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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Zhang & Chaudhuri, 2014

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

 $\begin{array}{l} \boldsymbol{A^2} \ (\textbf{Agnostic Active}) \\ \hline \text{for } t = 1, 2, \dots \ (\text{til stopping-criterion}) \\ 1. \ \textbf{sample } 2^t \ \text{unlabeled points } S \\ 2. \ \textbf{label points in } Q = \text{DIS}(\mathcal{H}) \cap S \\ 3. \ \textbf{optimize } \hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f) \\ 4. \ \textbf{reduce } \mathcal{H}: \ \text{remove all } f \ \text{with } \hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f})} \frac{d}{|Q|} \\ \textbf{output final } \hat{f} \end{array}$ 

Zhang & Chaudhuri, 2014

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

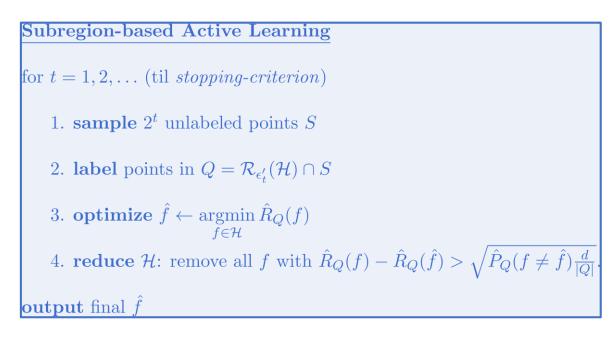
Subregion-based Active Learning
for $t = 1, 2, \dots$ (til stopping-criterion)
1. sample $2^t$ unlabeled points $S$
2. <b>label</b> points in $Q = \mathcal{R}_{\epsilon'_t}(\mathcal{H}) \cap S$
3. <b>optimize</b> $\hat{f} \leftarrow \underset{f \in \mathcal{H}}{\operatorname{argmin}} \hat{R}_Q(f)$
4. reduce $\mathcal{H}$ : remove all $f$ with $\hat{R}_Q(f) - \hat{R}_Q(\hat{f}) > \sqrt{\hat{P}_Q(f \neq \hat{f}) \frac{d}{ Q }}$ .
<b>output</b> 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  $\epsilon'$  carefully each round,  $R(\hat{f}) - R(f^*) \leq \epsilon$  at end

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

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



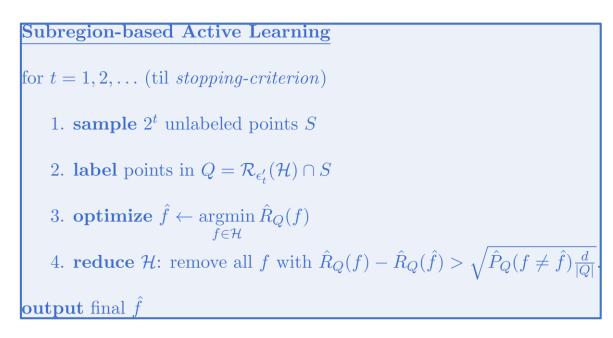
**Pick region**  $\mathcal{R}_{\epsilon'}(\mathcal{H})$  s.t.  $\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$ 

Zhang & Chaudhuri, 2014

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

**<u>Theorem</u>:** with **Bounded noise**,  $R(\hat{f}) \leq R(f^*) + \epsilon$  using # labels

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Zhang & Chaudhuri, 2014

**Pick region** 
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**<u>Theorem</u>:** with **Bounded noise**,  $R(\hat{f}) \leq R(f^*) + \epsilon$  using # labels

 $\approx \varphi_c d \log\left(\frac{1}{\epsilon}\right)$ Agnostic case:  $\varphi'_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(\mathbb{B}(f^*, 2\beta + r)))}{2\beta + r}$ Theorem:  $R(\hat{f}) \leq R(f^*) + \epsilon \text{ using } \# \text{ labels}$   $\approx \varphi'_c d \frac{\beta^2}{\epsilon^2}$ 

