# Learning Theory

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# Learning Theory

- We have explored **many** ways of learning from data
- But…
  – How good is our classifier, really?
  – How much data do I need to make it “good enough”?

# A simple setting

- Classification
  - m i.i.d. data points
  - **Finite** number of possible hypothesis (e.g., dec. trees of depth d)
- A learner finds a hypothesis *h*
- We are interested in:

$$\mathrm{error}_{\mathrm{train}} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(h(X_i) \neq Y_i)$$

$$\mathrm{error}_{\mathrm{true}} = \mathbb{P}(h(X) \neq Y)$$

# A simple setting

- Classification
  - m i.i.d. data points
  - **Finite** number of possible hypothesis (e.g., dec. trees of depth d)
- A learner finds a hypothesis *h* that is **consistent** with training data
  - Gets zero error in training, $\text{error}_{\text{train}}(h) = 0$
- What is the probability that *h* has more than $\varepsilon$ true error?
  - $\text{error}_{\text{true}}(h) \geq \varepsilon$



**Even if *h* makes zero errors in training data, may make errors in test**

# How likely is a bad hypothesis to get m data points right?

- Consider a bad hypothesis *h* i.e. $\text{error}_{\text{true}}(h) \geq \varepsilon$

- Probability that *h* gets one data point right

  $\leq 1 - \varepsilon$

- Probability that *h* gets *m* data points right

  $\leq (1 - \varepsilon)^m$

# How likely is a learner to pick a bad hypothesis?

- Usually there are many (say k) bad hypothesis in the class

  $h_1, h_2, \ldots, h_k$ s.t. $\text{error}(h_i) \geq \varepsilon$ $i = 1, \ldots, k$

- Probability that learner picks a bad hypothesis = Probability that some bad hypothesis is consistent with m data points

  Prob($h_1$ consistent with m data points OR
  $h_2$ consistent with m data points OR … OR
  $h_k$ consistent with m data points)

  $\leq$ Prob($h_1$ consistent with m data points) +
  Prob($h_2$ consistent with m data points) + … +
  Prob($h_k$ consistent with m data points)

  $\leq k(1-\varepsilon)^m$

Union bound

Loose but works

# How likely is a learner to pick a bad hypothesis?

- Usually there are many many (say k) bad hypothesis in the class

  $h_1, h_2, \ldots, h_k$ s.t. $\mathrm{error}(h_i) \geq \varepsilon$ $i = 1, \ldots, k$

- Probability that learner picks a bad hypothesis

  $\leq k\,(1-\varepsilon)^m \leq |H|\,(1-\varepsilon)^m \leq |H|\,e^{-\varepsilon m}$

  $|H| \rightarrow$ Size of hypothesis class

# PAC (Probably Approximately Correct) bound

- ***Theorem [Haussler'88]***: Hypothesis space *H* finite, dataset *D* with *m* i.i.d. samples, $0 < \varepsilon < 1$ : for any learned hypothesis *h* that is consistent on the training data:

$$P(\text{error}_{true}(h) \geq \epsilon) \leq |H|e^{-m\epsilon} \leq \delta$$

- Equivalently, with probability $\geq 1 - \delta$

$$\text{error}_{true}(h) \leq \epsilon$$

**Important: PAC bound holds for all *h*, but doesn't guarantee that algorithm finds best *h*!!!**

# Using a PAC bound

$$|H|e^{-m\epsilon} \le \delta$$

- Given ε and δ, yields sample complexity

  #training data, $m \ge \dfrac{\ln|H| + \ln\frac{1}{\delta}}{\epsilon}$

- Given m and δ, yields error bound

  error, $\epsilon \ge \dfrac{\ln|H| + \ln\frac{1}{\delta}}{m}$

# Limitations of Haussler's bound

- Consistent classifier

  h such that zero error in training, $\text{error}_{\text{train}}(h) = 0$

- Dependence on size of hypothesis space

$$m \geq \frac{\ln|H| + \ln\frac{1}{\delta}}{\epsilon}$$

  what if |H| too big or H is continuous (e.g. linear classifiers)?

