CS60020: Foundations of Algorithm Design and Machine Learning

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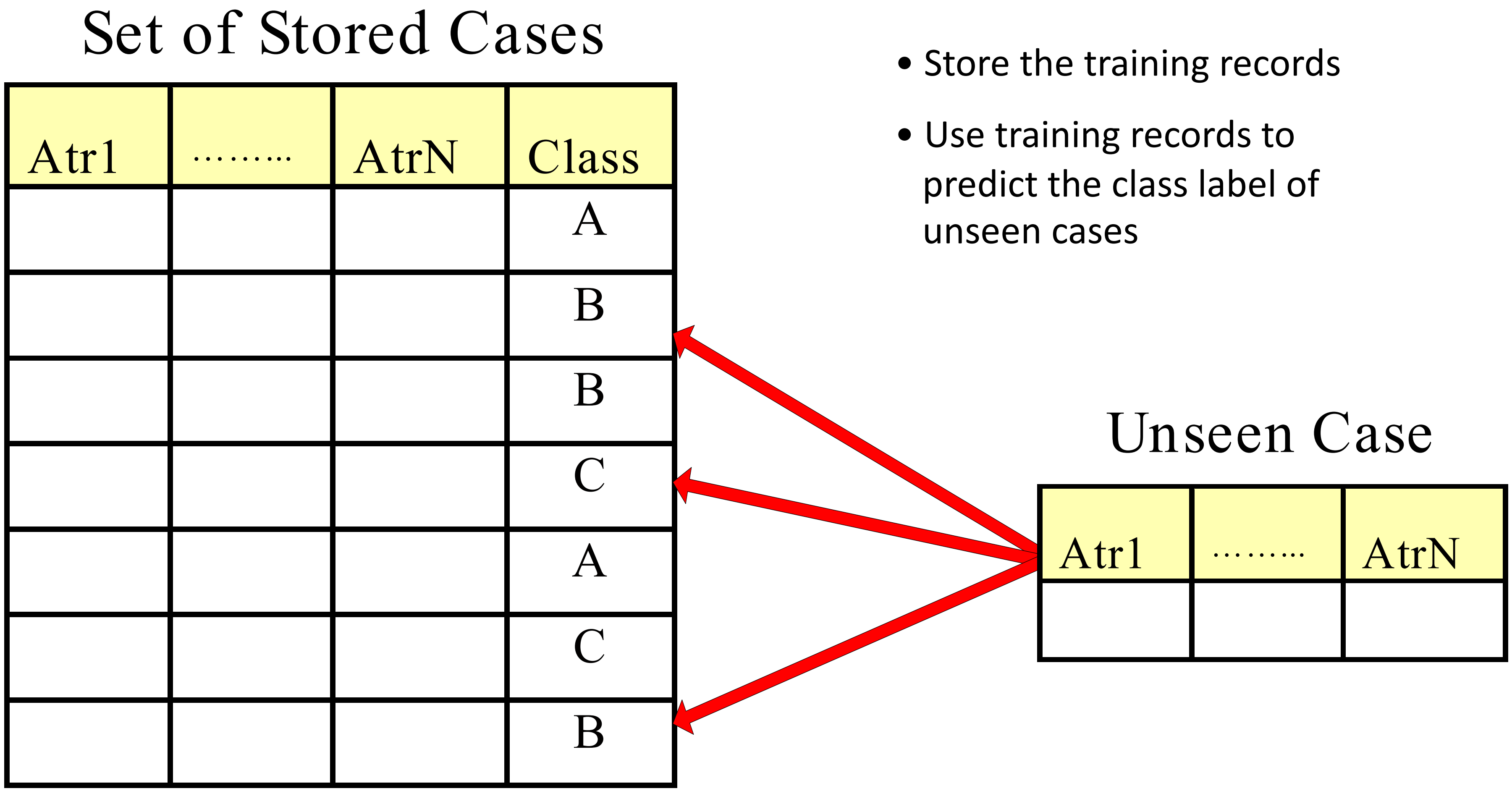
NON-PARAMETRIC MODELS