Zhang & Chaudhuri, 2014

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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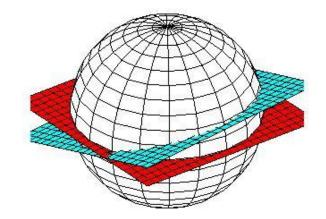
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Uniform  $P_X$  on *d*-dim sphere

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



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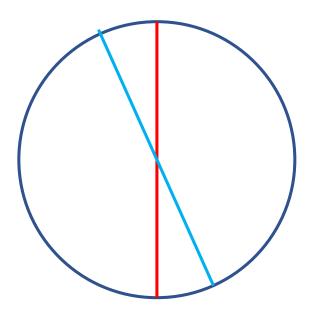
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Most projected prob mass toward middle



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

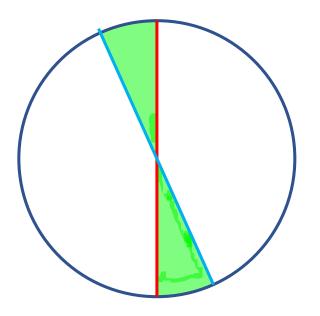
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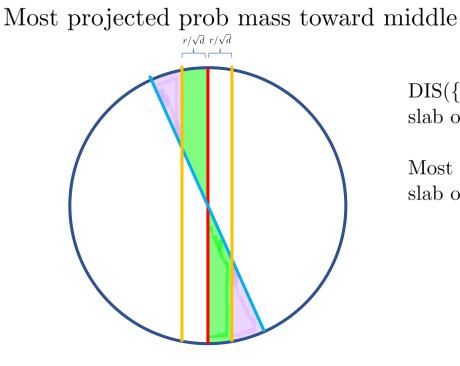
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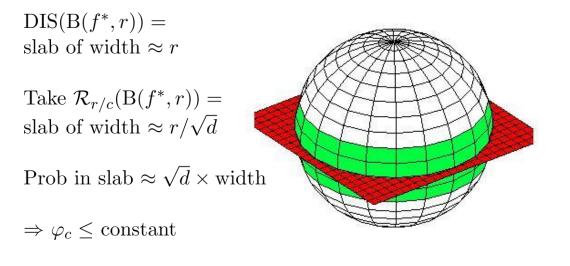
 $DIS(\{w, w^*\}) in$ <br/>slab of width  $\approx r$ 

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

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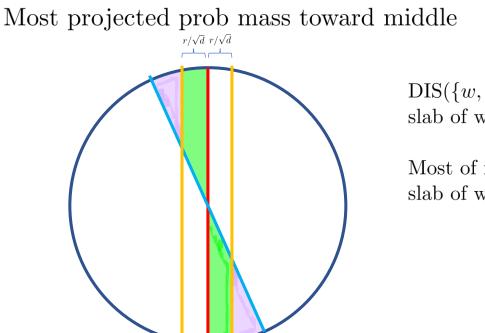
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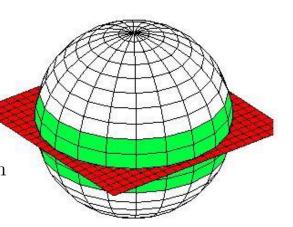
Margin-based Active Learning (Dasgupta, Kalai, Monteleoni, 2005; Balcan

 $DIS(B(f^*, r)) =$ <br/>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.  $\forall f, f' \in \mathcal{H}, P_X(x \notin \mathcal{R}_{\epsilon'}(\mathcal{H}) : f(x) \neq f'(x)) \leq \epsilon'.$ 

