Learning Theory

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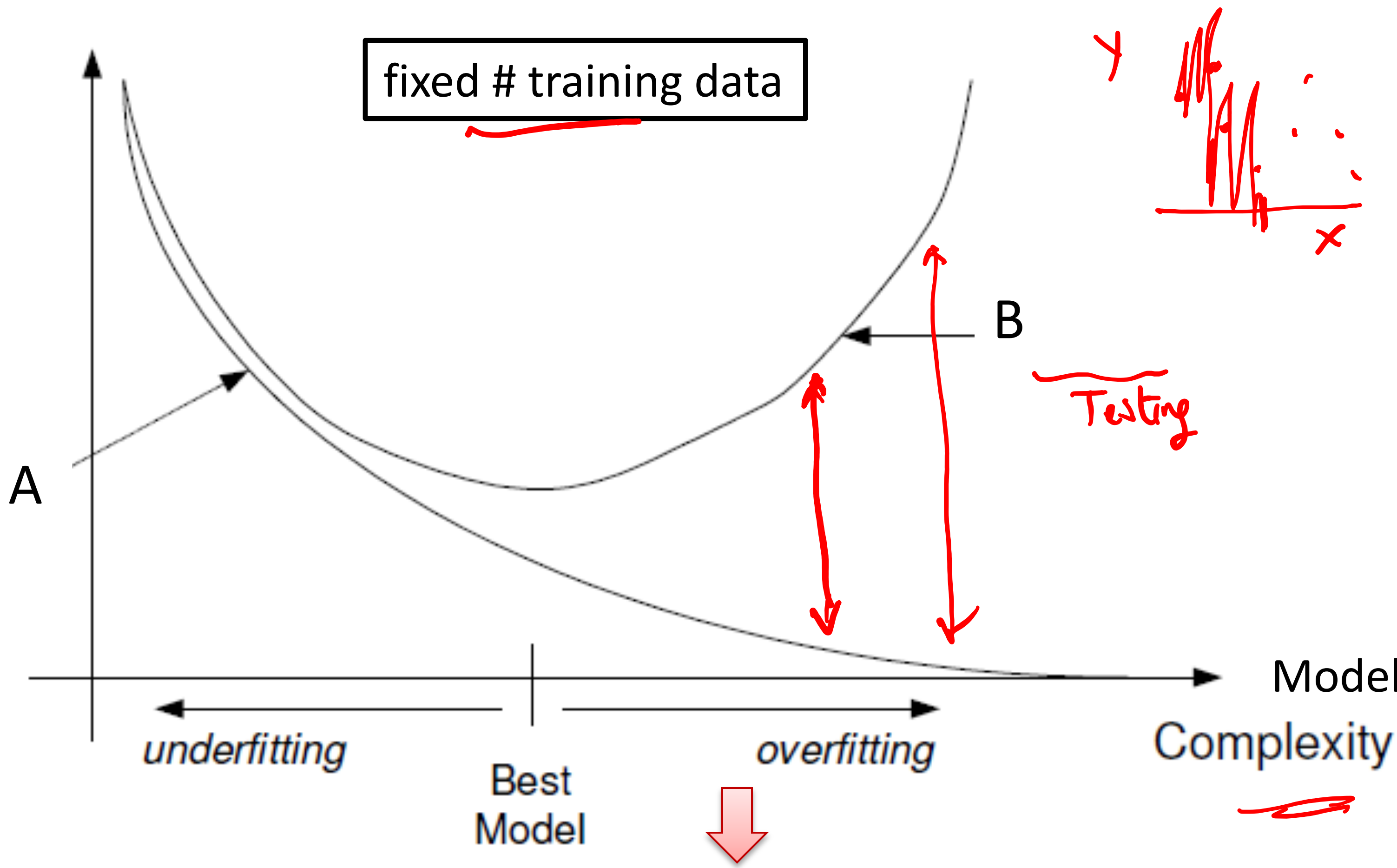
Training vs. Test Error

$\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$



Poll

Training error is no longer a good indicator of test error

Bias-Variance Tradeoff

- Why does test/validation error go down then up with increasing model complexity?

