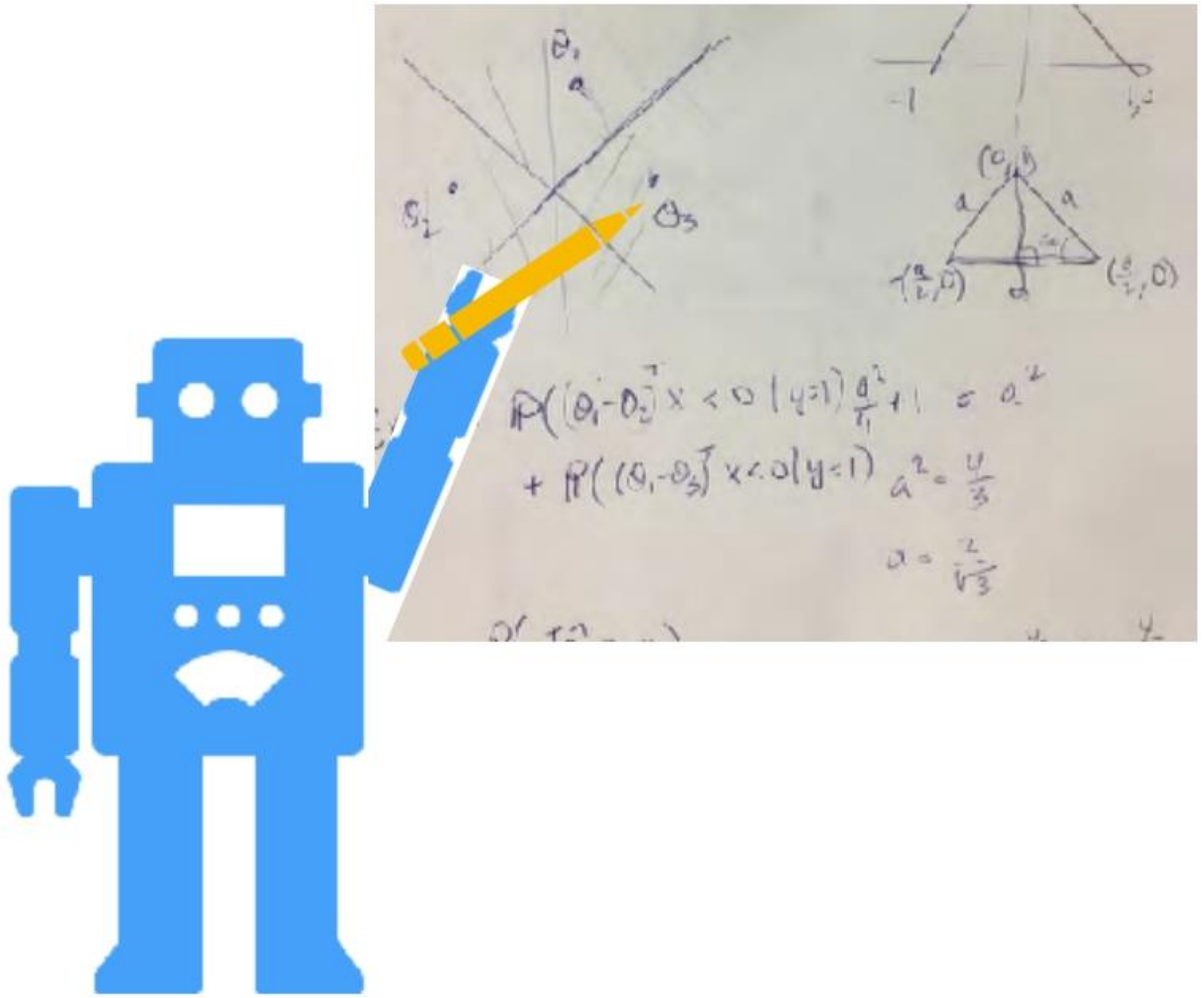
Active Learning from Theory to Practice



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ICML | 2019

Thirty-sixth International Conference on Machine Learning

Tutorial Outline

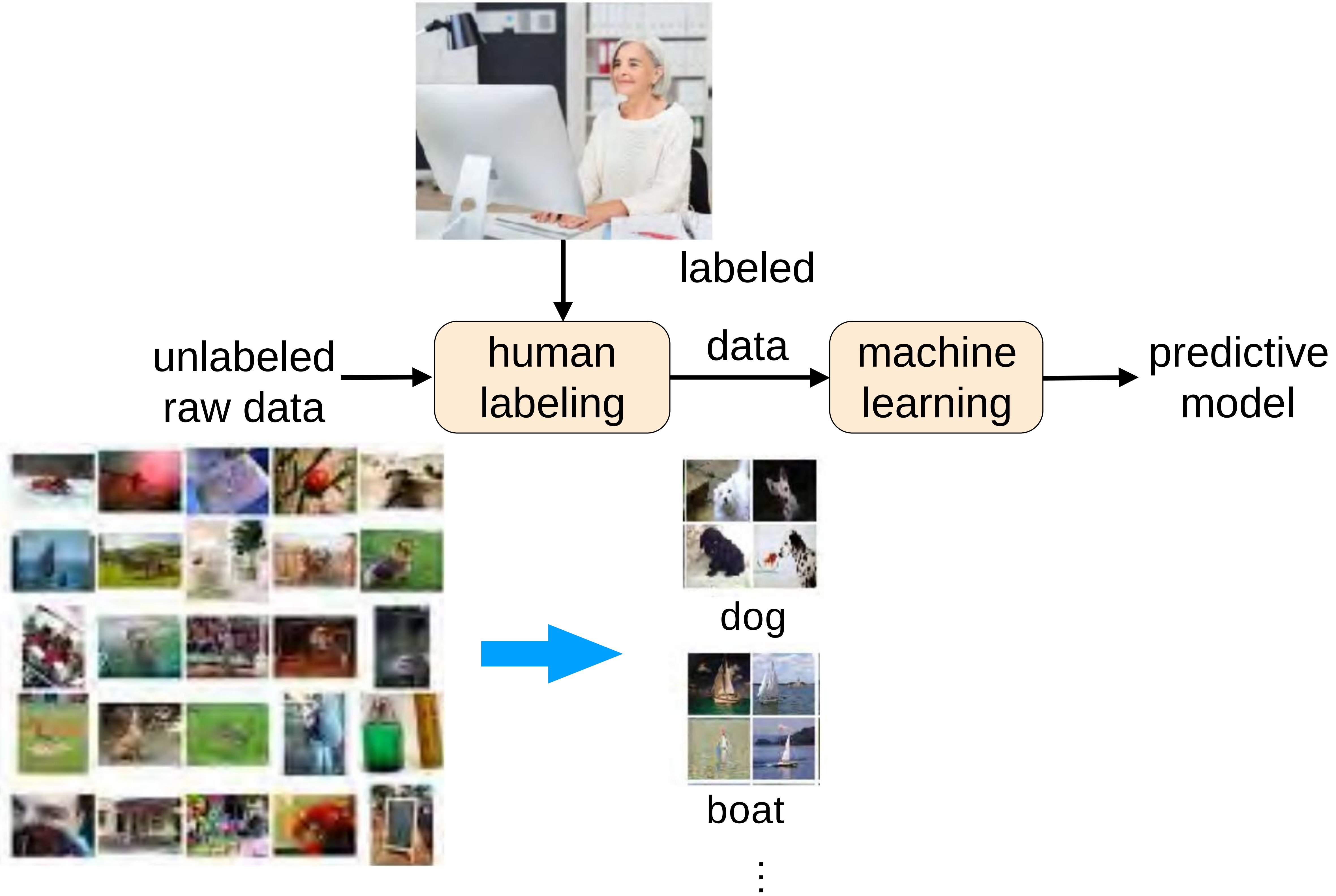
Part 1：Introduction to Active Learning

Part 2：Theory of Active Learning

Part 3：Advanced Topics and Open Problems

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

Conventional (Passive) Machine Learning



ALL SYSTEMS GO ?

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 AI-powered translation tool scores nearly identically to human translators

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

Forbes

Google's DeepMind Masters Atari Games

A computer that taught itself to play almost 50 video games including Space Invaders and Pong is being hailed as the pinnacle of artificial intelligence.

learned by playing more games than even my teenage son could stomach !

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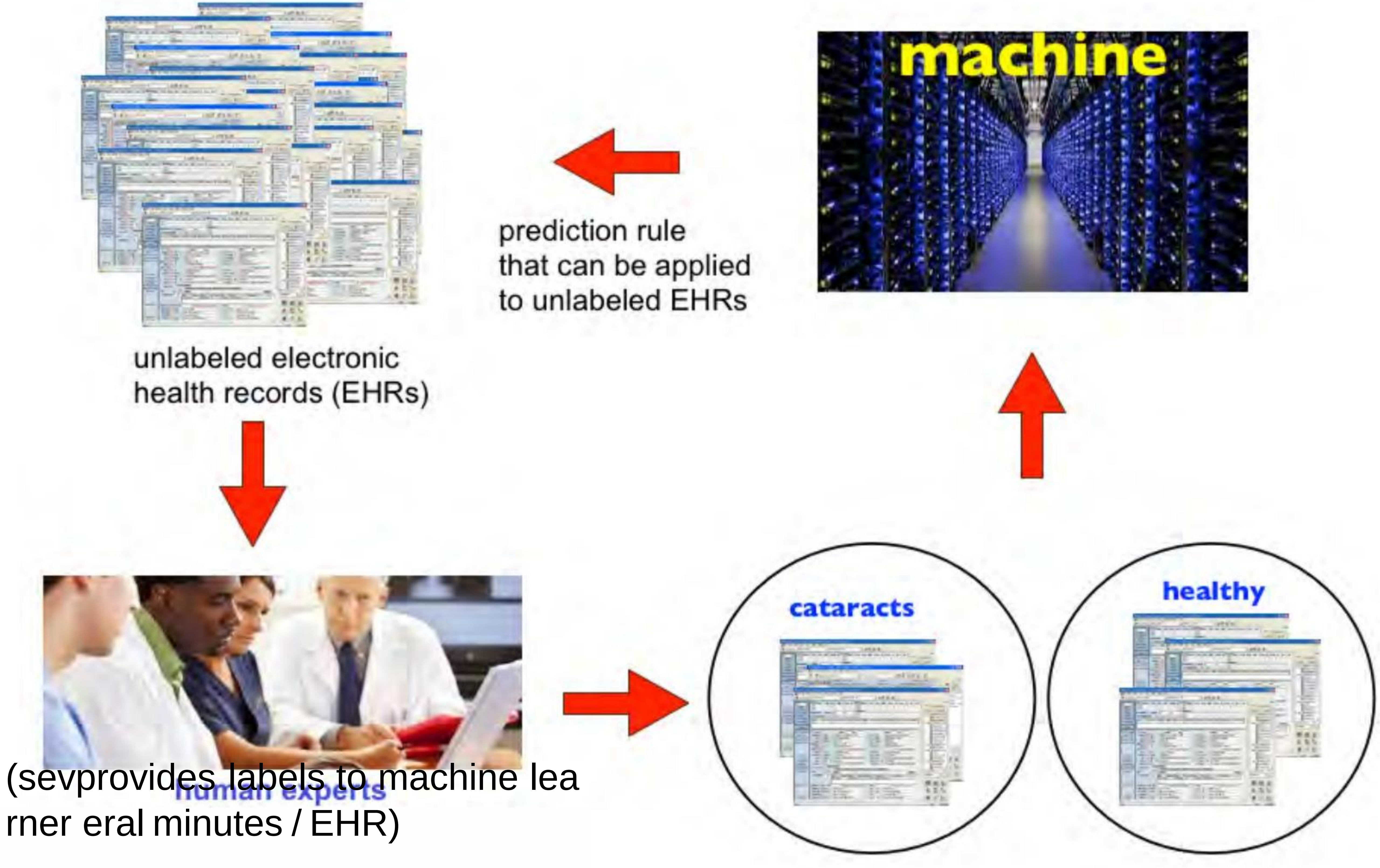
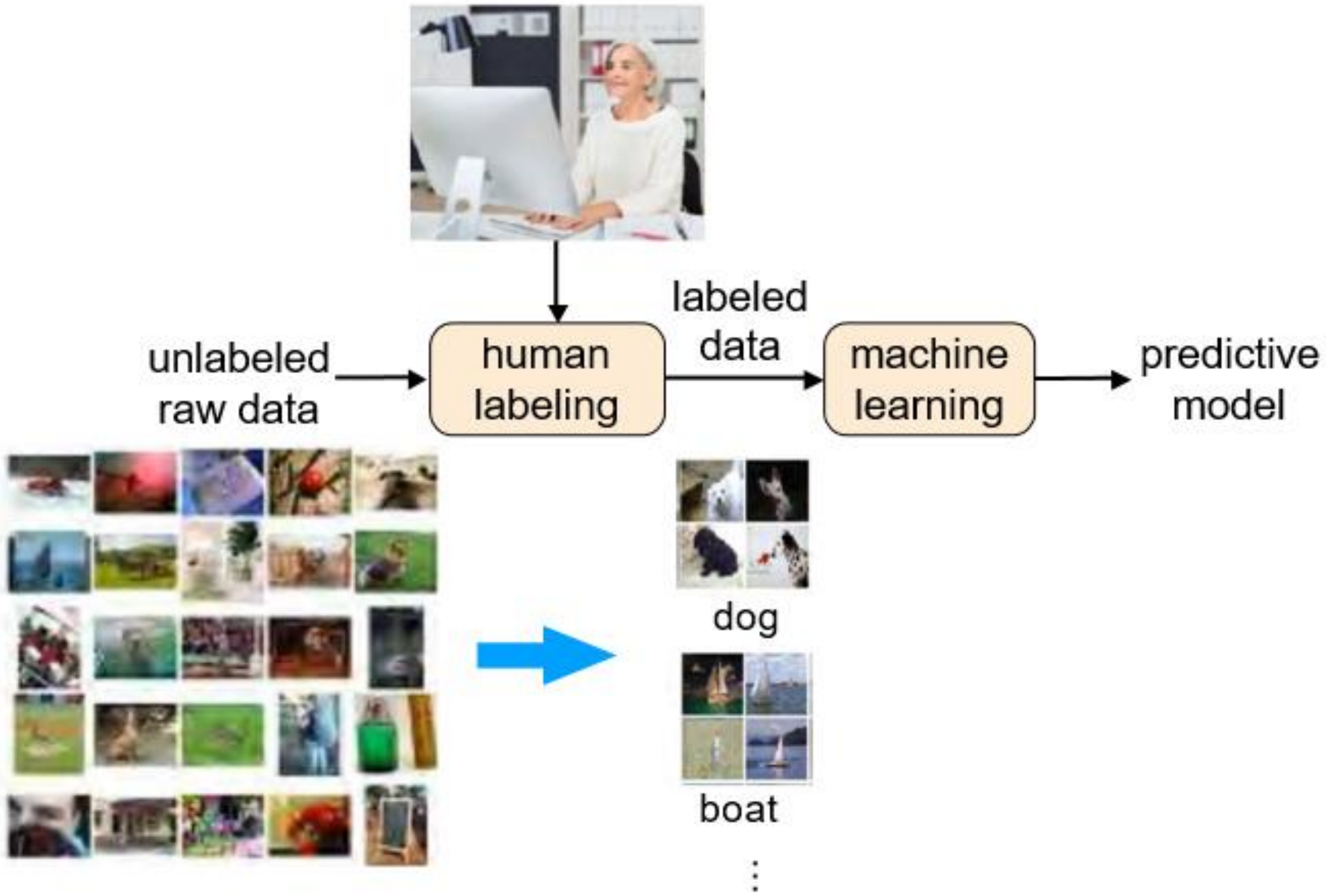
Can we train machines with less labeled data and less human supervision?

Motivating Appication

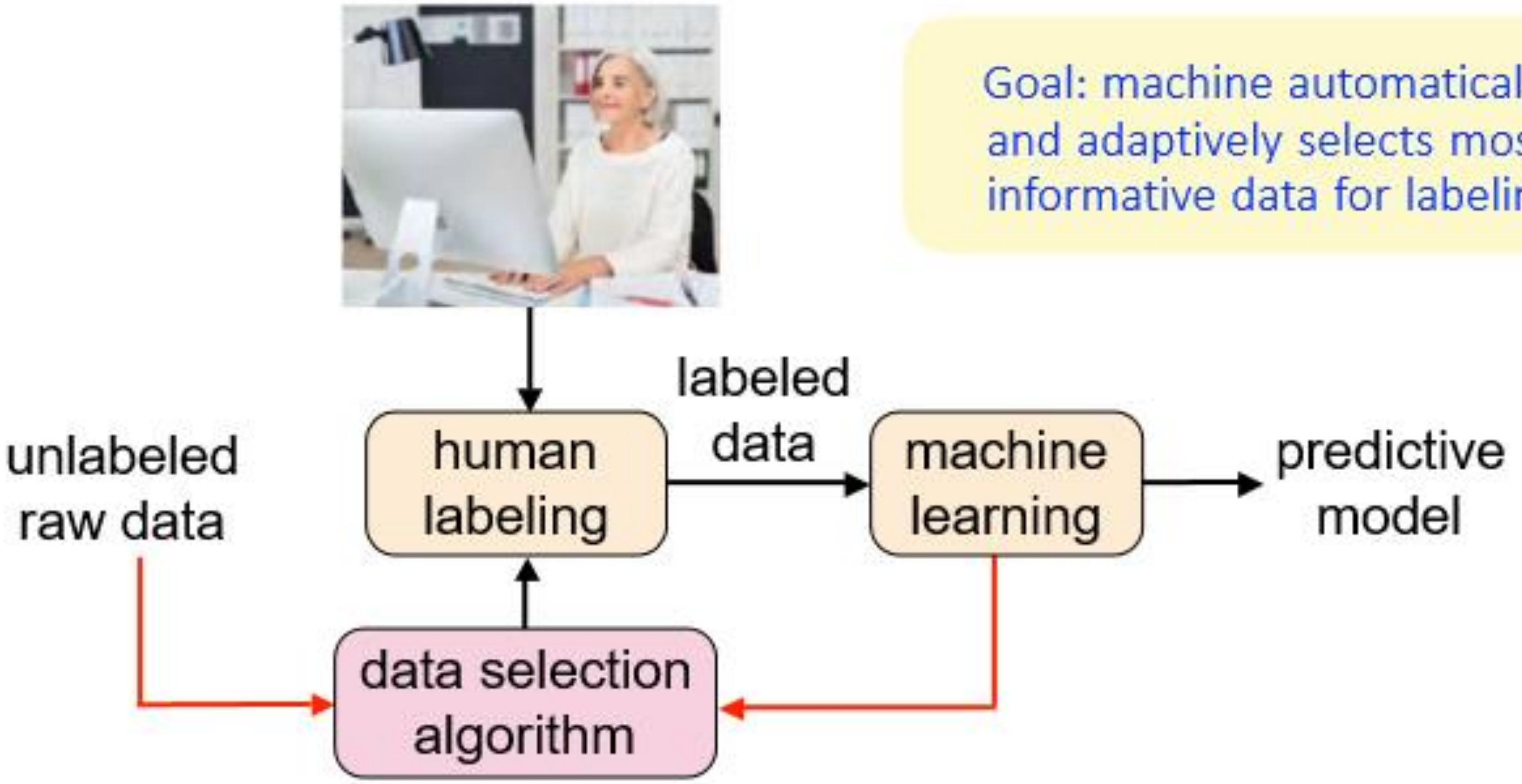


(sevprovides labels to machine lea
rner eral minutes / EHR)

Conventional Machine Learning (Passive)

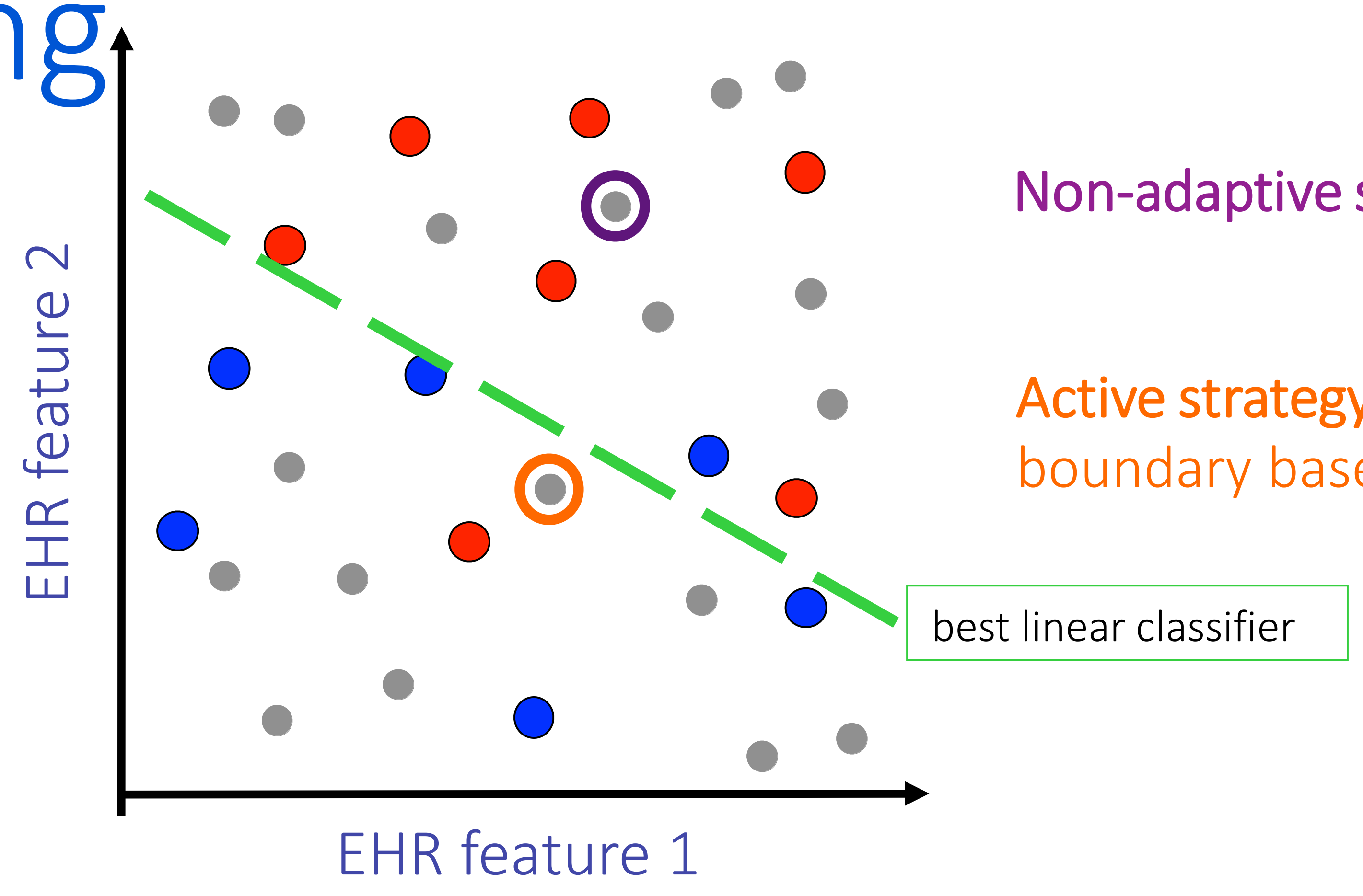


Active Machine Learning



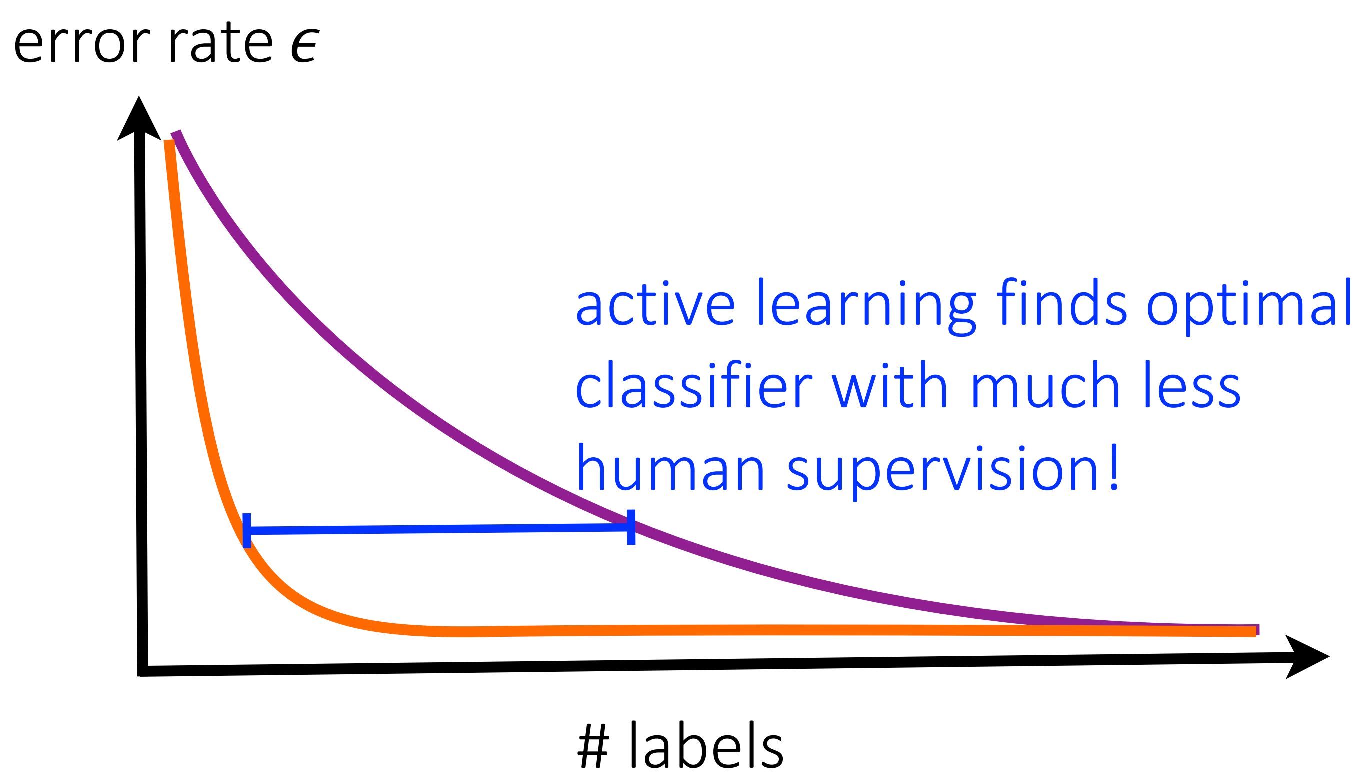
Goal: machine automatically and adaptively selects most informative data for labeling