# PAC bounds for finite hypothesis spaces

H - Finite hypothesis/classifier space

e.g. decision trees of depth k

histogram classifiers with binwidth h

With probability $\geq 1-\delta$,

1) For all $h \in H$ s.t. $\text{error}_{\text{train}}(h) = 0$,

$$\text{error}_{\text{true}}(h) \leq \varepsilon = \frac{\ln|H| + \ln\frac{1}{\delta}}{m}$$

Haussler's bound

# What if our classifier does not have zero error on the training data?

- A learner with zero training errors may make mistakes in test set
- What about a learner with $error_{train}(h) \neq 0$ in training set?
- The error of a hypothesis is like estimating the parameter of a coin!

$$error_{true}(h) := P(h(X) \neq Y) \equiv P(H=1) =: \theta$$

$$error_{train}(h) := \frac{1}{m}\sum_i \mathbf{1}_{h(X_i)\neq Y_i} \equiv \frac{1}{m}\sum_i Z_i =: \widehat{\theta}$$

# Hoeffding's bound for a single hypothesis

- Consider $m$ i.i.d. flips $x_1,\ldots,x_m$, where $x_i \in \{0,1\}$ of a coin with parameter $\theta$. For $0<\varepsilon<1$:

$$P\left(\left|\theta - \frac{1}{m}\sum_i x_i\right| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

- For a single hypothesis h

$$P\left(\left|\text{error}_{true}(h) - \text{error}_{train}(h)\right| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

# Hoeffding's bound for |H| hypotheses

- For each hypothesis $h_i$:

$$P\left(|\text{error}_{true}(h_i) - \text{error}_{train}(h_i)| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

- What if we are comparing |H| hypotheses?

  Union bound

- ***Theorem***: Hypothesis space *H* finite, dataset *D* with *m* i.i.d. samples, $0 < \varepsilon < 1$ : for any learned hypothesis $h \in H$:

$$P\left(|\text{error}_{true}(h) - \text{error}_{train}(h)| \geq \epsilon\right) \leq 2|H|e^{-2m\epsilon^2} \leq \delta$$

**Important: PAC bound holds for all *h*, but doesn't guarantee that algorithm finds best *h*!!!**

# Summary of PAC bounds for finite hypothesis spaces

With probability $\geq 1-\delta$,

1) For all $h \in H$ s.t. $\text{error}_{train}(h) = 0$,

$$\text{error}_{true}(h) \leq \varepsilon = \frac{\ln|H| + \ln\frac{1}{\delta}}{m}$$

$\boxed{\text{Haussler's bound}}$

2) For all $h \in H$

$$|\text{error}_{true}(h) - \text{error}_{train}(h)| \leq \varepsilon = \sqrt{\frac{\ln|H| + \ln\frac{1}{\delta}}{2m}}$$

$\boxed{\text{Hoeffding's bound}}$

# PAC bound and Bias-Variance tradeoff

$$P\left(|\text{error}_{true}(h) - \text{error}_{train}(h)| \geq \epsilon\right) \leq 2|H|e^{-2m\epsilon^2} \leq \delta$$

- Equivalently, with probability $\geq 1 - \delta$

$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$$

- Fixed m

| hypothesis space | $\text{error}_{train}(h)$ | $\sqrt{\frac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$ |
|---|---|---|
| complex | small | large |
| simple | large | small |