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

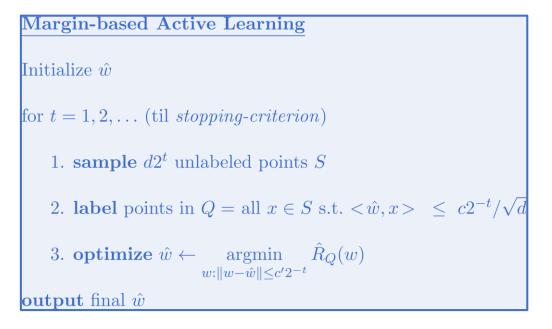
**<u>Theorem</u>:** with **Bounded noise**,  $R(\hat{f}) \leq R(f^*) + \epsilon$  using # labels  $\approx \varphi_c d \log(\frac{1}{\epsilon})$ 

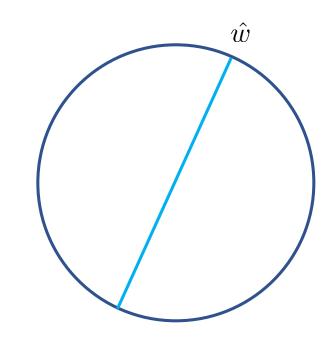
 $\Rightarrow \# \text{ labels} \approx d \log(\frac{1}{\epsilon}) \text{ suffice}$ 

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

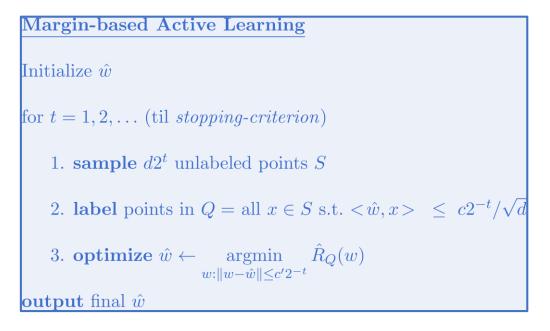
**Comparison:** 

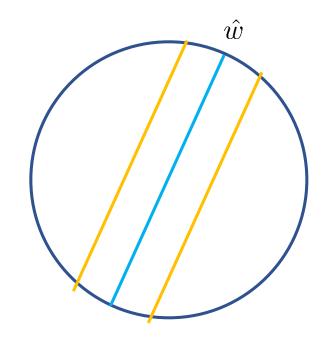
Recall  $\theta \approx \sqrt{d}$  $\Rightarrow A^2 \ \# \ \text{labels} \approx d^{3/2} \log(\frac{1}{\epsilon})$ 