Two sources of error:

e.g. Regression

function learnt on n data

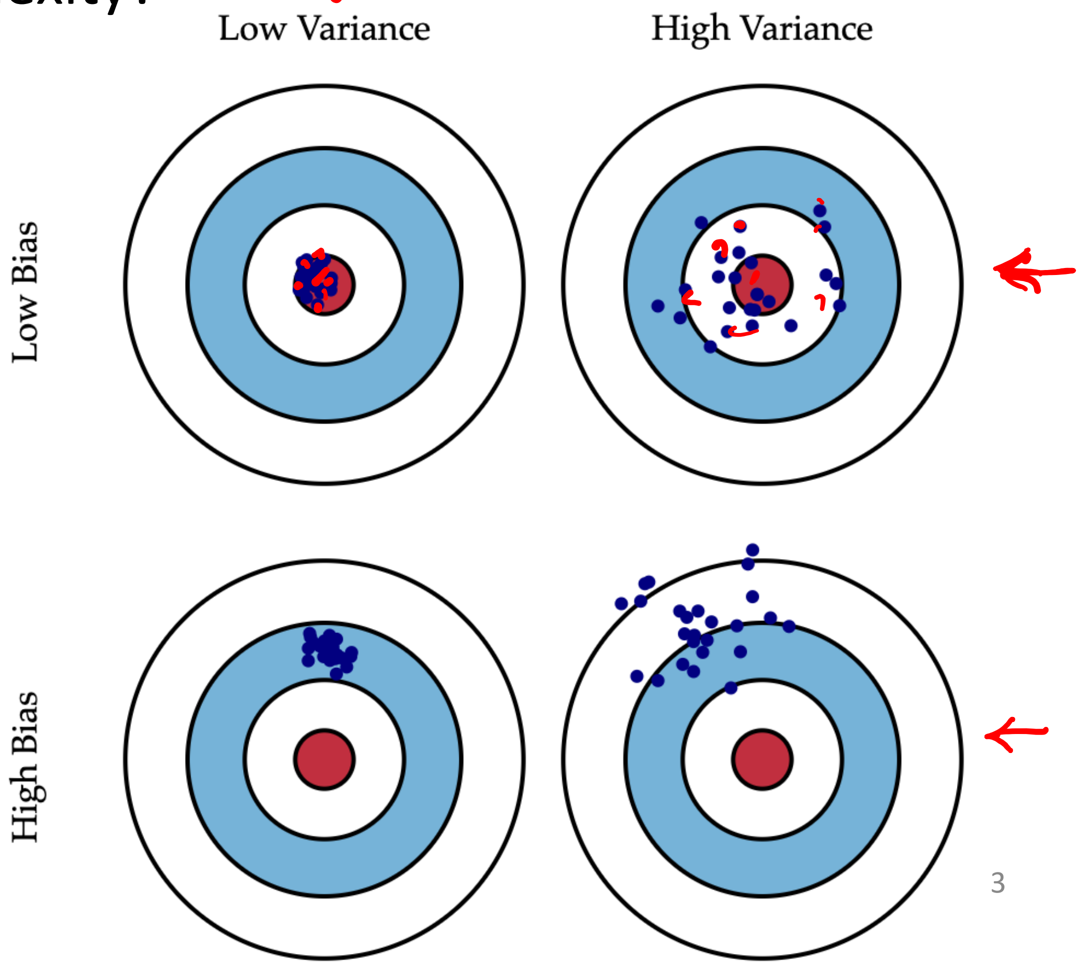
Bias

true function

$|E[f_n] - f^*|$

Variance

$E[|f_n - E[f_n]|^2]$

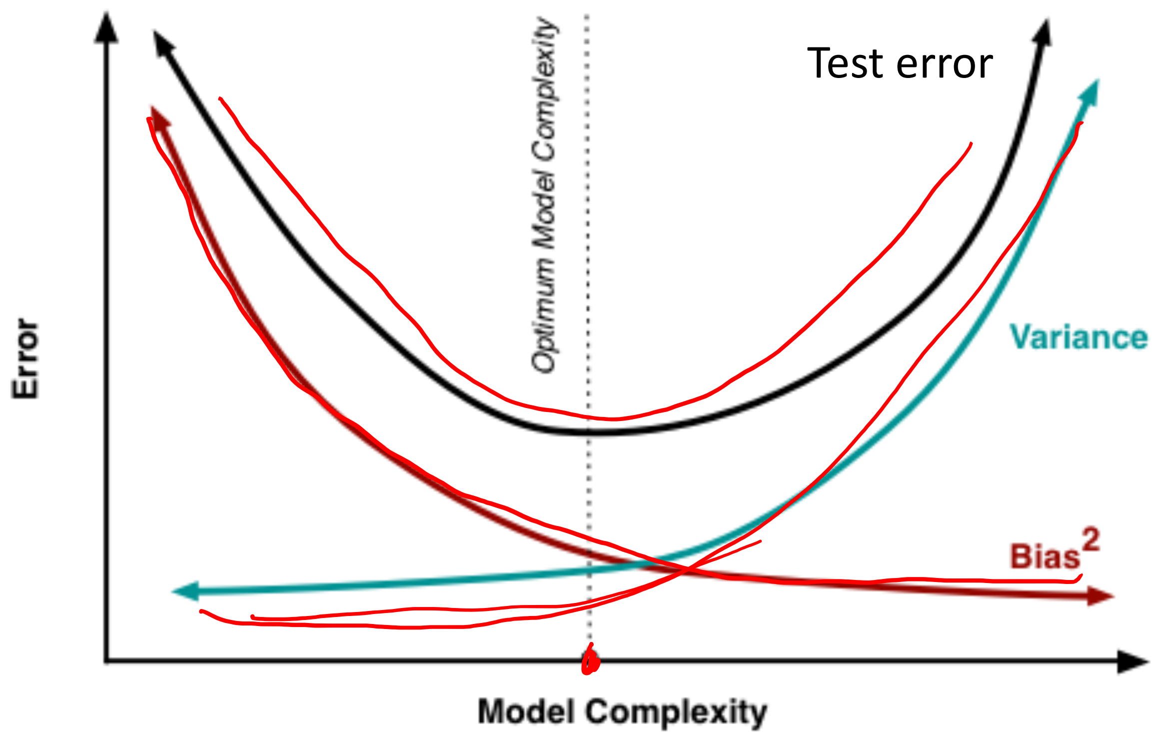


Bias-Variance Tradeoff

- Why does test/validation error go up with increasing model complexity?

err(f^*)

Mean square test error = Variance + Bias^2 + Irreducible error



Learning Theory

- We have explored **many** ways of learning from data
- But…
  - Can we certify how good is our classifier, really?
  - How much data do I need to make it "good enough"?

PAC Learnability

Probably Approximately Correct
δ ε

- True function space, F -
- Model space, H

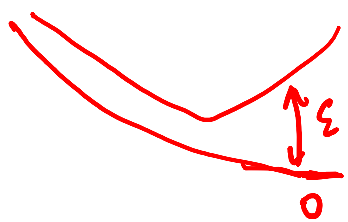
F is **PAC Learnable** by a learner using H if

there exists a learning algorithm s.t. for all functions in F, for all distributions over inputs, for all $0 < \varepsilon, \delta < 1$, with probability $> 1-\delta$, the algorithm outputs a model $h \in H$ s.t. $\text{error}_{\text{true}}(h) \leq \varepsilon$

in time and samples that are polynomial in $1/\varepsilon$, $1/\delta$.

A simple setting

- Classification
  - m i.i.d. data points
  - **Finite** number of possible classifiers in model class (e.g., dec. trees of depth d)
- Lets consider that a learner finds a classifier *h* that gets zero error in training
  - $\text{error}_{\text{train}}(h) = 0$
- What is the probability that *h* has more than ε true (= test) 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 classifier to get m data points right?

$P(h(X) \neq Y)$

- Consider a bad classifier *h* i.e. $\underline{error_{true}(h) \geq \varepsilon}$

- Probability that *h* gets one data point right

  $\leq 1 - \varepsilon$

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

  $\underline{\leq (1 - \varepsilon)^m}$

How likely is a learner to pick a bad classifier?

- Usually there are many (say k) bad classifiers in model class

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

- Probability that learner picks a bad classifier = Probability that some bad classifier gets 0 training error

  Prob(h_1 gets 0 training error OR

  h_2 gets 0 training error OR … OR

  h_k gets 0 training error)

  $P(A \text{ or } B) \leq P(A)+P(B)$

  $\leq$ Prob(h_1 gets 0 training error) +

  Prob(h_2 gets 0 training error) + … +

  Prob(h_k gets 0 training error)

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

Union bound

Loose but works

How likely is a learner to pick a bad classifier?

