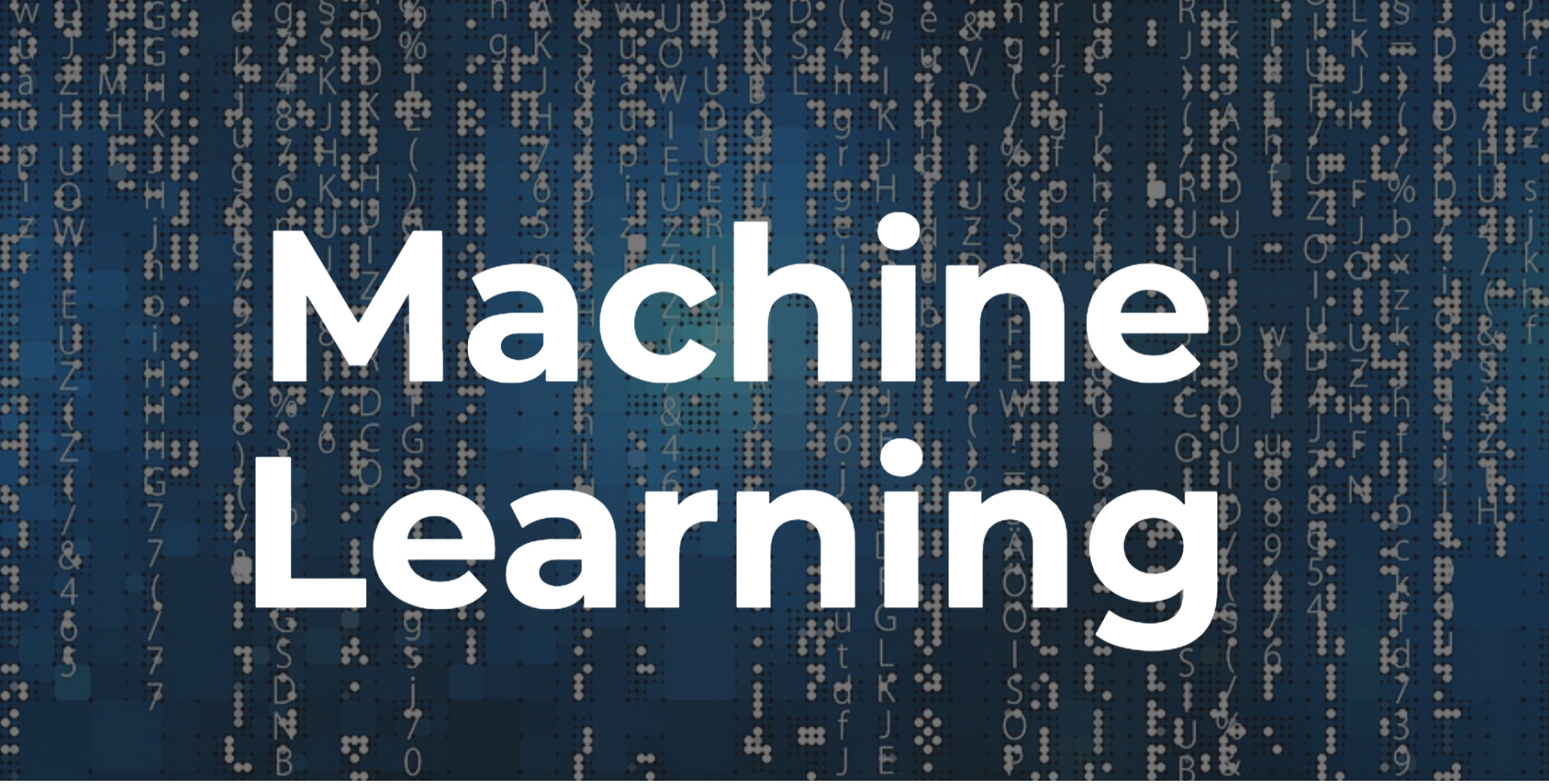


CSCI 4622 Fall 2019

Prof. Claire Monteleoni

Today: Lecture 6

- Overfitting vs. generalization
  - bias-variance tradeoff
- Model evaluation/selection
  - Validation, Cross-Validation

With credit to S. Dasgupta, C. Tan, T. Joachims

Greedy decision tree building

Start with all points in a single node

Repeat

    Pick the split with greatest benefit

Until ???

When to stop?

(i) When each leaf is pure?

(ii) When the tree is already pretty big?

(iii) When each leaf has uncertainty < some threshold?

Common strategy: keep going until leaves are pure (recall: this didn't work too well for us earlier…)

Then, shorten the tree by pruning, to correct the overfitting problem.

What is overfitting?

Data comes from some true underlying distribution D on X x Y.

[X = input space, Y = label space]

All we ever see are samples from D: training set, test set, etc.