Active Learning

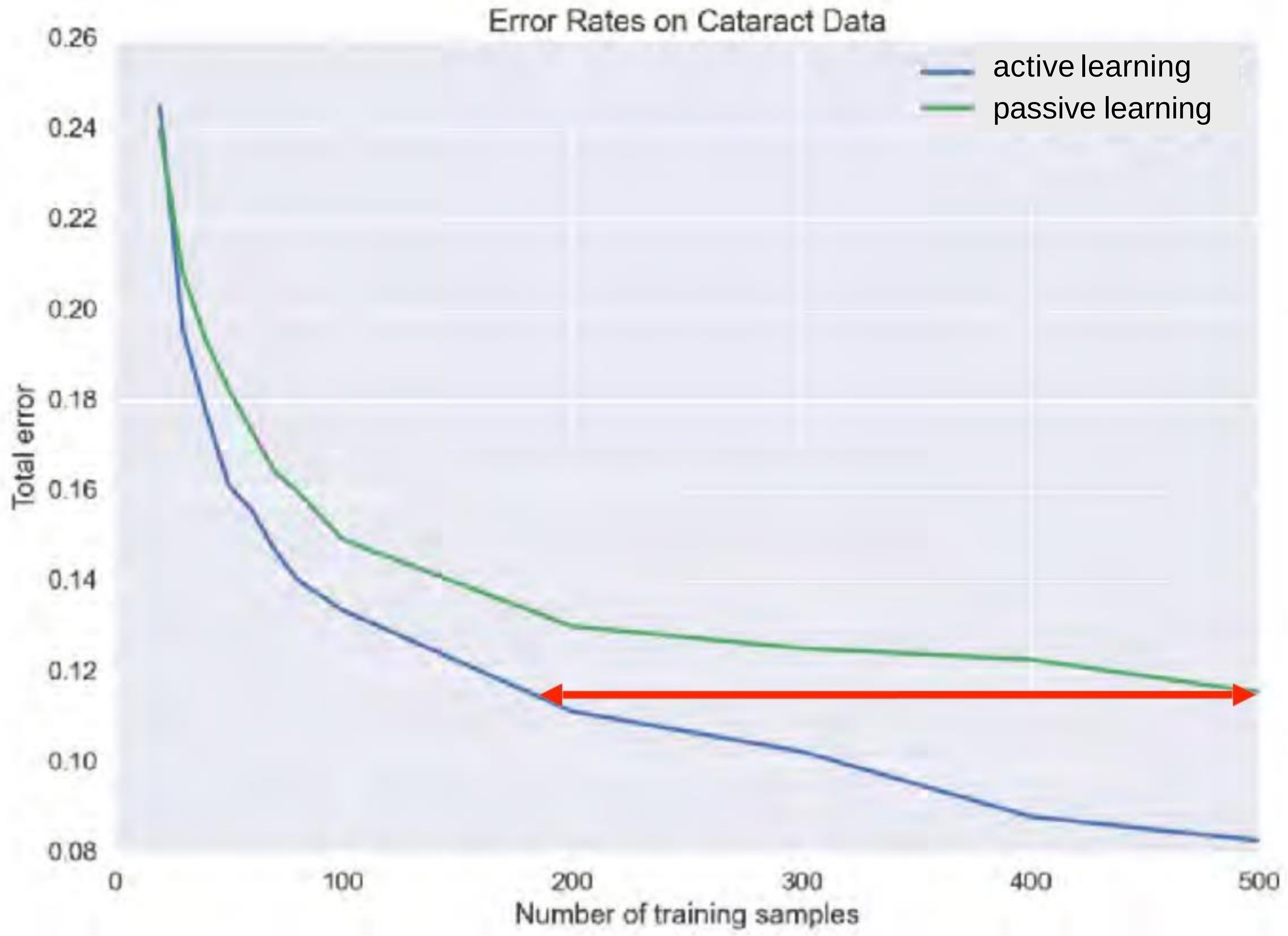


Non-adaptive strategy: Label a random sample

Active strategy: Label a sample near best decision boundary based on labels seen so far



Active Logistic Regression



11000 patient records

8000 positive

3000 negative

6182 Numerical Features

icd9 codes

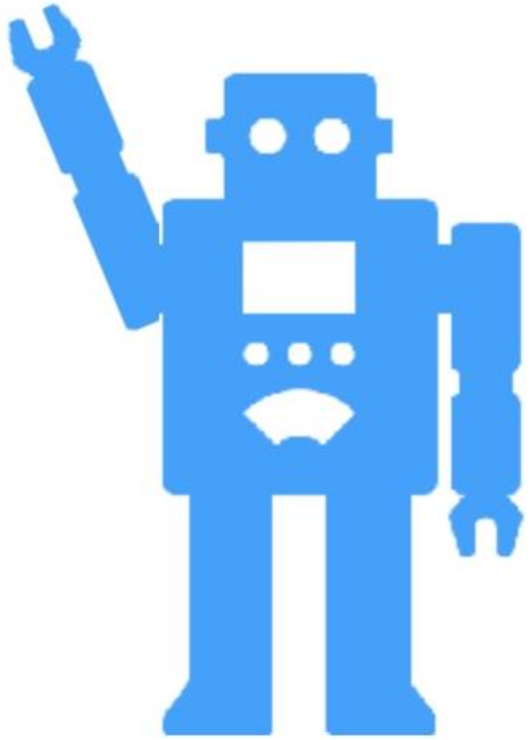
lab tests

patient data

Classification task: cataracts or healthy

less than half as many labeled examples needed by active learning

Principles of Active Learning



Meta-Algorithm for Active Learning

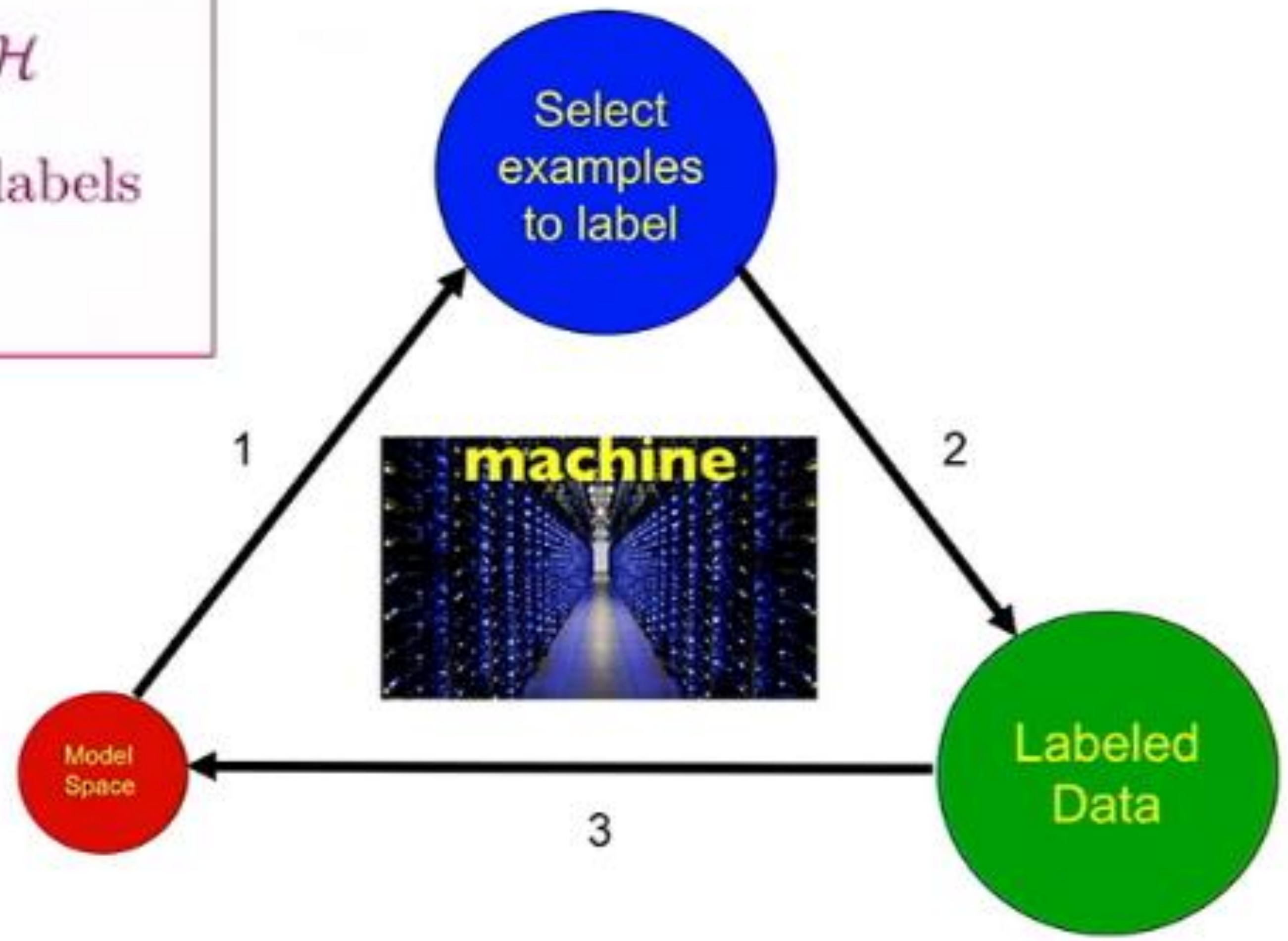
Version-Space (VS) Active Learning

initialize VS: $\mathcal{H}$ = all models/hypotheses

while (*stopping-criterion*) not met

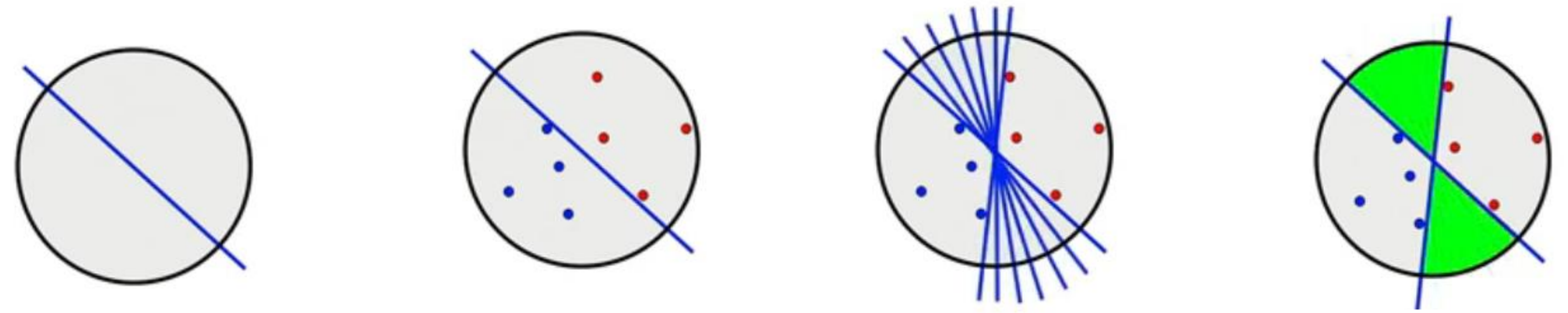
1. **sample** at random from available dataset
2. **label** only those samples that distinguish models in $\mathcal{H}$
3. **reduce** $\mathcal{H}$ by removing all models inconsistent with labels

output: best model in final $\mathcal{H}$

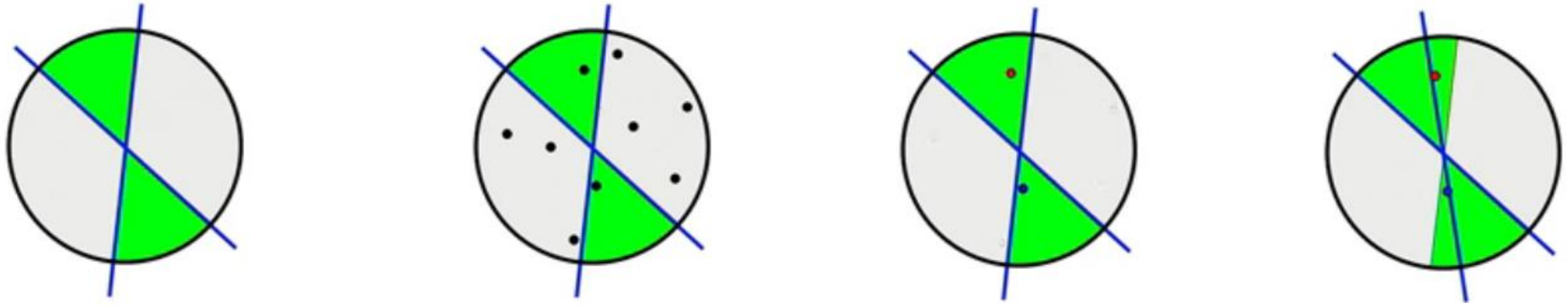


Disagreement-Based Active Learning

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



Region of disagreement



Machine will go and look at a large set of unlabeled examples remaining in that dataset.
It’s not going to label all of them but only label ones In green region (disagreement region)

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

Learning a 1-D Classifier

Unlabeled data

Label them, then we can find a linear classifier

After a few sample the binary search the active procedure has really nailed down where that decision boundary is.

binary search quickly finds decision boundary

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

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

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"

true risk

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

w.p. $\geq\; 1-\delta$

with probability

$n = sample\ size$
$\delta = confidence\ level$
$(0.01, infer\ 99\%\ confidence\ that\ this\ bound\ holds)$

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

$$\widehat{f} = \arg\min \widehat{R}(f)$$ rical risk minimizer

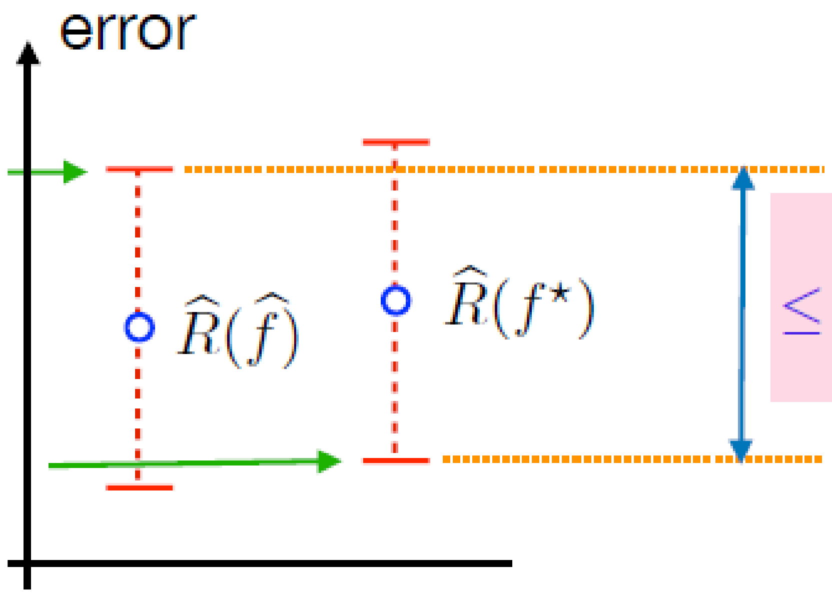
$\widehat{f}$ minimizes empirical risk:

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

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

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

$$R(\hat{f}) - R(f^*) \leqq \hat{R}(\hat{f}) - \hat{R}(f^*) + 12\sqrt{\frac{d\log(n/\delta)}{n}}$$

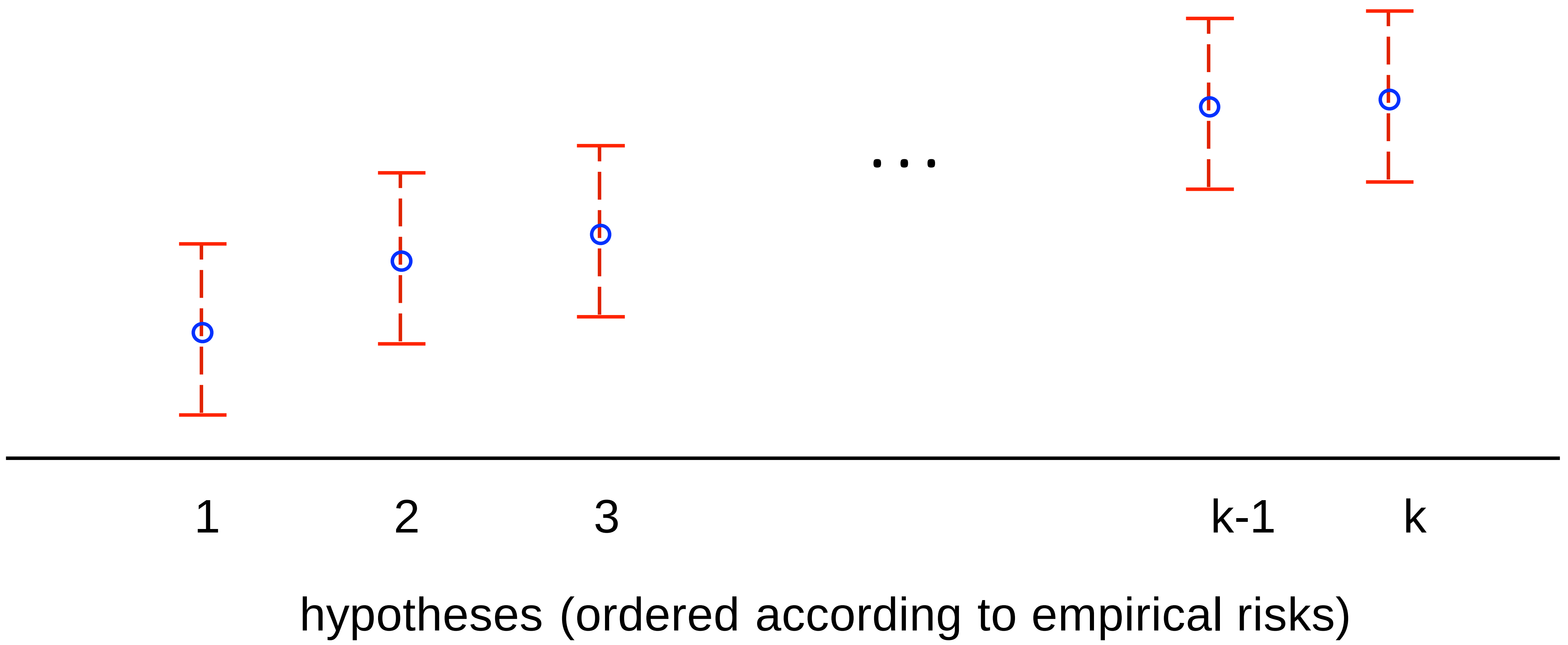


$$\leq \quad 12\sqrt{\frac{d\log(n/\delta)}{n}}$$

sufficient number of training examples:

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

Empirical Risks and Confidence Intervals



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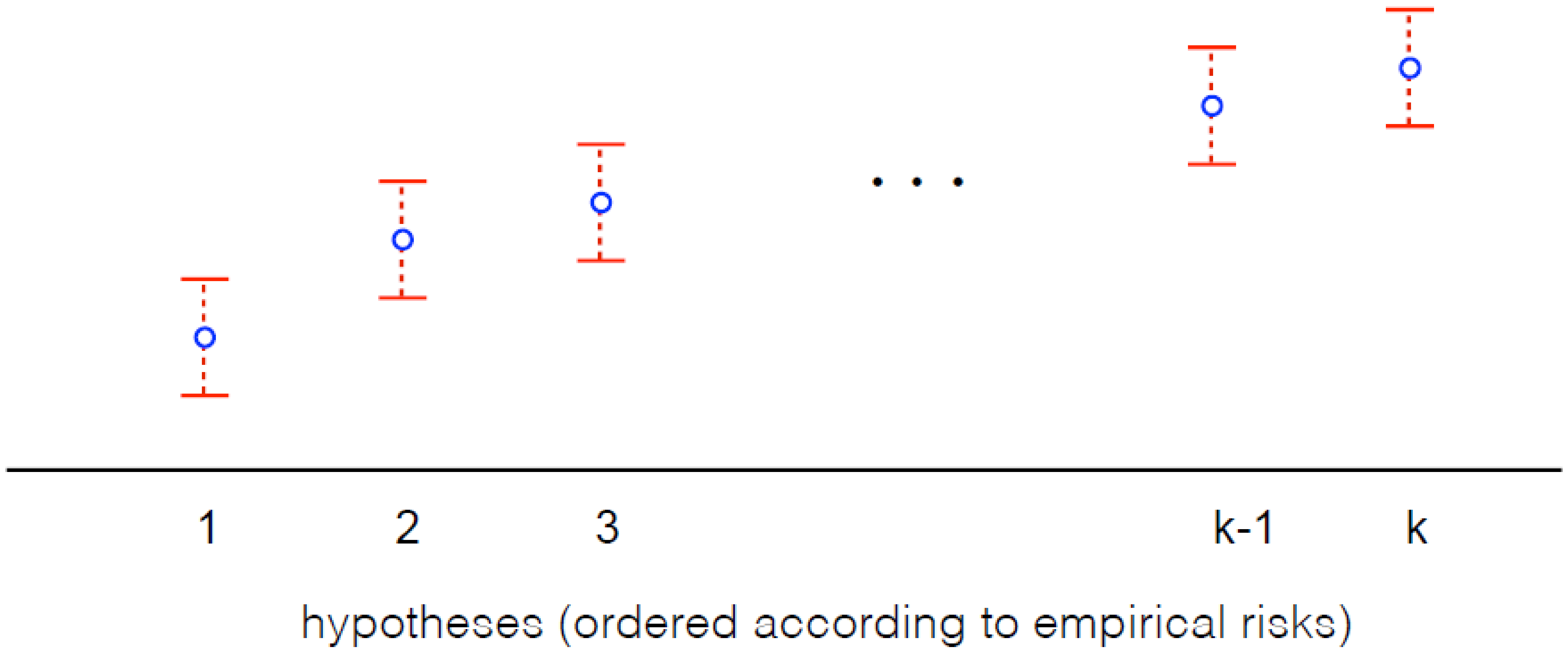
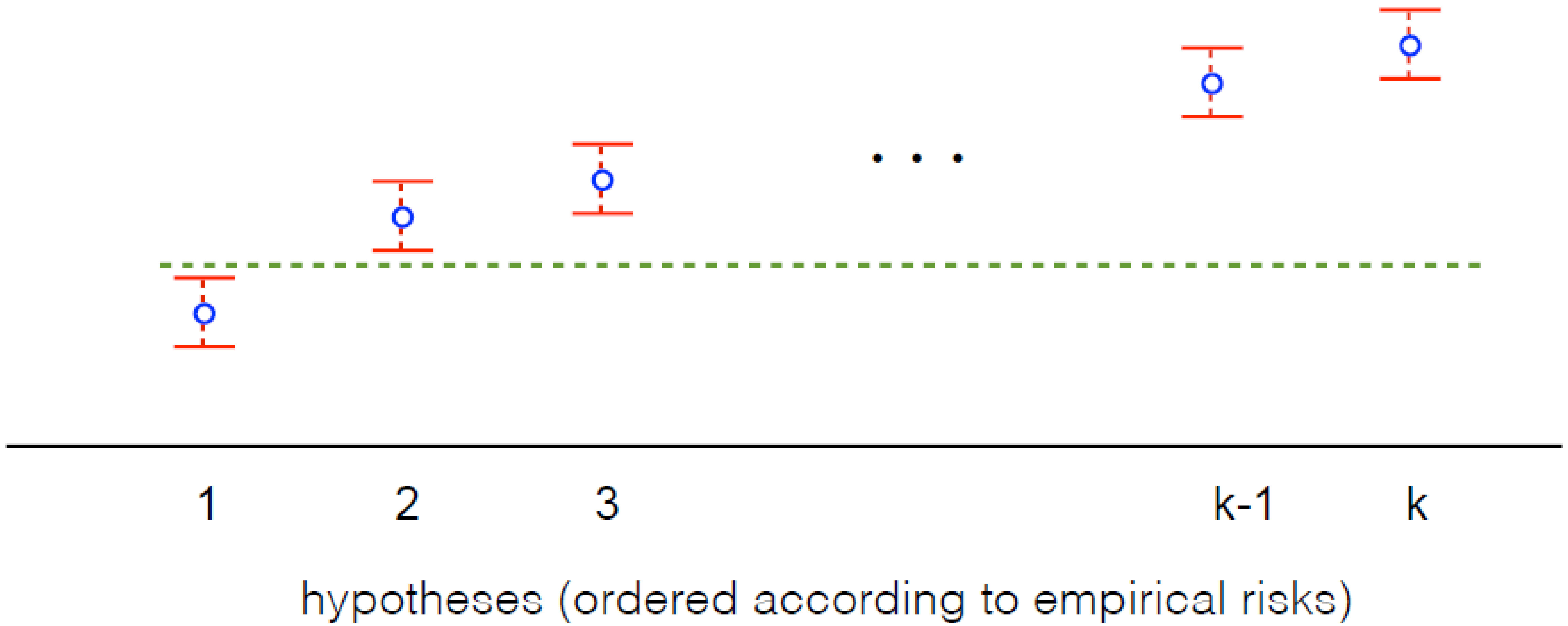


more training data $\Rightarrow$ smaller confidence intervals

Empirical Risks and Confidence Intervals



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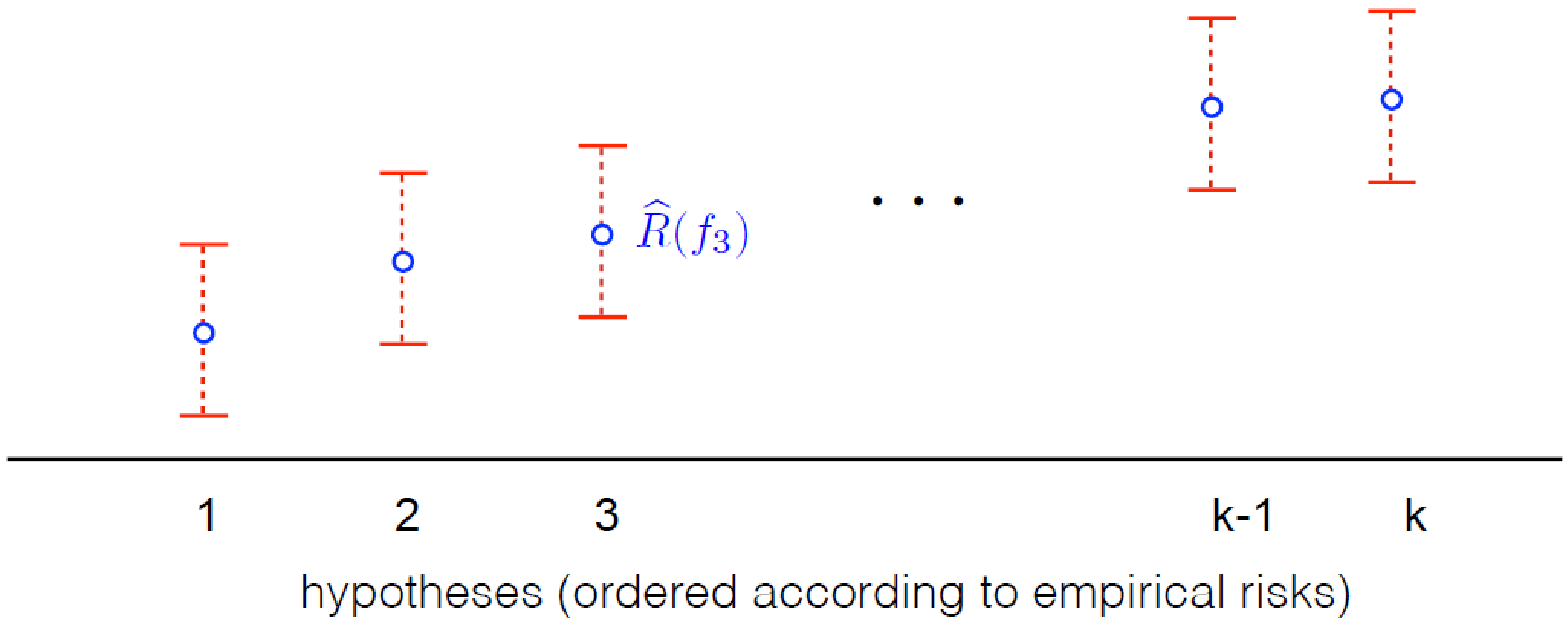
ERM is Wasting Labeled Examples



