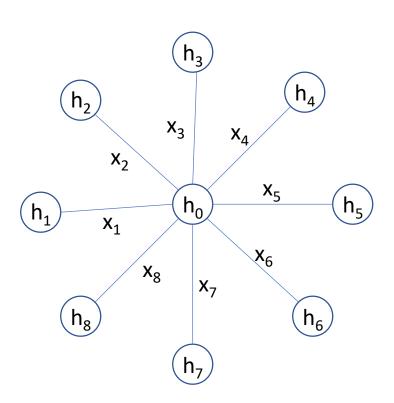
<u>Definition:</u> The **star number** \mathfrak{s} is the largest k s.t. $\exists h_0, h_1, \ldots, h_k \in \mathcal{H}$, $\exists x_1, \ldots, x_k \in \mathcal{X}$ s.t. $\forall i \in \{1, \ldots, k\}, \{x_j : h_i(x_j) \neq h_0(x_j)\} = \{x_i\}.$

Theorem: $\sup_{P_X} \sup_{f^* \in \mathcal{H}} \theta = \sup_{P_X} \sup_{f^* \in \mathcal{H}} \varphi_c = \sup_{P_X} \sup_{f^* \in \mathcal{H}} \tilde{\theta} = \min\{\mathfrak{s}, \frac{1}{\epsilon}\} =: \mathfrak{s}_{\epsilon}$

Corollary:

Bounded noise # labels $\approx \mathfrak{s}_{\epsilon} d \log(\frac{1}{\epsilon})$ Agnostic $(\beta = R(f^*))$ # labels $\approx \mathfrak{s}_{\beta} d \frac{\beta^2}{\epsilon^2}$

Achieved by A^2



(Hanneke & Yang, 2015; Hanneke, 2016)

Distribution-Free Analysis

 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

Can we do sample complexity analysis **without** distribution-dependence?

<u>Definition:</u> The **star number** \mathfrak{s} is the largest k s.t. $\exists h_0, h_1, \ldots, h_k \in \mathcal{H}$, $\exists x_1, \ldots, x_k \in \mathcal{X}$ s.t. $\forall i \in \{1, \ldots, k\}, \{x_j : h_i(x_j) \neq h_0(x_j)\} = \{x_i\}.$

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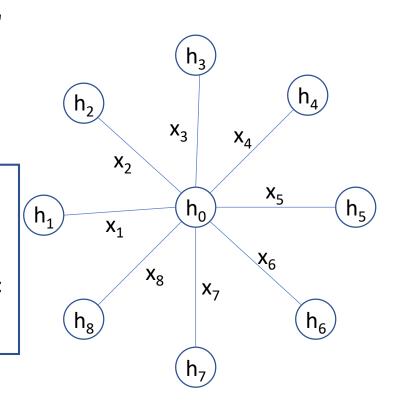
Corollary:

Bounded noise # labels $\approx \mathfrak{s}_{\epsilon} d \log(\frac{1}{\epsilon})$ Agnostic $(\beta = R(f^*))$ # labels $\approx \mathfrak{s}_{\beta} d \frac{\beta^2}{\epsilon^2}$

Achieved by A^2

Different alg., Bounded noise # labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

Near-matching lower bound: $\mathfrak{s}_{\epsilon} + d \log(\frac{1}{\epsilon})$



(Hanneke & Yang, 2015; Hanneke, 2016)

Distribution-Free Analysis

 $\theta, \varphi, \tilde{\theta}$ depend on f^*, P_X .

Can we do sample complexity analysis **without** distribution-dependence?

Definition: The **star number** \mathfrak{s} is the largest k s.t. $\exists h_0, h_1, \ldots, h_k \in \mathcal{H}$, $\exists x_1, \ldots, x_k \in \mathcal{X}$ s.t. $\forall i \in \{1, \ldots, k\}, \{x_j : h_i(x_j) \neq h_0(x_j)\} = \{x_i\}.$

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Corollary:

Bounded noise # labels $\approx \mathfrak{s}_{\epsilon} d \log(\frac{1}{\epsilon})$ Agnostic $(\beta = R(f^*))$ # labels $\approx \mathfrak{s}_{\beta} d \frac{\beta^2}{\epsilon^2}$

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Different alg., Bounded noise # labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

Near-matching lower bound: $\mathfrak{s}_{\epsilon} + d \log(\frac{1}{\epsilon})$