When we choose a classifier h: X → Y, we can talk about its error on the training set (x_1, y_1), …, (x_m, y_m):

$$\hat{\epsilon}(h) = \frac{1}{m} \sum_{i=1}^{m} \mathbf{1}(h(x_i) \neq y_i)$$

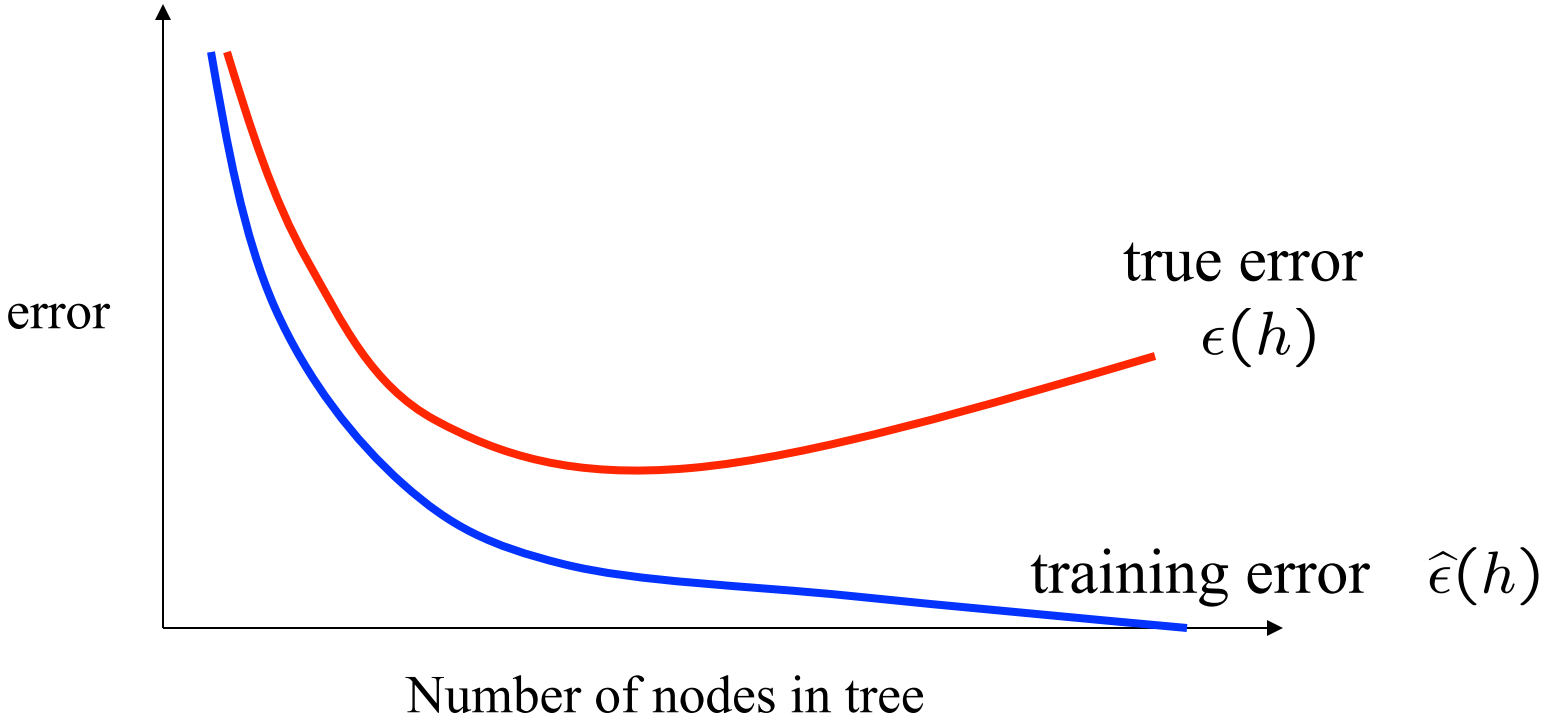
But we can also talk about its true error:

$$\epsilon(h) = \mathbf{P}_{(x,y)\sim D}(h(x) \neq y)$$

How are these two quantities related?

Overfitting: picture

E.g., building a decision tree

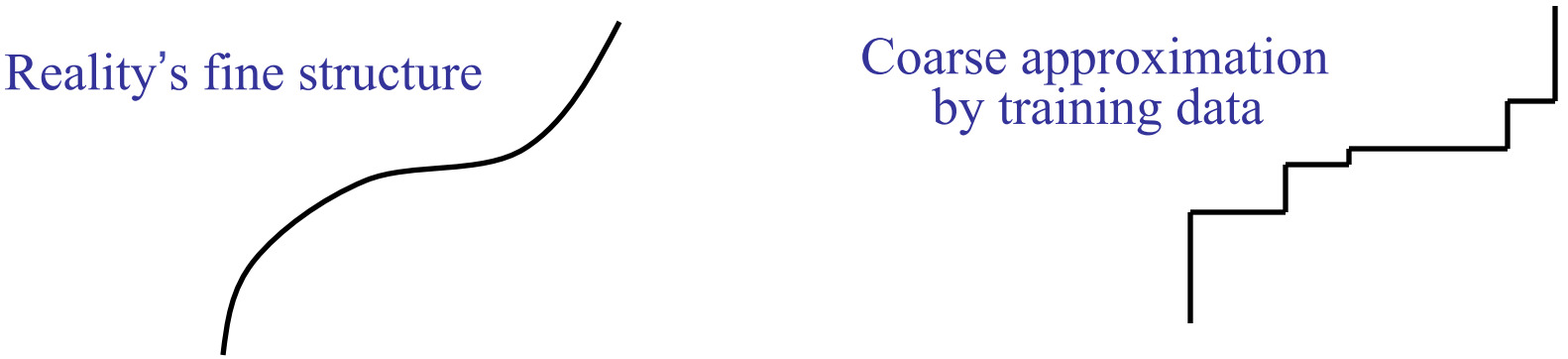


As we make our tree more and more complicated:

- The training error keeps going down
- but the true error stops improving and may even get worse!