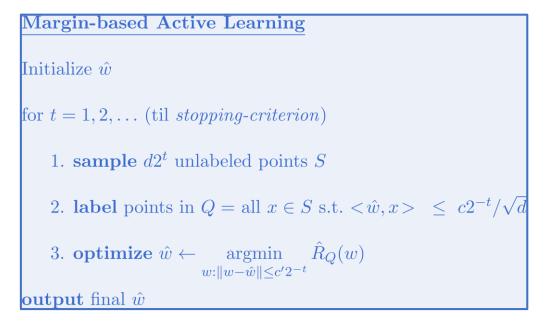


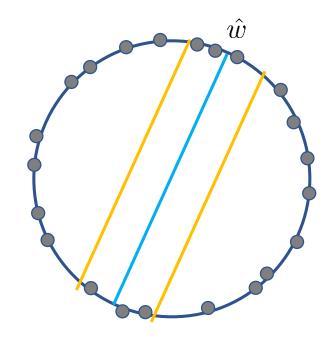
Uniform  $P_X$  on d-dim sphere



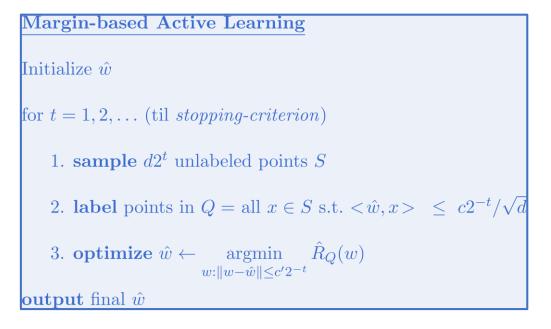


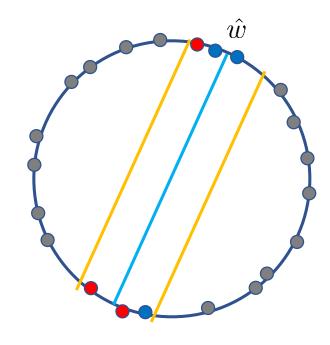
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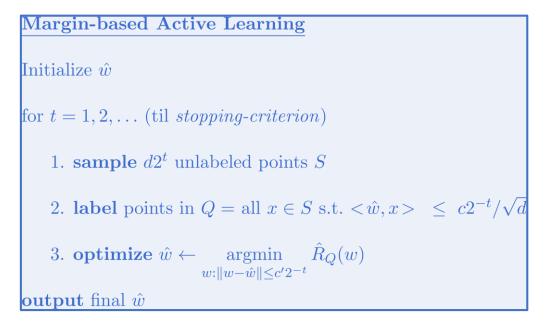


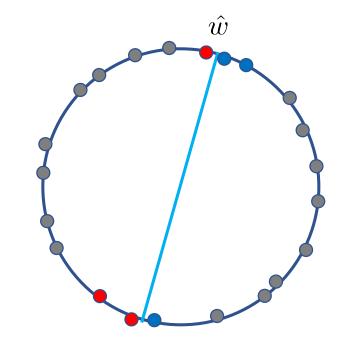
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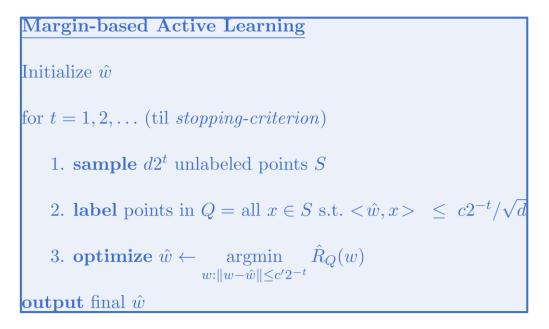


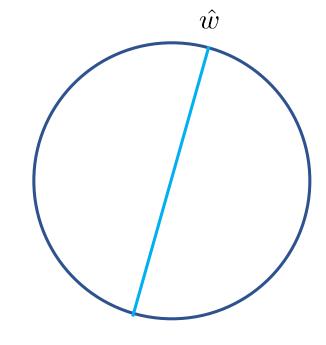
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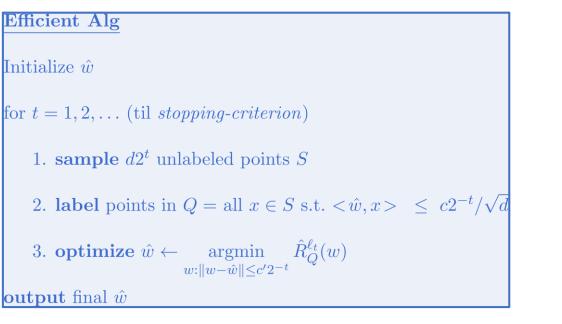
Uniform  $P_X$  on *d*-dim sphere **Theorem:** with **Bounded noise**,  $R(\hat{f}) \leq R(f^*) + \epsilon$  using # labels  $\approx d \log(\frac{1}{\epsilon})$ 

(also works for isotropic log-concave distributions)

## **Computational Efficiency**

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

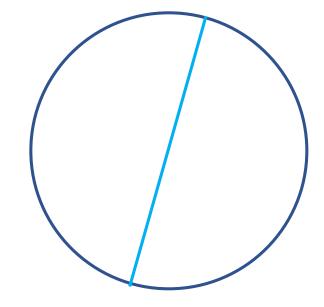
#### Uniform $P_X$ on d-dim sphere



Surrogate loss

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

#### Hinge loss slope changes each round



### **Computational Efficiency**

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

Uniform  $P_X$  on d-dim sphere

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

Efficient Alg

Initialize  $\hat{w}$ 

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

1. sample  $d2^t$  unlabeled points S

2. label points in 
$$Q = \text{all } x \in S \text{ s.t. } \langle \hat{w}, x \rangle \leq c 2^{-t} / \sqrt{c}$$