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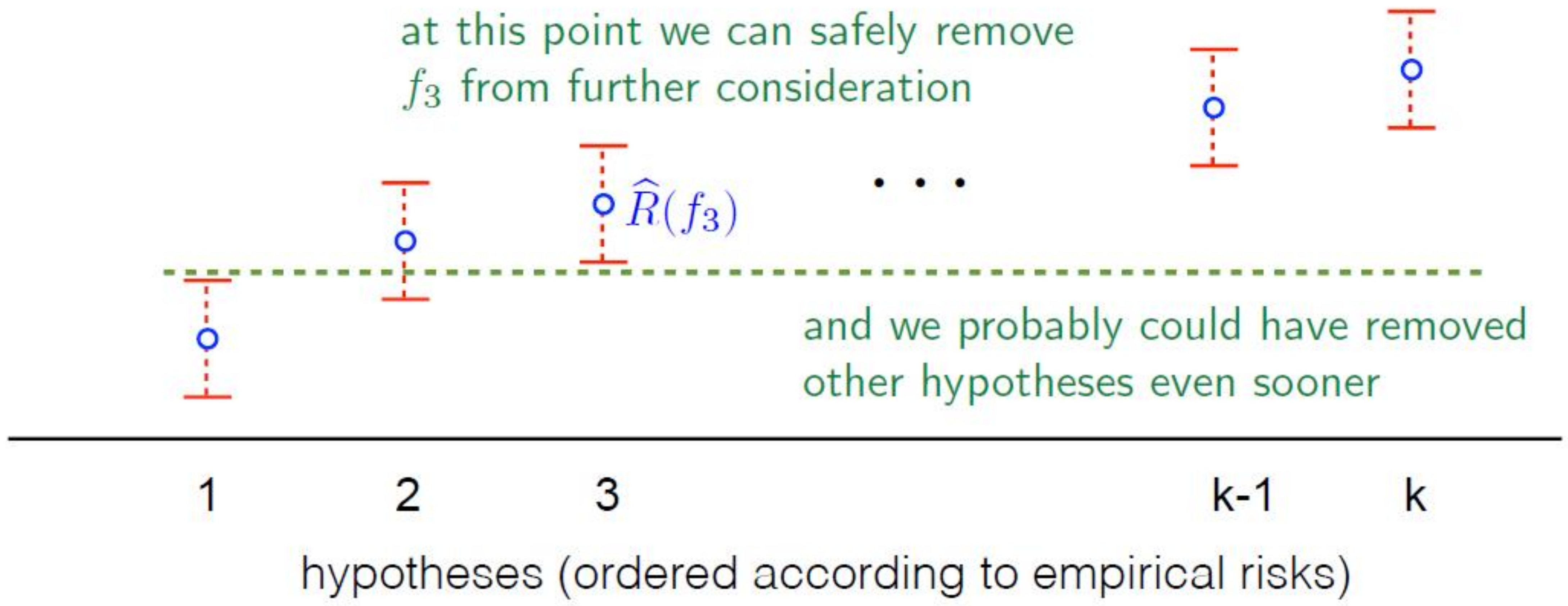
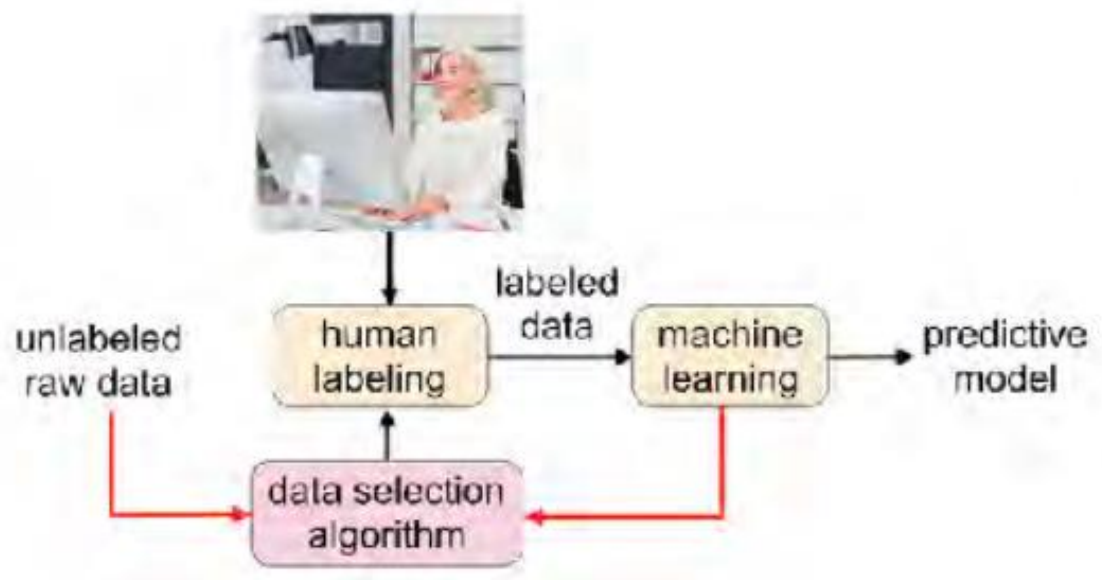


only require labels for examples that hypotheses 1 and 2 label differently (i.e., examples where they *disagree*)



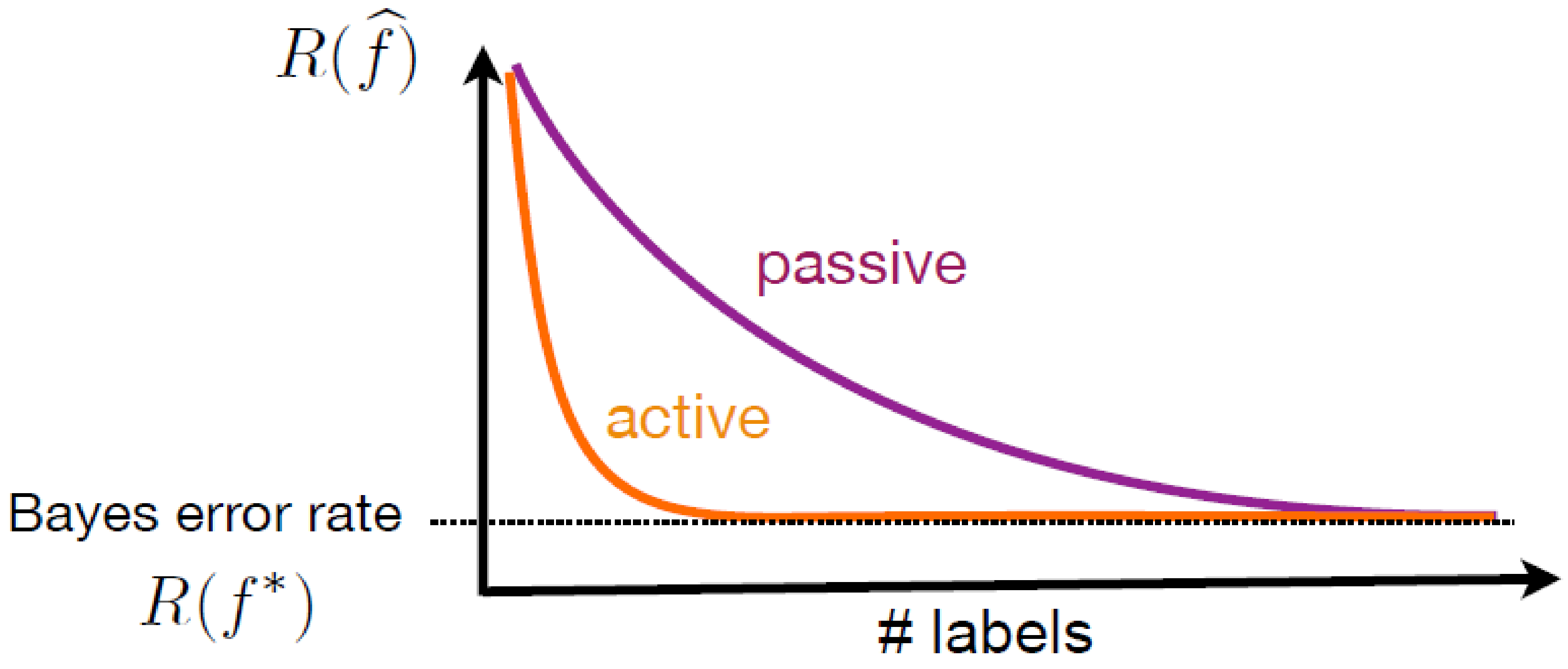
Active Binary Classification

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

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

passive $\quad \epsilon \sim \dfrac{d}{n}$ $\quad$ parametric rate

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



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

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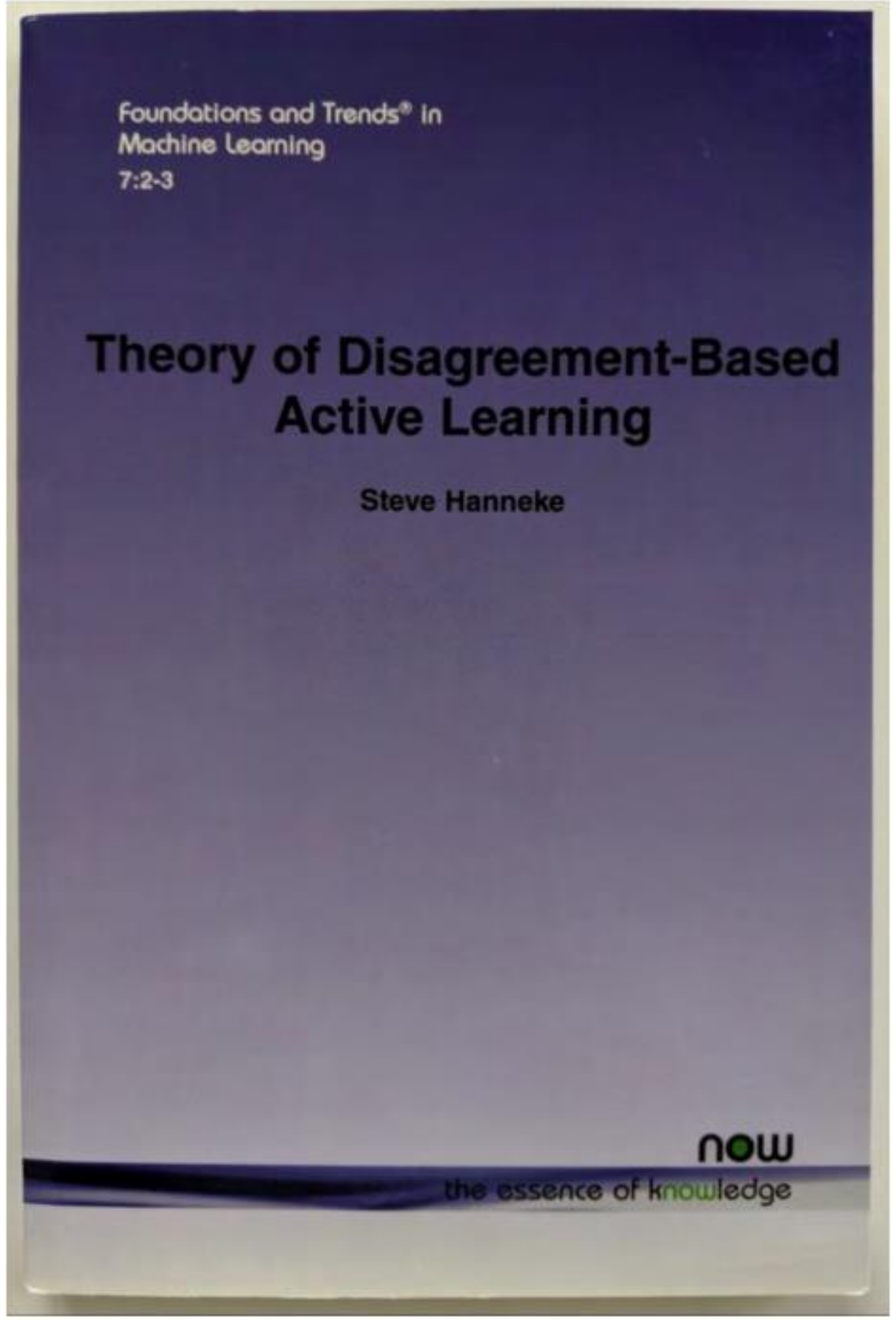
Agnostic Active Learning



Uniform Bernstein Inequality

Bernstein's inequality:

Just like the hoeffding bound

For m iid samples
$\forall f, f'$, 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:

VC dimension

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

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

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

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

Agnostic Active Learning

Balcan, Beygelzimer, & Langford (2006)

Region of disagreement:

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

The set of points such that there exists two classifiers in H that disagree on the label of that point

A^2 (Agnostic Active)

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

1. **sample** 2^t unlabeled points S
2. **label** points in $Q = \mathrm{DIS}(\mathcal{H}) \cap S$
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 $\hat{f}$

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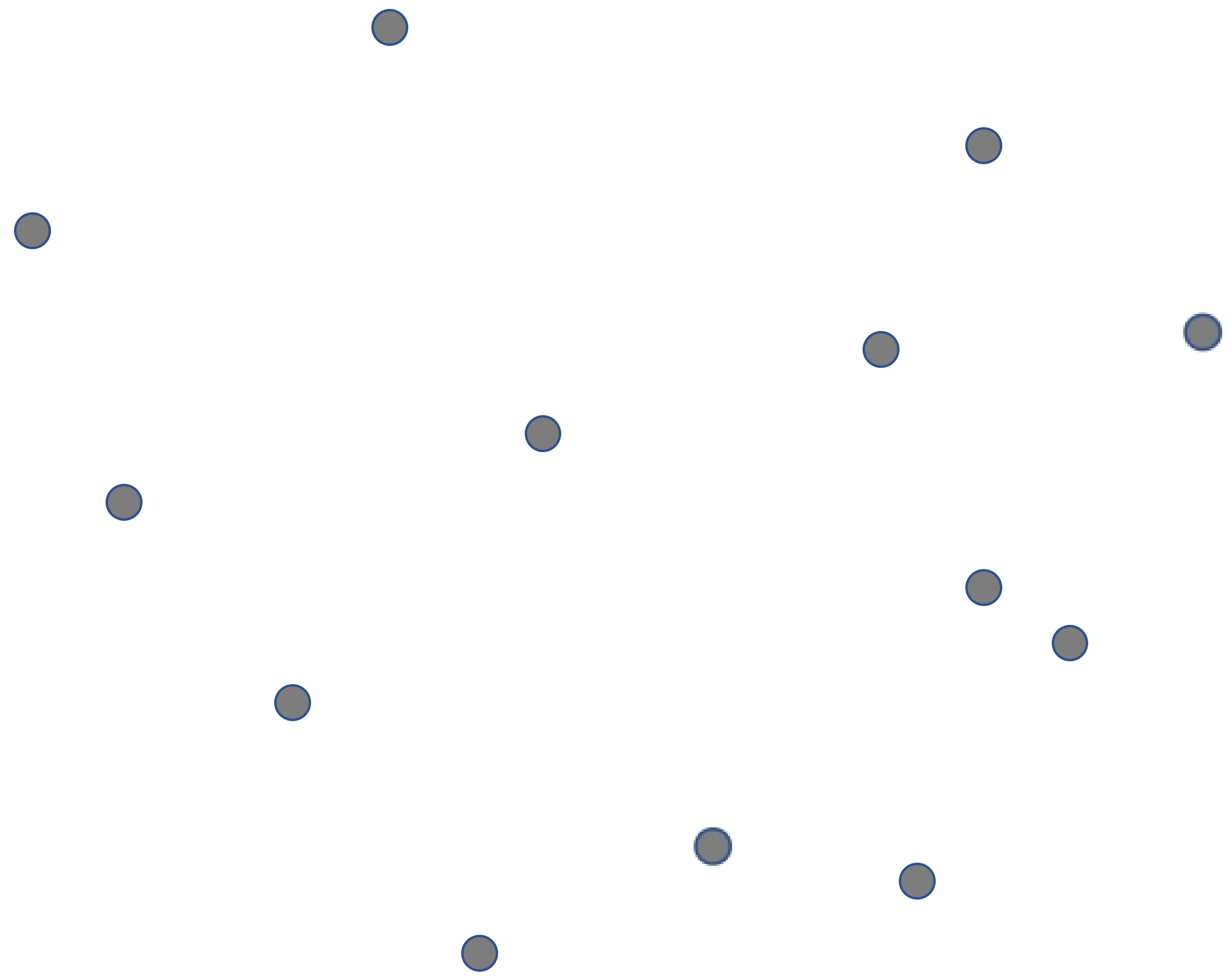

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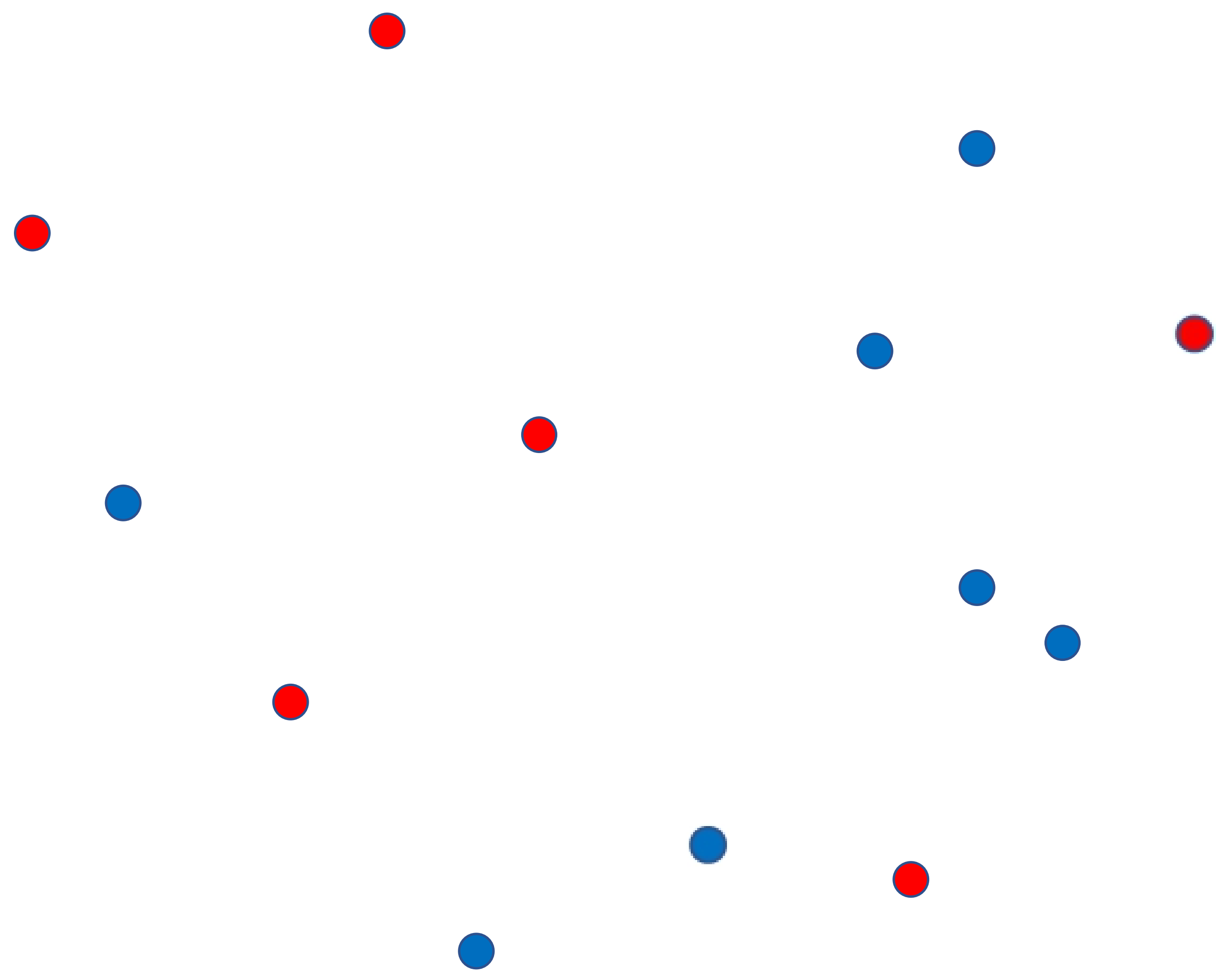

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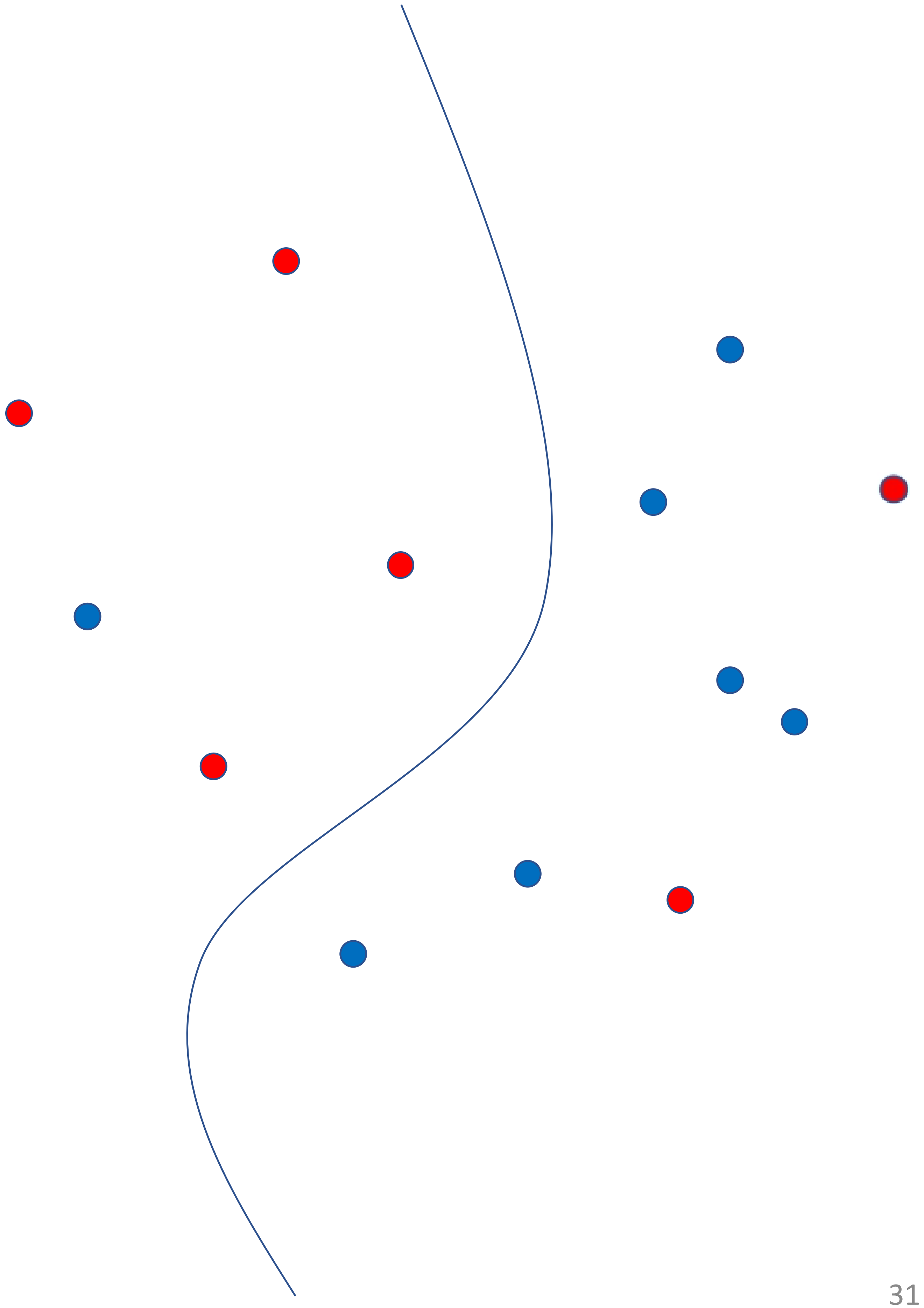