Overfitting: one perspective

1. The true underlying distribution D is the one whose structure we would like to capture
2. The training data reflects the structure of D, so it helps us.
3. But it also has **chance** structure of its own – we must try to avoid modeling this.



For instance: D = uniform distribution over {1,2,3,…,100}

Pick three training points: eg. 6, 12, 98.

They all happen to be even: but this is just chance structure.

It would be bad to build this into a classifier.

Overfitting: another perspective

"Fit a line to a point": absurd
"Fit a plane to two points": likewise

Moral: It is not good to use a model which is so complex that there isn't enough data to reliably estimate its parameters.

Decision tree pruning

[1] Split the training data S_{full} into two parts:

- A smaller training set S
- A validation set V (a model of reality, a surrogate test set)

[2] Learn a full decision tree, T, using training data set, S

[3] Then prune T using V:

Repeat

if there a node u in T such that removing the subtree rooted at u decreases the error on data set V:

T = T – {subtree rooted at u}

Of course, V has chance structure too, but its chance structure is unlikely to coincide with that of S.

Example: SPAM data set

4601 points, each corresponding to an email message

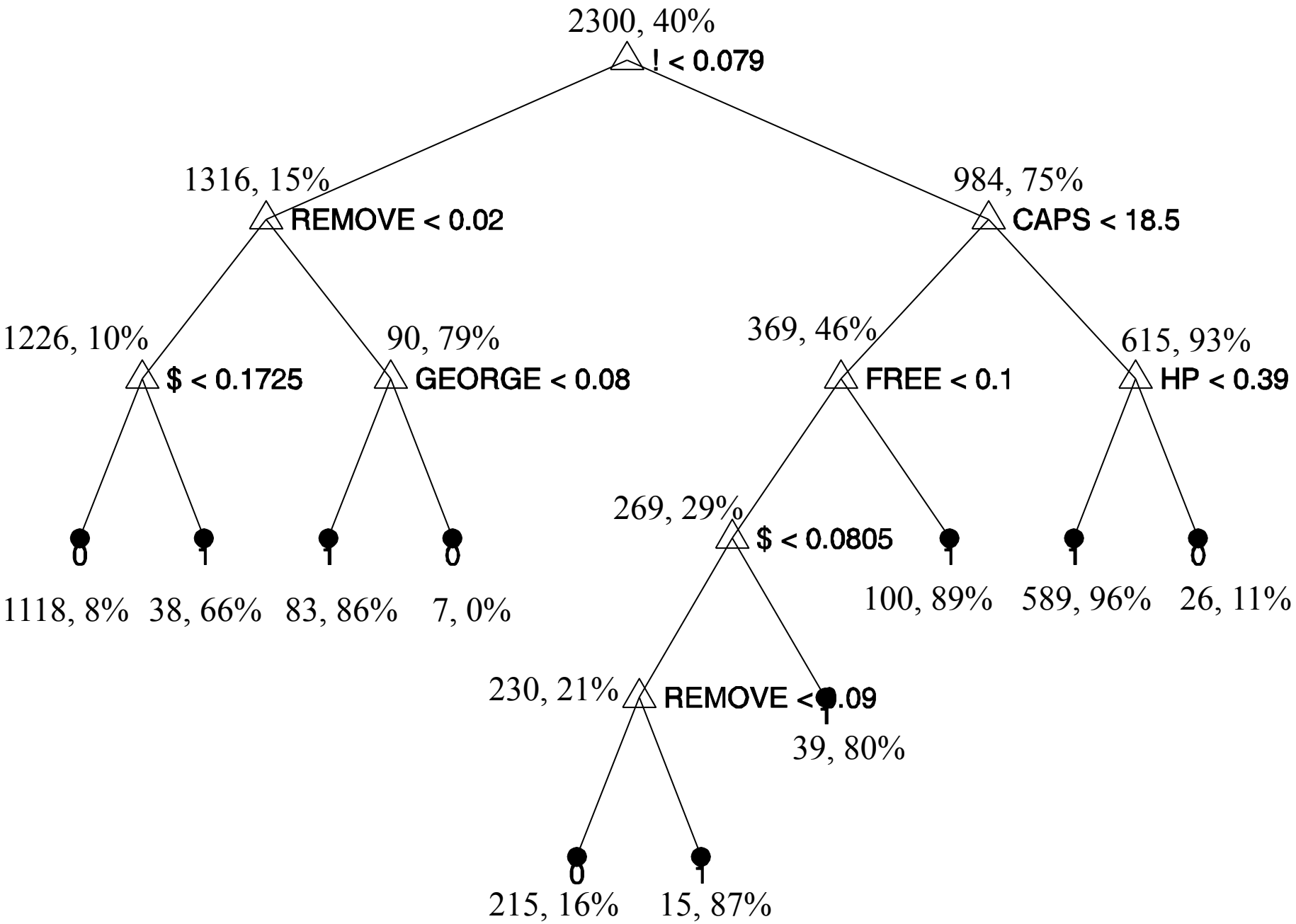
39.4% are SPAM

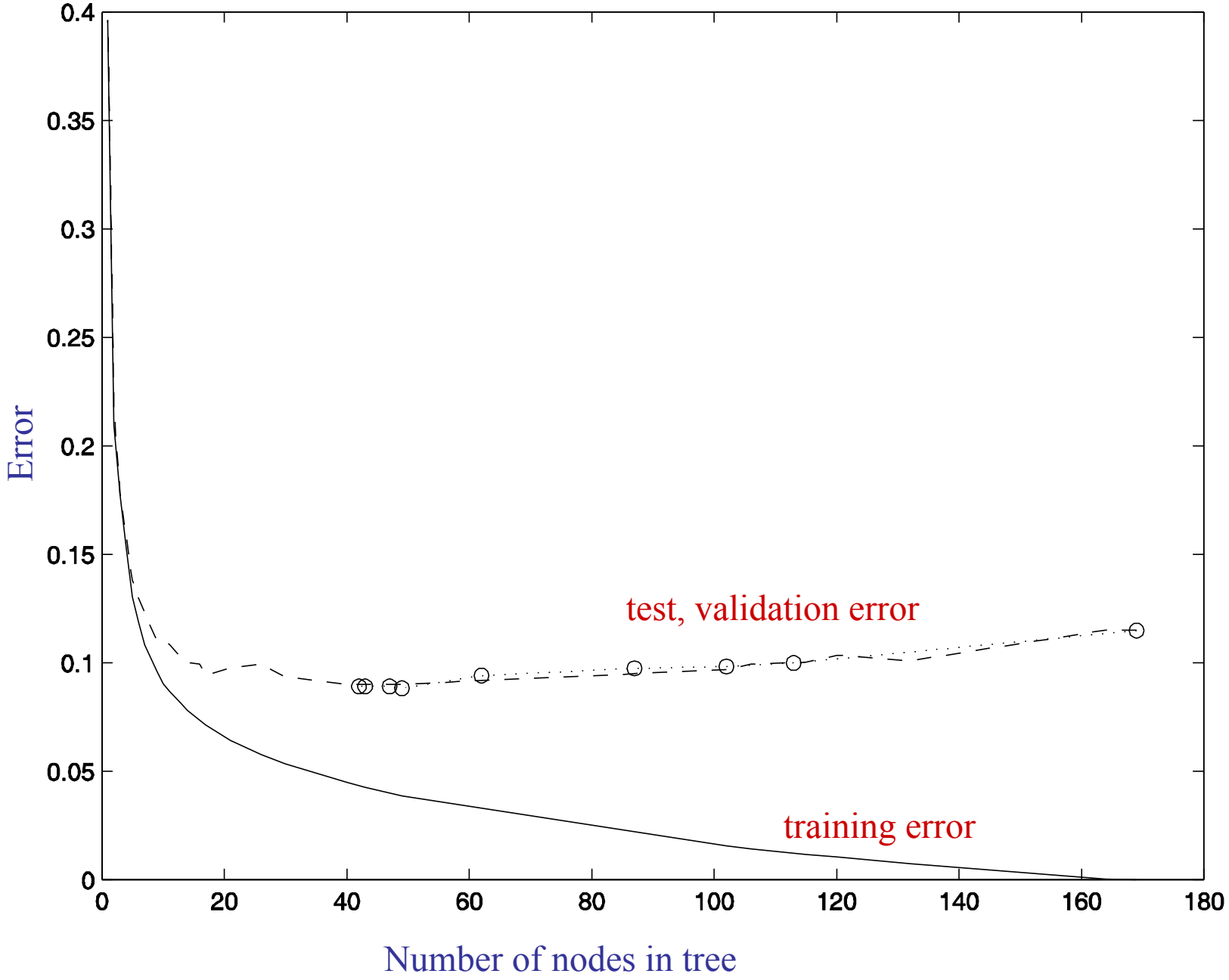
Each point has 57 features:

- 48 features check for specific words, eg. FREE
- 6 features check for specific characters, eg. !