Instance-Based Classifiers



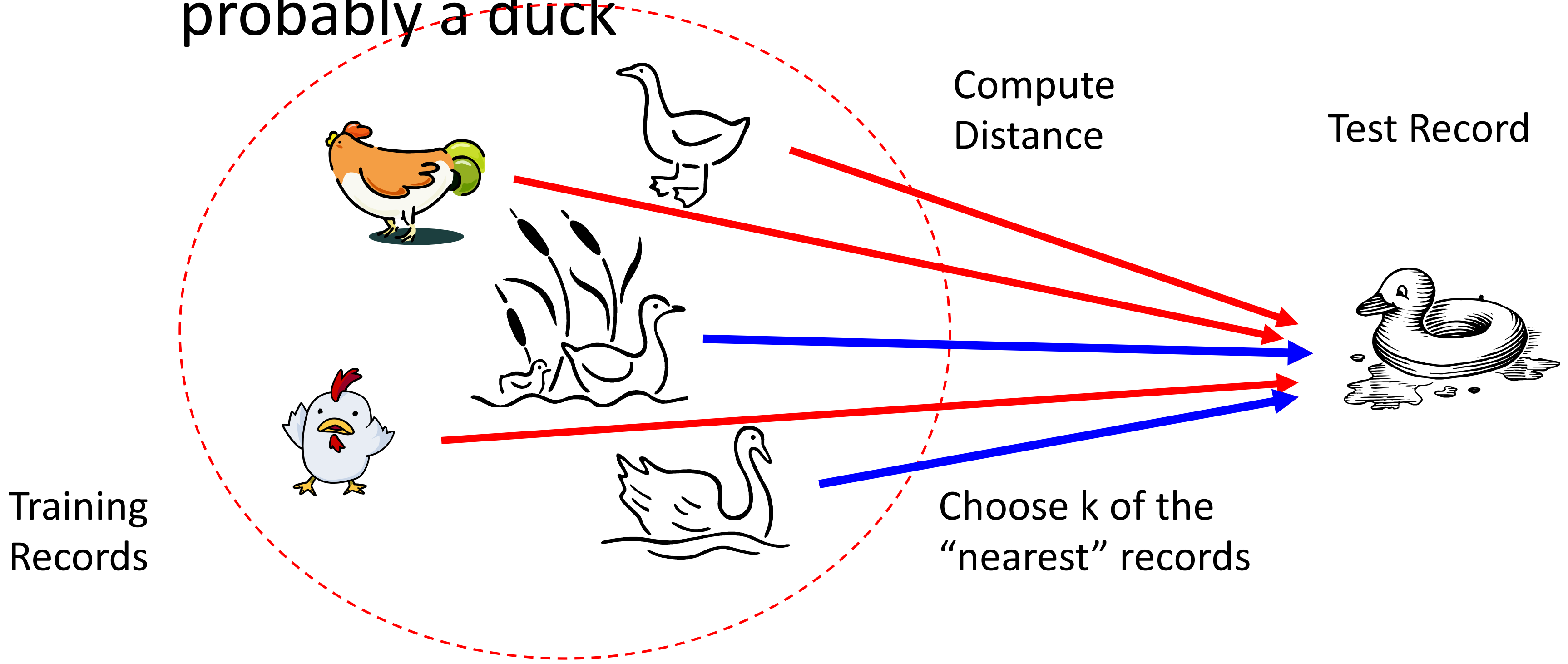
- Store the training records
- Use training records to predict the class label of unseen cases