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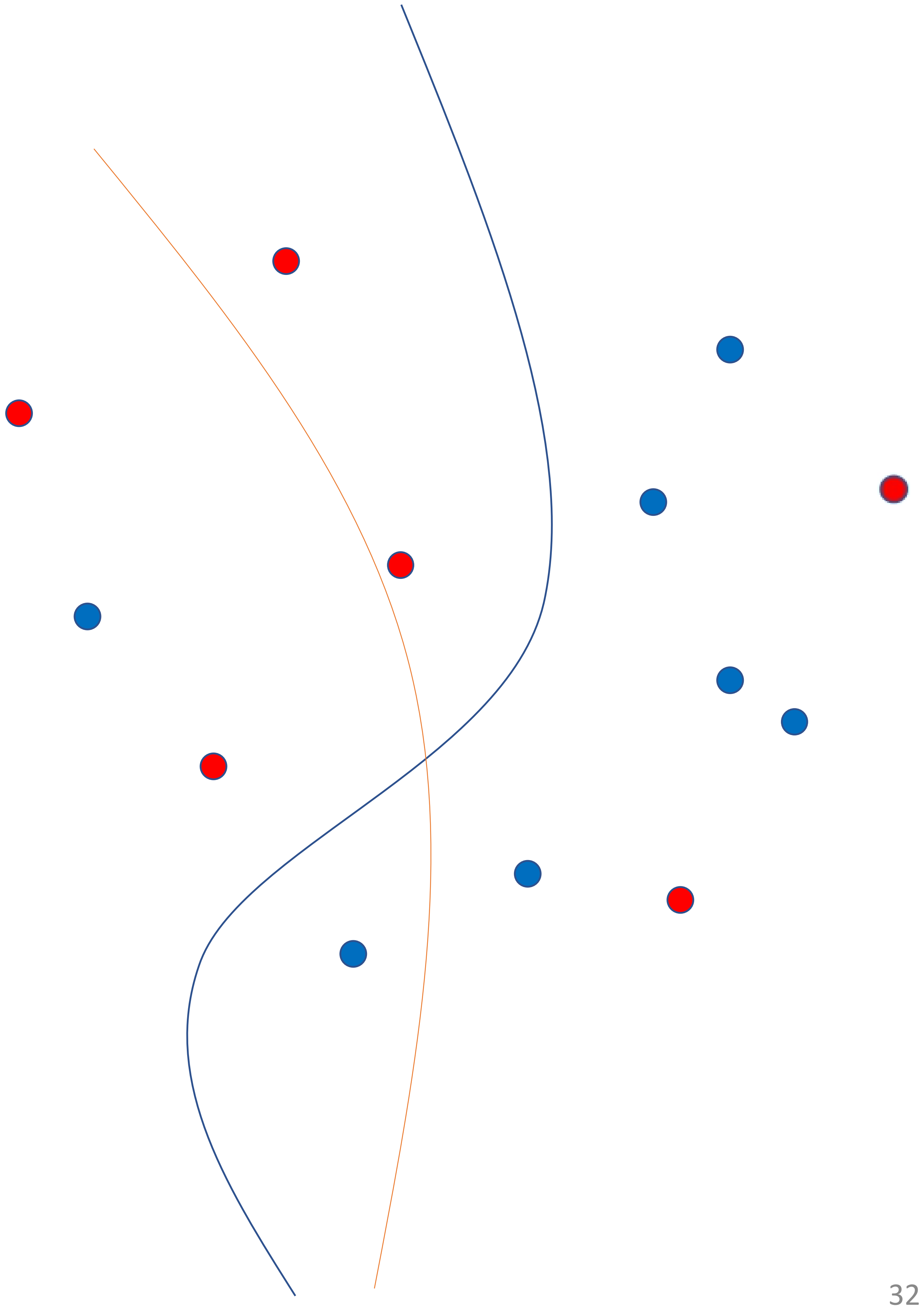

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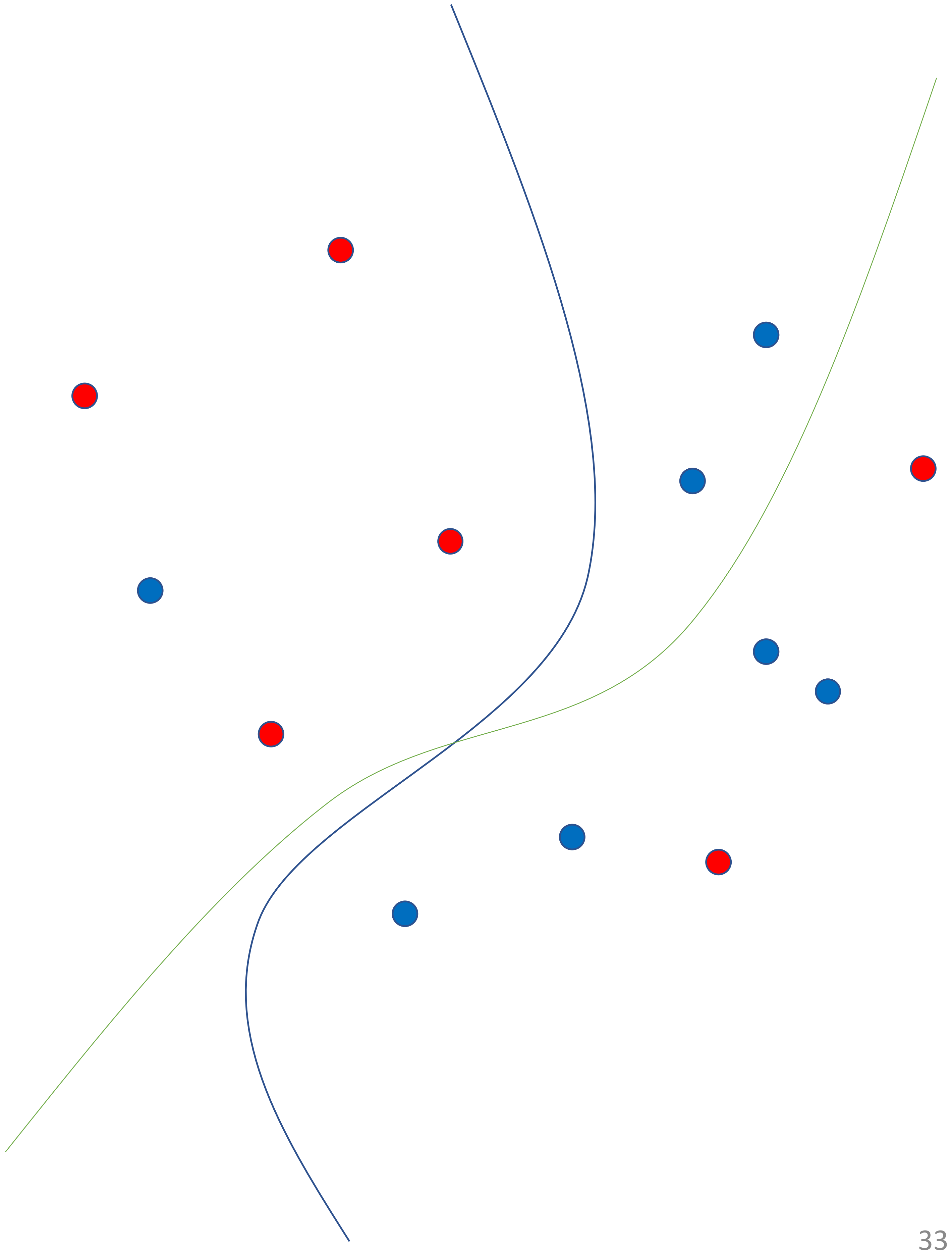

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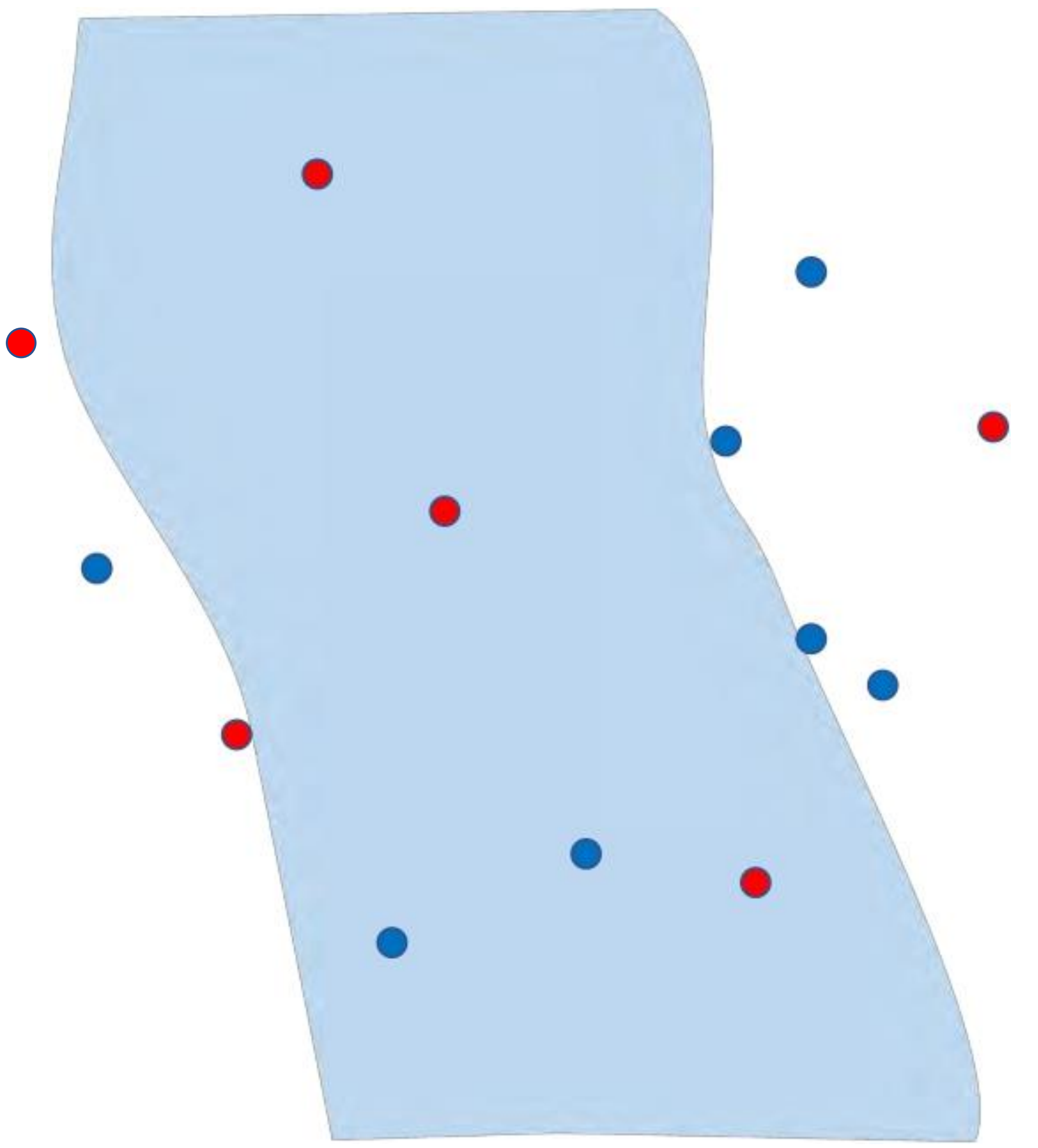

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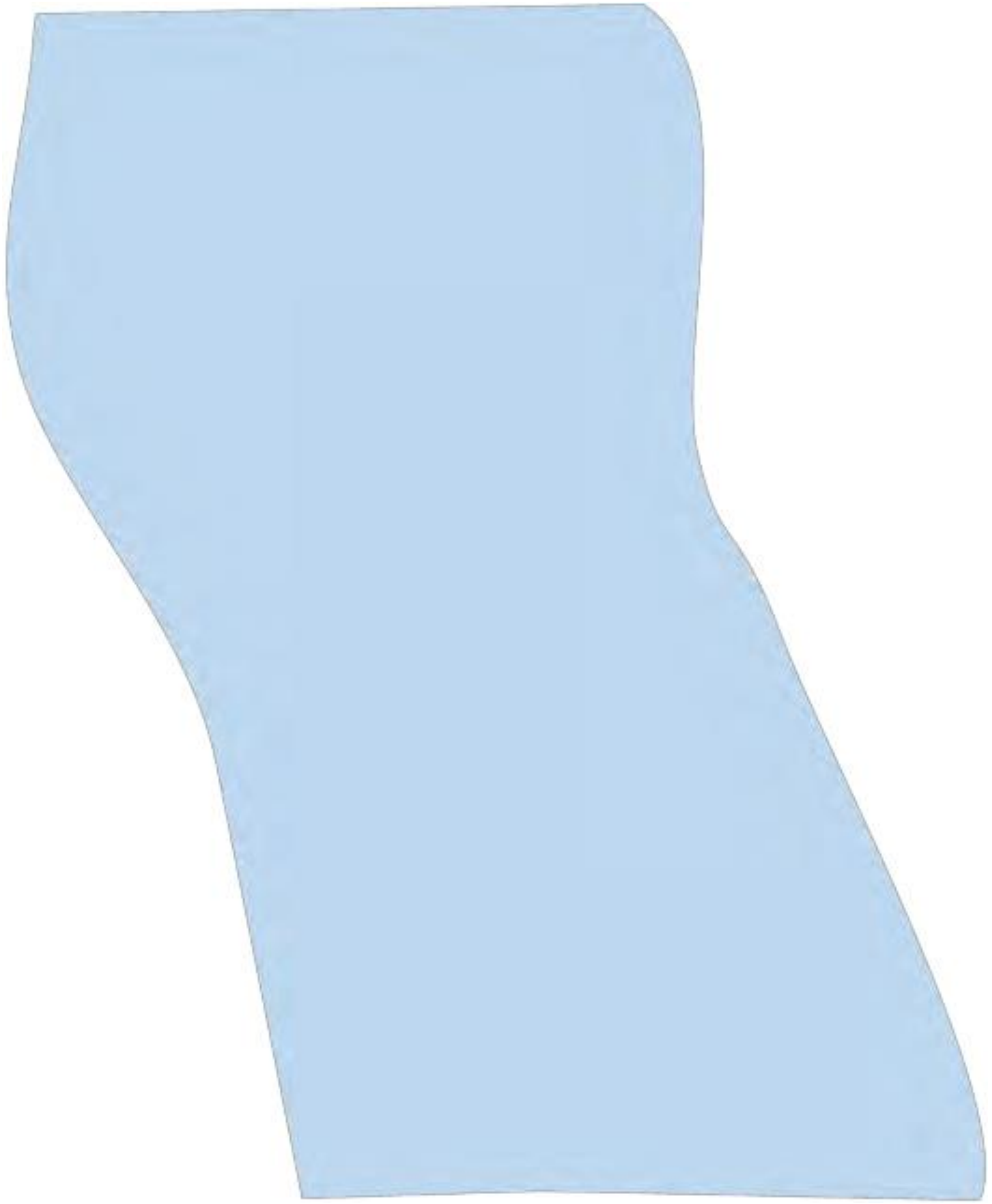

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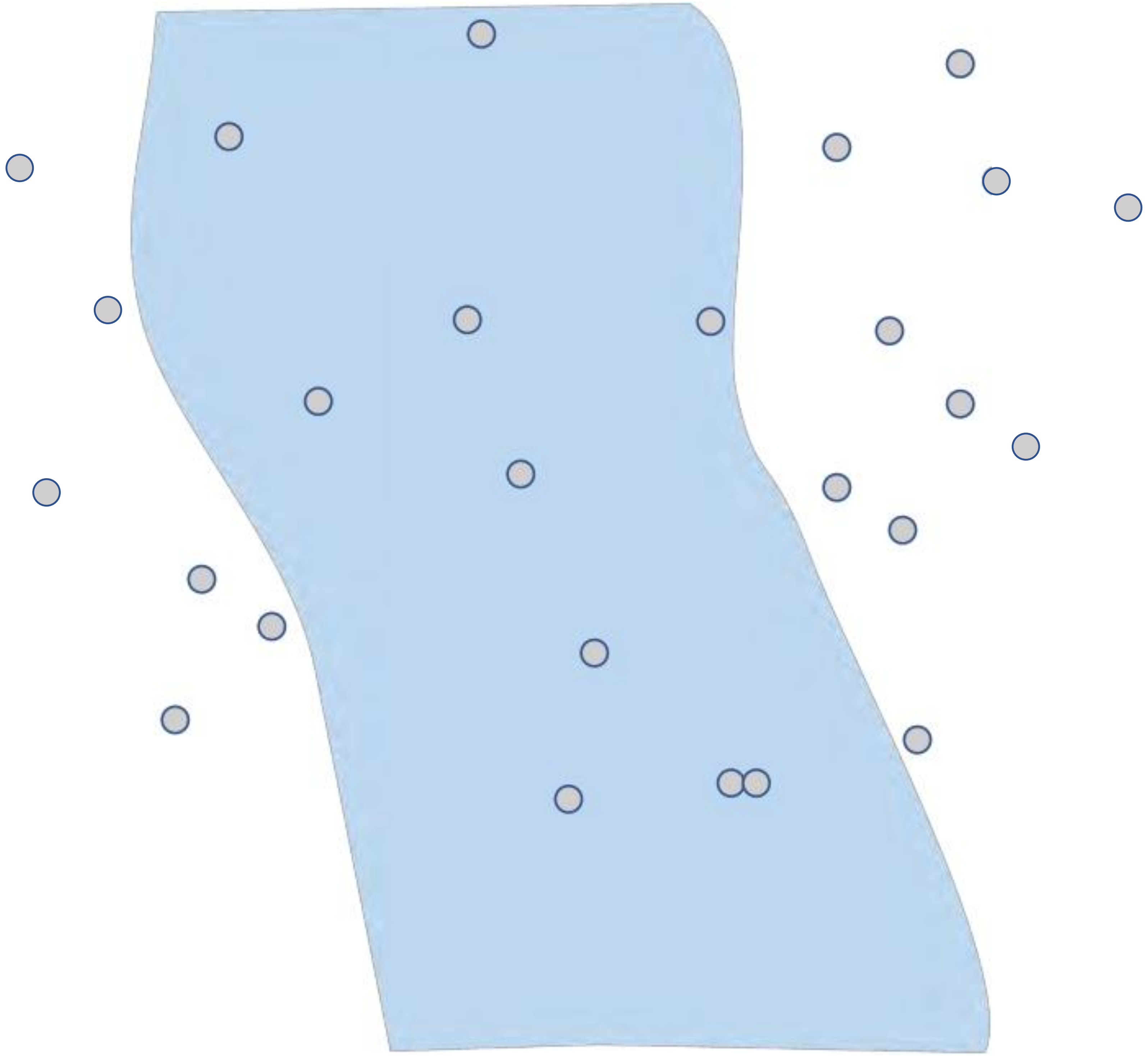

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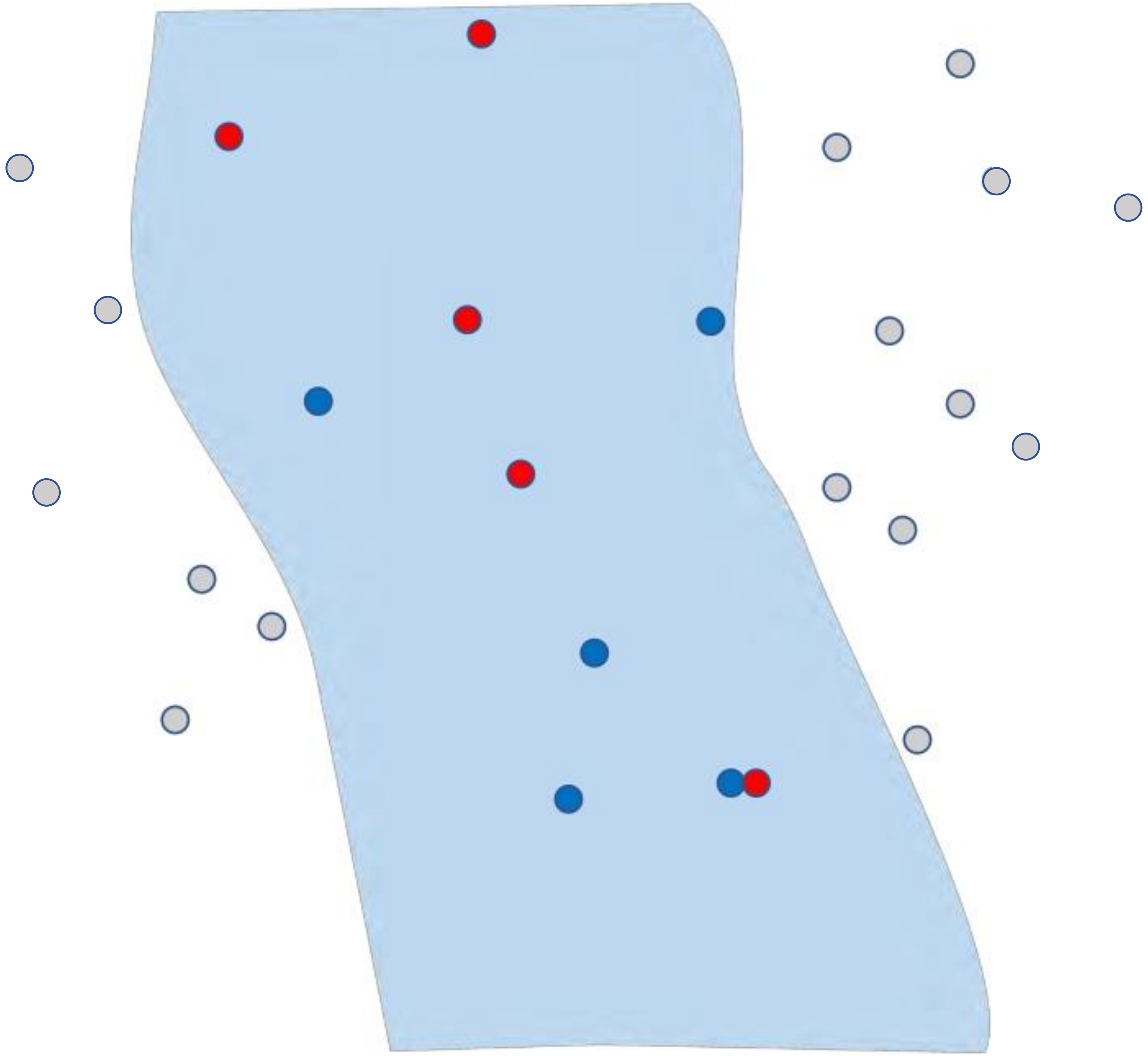

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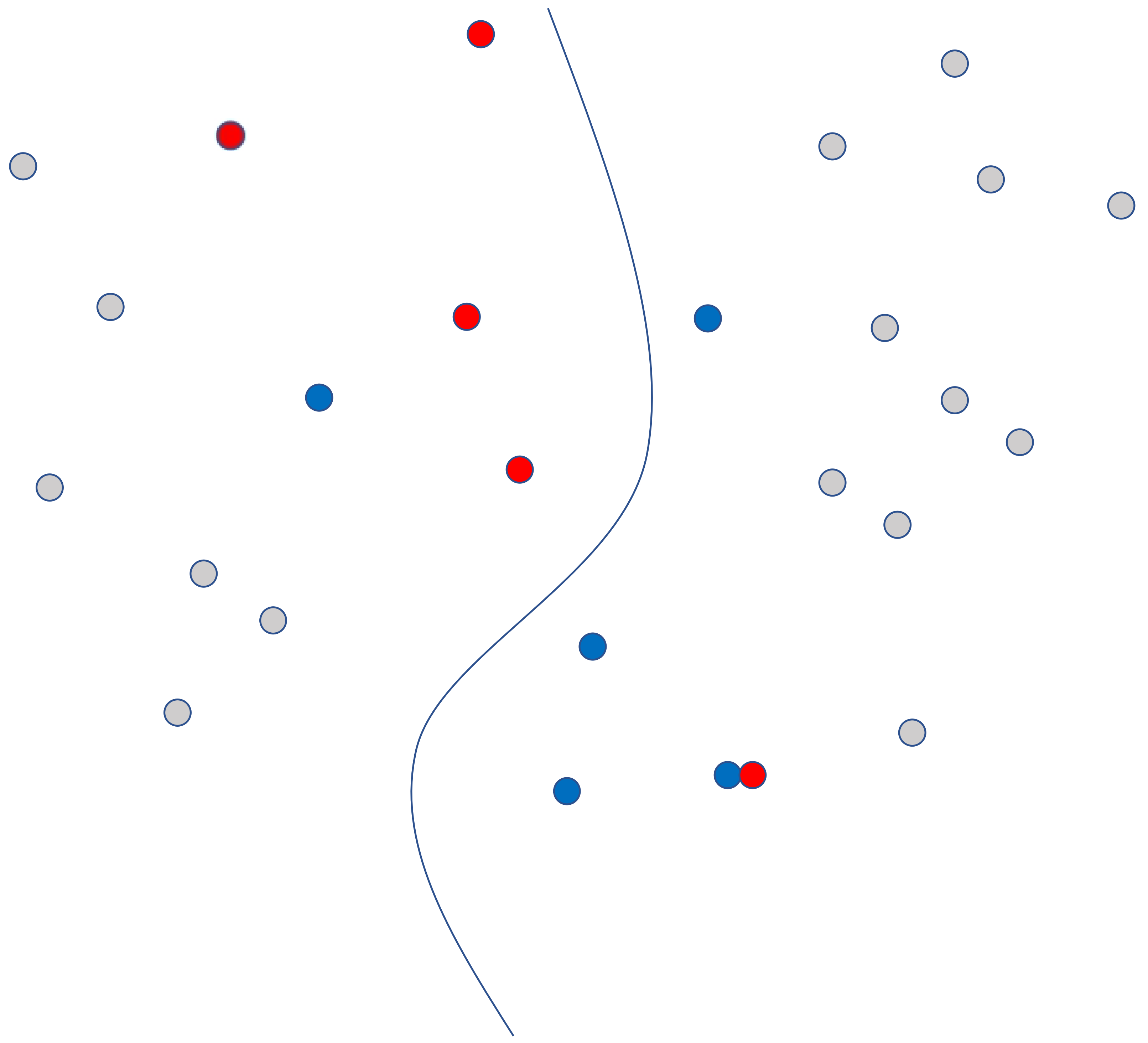