- 3 other features, eg. length of the longest run of capital letters

Randomly divide into three parts:

50%	training data
25%	validation
25%	testing


2300, 40%
! < 0.079
1316, 15%
REMOVE < 0.02
984, 75%
CAPS < 18.5
1226, 10%
$ < 0.1725
90, 79%
GEORGE < 0.08
369, 46%
FREE < 0.1
615, 93%
HP < 0.39
269, 29%
$ < 0.0805
230, 21%
REMOVE < 0.09
0
1
1
0
1
1
1
0
0
1
1118, 8%
38, 66%
83, 86%
7, 0%
100, 89%
589, 96%
26, 11%
39, 80%
215, 16%
15, 87%


0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
20
40
60
80
100
120
140
160
180
Error
Number of nodes in tree
test, validation error
training error

How accurate is the validation set?

How accurate are error estimates based on the validation set?

For any classifier h and underlying distribution D on X x Y:

"true error" $\text{err}(h) = \mathbf{P}_{(x,y)\sim D}(h(x) \neq y)$

"error on set S" $\text{err}(h, S) = \frac{1}{|S|} \sum_{(x,y)\in S} \mathbf{1}(h(x) \neq y)$

Suppose S is chosen i.i.d. (independent, identically distributed) from D. Then (over the random choices of S),

$$\mathbf{E}[\text{err}(h, S)] = \text{err}(h)$$

And the standard deviation of err(h,S) is about $1/\sqrt{|S|}$.

How accurate is the validation set?

Fix any h. Suppose S is chosen i.i.d. (independent, identically distributed) from D. Then (over the random choices of S),

$$\mathbf{E}[\text{err}(h, S)] = \text{err}(h)$$

And the standard deviation of err(h,S) is about $1/\sqrt{|S|}$

(i) In this scenario, S is used to assess the accuracy of a single, pre-specified classifier h.