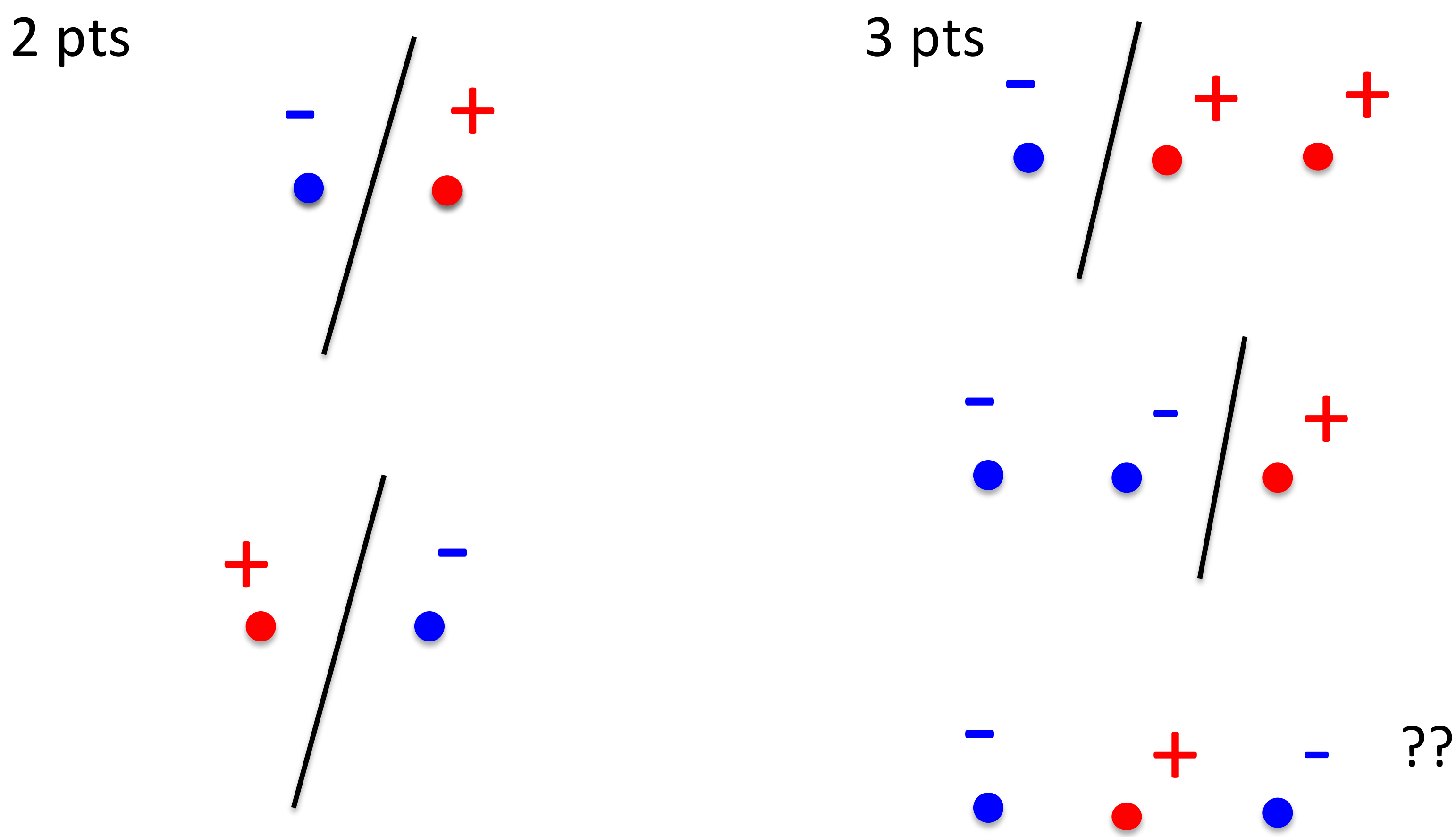
# What about continuous hypothesis spaces?

$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$$

- Continuous hypothesis space:
  - |H| = ∞
  - Infinite variance???

- **As with decision trees, complexity of hypothesis space only depends on maximum number of points that can be classified exactly (and not necessarily its size)!**