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

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

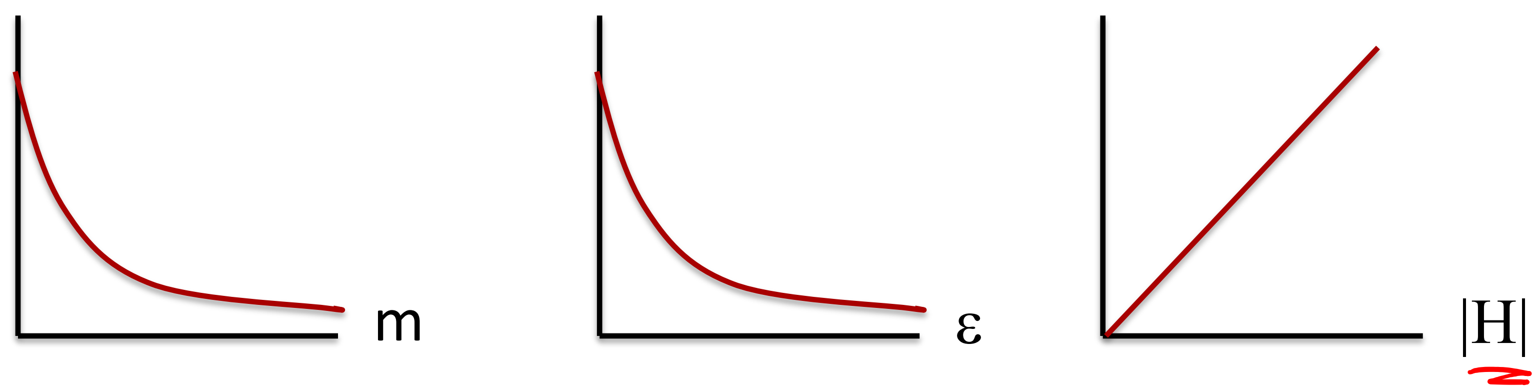
- Probability that learner picks a bad classifier

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

Size of model class

$e^{-x} = 1 - x + \frac{x^2}{2} \cdots$

$e^{-x} \geq 1 - x$



PAC (Probably Approximately Correct) bound

(ε, δ)

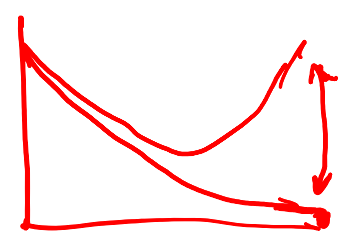
- ***Theorem [Haussler'88]***: Model class *H* finite, dataset *D* with *m* i.i.d. samples, $0 < \varepsilon < 1$: for any learned classifier *h* that gets 0 training error:

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

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

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

$= \text{error}_{train}(h)$



Important: PAC bound holds for all *h* with 0 training error, but doesn't guarantee that algorithm finds best *h*!!!

Using a PAC bound

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

- Given ε and δ, yields sample complexity

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

- Given m and δ, yields error bound

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

$|H| e^{-m\varepsilon} = \delta$

Poll

error train = 0

Assume m is the minimum number of training examples sufficient to guarantee that with probability 1 − δ a consistent learner using model class H will output a classifier with true error at worst ε.

Then a second learner that uses model space H' will require 2m training examples (to make the same guarantee) if |H' | = 2|H|.

A. True

B. False

If we double the number of training examples to 2m, the error bound ε will be halved.

C. True

D. False

Limitations of Haussler's bound

- Only consider classifiers with 0 training error

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

- Dependence on size of model class |H|

$$m = \frac{\ln \overset{\infty}{\underline{|H|}} + \ln \frac{1}{\delta}}{\epsilon}$$

$\to \infty$

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

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 classifier is like estimating the parameter of a coin!

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

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

Hoeffding’s bound for a single classifier

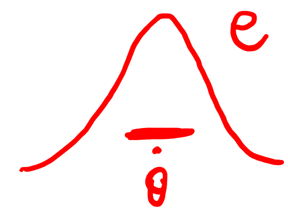
- Consider *m* i.i.d. flips $x_1,\ldots,x_m$, where $x_i \in \{0,1\}$ of a coin with parameter θ. For $0<\varepsilon<1$:

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

- Central limit theorem:

x_i mean θ, var σ^2

$$\frac{1}{m}\sum_i x_i \xrightarrow{m\to\infty} \mathcal{N}\left(\theta, \frac{\sigma^2}{m}\right)$$



$e^{-\frac{\varepsilon^2 m}{2\sigma^2}}$

$$\sqrt{m}\left(\frac{1}{m}\sum_i x_i - \theta\right) \xrightarrow[m\to\infty]{} \mathcal{N}(0,\sigma^2)$$

Hoeffding's bound for a single classifier

- Consider m i.i.d. flips $x_1,\ldots,x_m$, where $x_i \in \{0,1\}$ of a coin with parameter θ. 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 classifier 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| classifiers

- For each classifier 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| classifiers?