Can the same S be used to check many classifiers simultaneously?

Answer: VC theory

(ii) In particular, if h was created using S as a training set, then the above scenario does not apply. In such situations, err(h,S) might be a very poor estimate of err(h).

Example

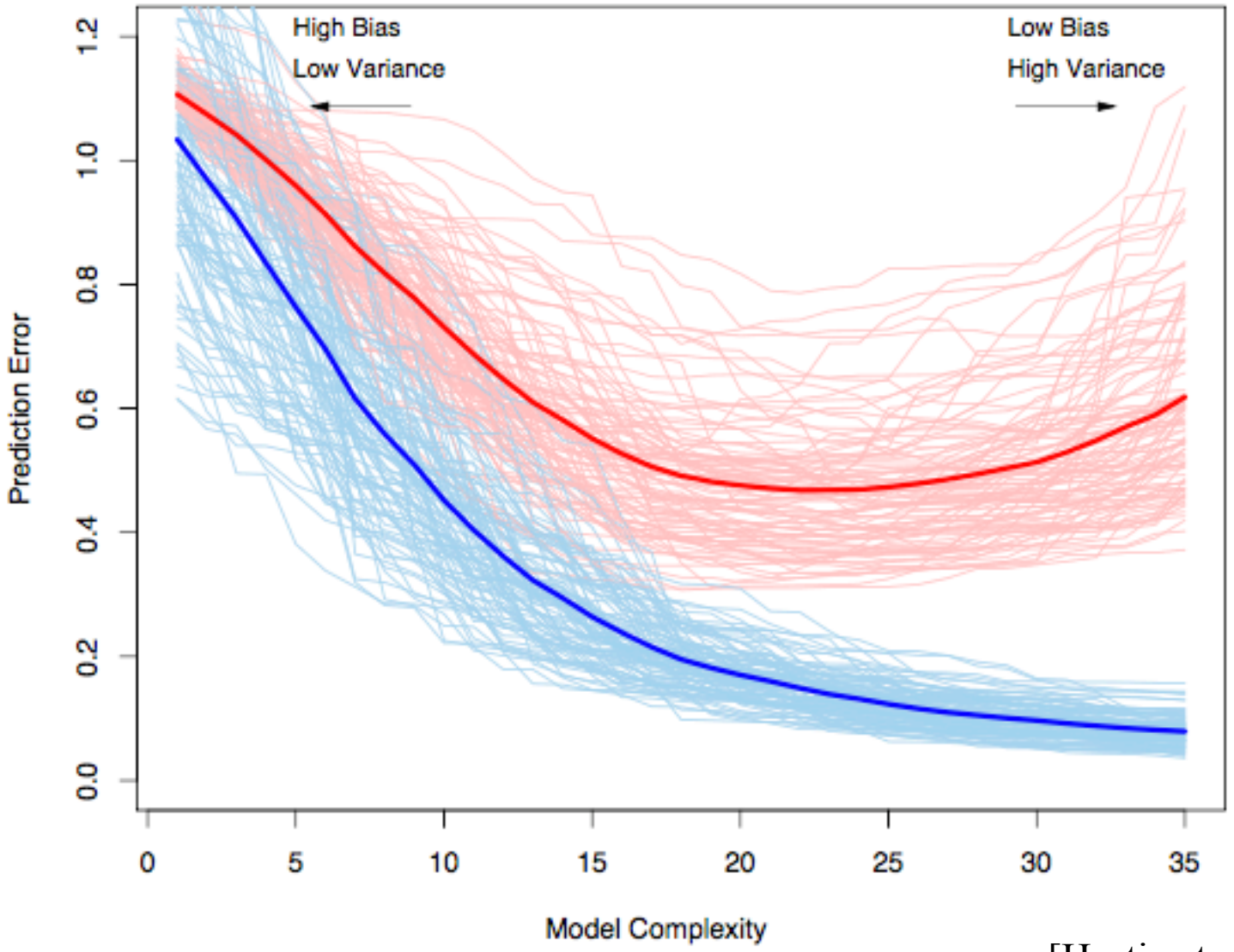
Predict flu trends using search-engine queries

- X: search-engine query data
- Y: fraction of population with flu

- S_{train} = all data before 2012

- S_{test} = all data in 2012

Example



Test error

Training error

[Hastie et al., 2001. Fig. 7.1]