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

**output** final  $\hat{w}$ 

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

(Hanneke, 2009, 2012)

## Shattering-Based Active Learning

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

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

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

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Shattering-based Active Learning for t = 1, 2, ... (til stopping-criterion) 1. sample  $2^t$  unlabeled points S2. 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. 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	
for $t = 1, 2, \dots$ (til <i>stopping-criterion</i> )	
1. sample $2^t$ unlabeled points $S$	]
2. <b>label</b> 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 $\hat{y}_x := \operatorname*{argmax}_y P_X^k (A \in \mathcal{X}^k : \mathcal{H}_{x,y} \text{ shatters } A   \mathcal{H} \text{ shatters } A) \blacktriangleleft$	]
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<b>output</b> final $\hat{f}$	

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

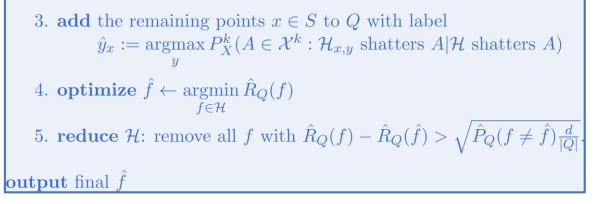
Denote 
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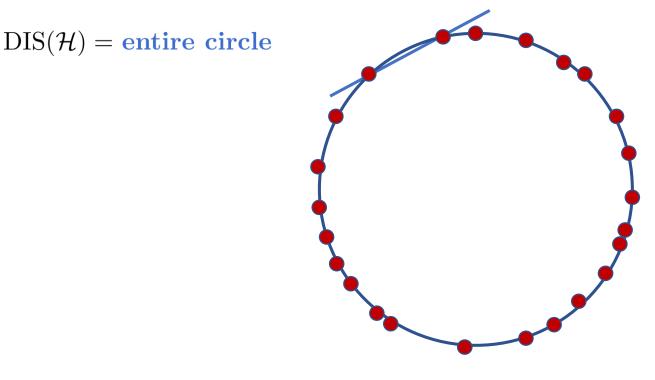
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**Example:** Linear separators, Uniform  $P_X$  on circle Suppose true labels are **all** -1



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3. add the remaining points x ∈ S to Q with label ŷ<sub>x</sub> := argmax P<sup>k</sup><sub>X</sub>(A ∈ X<sup>k</sup> : H<sub>x,y</sub> shatters A|H shatters A)
4. optimize f̂ ← argmin R̂<sub>Q</sub>(f)
5. reduce H: remove all f with R̂<sub>Q</sub>(f) - R̂<sub>Q</sub>(f̂) > √P̂<sub>Q</sub>(f ≠ f̂) d/|Q|
output final f̂ **Example:** Linear separators, Uniform  $P_X$  on circle Suppose true labels are **all** -1

DIS $(\mathcal{H}) =$  entire circle Try k = 1Given sample xRand x' probably not close Can't shatter  $\{x, x'\}$ without a lot of points wrong So 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  $\mathcal{H}$ 

Shattering-based Active Learning

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

1. sample  $2^t$  unlabeled points S

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

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output final f̂

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

 $DIS(\mathcal{H}) = entire circle$ Try k = 1random x' $(A = \{x'\})$ Given sample xRand x' probably not close Can't shatter  $\{x, x'\}$ sample point xwithout a lot of points wrong So won't query x $DIS(\mathcal{H}_{x,-1})$  still entire circle (minus x)  $DIS(\mathcal{H}_{x,+1})$  small region  $\Rightarrow \hat{y}_x = -1$ 