# How many points can a linear boundary classify exactly? (1-D)

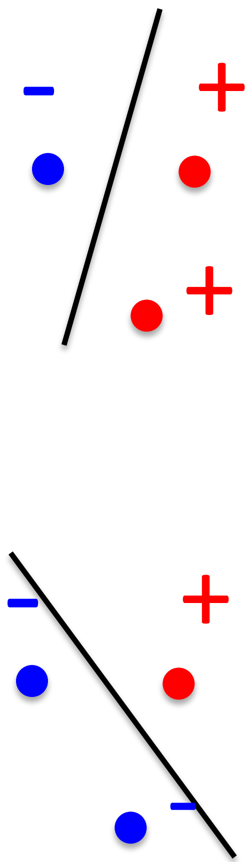




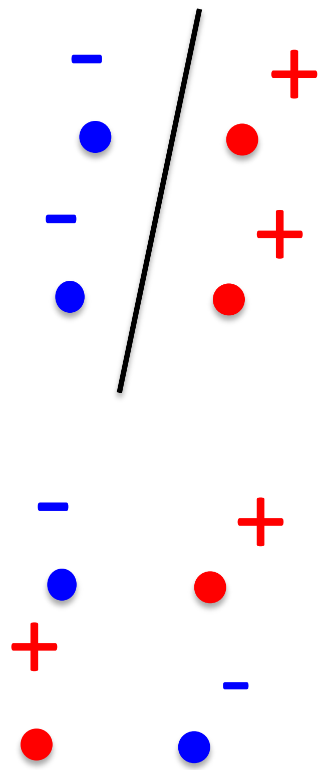

There exists placement s.t. all labelings can be classified

# How many points can a linear boundary classify exactly? (2-D)

3 pts




4 pts

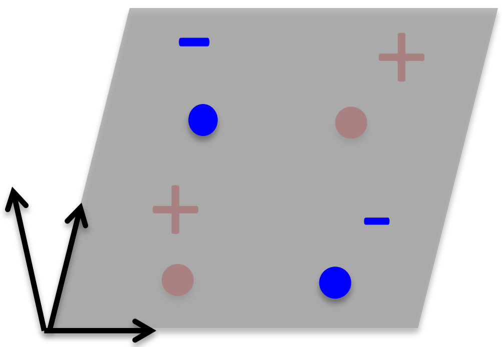



??



There exists placement s.t. all labelings can be classified

# How many points can a linear boundary classify exactly? (d-D)




d+1 pts

How many parameters in linear Classifier in d-Dimensions?

$$w_0 + \sum_{i=1}^{d} w_i x_i$$

d+1



There exists placement s.t. all labelings can be classified

# PAC bound using VC dimension

- Number of training points that can be classified exactly is VC dimension!!!
  - Measures relevant size of hypothesis space, as with decision trees with k leaves

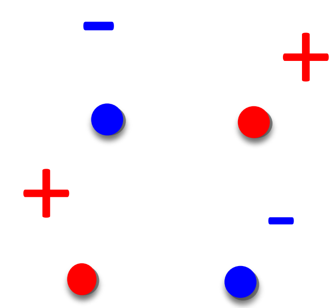
$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + 8\sqrt{\frac{VC(H)\left(\ln\frac{m}{VC(H)}+1\right)+\ln\frac{8}{\delta}}{2m}}$$

Instead of ln|H|

# VC dimension

Definition: VC dimension of a hypothesis space H is the maximum number of points such that there exists a hypothesis in H that is consistent with (can correctly classify) any labeling of the points.

- You pick set of points
- Adversary assigns labels
- You find a hypothesis in H consistent with the labels




If VC(H) = k, then for all k+1 points, there exists a labeling that cannot be shattered (can't find a hypothesis in H consistent with it)

# PAC bound using VC dimension

- Number of training points that can be classified exactly is VC dimension!!!
  - Measures relevant size of hypothesis space, as with decision trees with k leaves
  - Bound for infinite dimension hypothesis spaces:

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

$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + 8\sqrt{\frac{VC(H)\left(\ln \frac{m}{VC(H)} + 1\right) + \ln \frac{8}{\delta}}{2m}}$$

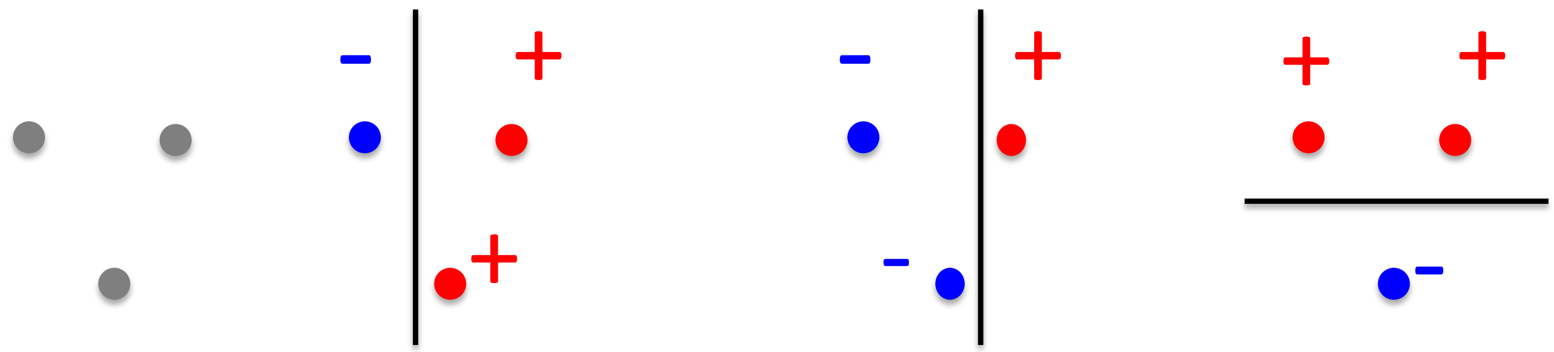
| linear classifiers | | |
|---|---|---|
| 2D | large | small |
| 10,000 D | small | large |

# Examples of VC dimension

- Linear classifiers:
  - VC(H) = d+1, for *d* features plus constant term

# Another VC dim. example - What can we shatter?

- What's the VC dim. of decision stumps in 2d?