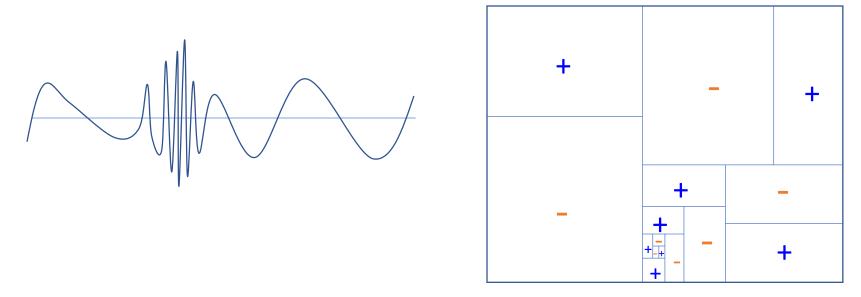
Open Question:

Agnostic $(\beta = R(f^*))$ # labels $\approx d \frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$?

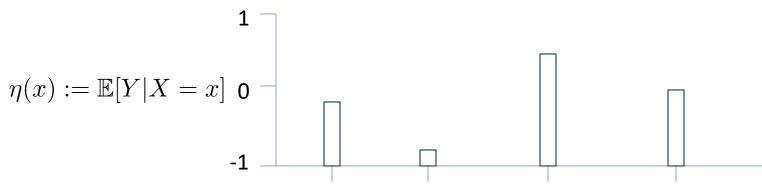
lower bound:
$$d\frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon} + d\log(\frac{1}{\epsilon})$$

Adapting to Heterogeneous Noise

So far: Active learning for spatial heterogeneity of opt function:



Also consider: Spatial heterogeneity of **noise**:



(Hanneke & Yang, 2015)

Active Learning with TicToc

```
Algorithm: \mathbb{A}(n)
Input: Label budget n
Output: Classifier \hat{f}_n.

1. \mathbb{L} \leftarrow \{\}
2. For m = 1, 2, ...
3. X_{s_m} \leftarrow \text{GetSeed}(\mathbb{L}, m) \leftarrow
4. \mathcal{L}_m \leftarrow \text{TicToc}(X_{s_m}, m) \leftarrow
5. if \mathcal{L}_m exists, \mathbb{L} \leftarrow \mathbb{L} \cup \{(s_m, \mathcal{L}_m)\}
6. If we've made n queries
7. Return \hat{f}_n \leftarrow \text{Learn}(\mathbb{L}) \leftarrow
An active learning alg.

(e.g. \mathbb{A}^2)

Main new part

A passive learning alg.
```

Active Learning with TicToc

```
Algorithm: \mathbb{A}(n)
Input: Label budget n
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7. Return \hat{f}_n \leftarrow \text{Learn}(\mathbb{L})
```

```
Denote \eta(x) = \mathbb{E}[Y|X=x]
Suppose f^* is the global optimal function: f^*(x) = \text{sign}(\eta(x))
```

```
TICTOC(X, m):
Query X (or nearby) to try to guess f^*(X)
If can figure it out, return that label
If can't figure it out by \tau_m queries give up (don't return a label)
```

Focus queries on less-noisy points.

Double advantage:

• Focusing on the points we actually care about:

$$R(f|x) - R(f^*|x) = |\eta(x)|\mathbb{I}[f(x) \neq f^*(x)]$$

(small $|\eta(x)| \Rightarrow$ not much effect on $R(f|x)$ if $f(x) = f^*(x)$ or not).

• And those points require fewer queries to determine $f^*(X_i)!$

$$\sim \frac{1}{\eta(X_i)^2}$$
 queries to determine $f^*(X_i)$.

Active Learning with TicToc

```
Algorithm: \mathbb{A}(n)

Input: Label budget n

Output: Classifier \hat{f}_n.

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

3. X_{s_m} \leftarrow \text{GETSEED}(\mathbb{L}, m)

4. \mathcal{L}_m \leftarrow \text{TICTOC}(X_{s_m}, m)

5. if \mathcal{L}_m exists, \mathbb{L} \leftarrow \mathbb{L} \cup \{(s_m, \mathcal{L}_m)\}

6. If we've made n queries

7. Return \hat{f}_n \leftarrow \text{LEARN}(\mathbb{L})
```

Theorem: Bounded noise: # labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

Denote $\eta(x) = \mathbb{E}[Y|X=x]$ Suppose f^* is the **global** optimal function: $f^*(x) = \text{sign}(\eta(x))$

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 queries to determine $f^*(X_i)$.

Active Learning with TicToc

Algorithm: $\mathbb{A}(n)$

Input: Label budget n

Output: Classifier \hat{f}_n .