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$$\begin{split} \theta^{(k)} &:= \sup_{r > \epsilon} \frac{P_X^k(A \in \mathcal{X}^k : \mathbb{B}(f^*, r) \text{ shatters } A)}{r} \\ \tilde{d} &:= \min \left\{ k : P_X^k(A \in \mathcal{X}^k : \mathbb{B}(f^*, r) \text{ shatters } A) \xrightarrow[r \to 0]{} \right\} \\ \tilde{\theta} &:= \theta^{(\tilde{d})} \\ \hline \mathbf{Theorem:} \text{ For Bounded noise, } R(\hat{f}) \leq R(f^*) + \epsilon \\ &\text{with } \# \text{ labels} \\ &\approx C \tilde{\theta} d \log(\frac{1}{\epsilon}) \end{split}$$

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# Shattering-Based Active Learning

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Shattering-based Active Learning

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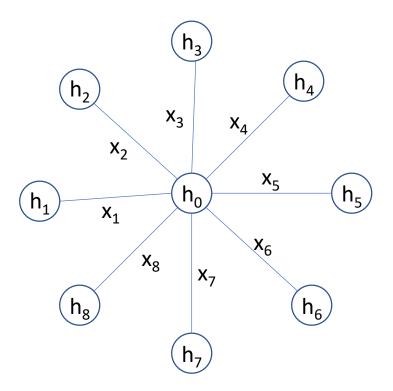
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Up Next: Distribution-free Analysis

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

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

**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.  $\forall i \in \{1, \ldots, k\}, \{x_j : h_i(x_j) \neq h_0(x_j)\} = \{x_i\}.$ 



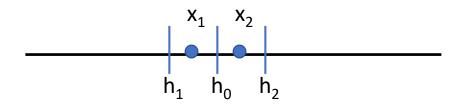
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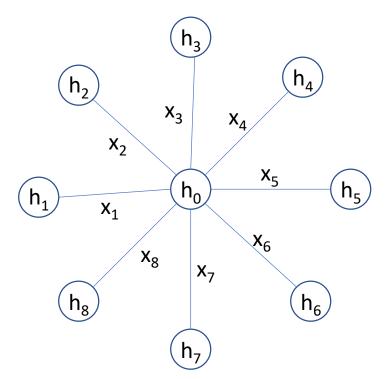
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**Example:** Thresholds:  $f(x) = \mathbb{I}[x \ge t]$ .





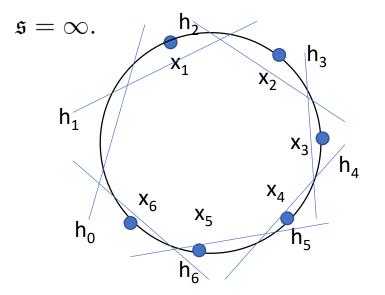


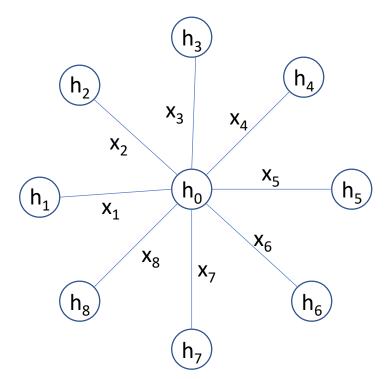
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**Example:** Linear Separators in  $\mathbb{R}^n$ ,  $n \ge 2$ :