Instance Based Classifiers

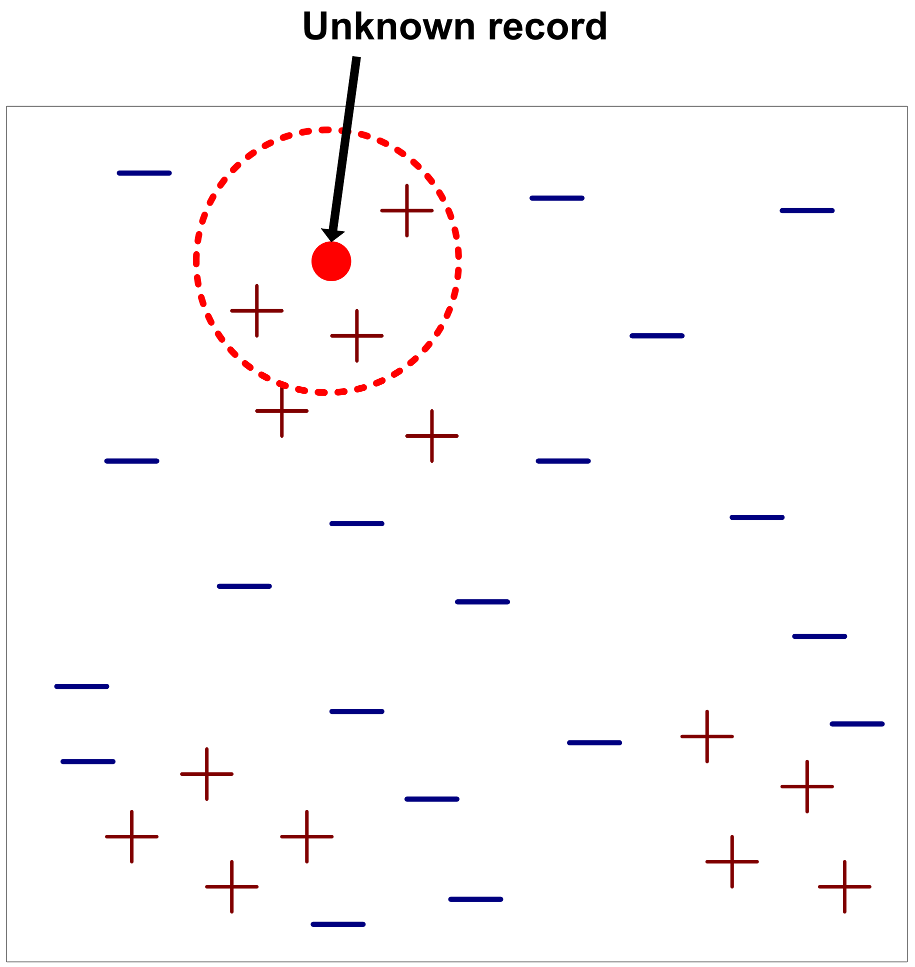
- Examples:
  - Rote-learner
    - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
  - Nearest neighbor
    - Uses k “closest” points (nearest neighbors) for performing classification

Nearest Neighbor Classifiers

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it's probably a duck



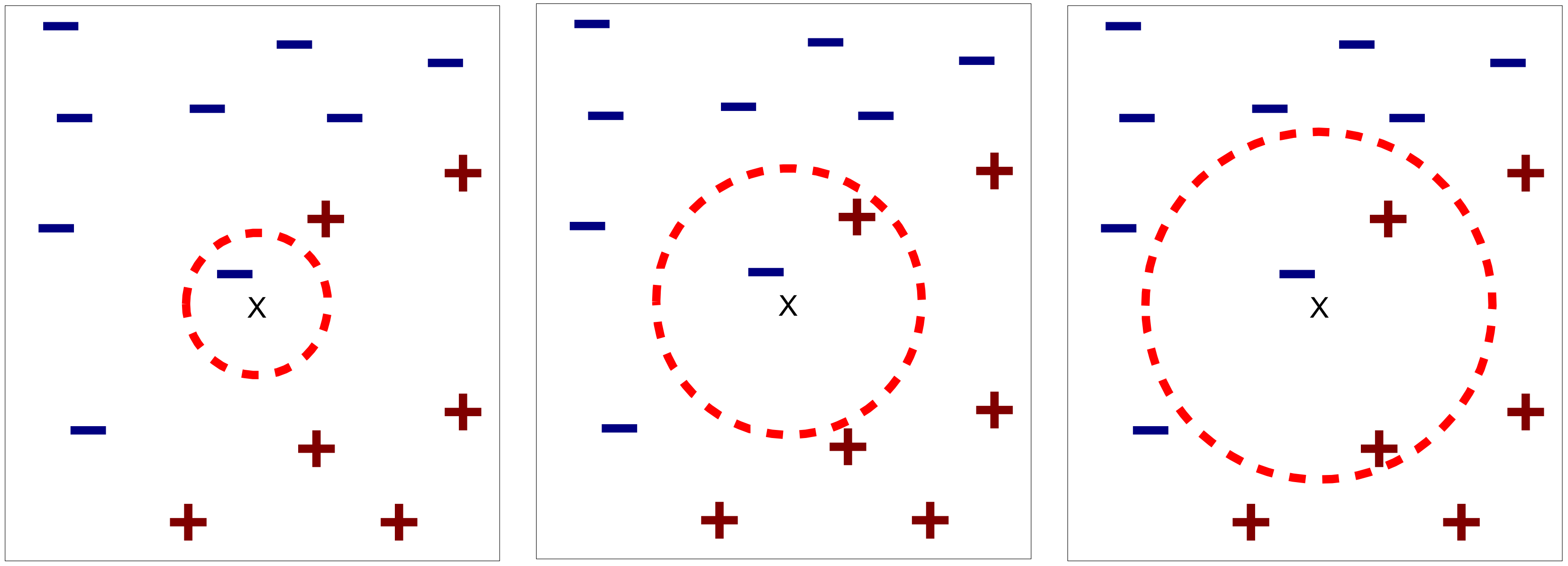
Nearest-Neighbor Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric to compute distance between records
  - The value of *k*, the number of nearest neighbors to retrieve