  Union bound

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

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

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

Summary of PAC bounds for finite model classes

With probability ≥ 1-δ,

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

2) For all $h \in H$

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

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 $\geq 1 - \delta$

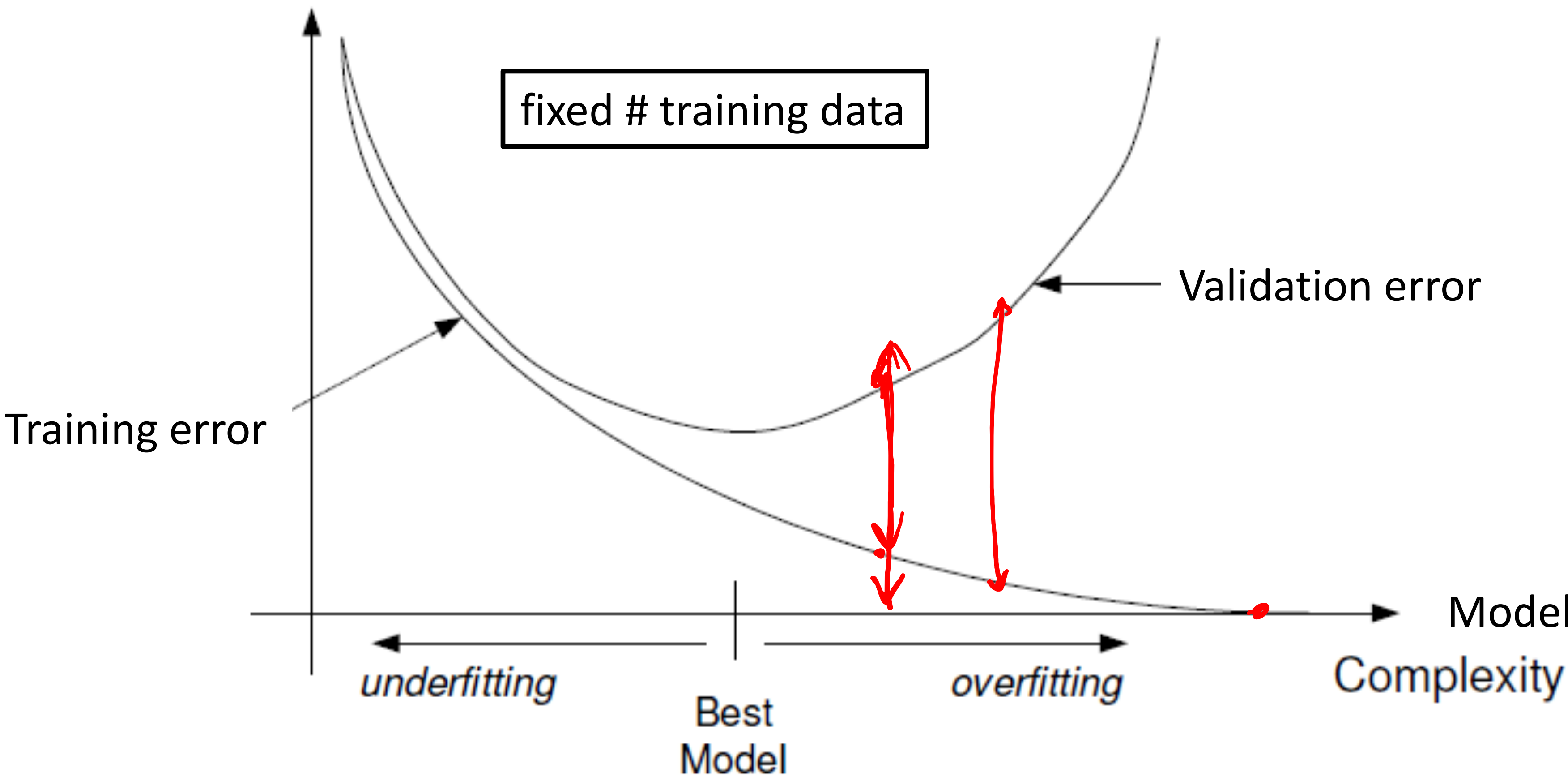
$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$$