- 1. $\mathbb{L} \leftarrow \{\}$
- 2. For m = 1, 2, ...
- 3. $X_{s_m} \leftarrow \text{GetSeed}(\mathbb{L}, m)$
- 4. $\mathcal{L}_m \leftarrow \text{TicToc}(X_{s_m}, m)$
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- 6. If we've made n queries
- 7. Return $\hat{f}_n \leftarrow \text{Learn}(\mathbb{L})$

Theorem: Agnostic $(\beta = R(f^*))$

and suppose $f^* = \text{global best}$:

labels

$$\approx d \frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$$

Confirms agnostic sample complexity conjecture but with extra assumption $f^* = \text{global opt.}$

Near-match lower bound: $d\frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon} + d\log(\frac{1}{\epsilon})$

Denote $\eta(x) = \mathbb{E}[Y|X=x]$

Suppose f^* is the **global** optimal function: $f^*(x) = \text{sign}(\eta(x))$

 $\mathrm{TicToc}(X,m)$:

Query X (or nearby) to try to guess $f^*(X)$

If can figure it out, return that label

If can't figure it out by τ_m queries give up (don't return a label)

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Double advantage:

• Focusing on the points we actually care about:

$$R(f|x) - R(f^{\star}|x) = |\eta(x)|\mathbb{I}[f(x) \neq f^{\star}(x)]$$

(small $|\eta(x)| \Rightarrow$ not much effect on R(f|x) if $f(x) = f^*(x)$ or not).

• And those points require fewer queries to determine $f^*(X_i)!$

$$\sim \frac{1}{\eta(X_i)^2}$$
 queries to determine $f^*(X_i)$.

Principles of Active Learning

- 1. Query in dense regions where \hat{f} could disagree a lot with f^*
- 2. Query in regions with low noise

The alg. adapts to heterogeneity in the noise.

Let's try it with a model that explicitly describes heterogeneous noise:

Tsybakov Noise

Denote $\eta(x) = \mathbb{E}[Y|X=x]$

Definition: (Tsybakov noise) $f^{\star}(x) = \operatorname{sign}(\eta(x))$ and $\exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$ $P_X(x: |\eta(x)| \leq \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$

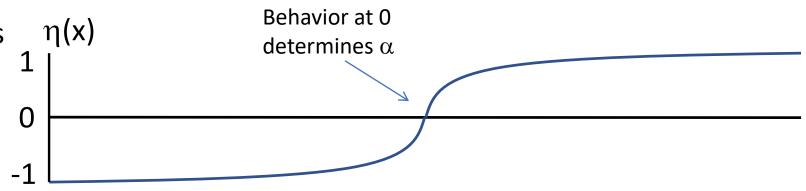
(Tsybakov, 2004; Mammen & Tsybakov 1999)

Denote
$$\eta(x) = \mathbb{E}[Y|X=x]$$

Definition: (Tsybakov noise) $f^{\star}(x) = \operatorname{sign}(\eta(x))$ and $\exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$ $P_X(x: |\eta(x)| \leq \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$

Example:

Thresholds



(unif. distrib)

Denote $\eta(x) = \mathbb{E}[Y|X=x]$

Definition: (Tsybakov noise)

$$f^{\star}(x) = \operatorname{sign}(\eta(x)) \text{ and } \exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$$

$$P_X(x : |\eta(x)| \le \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$$

Passive OPT: $\tilde{\Theta}\left(\frac{d}{\epsilon^{2-\alpha}}\right)$.

Active OPT:
$$\begin{cases} \frac{d}{\epsilon^{2-2\alpha}} & \text{if } 0 < \alpha \le 1/2\\ \min\left\{\frac{d}{\epsilon^{2-2\alpha}} \left(\frac{\mathfrak{s}}{d}\right)^{2\alpha-1}, \frac{d}{\epsilon}\right\} & \text{if } 1/2 < \alpha < 1 \end{cases}.$$

$$\sim \begin{cases} rac{1}{arepsilon^{2-2lpha}}, & ext{if } \mathfrak{s} < \infty \ rac{1}{arepsilon}, & ext{if } \mathfrak{s} = \infty \end{cases}.$$

Active Opt \ll Passive Opt. (always)

(Massart & Nédélec, 2006)

(Hanneke & Yang, 2015)

Conclusions

- Many proposals for going beyond Disagreement-based Active Learning
- Each exhibits improvements in certain cases
- We still don't know the optimal agnostic active learning algorithm

$$d\frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d}\log(\frac{1}{\epsilon})$$

Questions?

Further reading:

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