Agnostic Active Learning

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

A^2 (Agnostic Active)

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

1. **sample** 2^t unlabeled points S
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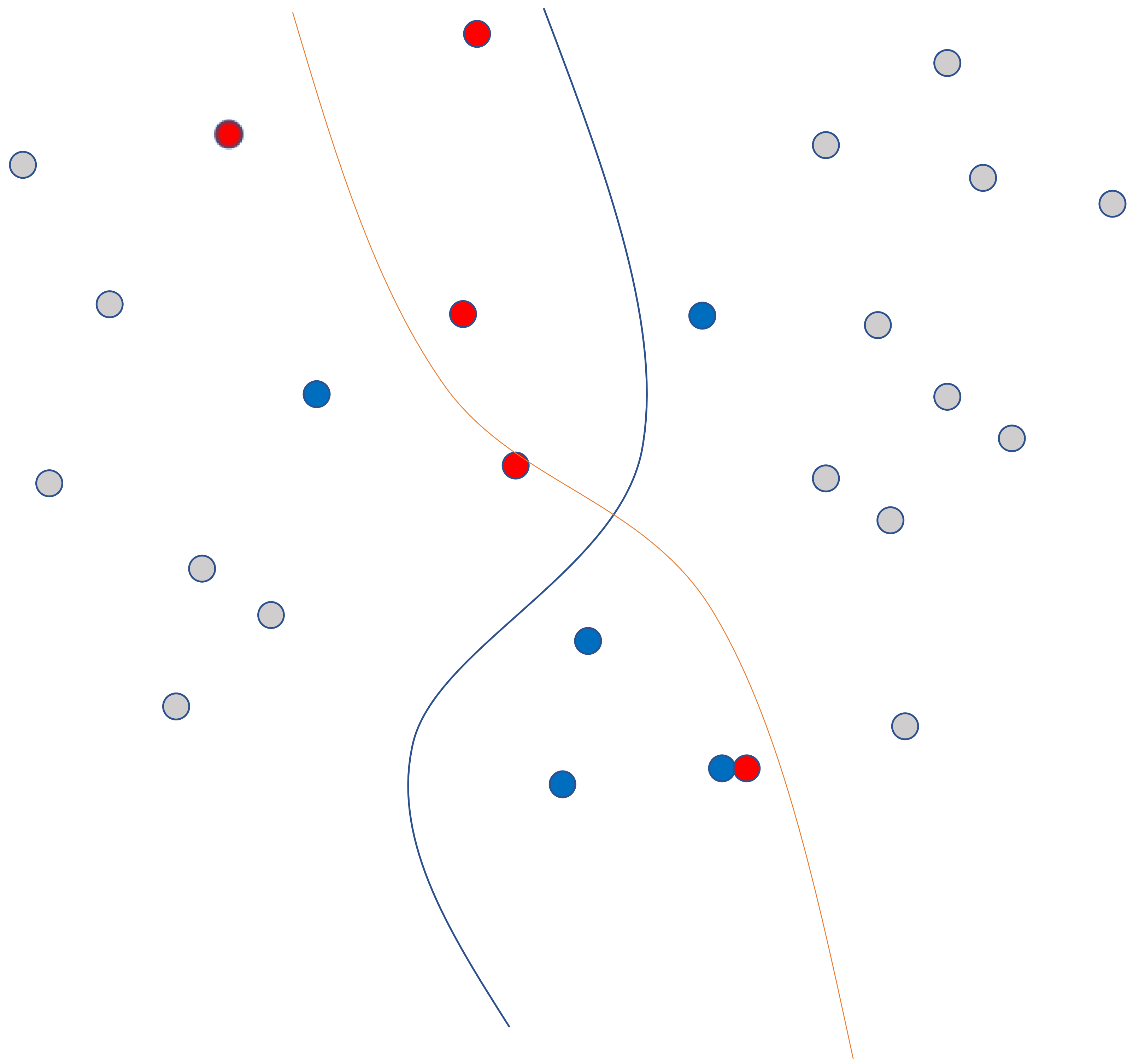

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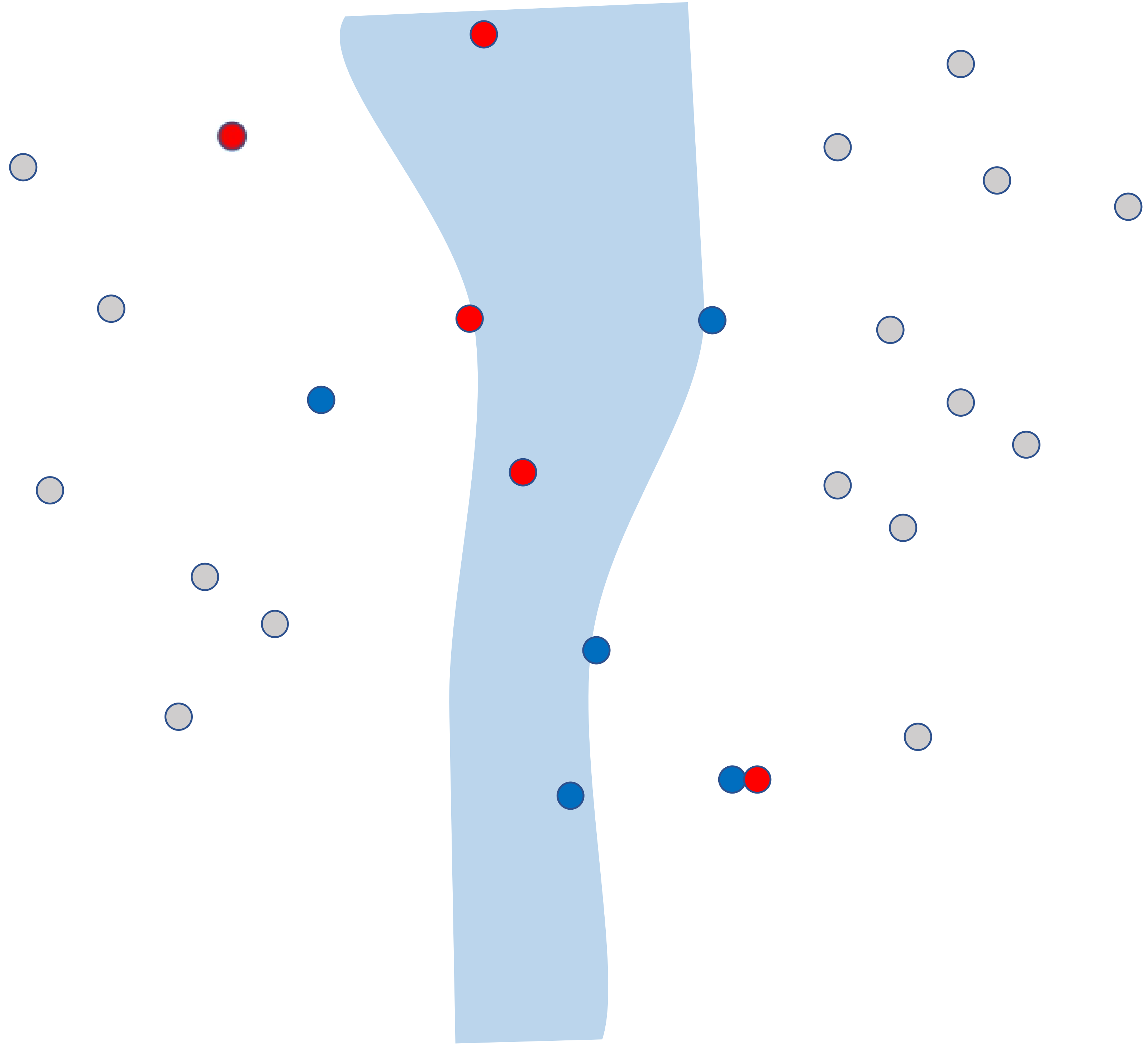

Agnostic Active Learning

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$\mathcal{A}^2$ (Agnostic Active)

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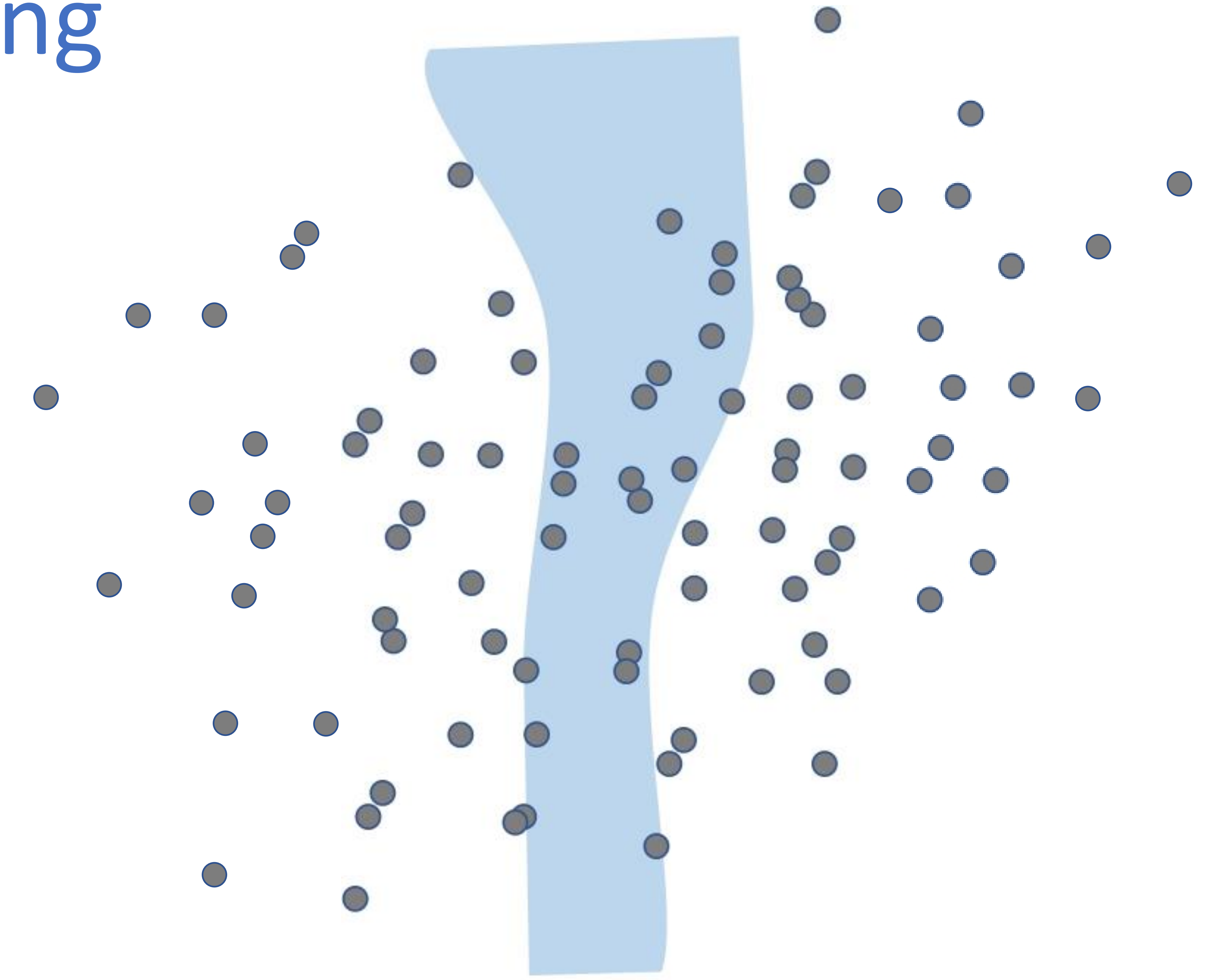

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A^2 (Agnostic Active)

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output final $\hat{f}$

The point:

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

This difference is at most 0

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

$\Rightarrow$ ***f^** never removed.**

Agnostic Active Learning

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

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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.**

Next: **How many labels does it use?**

Sample Complexity Analysis

Hanneke (2007,...)

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

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

Disagreement coefficient:

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

https://pdfs.semanticscholar.org/0626/241872b8def3e517e3af8acd12c5107c8c1a.pdf

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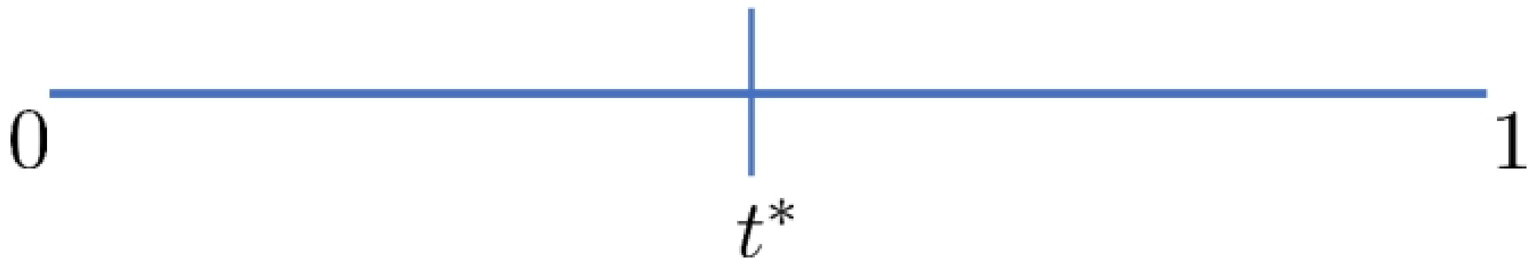
Example: **Thresholds**, P_X Uniform$(0, 1)$

$f(x) = \mathbb{I}[x \geq t]$



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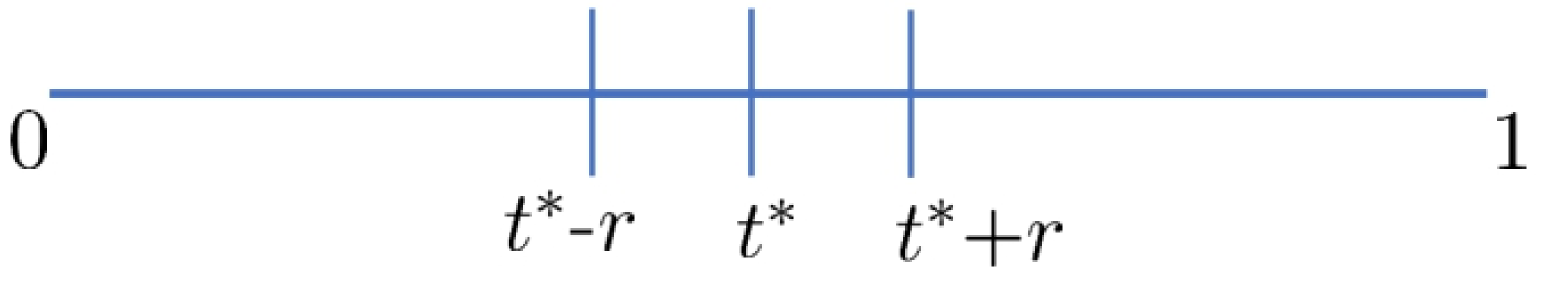

$\mathrm{DIS}(\mathrm{B}(f^*, r)) = [t^* - r, t^* + r)$

$P_X(\mathrm{DIS}(\mathrm{B}(f^*, r))) = 2r$

$\theta = 2$

Sample Complexity Analysis

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

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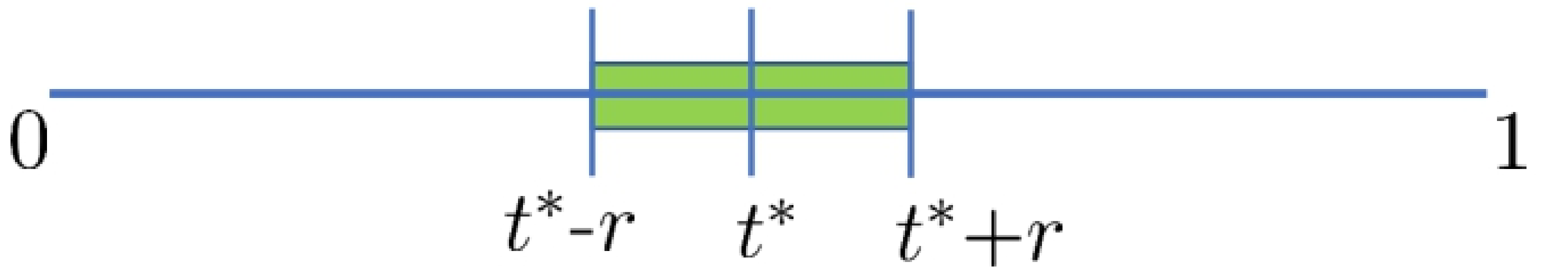

$$\mathrm{DIS}(\mathrm{B}(f^*, r)) = [t^* - r, t^* + r)$$

$$P_X(\mathrm{DIS}(\mathrm{B}(f^*, r))) = 2r$$

$$\Rightarrow \theta = 2$$

Sample Complexity Analysis

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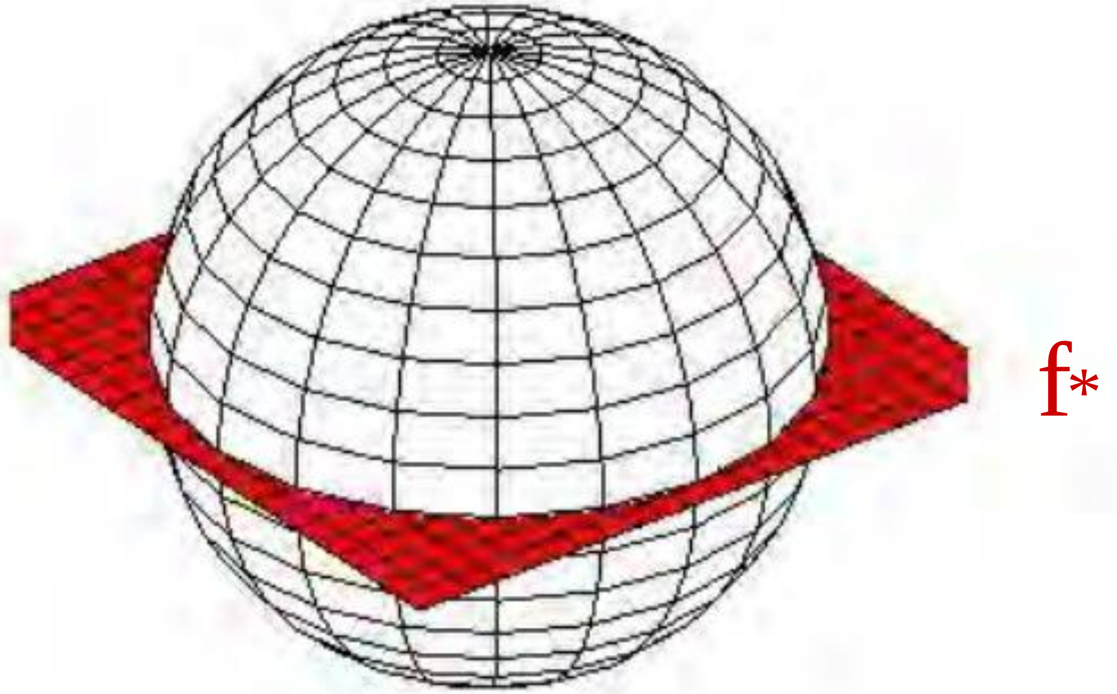
Example: homog. linear separators (bias 0), n dimensions, uniform P_X on sphere.



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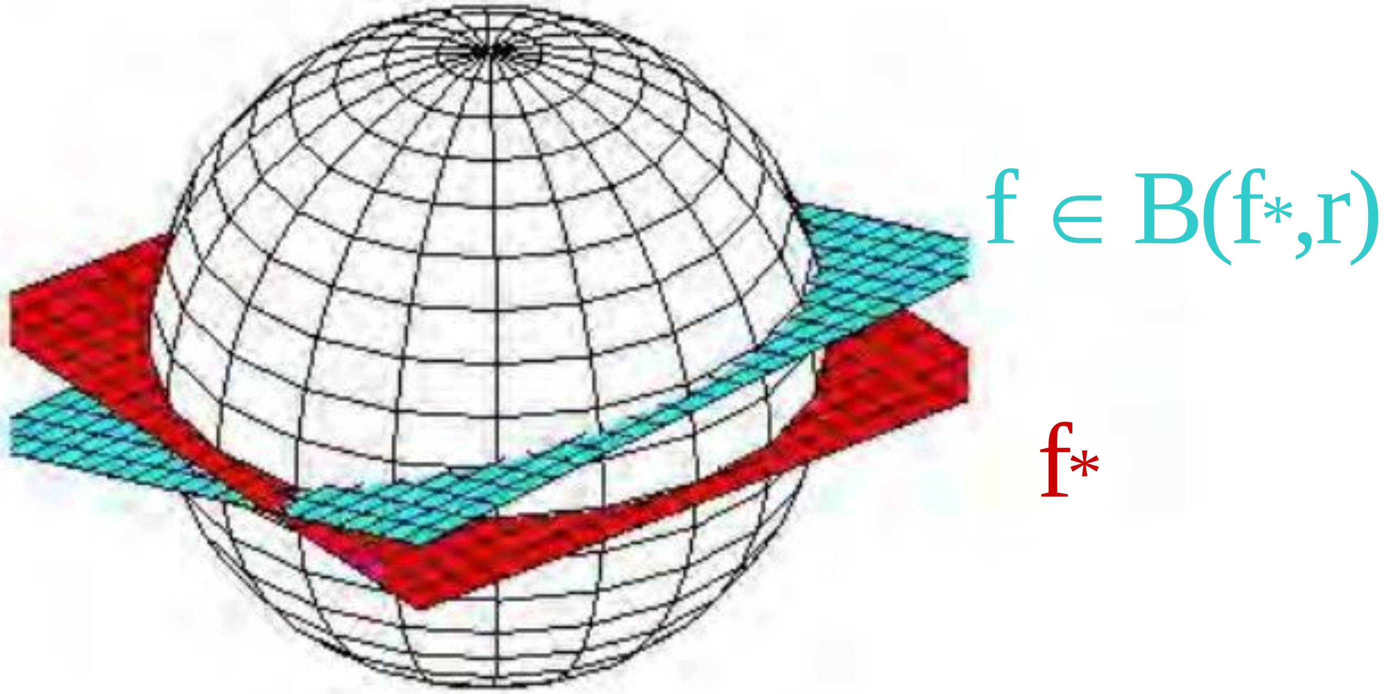

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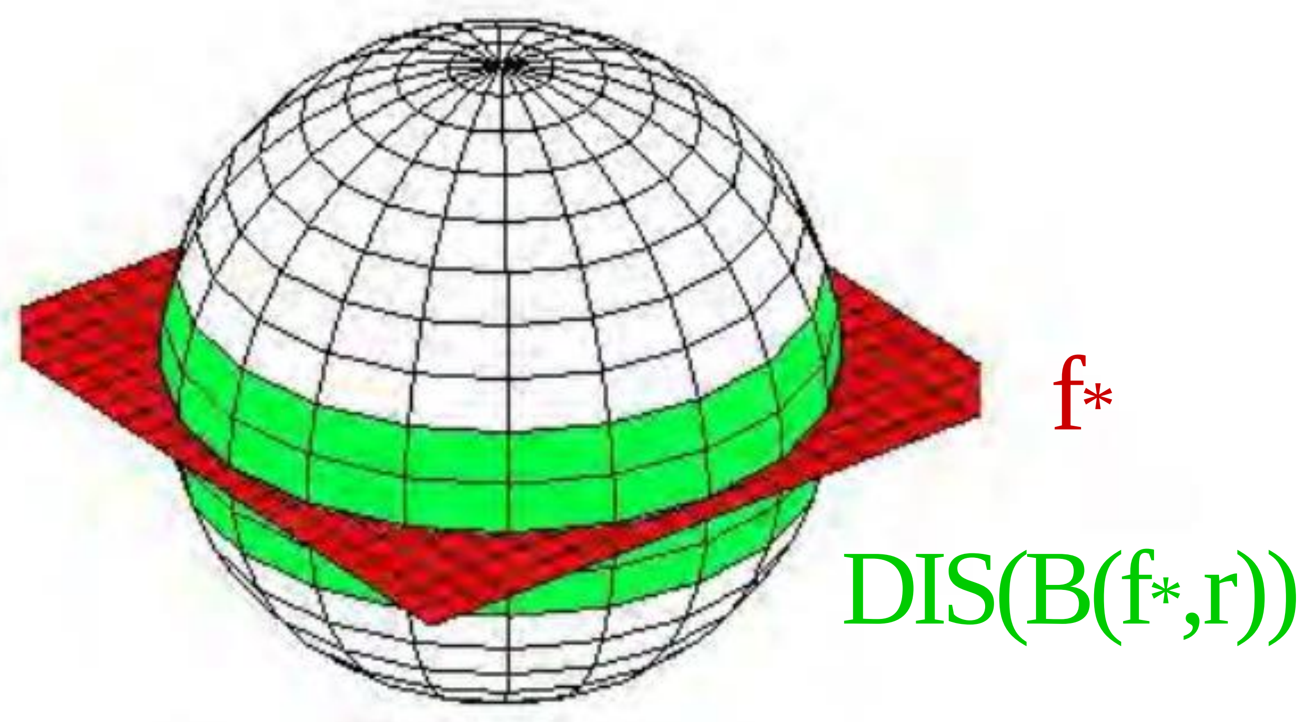

Sample Complexity Analysis

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

Example: homog. linear separators (bias 0),

DIS(B(.