- Fixed m

Model class		
complex	small	large
simple	large	small

Training vs. Test Error

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



What about the size of the model class?

$$2|H|e^{-2m\epsilon^2} \leq \delta$$

- Sample complexity

$$m = \frac{1}{2\epsilon^2}\left(\ln|H| + \ln\frac{2}{\delta}\right)$$

- How large is the model class?
  - Number of binary decision trees of depth k = 2^{2^k}

    m is exponential in depth k $\ln|2^{2^k}| \simeq 2^k$

    BUT given m points, decision tree can't get too big
  - Number of binary decision trees with k leaves = 2^k

    m is linear in number of leaves k $\ln 2^k \simeq k$

Number of decision trees of depth k

$$m \geq \frac{1}{2\epsilon^2}\left(\ln|H| + \ln\frac{2}{\delta}\right)$$

Recursive solution:

Given *n* **binary** attributes features

H_k = Number of **binary** decision trees of depth k

$H_0 = 2$

H_k = (#choices of root attribute)

*(# possible left subtrees)

*(# possible right subtrees) $= n * \underbrace{H_{k-1}} * H_{k-1}$

Write $L_k = \log_2 H_k$

$|H_k| \sim 2^{L_k} \sim 2^{2^k}$

$L_0 = 1$

$L_k = \log_2 n + 2L_{k-1} = \log_2 n + 2(\log_2 n + 2L_{k-2})$

$= \log_2 n + 2\log_2 n + 2^2\log_2 n + \ldots + 2^{k-1}(\log_2 n + 2L_0)$

So $L_k = (2^k-1)(1+\log_2 n) + 1$

PAC bound for decision trees of depth k

log |H|

$$m \geq \frac{\ln 2}{2\epsilon^2}\left((2^k - 1)(1 + \log_2 n) + 1 + \log_2 \frac{2}{\delta}\right)$$

- Bad!!!
  - Number of points is exponential in depth k!

- But, for *m* data points, decision tree can't get too big…

Number of leaves never more than number data points, so we are over-counting a lot!

Number of decision trees with k leaves

$$m \geq \frac{1}{2\epsilon^2}\left(\ln|H| + \ln\frac{2}{\delta}\right)$$

H_k = Number of binary decision trees with k leaves

H_1 =2

H_k = (#choices of root attribute) *

[(# left subtrees wth 1 leaf)*(# right subtrees wth k-1 leaves)

+ (# left subtrees wth 2 leaves)*(# right subtrees wth k-2 leaves)

+ …

+ (# left subtrees wth k-1 leaves)*(# right subtrees wth 1 leaf)]

$H_k = n\sum_{i=1}^{k-1} H_i H_{k-i}$ = $n^{k-1}\ C_{k-1}$ (C_{k-1} : Catalan Number)

Loose bound (using Sterling's approximation):

$$H_k \leq n^{k-1} 2^{2k-1}$$

Number of decision trees

- With k leaves

$$m \geq \frac{1}{2\epsilon^2}\left(\ln|H| + \ln\frac{2}{\delta}\right)$$

$$\log_2 H_k \leq (k-1)\log_2 n + 2k - 1$$

linear in k

number of points m is linear in #leaves

- With depth k

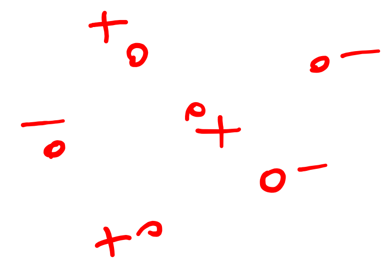
$$\log_2 H_k = (2^k-1)(1+\log_2 n) + 1$$

exponential in k

number of points m is exponential in depth

What did we learn from decision trees?

- VC dimension
- Rademacher complexity



- Moral of the story:

  Complexity of learning not measured in terms of size of model space, but in maximum *number of points* that can be correctly classified using a model from that space

<u>Next class:</u> Use this idea to define complexity of infinite model spaces e.g. linear classifiers, neural nets, …