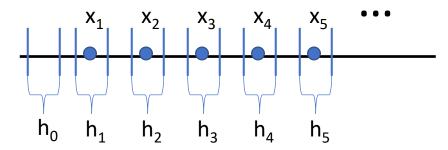
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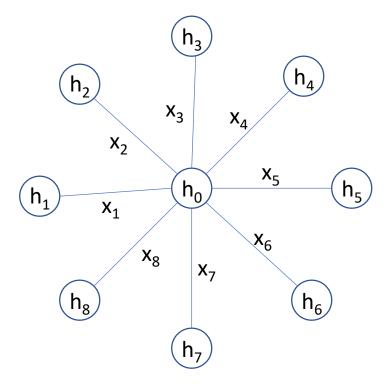
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```
Example: Intervals: x \mapsto \mathbb{I}[a \le x \le b]
```





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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**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  $A^2$ 

h<sub>3</sub> h₄  $h_2$ X<sub>3</sub> X₄  $X_2$ Χ<sub>5</sub> ۰ h<sub>0</sub> , h<sub>5</sub> h<sub>1</sub> ' **X**<sub>1</sub> ×<sub>6</sub> X<sub>8</sub>  $X_7$ h<sub>6</sub> h<sub>8</sub>  $h_7$ 

(Hanneke & Yang, 2015; Hanneke, 2016)

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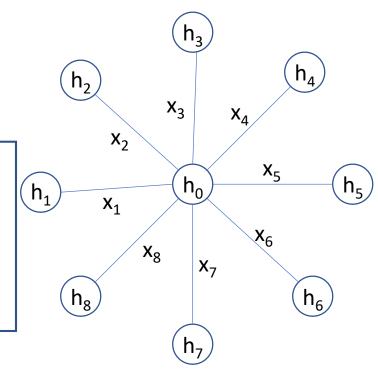
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Different alg., Bounded noise # labels  $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$ 

Near-matching **lower bound**:  $\mathfrak{s}_{\epsilon} + d \log(\frac{1}{\epsilon})$  (Hanneke & Yang, 2015; Hanneke, 2016)



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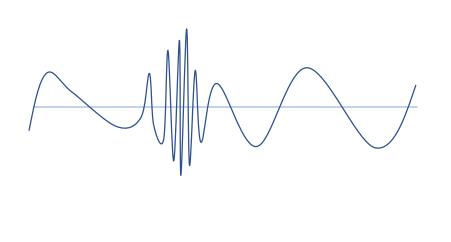
Near-matching **lower bound**:  $\mathfrak{s}_{\epsilon} + d \log(\frac{1}{\epsilon})$   $\begin{array}{l} \begin{array}{l} \begin{array}{l} \textbf{Open Question:} \\ \hline \text{Agnostic } (\beta = R(f^*)) \\ \# \text{ labels} \\ \approx d \frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon}) \end{array} \end{array}$ 

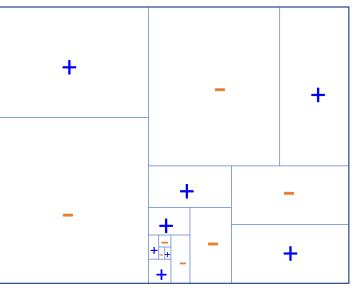
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(Hanneke & Yang, 2015; Hanneke, 2016)

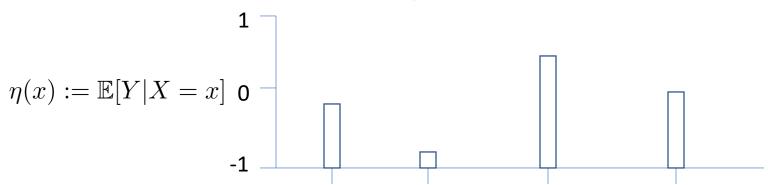
#### Adapting to Heterogeneous Noise

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



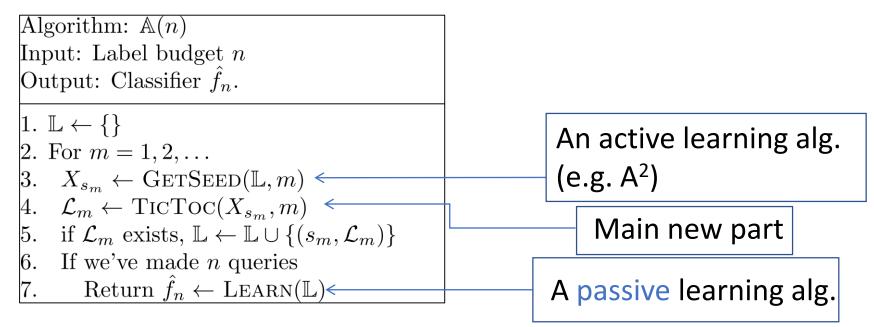


Also consider: Spatial heterogeneity of **noise**:



(Hanneke & Yang, 2015)

## Active Learning with TicToc



# Active Learning with TicToc

Algorithm:  $\mathbb{A}(n)$ Input: Label budget nOutput: 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  $\hat{f}_n \leftarrow \text{LEARN}(\mathbb{L})$  Denote  $\eta(x) = \mathbb{E}[Y|X = x]$ Suppose  $f^*$  is the **global** optimal function:  $f^*(x) = \operatorname{sign}(\eta(x))$ 