Disagr

$$\theta_{h^*} = \sup_r \frac{Pr(DIS(B(h^*, r)))}{r} = \frac{2r}{r} = 2.$$

With the exception of very nice situations (uniform distribution, symmetric geometry, etc.) the disagreement coefficient is often impossible to calculate. Below are the disagreement coefficients for some classes of problems:

- Thresholds on $\mathbb{R}$: $\theta = 2$.
- Homogeneous hyperplanes in $\mathbb{R}^d$ with data uniformly distributed on a sphere: $\theta \leq \sqrt{d}$
- General hyperplanes in $\mathbb{R}^d$ with the data density bounded below: $\theta = O(d)$
- Intervals $[a, b]$ on $\mathbb{R}$: $\theta = \infty$

r))

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

$$\Rightarrow \qquad \boldsymbol{\theta \propto \sqrt{n}}.$$

Sample Complexity Analysis

Hanneke (2007,…)

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

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

Disagreement coefficient:

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https://pdfs.semanticscholar.org/0626/241872b8def3e517e3af8acd12c5107c8c1a.pdf

Sample Complexity Analysis

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	$\frac{d}{\epsilon}$	$\frac{d}{n}$
Active	$d\theta \log(\frac{1}{\epsilon})$	$e^{-n/d\theta}$

Sample Complexity Analysis

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

A^2 (Agnostic Active)

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

1. **sample** 2^t unlabeled points S
2. **label** points in $Q = \mathrm{DIS}(\mathcal{H}) \cap S$
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 $\hat{f}$

Bounded noise:

$$R(f) - R(f^*) = \int_{f \neq f^*} (P(Y = f^*(X)|X) - P(Y \neq f^*(X)|X)) \mathrm{d}P_X$$
$$\geq (1 - 2\beta) P_X(f \neq f^*)$$

Theorem: $P(Y \neq f^*(X)|X) \leq \beta$. $R(\hat{f}) \leq R(f^*) + \epsilon$ with

$$\#\text{ labels} \approx d\theta \log(\tfrac{1}{\epsilon}).$$

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

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

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

Sample Complexity Analysis

Agnostic Learning: (no assumptions)

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

	Sample Complexity: $R(\hat{f}) \leq R(f^*) + \epsilon$	Excess Error: n labels
Passive	$d\frac{\beta}{\epsilon^2}$	$\sqrt{\frac{d\beta}{n}}$
Active	$d\theta\frac{\beta^2}{\epsilon^2}$	$\sqrt{\frac{d\beta^2\theta}{n}}$

Sample Complexity Analysis

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

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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 $\hat{f}$

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

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

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

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

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

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

$\square$

Sample Complexity Analysis

When is θ small?

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

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

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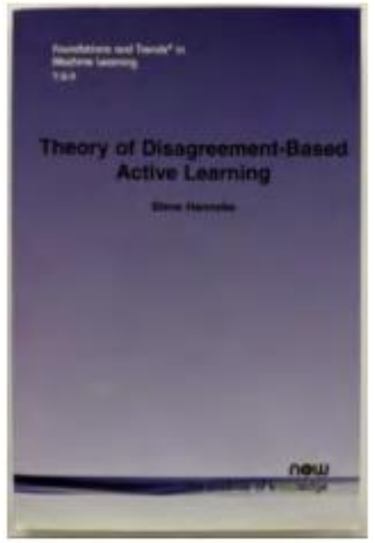
Passive	$d\frac{\beta}{\epsilon^2}$	$\sqrt{\frac{d\beta}{n}}$
Active	$d\theta\frac{\beta^2}{\epsilon^2}$	$\sqrt{\frac{d\beta^2\theta}{n}}$

Lots more →



Stopping Criterion

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

A^2 (Agnostic Active)

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

1. **sample** 2^t unlabeled points S
2. **label** points in $Q = \mathrm{DIS}(\mathcal{H}) \cap S$
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 $\hat{f}$

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 $m = 1, 2, \ldots$ (til *stopping-criterion*)

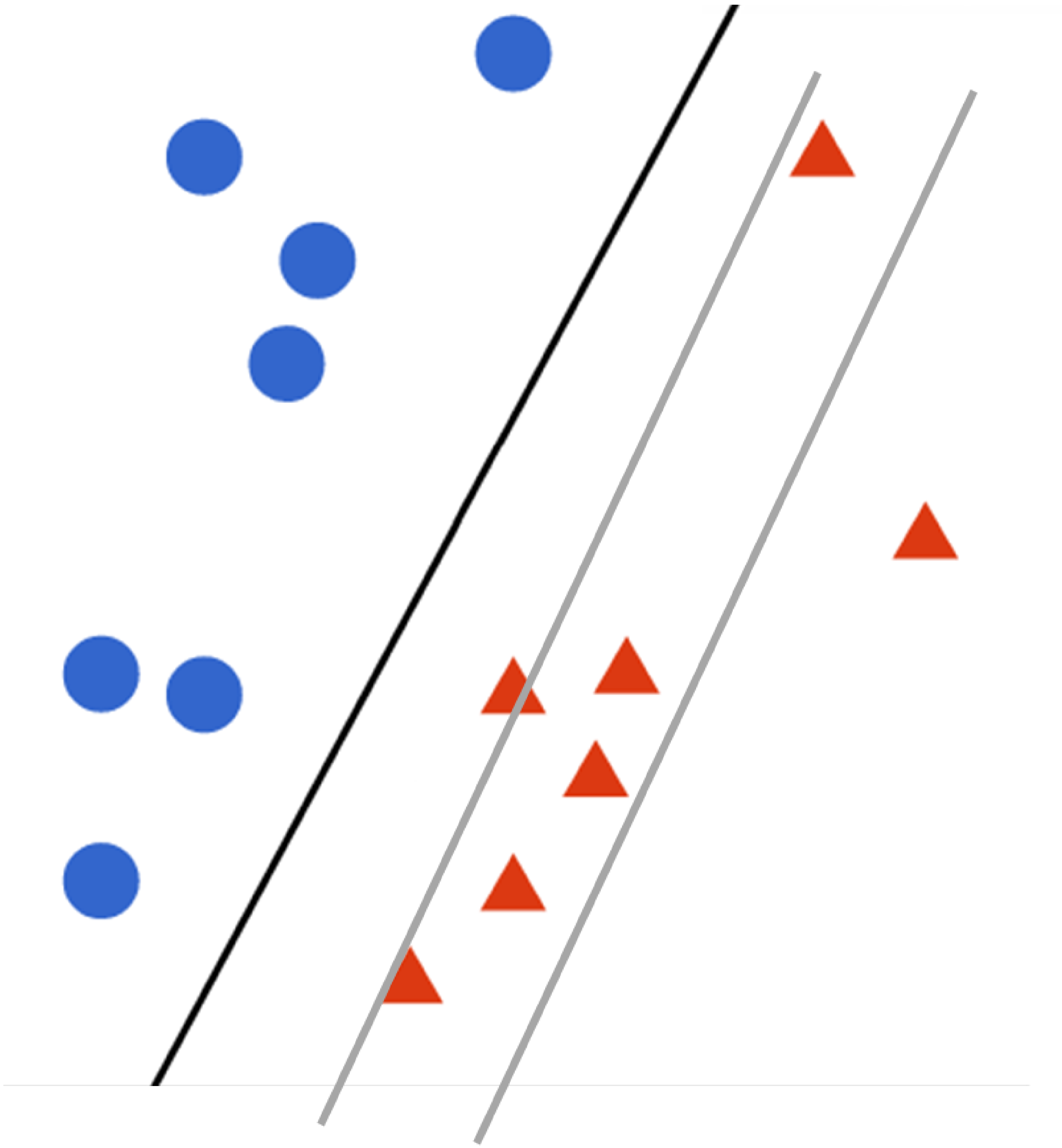
1. **sample** a random point x
2. **optimize** $\forall y,\ \hat{f}_y \leftarrow \underset{f \in \mathcal{H}: f(x)=y}{\operatorname{argmin}}\ \hat{R}_Q(f)$
3. if $|\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \leq \sqrt{\hat{P}_Q(\hat{f}_- \neq \hat{f}_+)\frac{d}{|Q|}}$

   then **label** x, add it to Q

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

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

http://www.cs.columbia.edu/~djhsu/papers/dissertation.pdf



Hanneke & Yang (2012)

- 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, ...)

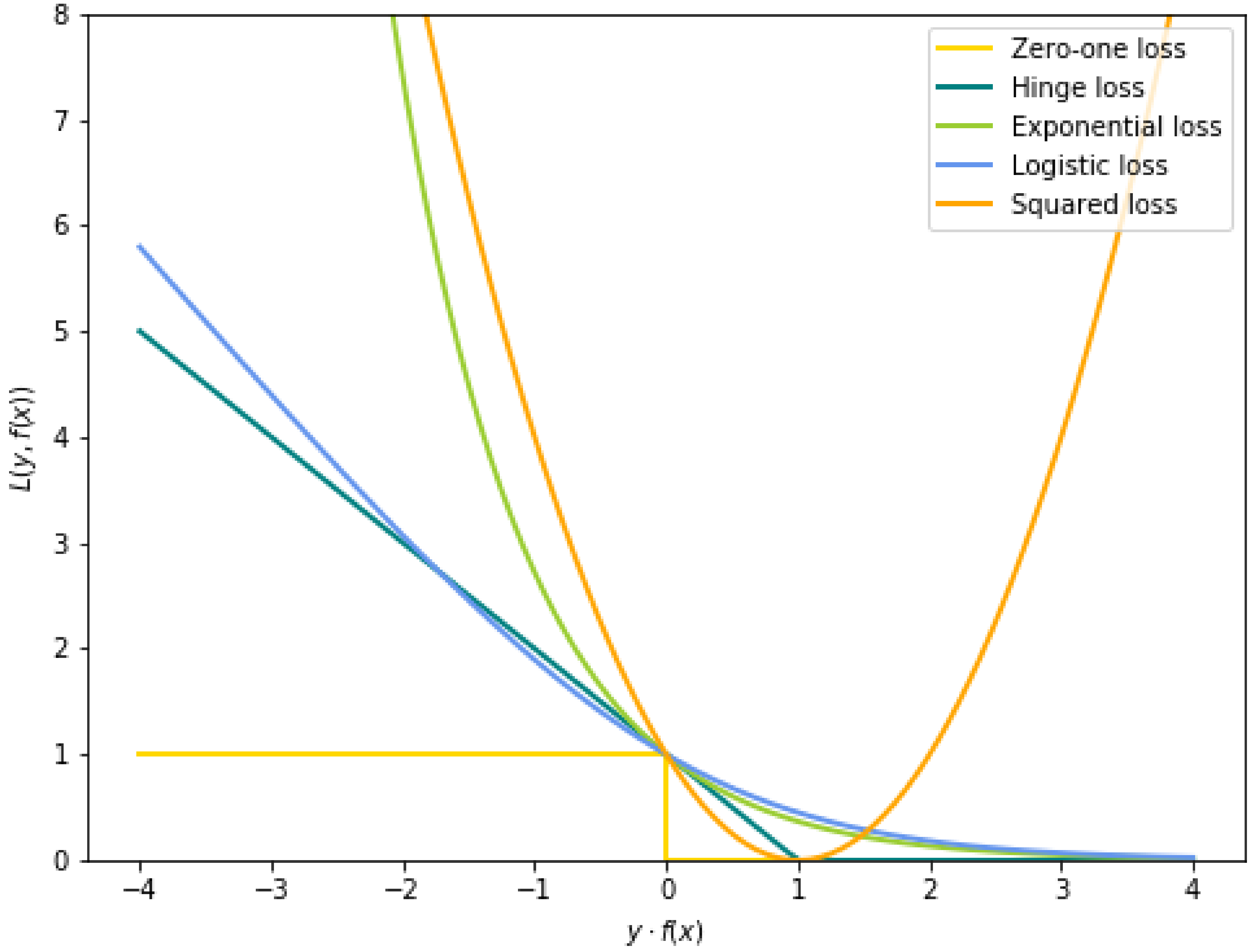
Now $\mathcal{H}$ is **real-valued** functions
$\hat{R}^{\ell}_{Q}(f) = \frac{1}{|Q|} \sum_{(x,y)\in Q} \ell(f(x), y)$

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

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

https://arxiv.org/pdf/1207.3772.pdf

Surrogate Loss



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
$p_x = \mathbb{I}\left[\, |\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \leq \sqrt{\hat{P}_Q(\hat{f}_+ \neq \hat{f}_-)\frac{d}{|Q|}}\,\right]$

https://arxiv.org/pdf/0812.4952.pdf

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

- **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
$p_x = \mathbb{I}\left[|\hat{R}_Q(\hat{f}_+) - \hat{R}_Q(\hat{f}_-)| \leq \sqrt{\hat{P}_Q(\hat{f}_+ \neq \hat{f}_-) \frac{d}{|Q|}} \right]$
- 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
- Distribution-Free Analysis, Optimality
- TicToc: Adapting to Heterogeneous Noise

Tutorial on Active Learning: Theory to Practice

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ICML | 2019
Thirty-sixth International Conference on Machine Learning

Subregion-Based Active Learning

Zhang & Chaudhuri, 2014

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

A^2 (Agnostic Active)

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

1. **sample** 2^t unlabeled points S
2. **label** points in $Q = \mathrm{DIS}(\mathcal{H}) \cap S$
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 $\hat{f}$

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

Subregion-based Active Learning

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

1. **sample** 2^t unlabeled points S
2. **label** points in $Q = \mathcal{R}_{\epsilon'_t}(\mathcal{H}) \cap S$
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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 $\hat{f}$

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,
$R(\hat{f}) - R(f^*) \leq \epsilon$ at end

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

https://arxiv.org/pdf/1407.2657.pdf

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Zhang & Chaudhuri, 2014

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

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

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

$$\approx \varphi_c d \log\left(\tfrac{1}{\epsilon}\right)$$

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Theorem: with **Bounded noise**,
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$$\approx \varphi_c d \log\left(\frac{1}{\epsilon}\right)$$

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

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

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

Subregion-Based Active Learning

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**

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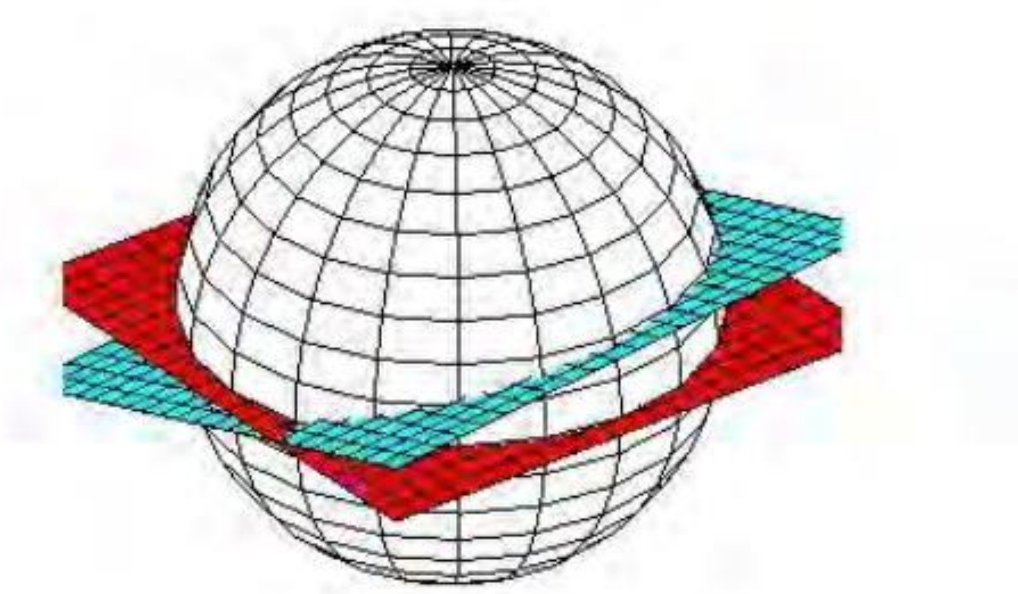
Uniform P_X on d-dim sphere

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



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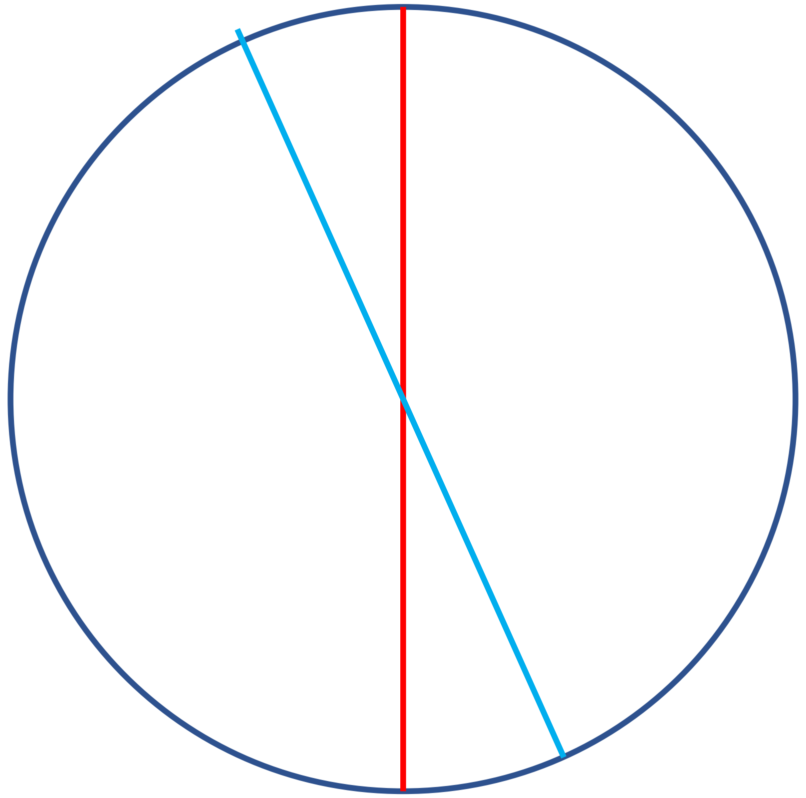
Uniform P_X on d-dim sphere

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

Most projected prob mass toward middle



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

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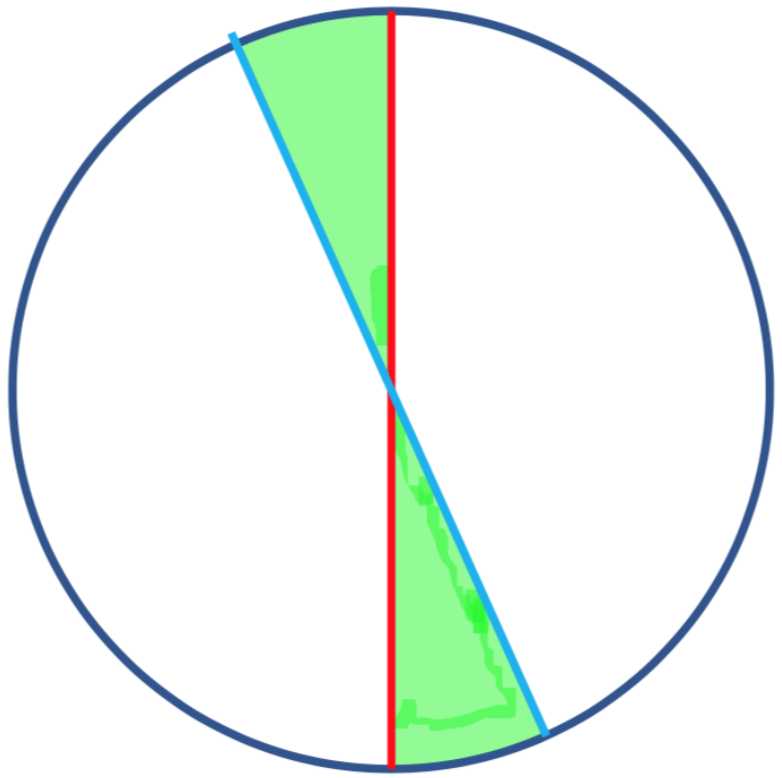

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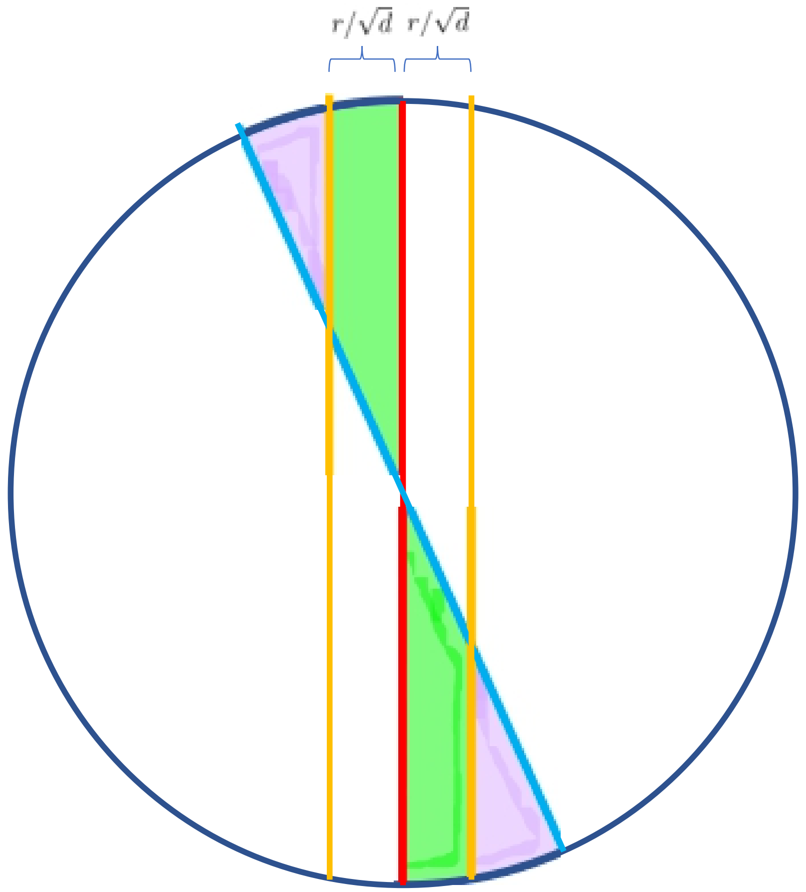


DIS($\{w, w^*\}$) in
slab of width $\approx r$

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**

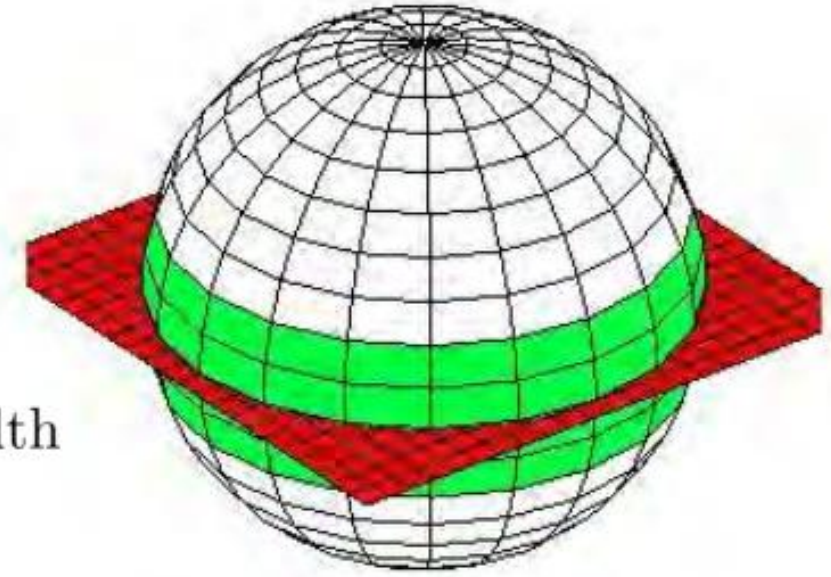
  Margin-based Active Learning
  (Dasgupta, Kalai, Monteleoni, 2005; Balcan, Broder, Zhang, 2007; ...)

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

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

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

$\Rightarrow \varphi_c \leq$ constant



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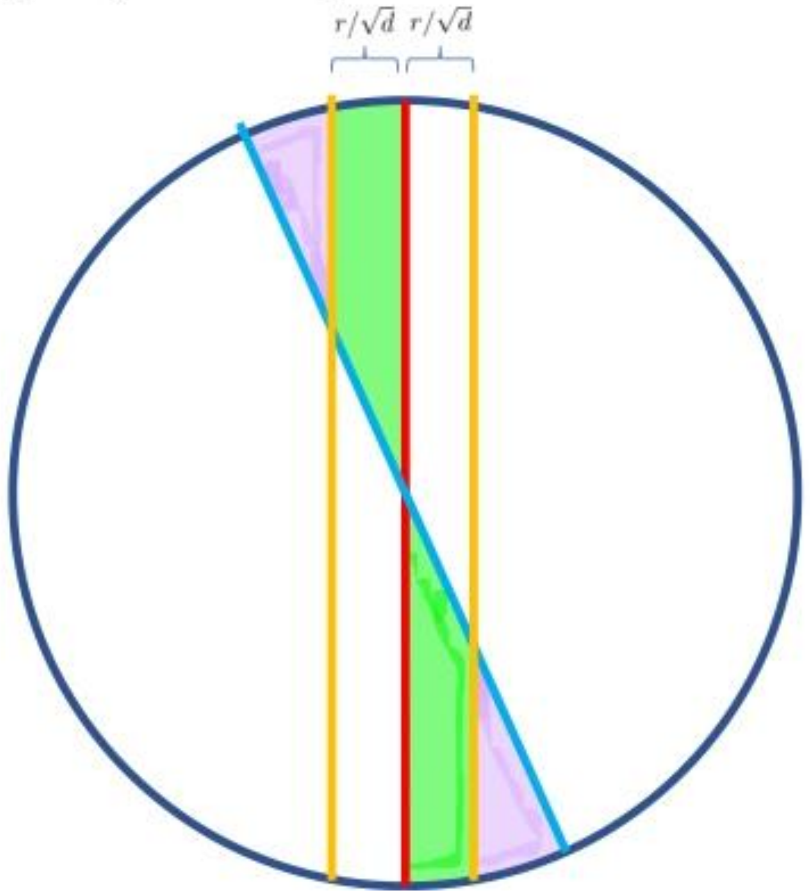
Uniform P_X on d-dim sphere

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

Most projected prob mass toward middle



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

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

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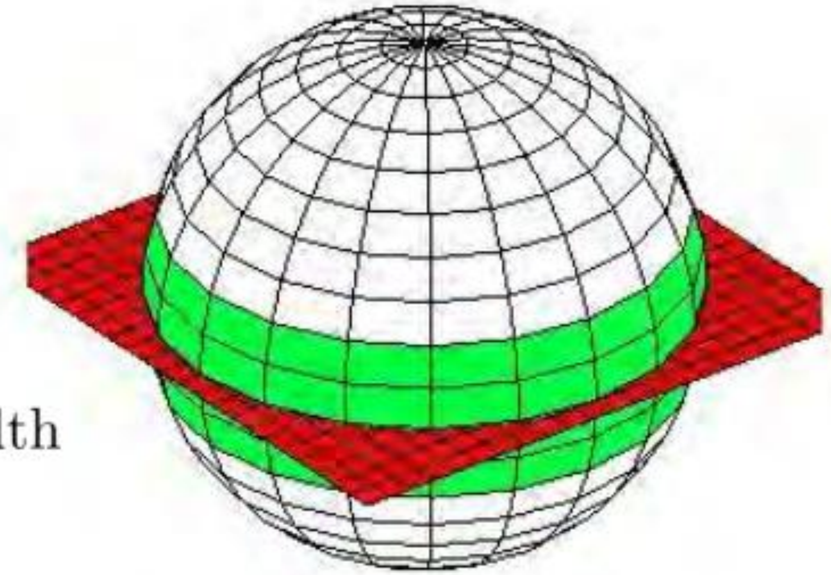

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$$\varphi_c := \sup_{r > \epsilon} \frac{P_X(\mathcal{R}_{r/c}(\mathrm{B}(f^*,r)))}{r}$$

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

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

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

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

Margin-Based Active Learning

(Balcan, Broder, Zhang, 2007; ...)