Bias-Variance Error Decomposition

If we assume all data points (x,y) obey: $y = f(x) + \epsilon$

where: $\mathrm{E}[\epsilon] = 0$

$\mathrm{Var}(\epsilon) = \sigma^2$

Then, $\mathrm{Err_h}(x) = \mathrm{E}[(y - h(x))^2 | X = x]$

$= \sigma^2 + \mathrm{Var}[h] + (\mathrm{Bias}[h])^2$

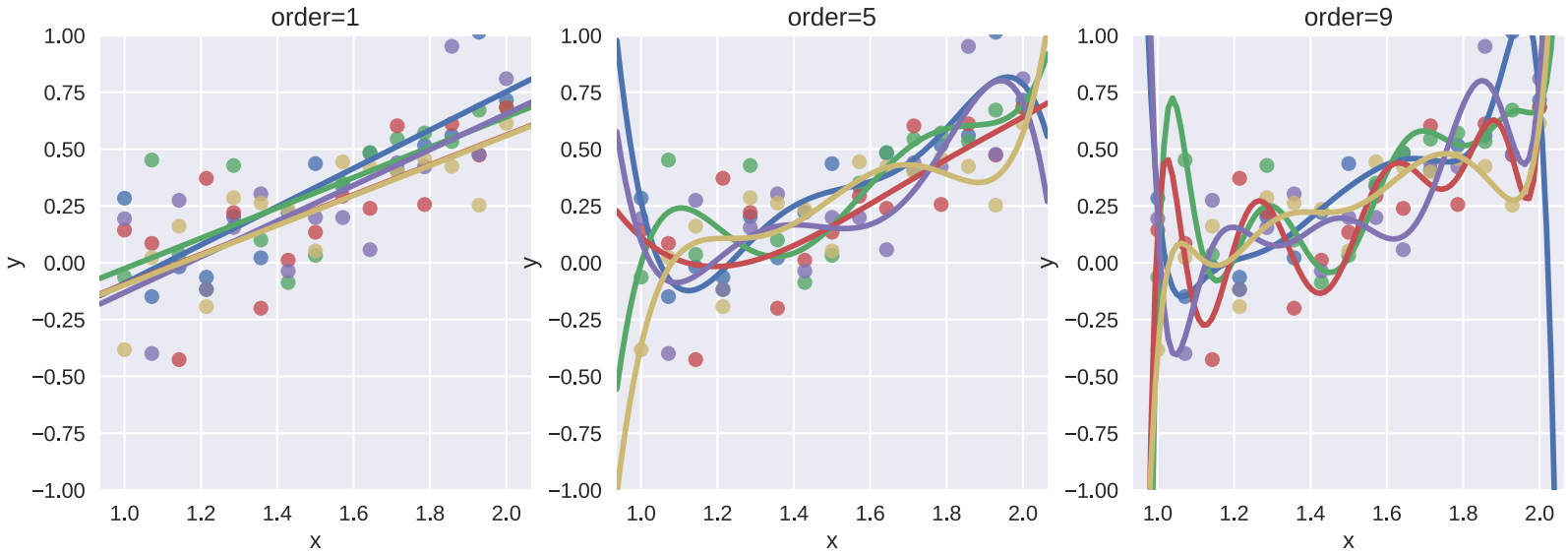
Irreducible error (can't be changed by choice of h)

where: $\mathrm{Var}[h] = \mathrm{E}[h(x)^2] - \mathrm{E}[h(x)]^2$

$\mathrm{Bias}[h] = (f(x) - \mathrm{E}[h(x)])$

NOTE: All expectations are w.r.t. the random training set *h* is learned from, NOT *x*.

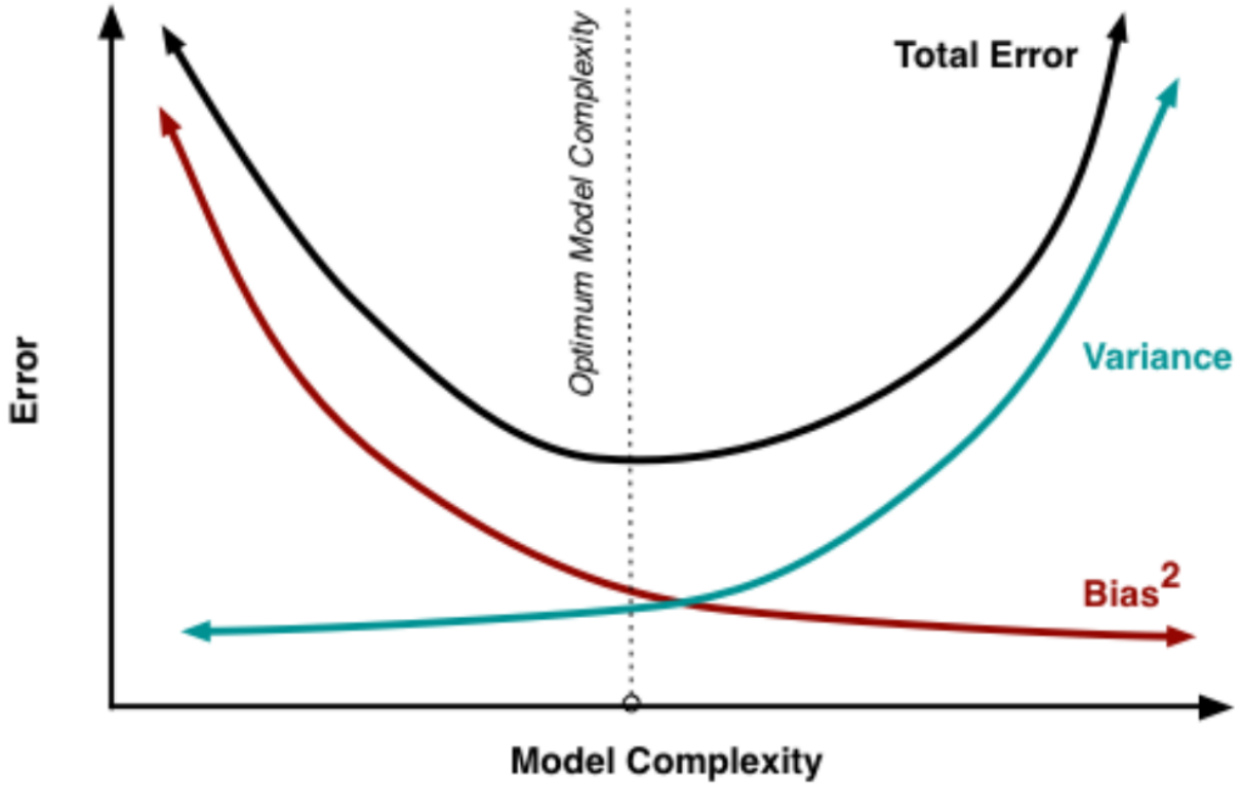
Example



Increasing the order of the polynomial model used to fit the data increases model complexity, eventually leading to overfitting.