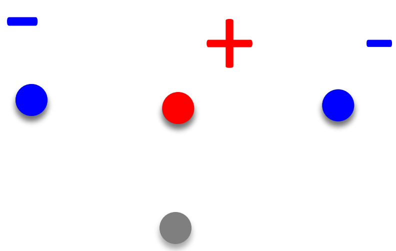

VC(H) ≥ 3

# Another VC dim. example - What can't we shatter?

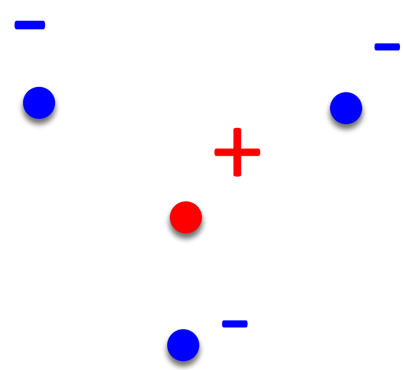
- What's the VC dim. of decision stumps in 2d?

If VC(H) = 3, then for all placements of 4 pts, there exists a labeling that can't be shattered

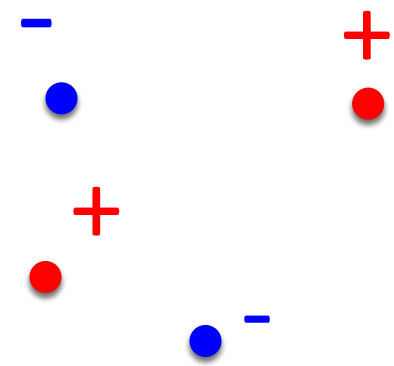
3 collinear



1 in convex hull of other 3



quadrilateral



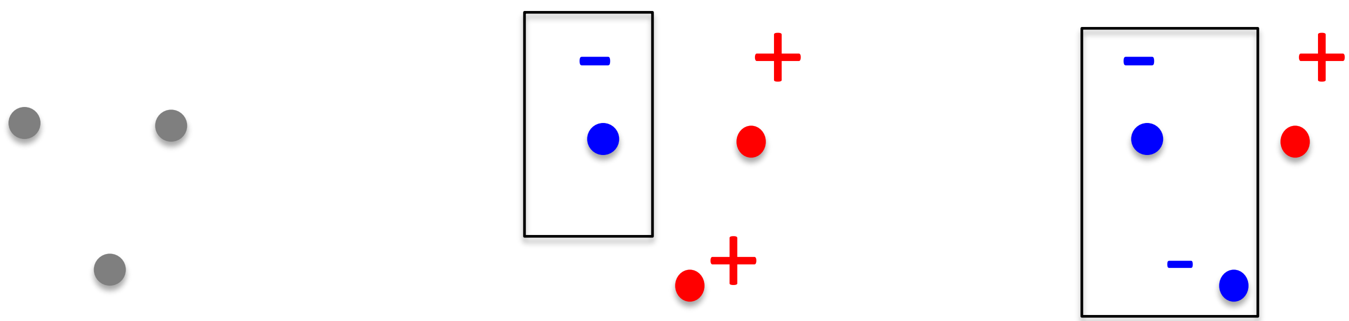
# Examples of VC dimension

- Linear classifiers:
  - VC(H) = d+1, for *d* features plus constant term

- Decision stumps: VC(H) = d+1 (3 if d=2)