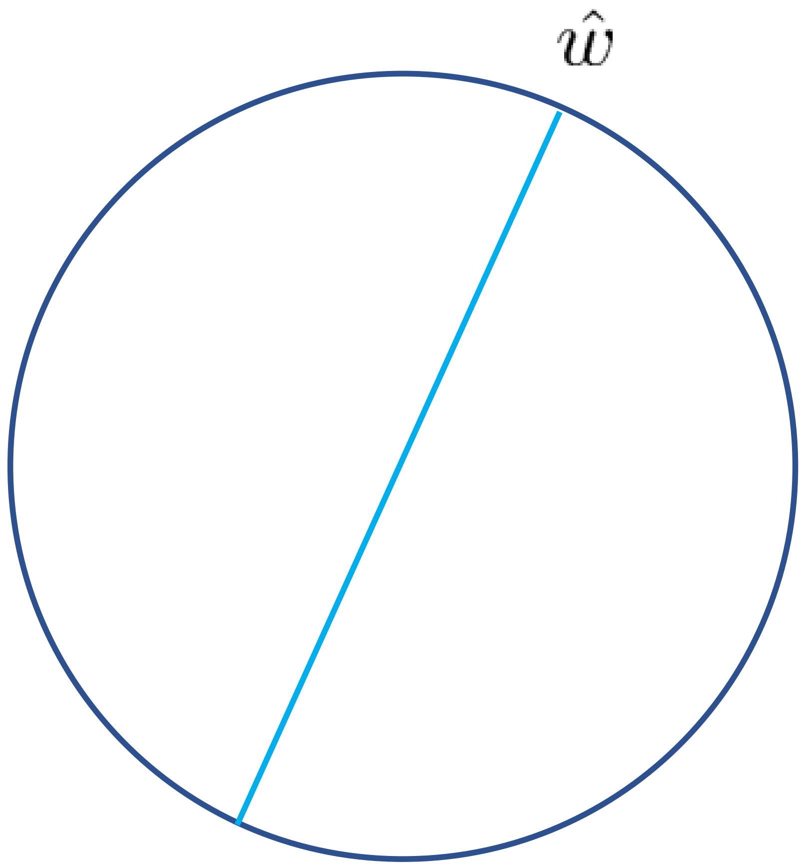
Margin-based Active Learning

Initialize $\hat{w}$

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

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

output final $\hat{w}$



Uniform P_X on d-dim sphere

http://tongzhang-ml.org/papers/colt07-active.pdf

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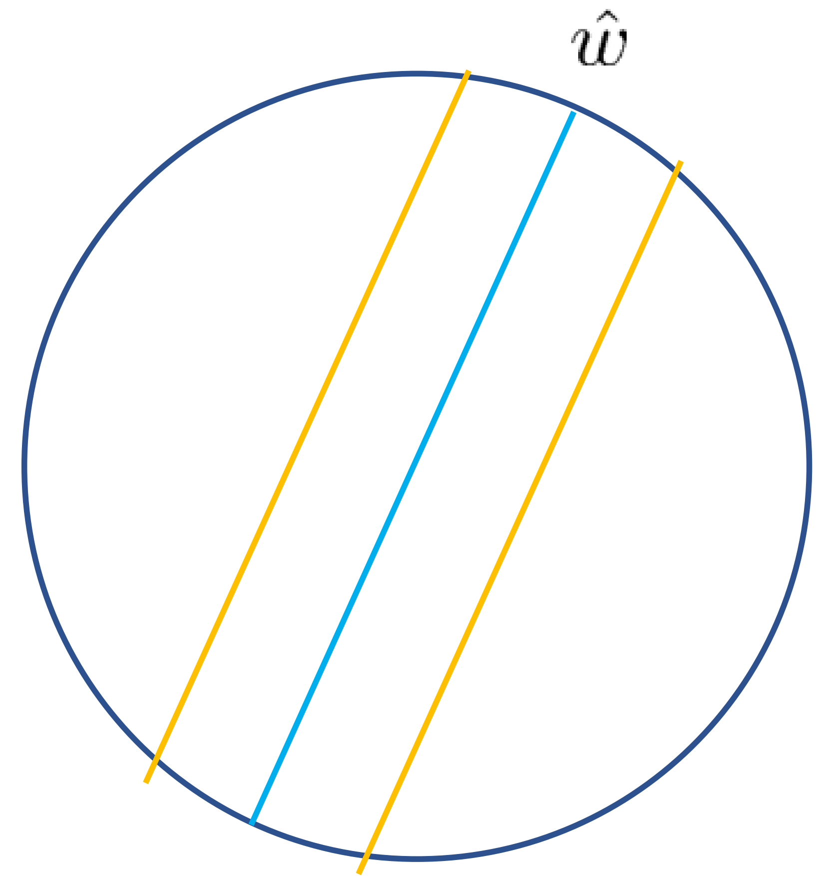

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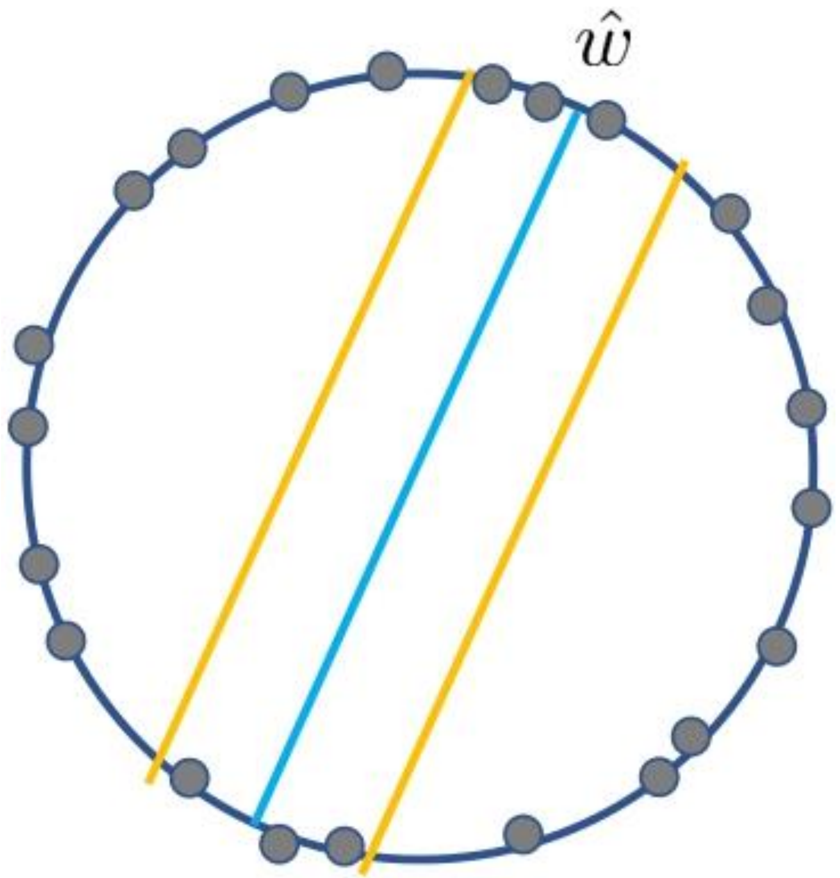

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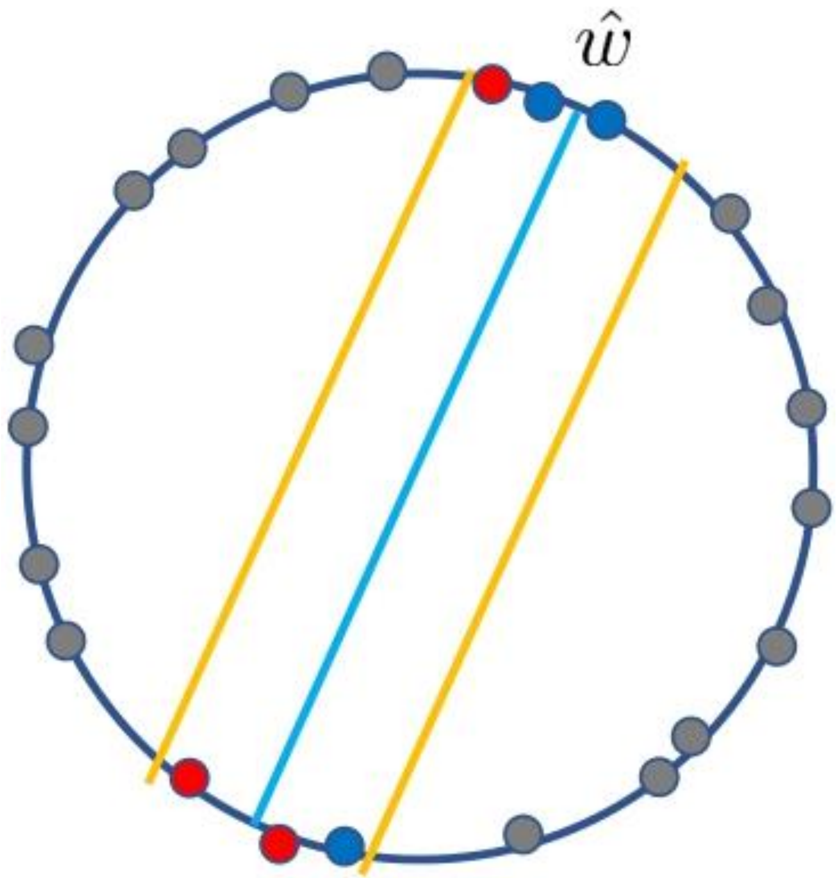

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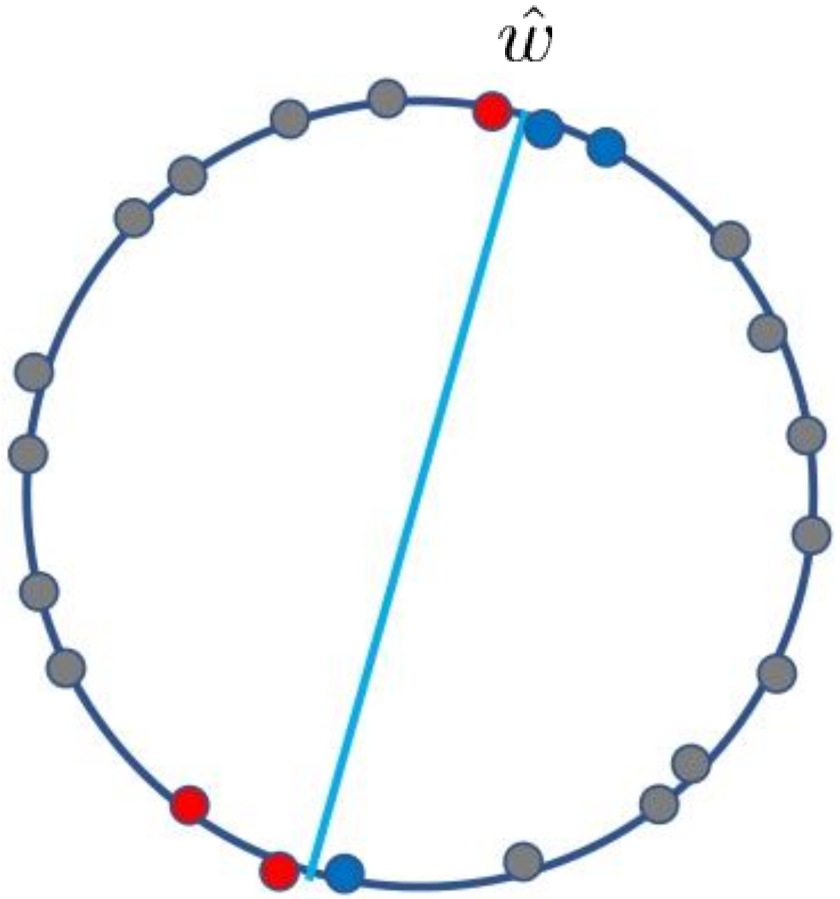

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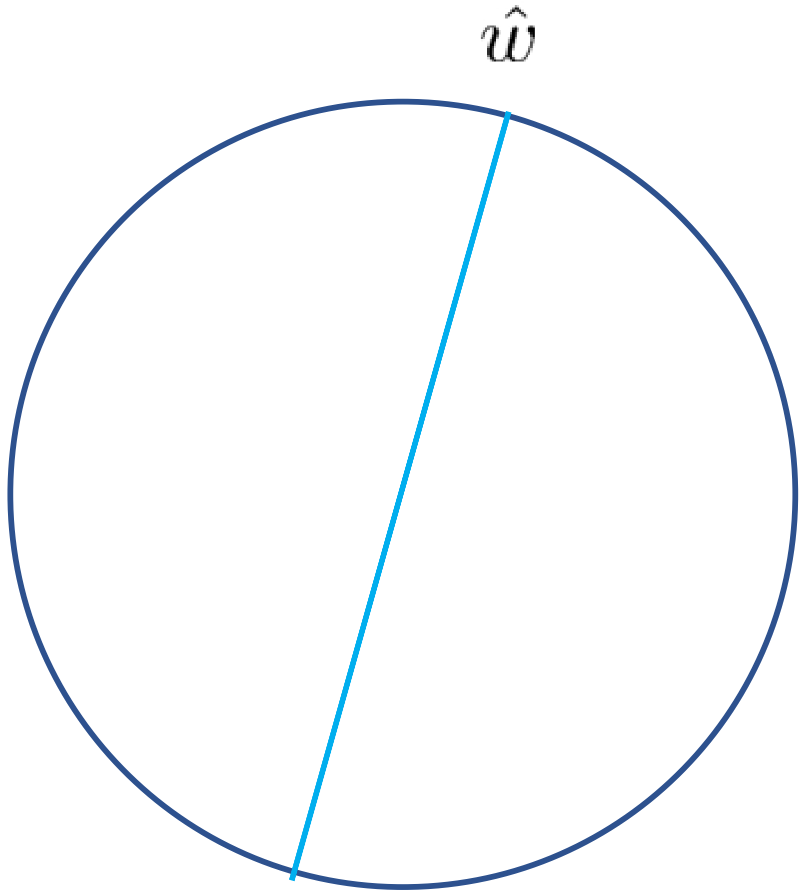


Uniform P_X on d-dim sphere

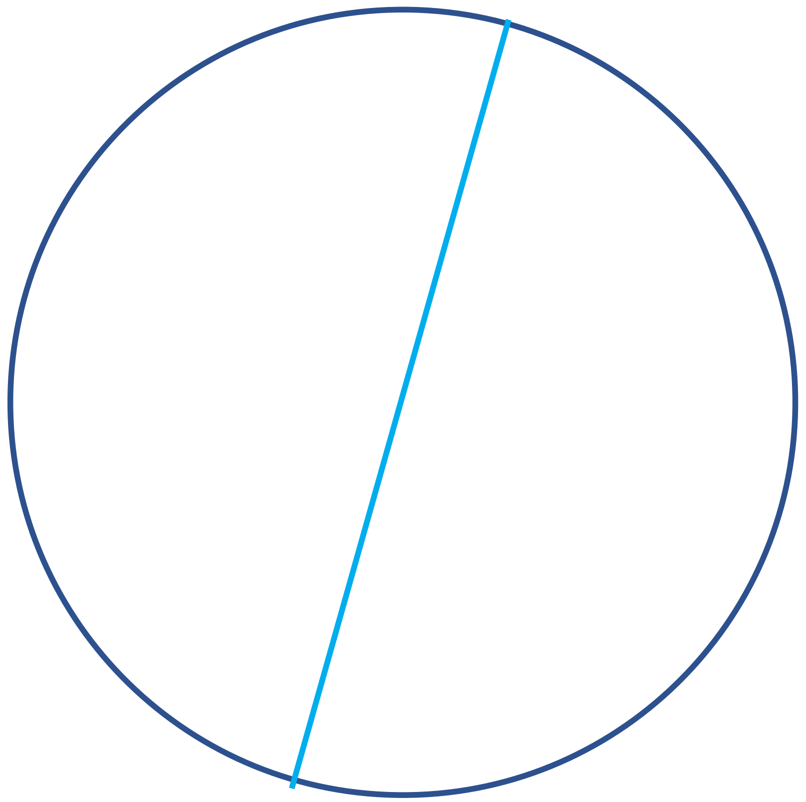
Theorem: with **Bounded noise**,
$R(\hat{f}) \leq R(f^*) + \epsilon$ using # labels
$$\approx d \log\left(\frac{1}{\epsilon}\right)$$

(also works for isotropic log-concave distributions)

Computational Efficiency

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

Uniform P_X on d-dim sphere



Efficient Alg

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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

https://arxiv.org/pdf/1503.03594.pdf

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

Uniform P_X on d-dim sphere

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

Computational Efficiency

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

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2. **label** points in $Q =$ all $x \in S$ s.t. $<\hat{w}, x> \;\leq\; c2^{-t}/\sqrt{d}$
3. **optimize** $\hat{w} \leftarrow \underset{w:\|w-\hat{w}\| \leq c' 2^{-t}}{\operatorname{argmin}} \hat{R}_Q^{\ell_t}(w)$

output final $\hat{w}$

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
$$\approx d \log\left(\tfrac{1}{\epsilon}\right)$$
and running in polynomial time

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

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

(also works for isotropic log-concave distributions)

Up Next:
Distribution-free Analysis

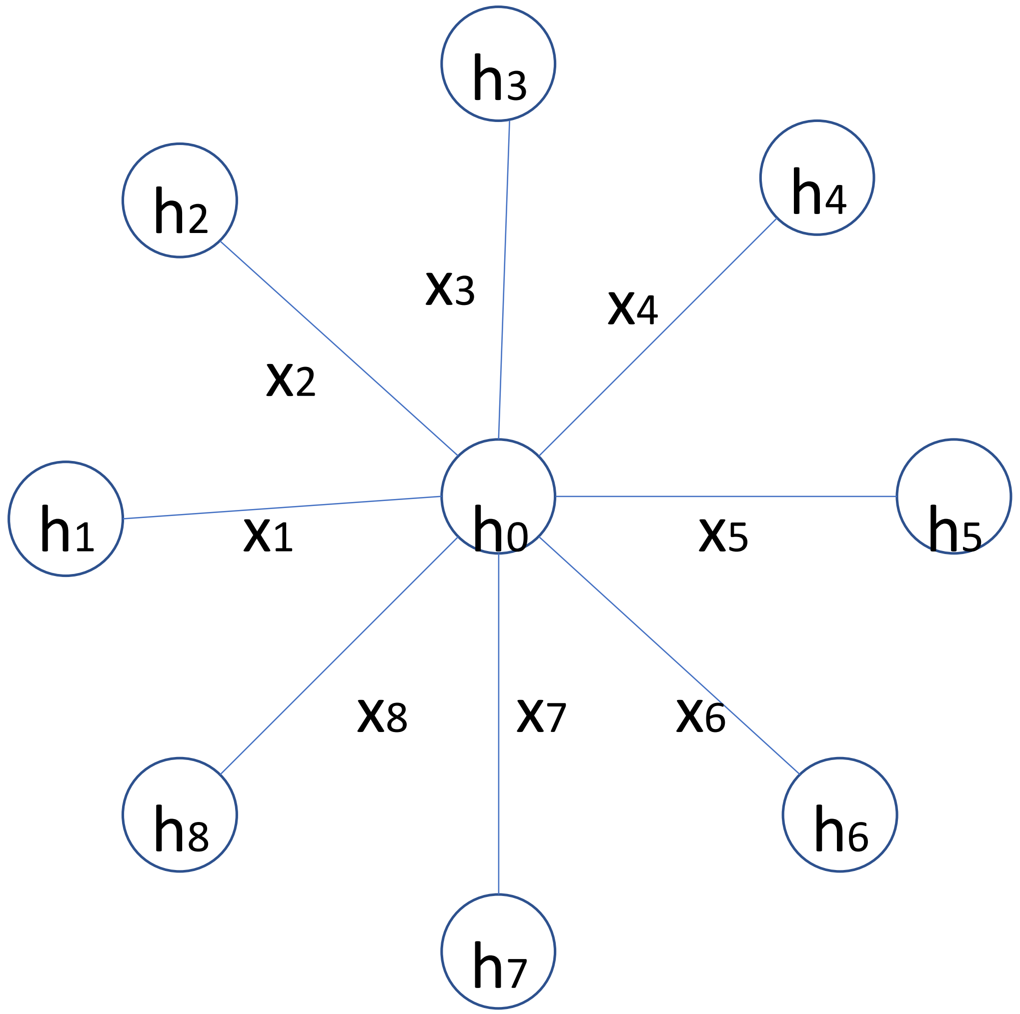
Distribution-Free Analysis

(Hanneke & Yang, 2015)

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



https://arxiv.org/pdf/1410.0996.pdf

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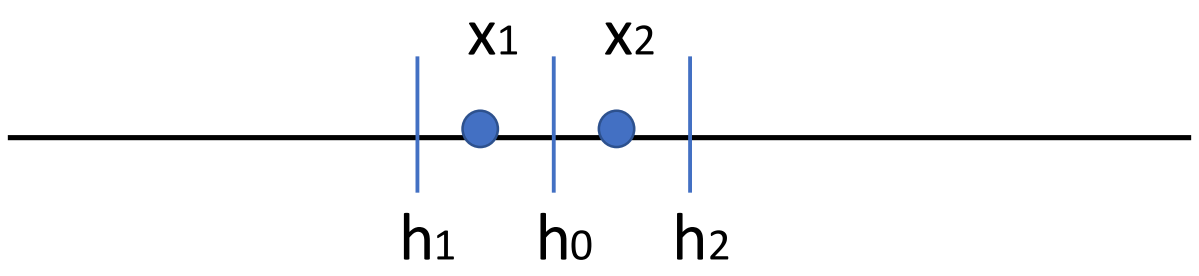
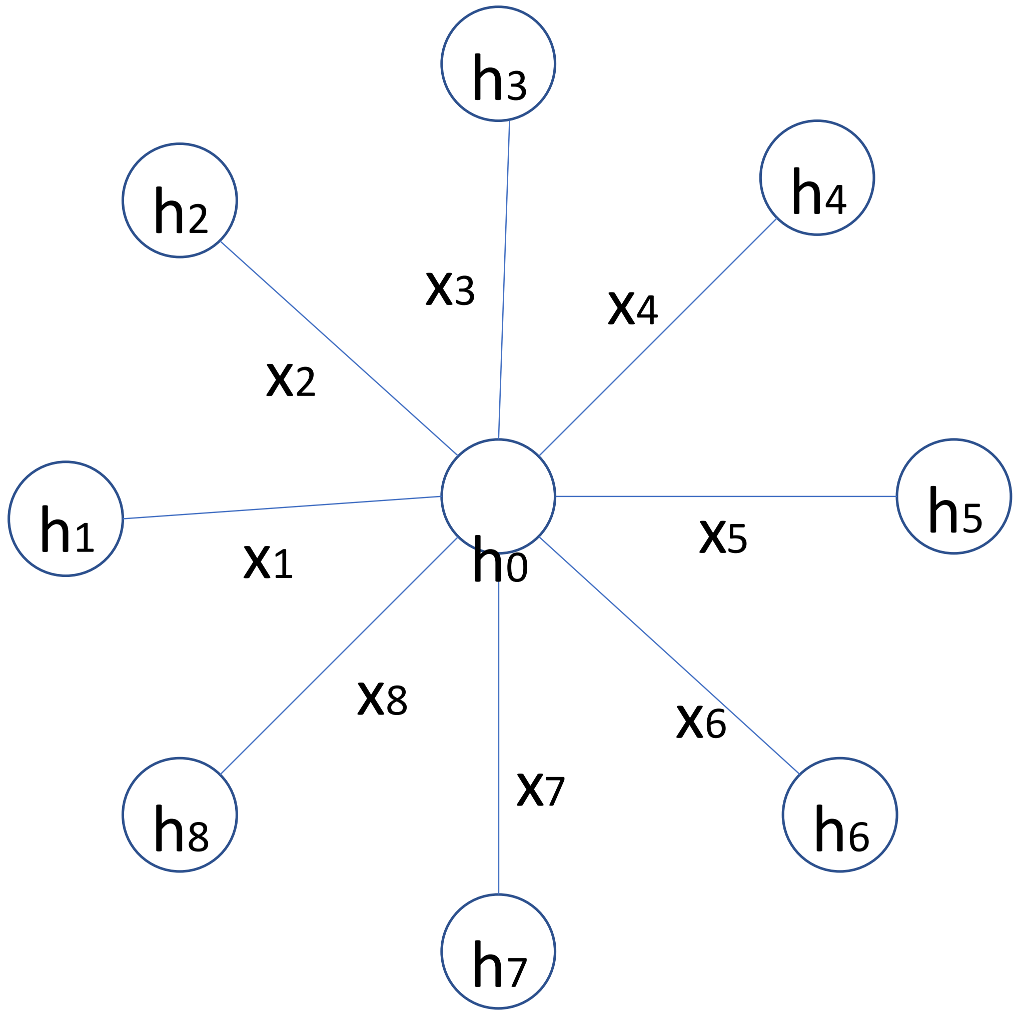
Example: Thresholds: $f(x) = \mathbb{I}[x \geq t]$.

$\mathfrak{s} = 2$.