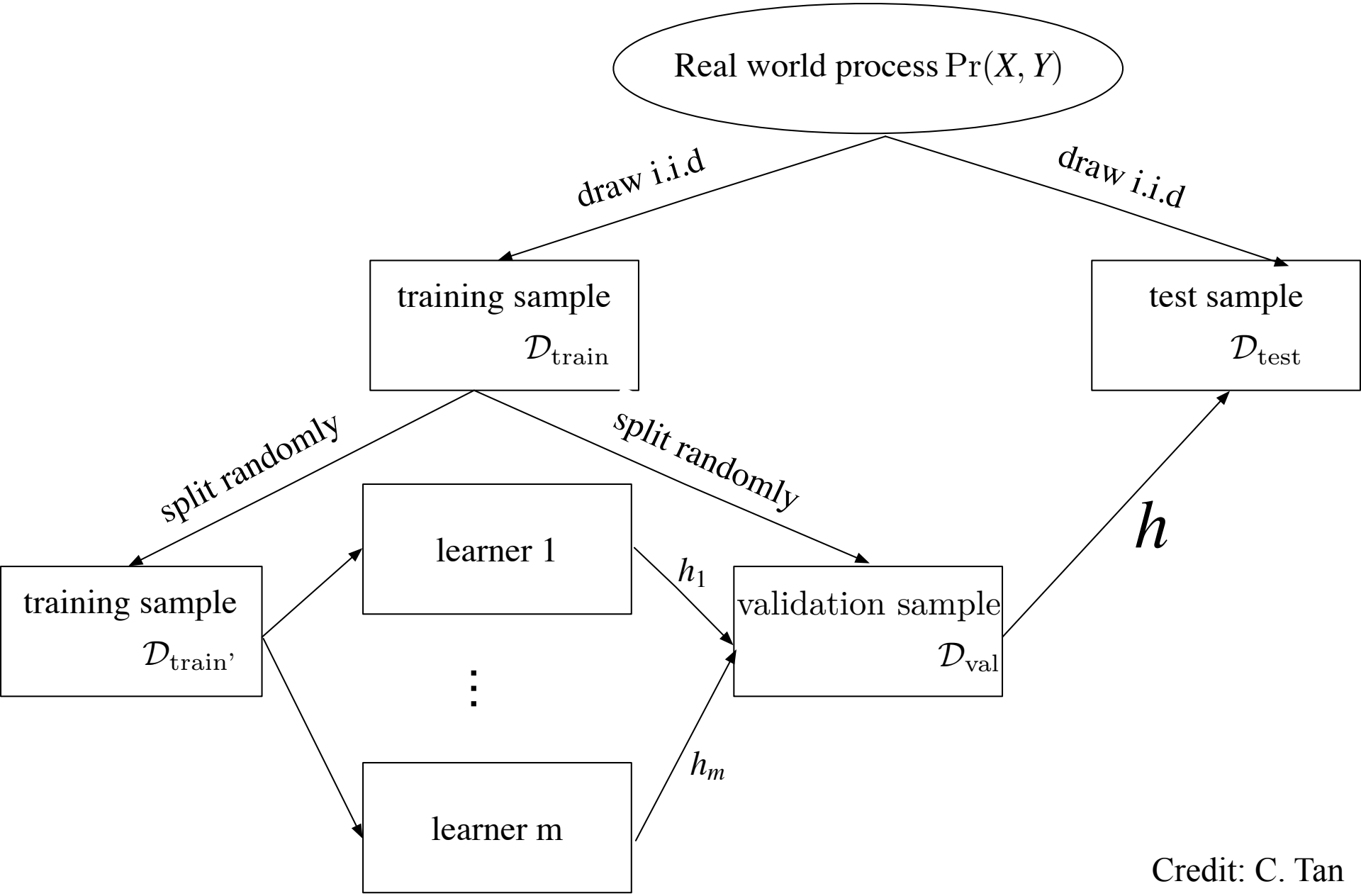
Credit: C. Tan

Bias-Variance Tradeoff



Credit:
http://scott.fortmann-roe.com/docs/BiasVariance.html

Model Selection



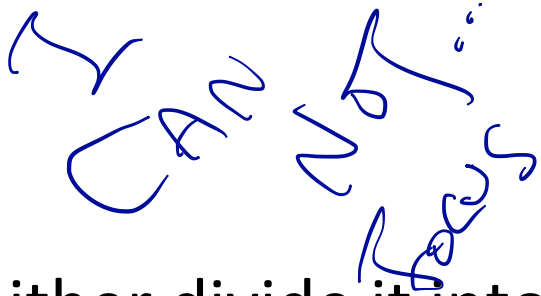
Credit: C. Tan

Managing data sets: Train v. Test

- In general, you should have a separate training set and test set.
- Ideally they will be drawn from the same distribution.
- E.g. randomly permute your entire input data set, then fix T, and use all (x_t,y_t) for $t < T$ for Train, and the remaining data for Test.