# Another VC dim. example - What can we shatter?

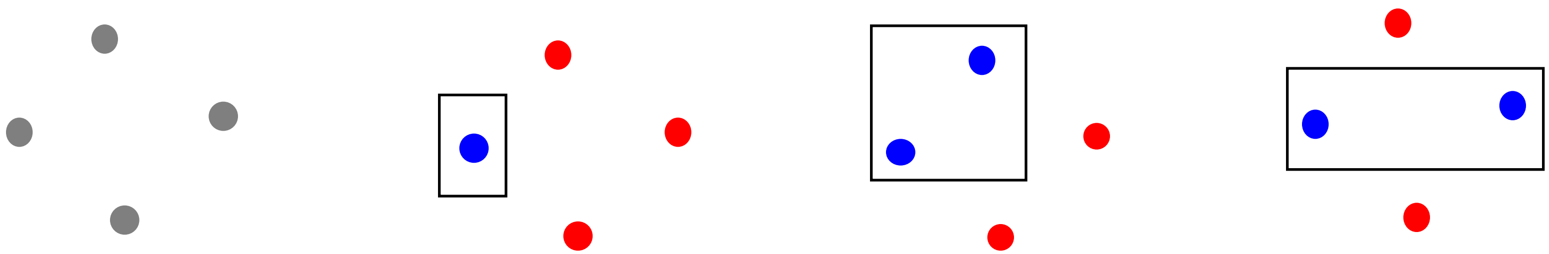
- What's the VC dim. of axis parallel rectangles in 2d? sign(1- 2*$\mathbf{1}_{x \in \text{rectangle}}$)

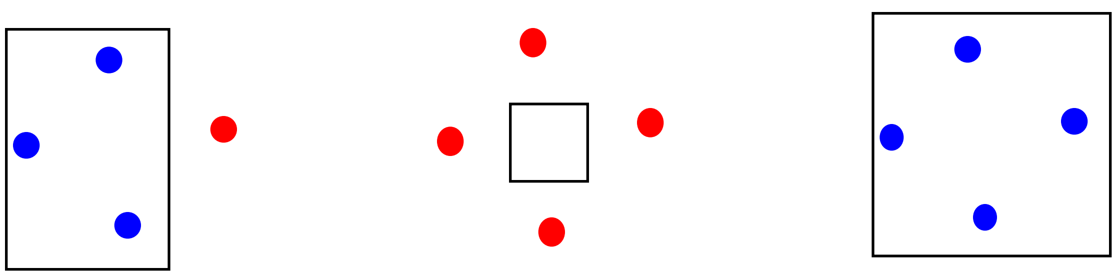



VC(H) ≥ 3

# Another VC dim. example - What can't we shatter?

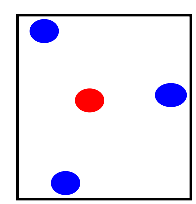
- What's the VC dim. of axis parallel rectangles in 2d? $\text{sign}(1 - 2*\mathbf{1}_{x \in \text{rectangle}})$





$VC(H) \geq 4$

- Some placement of 4 pts can't be shattered

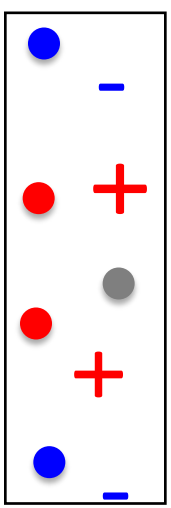


# Another VC dim. example - What can't we shatter?

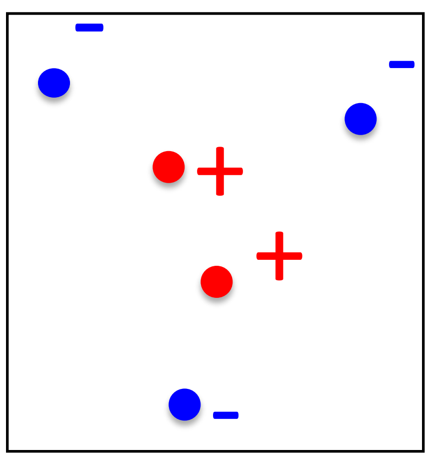
- What's the VC dim. of axis parallel rectangles in 2d? $\quad \text{sign}(1- 2*\mathbf{1}_{x \in \text{rectangle}})$

  If VC(H) = 4, then for all placements of 5 pts, there exists a labeling that can't be shattered