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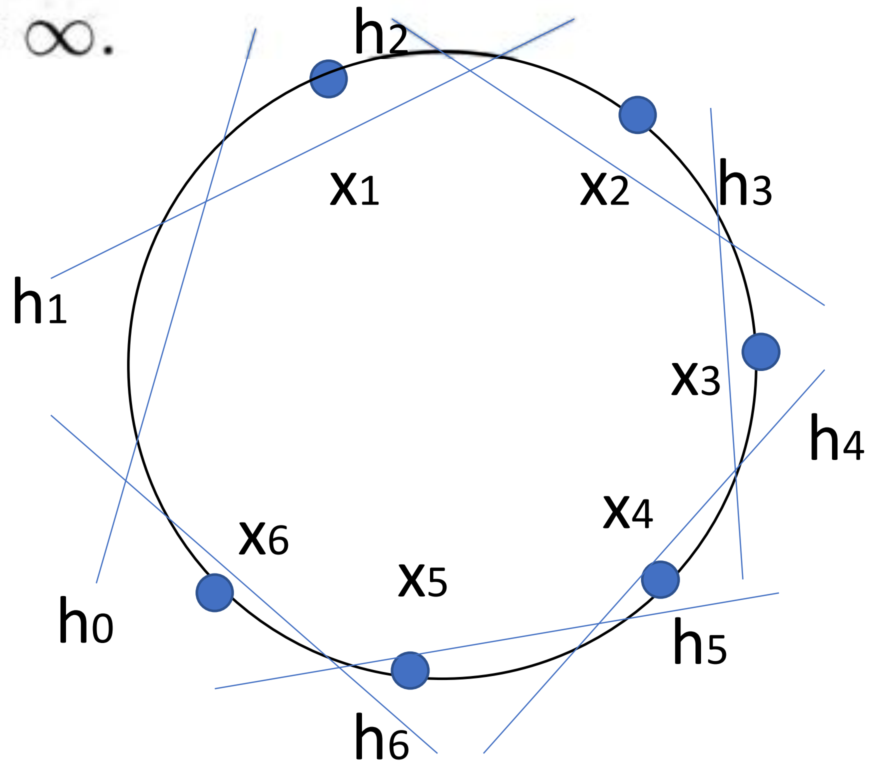
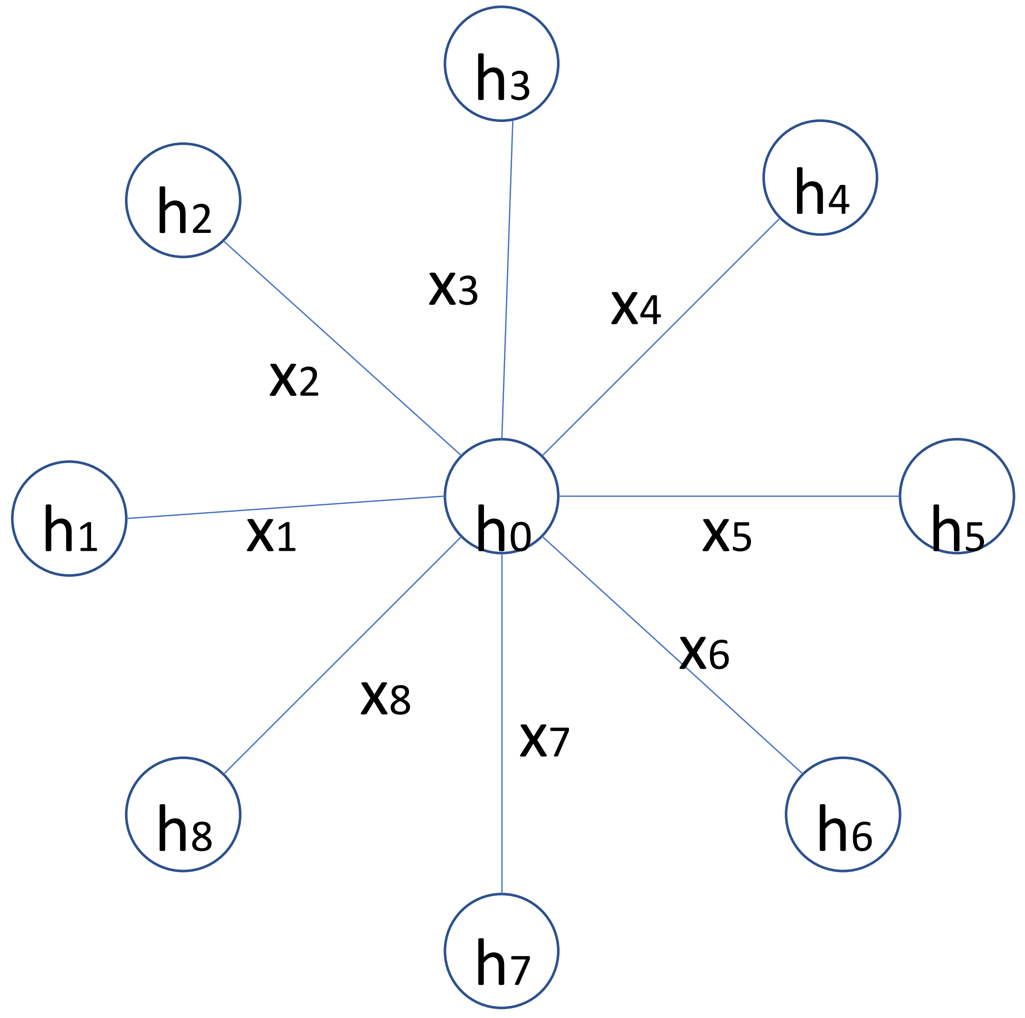
Example: Linear Separators in $\mathbb{R}^n$, $n \geq 2$:

$\mathfrak{s} = \infty$.





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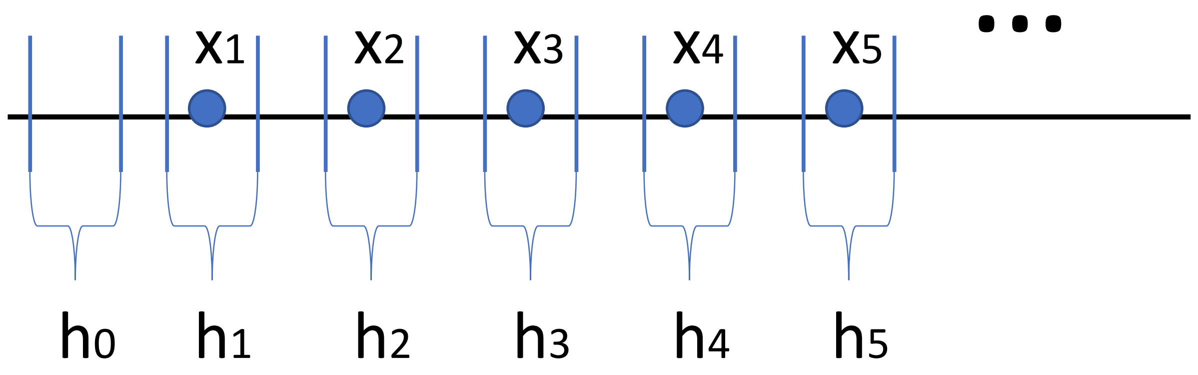
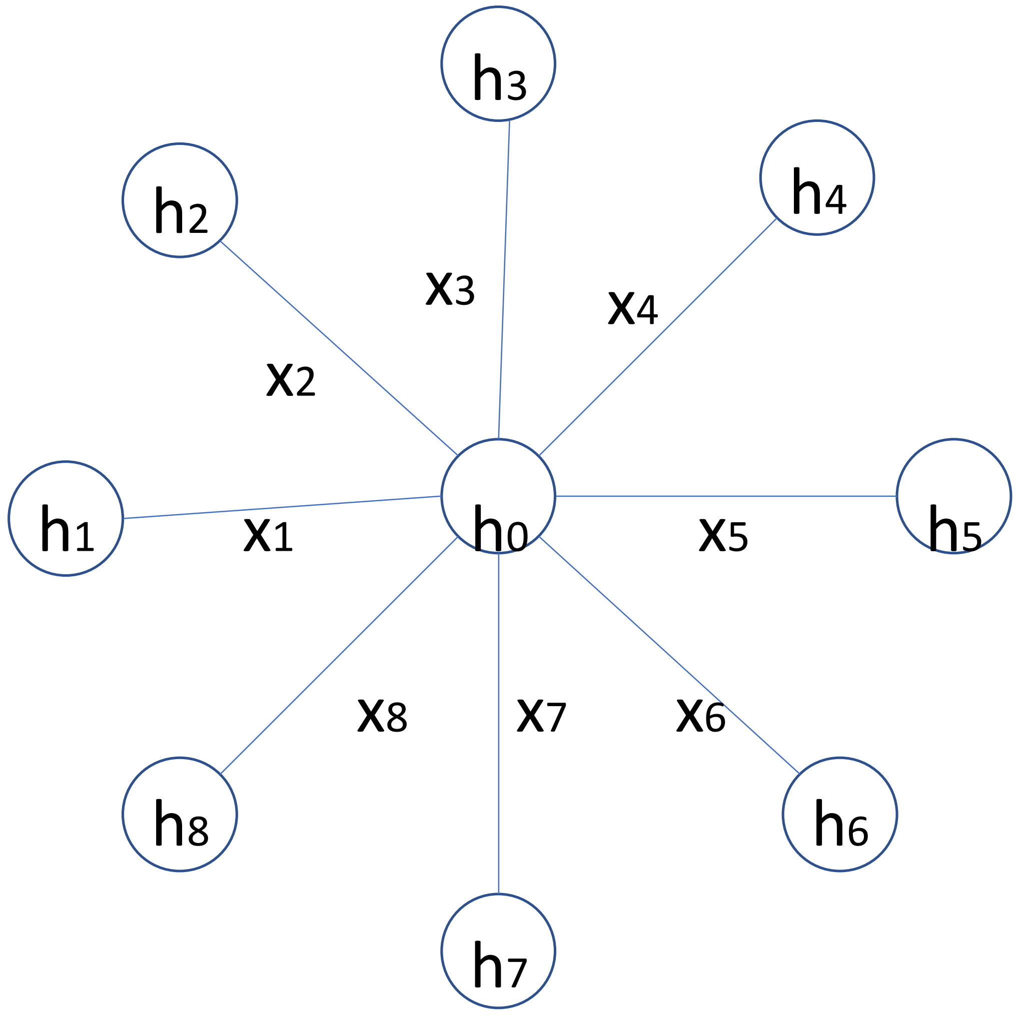
Example: Intervals: $x \mapsto \mathbb{I}[a \leq x \leq b]$

$\mathfrak{s} = \infty$.





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

Distribution-Free Analysis

(Hanneke & Yang, 2015; Hanneke, 2016)

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

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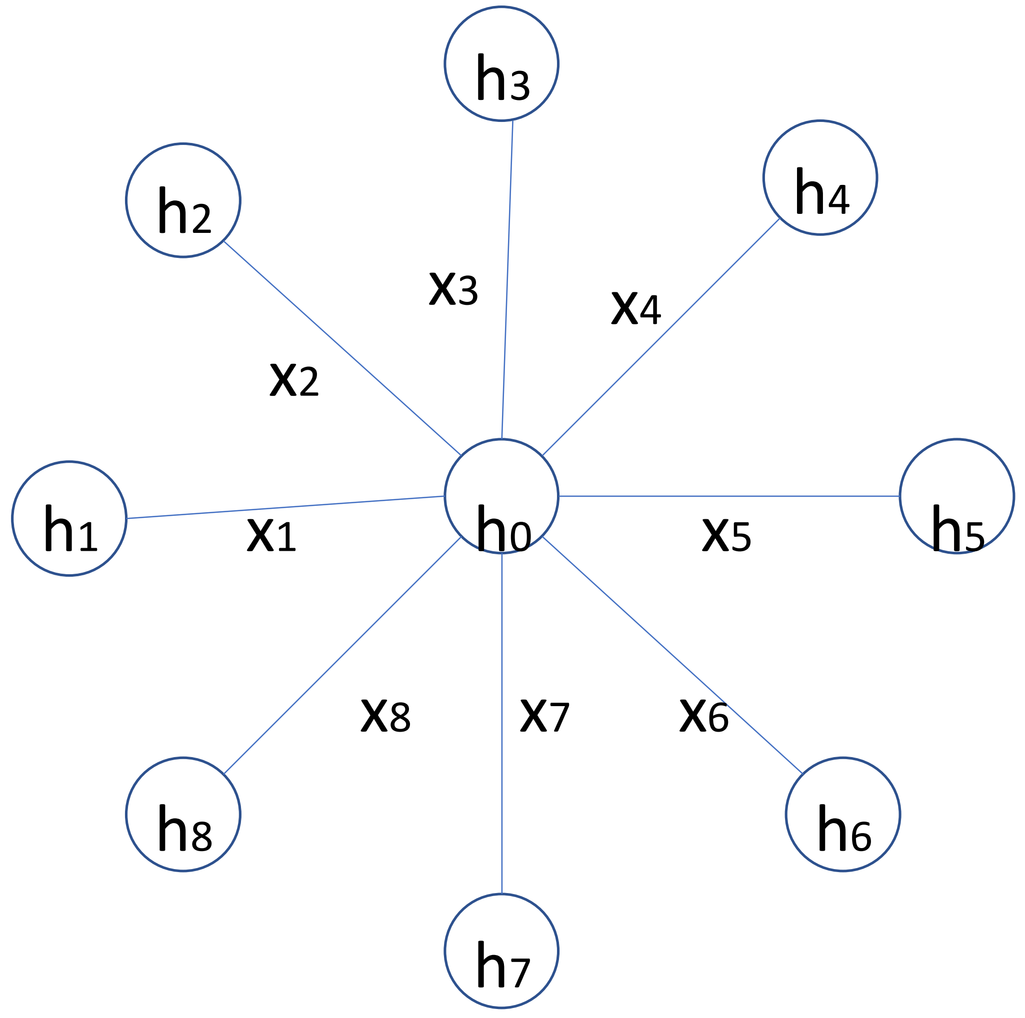

Theorem: $\sup_{P_X} \sup_{f^* \in \mathcal{H}} \theta = \sup_{P_X} \sup_{f^* \in \mathcal{H}} \varphi_c = \sup_{P_X} \sup_{f^* \in \mathcal{H}} \tilde{\theta} = \min\{\mathfrak{s}, \frac{1}{\epsilon}\} =: \mathfrak{s}_\epsilon$

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

Distribution-Free Analysis

(Hanneke & Yang, 2015; Hanneke, 2016)

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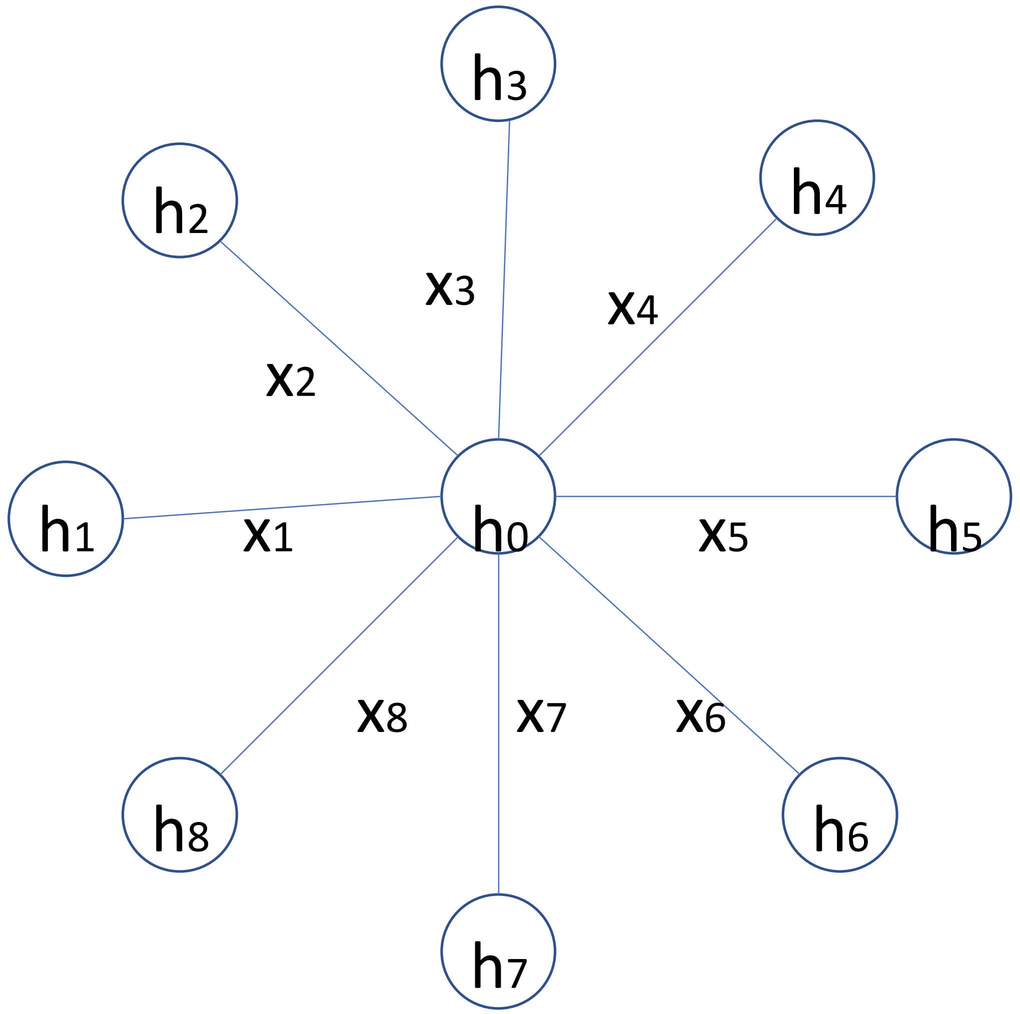
Different alg., Bounded noise
labels $\approx \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$

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



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Near-matching **lower bound**:

$\mathfrak{s}_\epsilon + d \log(\frac{1}{\epsilon})$

Open Question:

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

labels

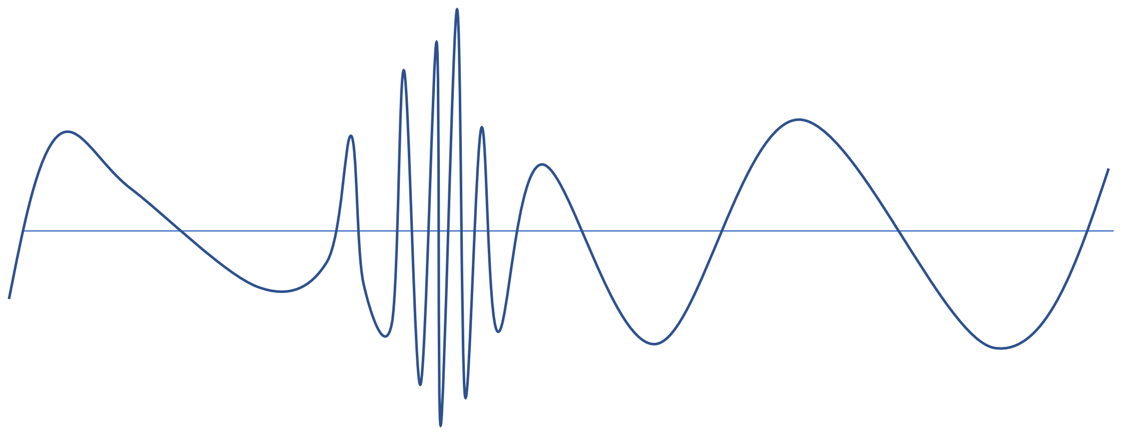
$\approx d \frac{\beta^2}{\epsilon^2} + \mathfrak{s}_{\epsilon/d} \log(\frac{1}{\epsilon})$ **?**

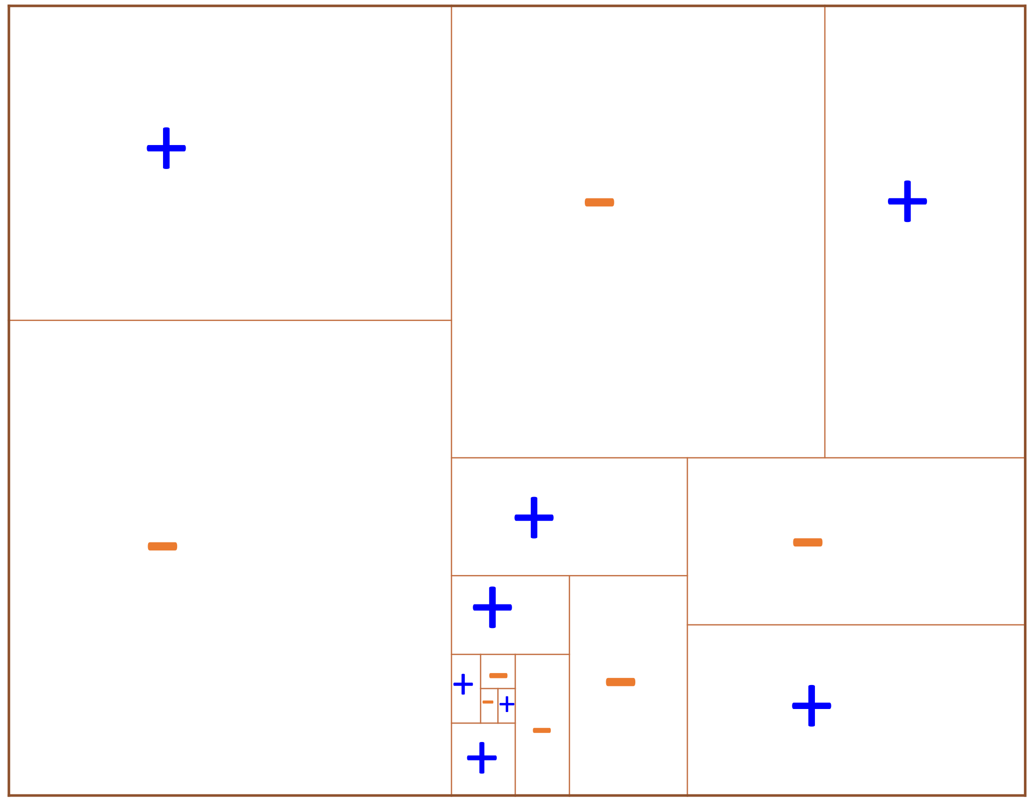
lower bound:

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

Adapting to Heterogeneous Noise

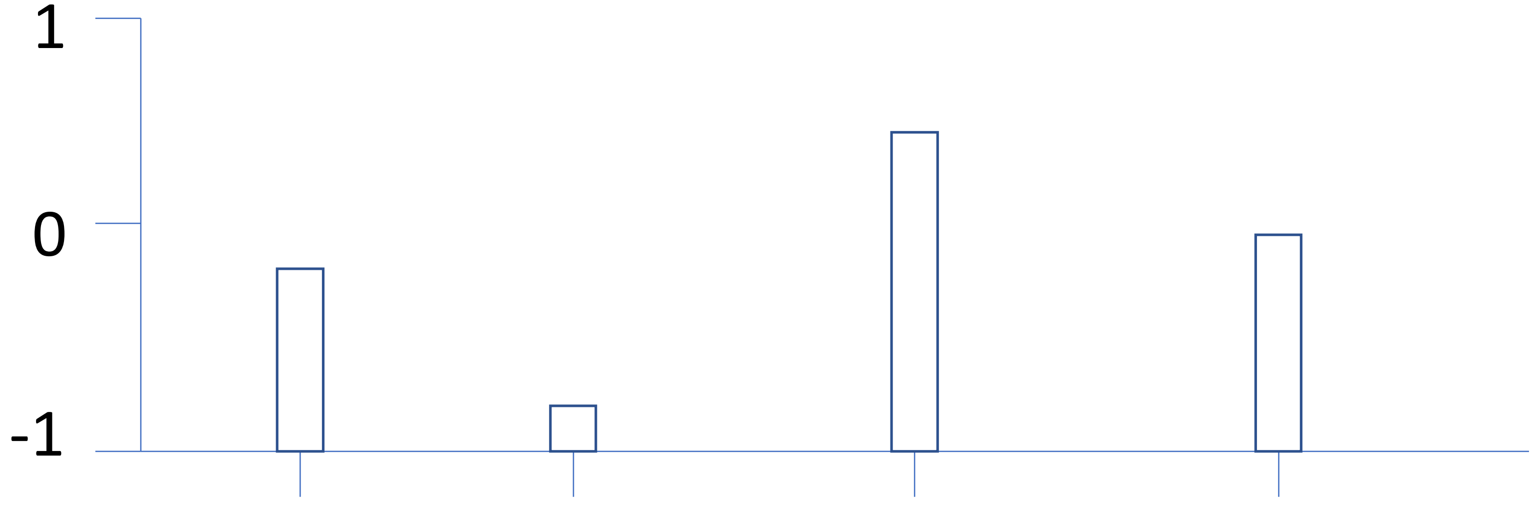
So far: Active learning for spatial heterogeneity of **opt function**:





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

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



Active Learning with TicToc

(Hanneke & Yang, 2015)

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

$\mathbb{L} \leftarrow \{\}$
For $m = 1, 2, \ldots$
  $X_{s_m} \leftarrow \textsc{GetSeed}(\mathbb{L}, m)$
  $\mathcal{L}_m \leftarrow \textsc{TicToc}(X_{s_m}, m)$
  if $\mathcal{L}_m$ exists, $\mathbb{L} \leftarrow \mathbb{L} \cup \{(s_m, \mathcal{L}_m)\}$
  If we've made n queries
    Return $\hat{f}_n \leftarrow \textsc{Learn}(\mathbb{L})$

An active learning alg. (e.g. A^2)

Main new part

A passive learning alg.

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7. Return $\hat{f}_n \leftarrow \textsc{Learn}(\mathbb{L})$

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

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

$\textsc{TicToc}(\boldsymbol{X}, \boldsymbol{m})$:
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 $f^\star(X_i)$!

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

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

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1. $\mathbb{L} \leftarrow \{\}$ 2. For $m = 1, 2, \ldots$ 3. $X_{s_m} \leftarrow \textsc{GetSeed}(\mathbb{L}, m)$ 4. $\mathcal{L}_m \leftarrow \textsc{TicToc}(X_{s_m}, m)$ 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 $\hat{f}_n \leftarrow \textsc{Learn}(\mathbb{L})$

Theorem: Agnostic ($\beta = R(f^*)$)
and suppose $f^* =$ global best:
labels

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

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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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

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**

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

Questions?

Further reading:

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