 $\frac{\text{TicToc}(X, m)}{\text{Query } X \text{ (or nearby) to try to guess } f^*(X)}$ 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:

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

(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  $f^{\star}(X_i)!$ 

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

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**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:  $f^*(x) = \operatorname{sign}(\eta(x))$ 

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**<u>Theorem</u>:** Agnostic  $(\beta = R(f^*))$ and suppose  $f^* =$  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  $f^* =$  global opt.

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

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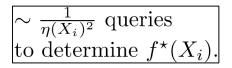
Double advantage:

• 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  $f^*(X_i)!$ 



## 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

#### Tsybakov Noise

The alg. adapts to heterogeneity in the noise.

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

Tsybakov Noise

#### Tsybakov Noise

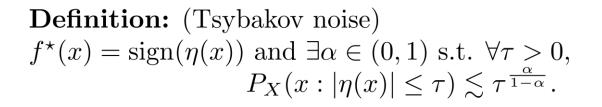
Denote  $\eta(x) = \mathbb{E}[Y|X = x]$ 

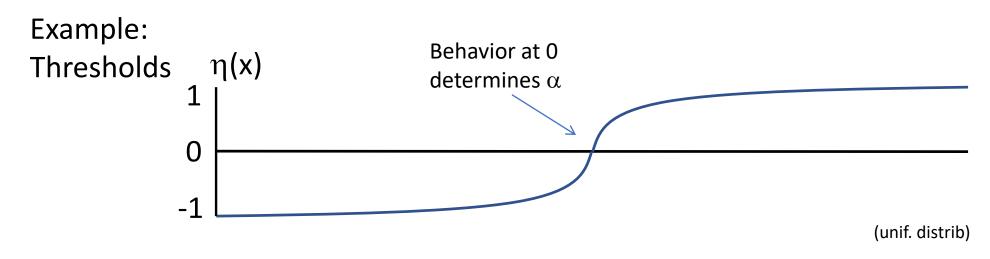
**Definition:** (Tsybakov noise)  $f^{\star}(x) = \operatorname{sign}(\eta(x)) \text{ and } \exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$  $P_X(x : |\eta(x)| \le \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$  (Tsybakov, 2004; Mammen & Tsybakov 1999)

(Tsybakov, 2004; Mammen & Tsybakov 1999)

## Tsybakov Noise

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





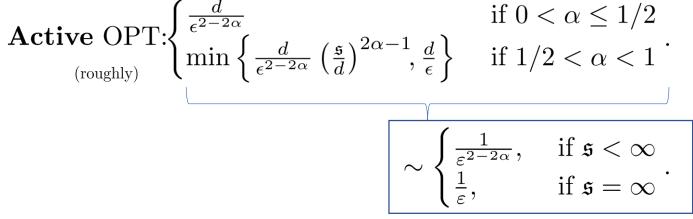
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**Definition:** (Tsybakov noise)  $f^{\star}(x) = \operatorname{sign}(\eta(x)) \text{ and } \exists \alpha \in (0,1) \text{ s.t. } \forall \tau > 0,$  $P_X(x : |\eta(x)| \le \tau) \lesssim \tau^{\frac{\alpha}{1-\alpha}}.$ 

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

(Massart & Nédélec, 2006)



(Hanneke & Yang, 2015)

Active Opt  $\ll$  Passive Opt. (always)

#### 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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