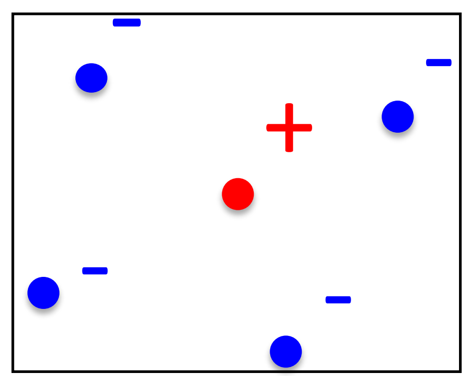
4 collinear



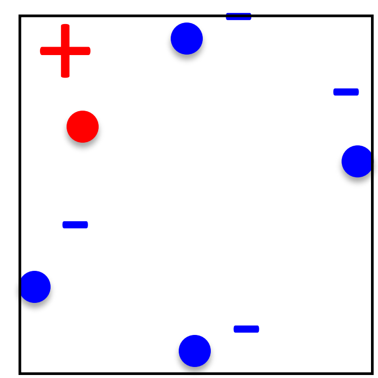
2 in convex hull of other 3



1 in convex hull of other 4



pentagon



# Examples of VC dimension

- Linear classifiers:
  - VC(H) = d+1, for *d* features plus constant term

- Decision stumps: VC(H) = d+1

- Axis parallel rectangles: VC(H) = 2d (4 if d=2)

- 1 Nearest Neighbor: VC(H) = $\infty$

# VC dimension and size of hypothesis space

- To be able to shatter m points, how many hypothesis do we need?

$$2^m \text{ labelings} \quad \Rightarrow \quad |H| \geq 2^m$$

Given $|H|$ hypothesis can hope to shatter max $m = \log_2|H|$ points

$$VC(H) \leq \log_2|H|$$

So VC bound is tighter.

# Summary of PAC bounds

With probability $\geq 1-\delta$,

1) for all $h \in H$ s.t. $\text{error}_{train}(h) = 0$,

$$\text{error}_{true}(h) \leq \varepsilon = \frac{\ln |H| + \ln \frac{1}{\delta}}{m}$$

2) for all $h \in H$,

$$|\text{error}_{true}(h) - \text{error}_{train}(h)| \leq \varepsilon = \sqrt{\frac{\ln |H| + \ln \frac{1}{\delta}}{2m}}$$

Finite hypothesis space

3) for all $h \in H$,

$$|\text{error}_{true}(h) - \text{error}_{train}(h)| \leq \varepsilon = 8\sqrt{\frac{VC(H)\left(\ln \frac{m}{VC(H)} + 1\right) + \ln \frac{8}{\delta}}{2m}}$$

Infinite hypothesis space

# Limitation of VC dimension

- Hard to compute for many hypothesis spaces

  VC(H) ≥ lower bound (easy)

  VC(H) = … (HARD!)

  For all placements of VC(H)+1 points, there exists a labeling that can't be shattered

- Too loose for many hypothesis spaces

  linear SVMs, VC dim = d+1 (d features)

  kernel SVMs, VC dim = ??

  = $\infty$ (Gaussian kernels)

Suggests Gaussian kernels are really BAD!!

# Summary of PAC bounds

With probability ≥ 1-δ,

1) for all h ∈ H s.t. $error_{train}(h) = 0$,

$$error_{true}(h) \le \varepsilon = \frac{\ln |H| + \ln \frac{1}{\delta}}{m}$$

2) for all h ∈ H,

$$|error_{true}(h) - error_{train}(h)| \le \varepsilon = \sqrt{\frac{\ln |H| + \ln \frac{1}{\delta}}{2m}}$$

Finite hypothesis space

3) for all h ∈ H,

$$|error_{true}(h) - error_{train}(h)| \le \varepsilon = 8\sqrt{\frac{VC(H)\left(\ln \frac{m}{VC(H)} + 1\right) + \ln \frac{8}{\delta}}{2m}}$$