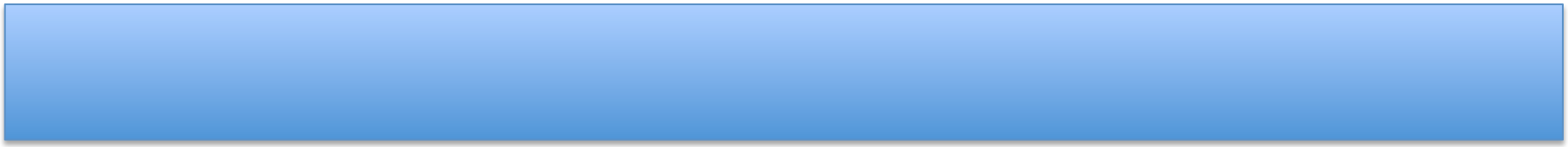
Managing data sets: Train v. Test

- First create the holdout data set, the Test set, for computing the final test error. For best performance it will be a (labeled) dataset from the same distribution as the Training set.
  - E.g. technique on previous slide.

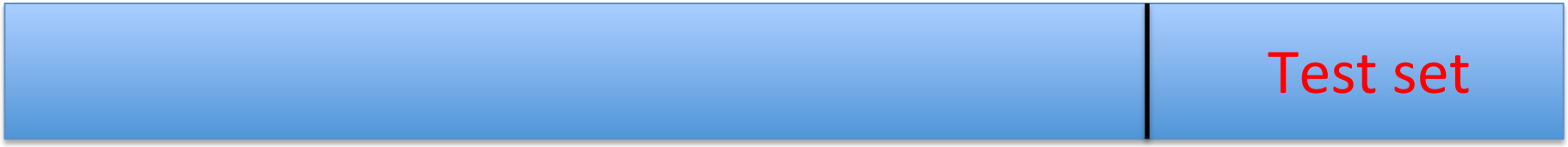


- With the remaining data set, you can either divide it into two parts for Train and Validation, as specified on the previous slide, or you can run Cross-Validation on it.
  - This is for model selection / parameter tuning

- Whole data set:



- Separate the test set, and hold it out:



- From the remaining data, use part for Validation:

- Or run cross validation to train and fit parameters:

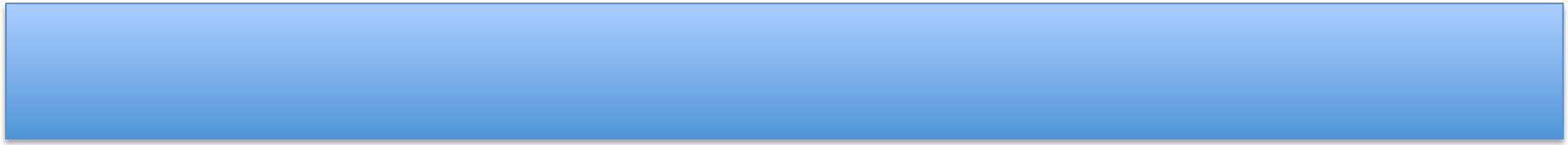
Cross validation: motivation

- To get a more robust estimate of the error rate, we should run more experiments, and average the error rates over the experiments.

- If we have a huge amount of labeled data, we can run several disjoint experiments (e.g. further split Train and Test into more data sets) and average the test error over the results. This is usually not the case.
  - Instead we do Cross-Validation.

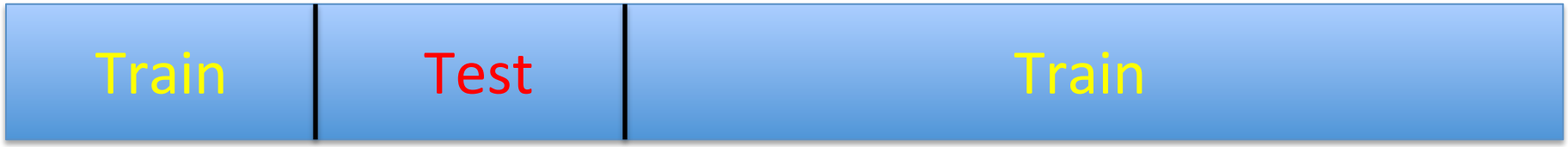
N-fold Cross-validation

- Cross validation data set:



- Fold 1:

- Fold 2:



- …
- Fold n

N-fold cross-validation

- Fix N, for example 5 or 10.
- Run N experiments. In each experiment, 1/N fraction of the data is used for Test and the remaining data is used for Train. The Test sets over the N experiments are disjoint, and the Train sets are overlapping.
- Average the Test error over the N experiments.
- Note: different classifiers will likely be learned in each experiment, as the Train sets differ slightly.

Leave-one-out cross-validation

- N is set to the size of the data set. For each experiment, Test consists of the i-th point, and Train consists of all points exept the i-th point.
- Average the test error over the N experiments.

Model selection / Parameter tuning

- For each meta-parameter, e.g. *k* in *k*-NN, explore a range of parameter values. Log-search can be performed by doubling, or halving the value of the parameter.

- On the tuning data set (a.k.a. Validation set, or CV on the training data), try to find the "knee" in the curve: the parameter setting such that the tuning test error is minimized, before increasing again.