4) For all h ∈ H,

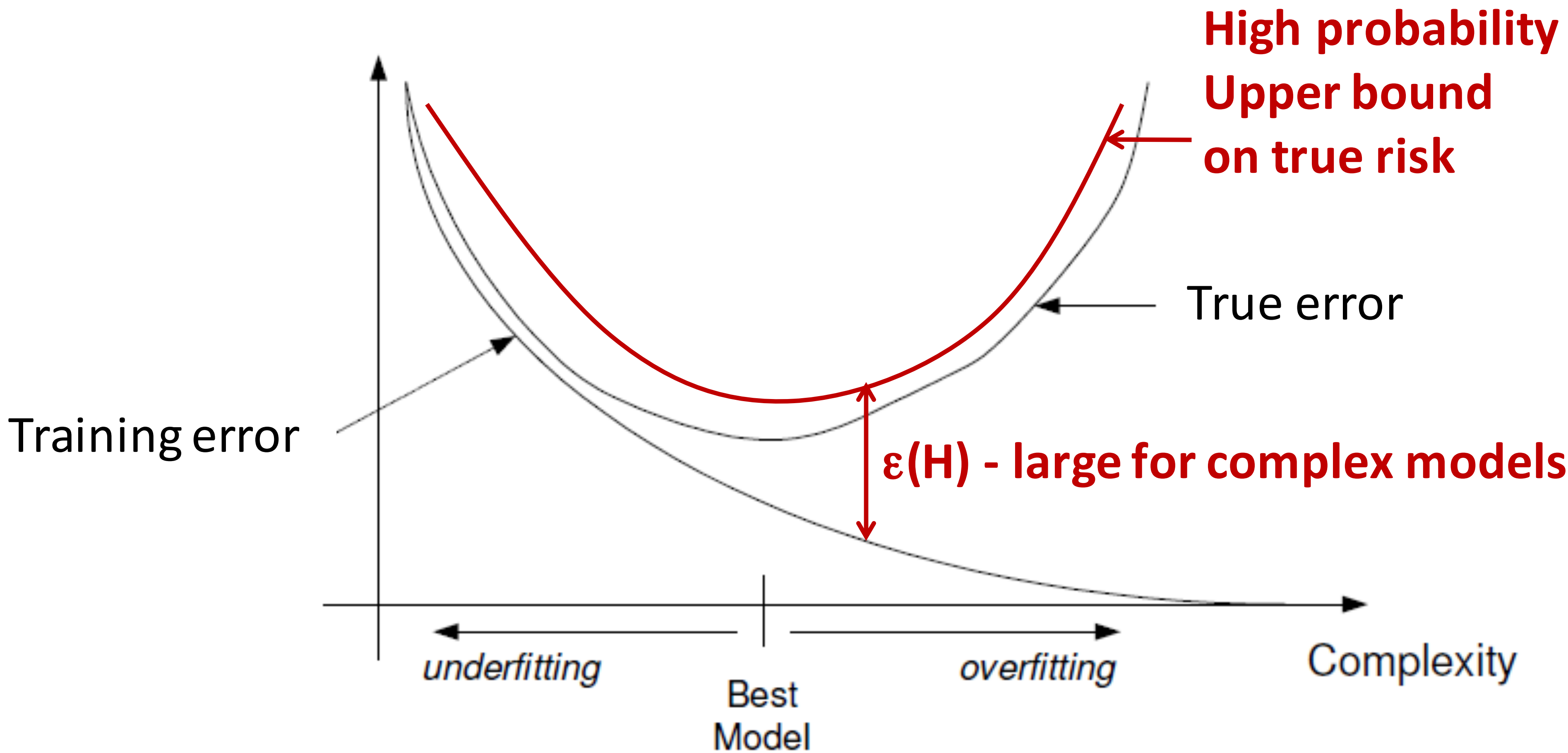
$$|error_{true}(h) - error_{train}(h)| \le \varepsilon = \widehat{R}_m(H) + 3\sqrt{\frac{\log(2/\delta)}{m}}$$

Infinite hypothesis space

# PAC Bounds

With probability $\geq 1-\delta$, for all $h \in H$,

$$|error_{true}(h) - error_{train}(h)| \leq \varepsilon(H)$$



# PAC Learnability

- Target concept class C – true function space
- Hypothesis class H – model space

C is ***PAC Learnable*** by a learner using H if

there exists a learning algorithm s.t. for all concepts in C, for all distributions over inputs, for all $0 < \varepsilon, \delta < 1$,

with probability $> 1-\delta$, the algorithm outputs a hypothesis $h \in H$ s.t.

$error_{true}(h) \leq \varepsilon$

in time that is polynomial in $1/\varepsilon$, $1/\delta$ and n.

# What you need to know

- PAC bounds on true error in terms of empirical/training error and complexity of hypothesis space
- Complexity of the classifier depends on number of points that can be classified exactly
  - Finite case – Number of hypothesis
  - Infinite case – VC dimension, Rademacher complexity
- Other bounds – Margin based, Mistake bounds, …