- To classify an unknown record:
  - Compute distance to other training records
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Definition of Nearest Neighbor



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

Nearest Neighbor Classification

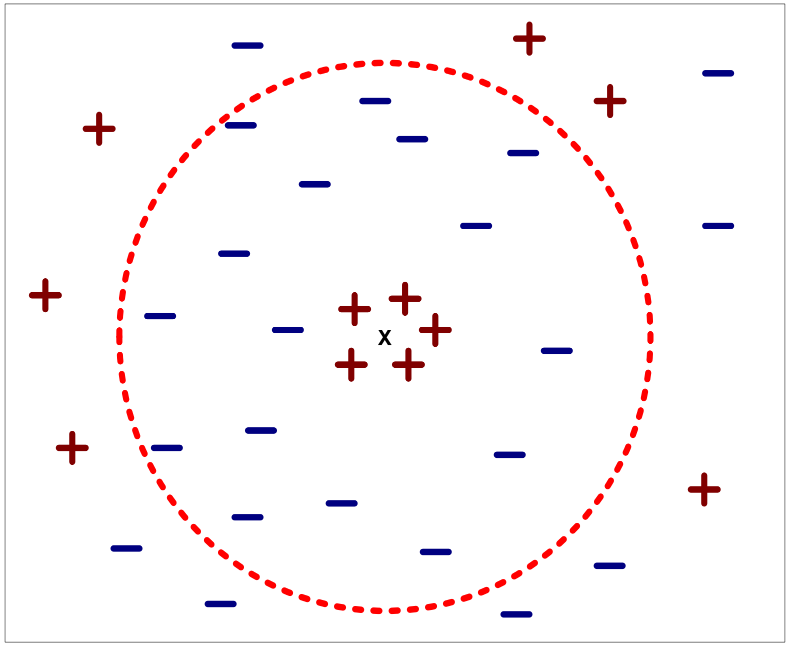
- Compute distance between two points:
  - Euclidean distance

$$d(p,q) = \sqrt{\sum_i (p_i - q_i)^2}$$

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - Weigh the vote according to distance
    - weight factor, $w = 1/d^2$

Nearest Neighbor Classification…

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



Nearest Neighbor Classification…

- Scaling issues
  - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
  - Example of an attribute dominating distance computation:
    - height of a person may vary from 1.5m to 1.8m
    - weight of a person may vary from 90lb to 300lb
    - income of a person may vary from $10K to $1M

The K-Nearest Neighbor Method

- K neighbors in training data to the input data x: break ties arbitrarily
- All k neighbors will vote: majority wins
- Extension:
  - Weighted KNN

"K" is a variable:

  - Often we experiment with different values of K=1, 3, 5, to find out the optimal one

- Why is KNN important?
  - Often a baseline
  - Must beat this one to claim innovation
- Applications of KNN
  - Document similarity

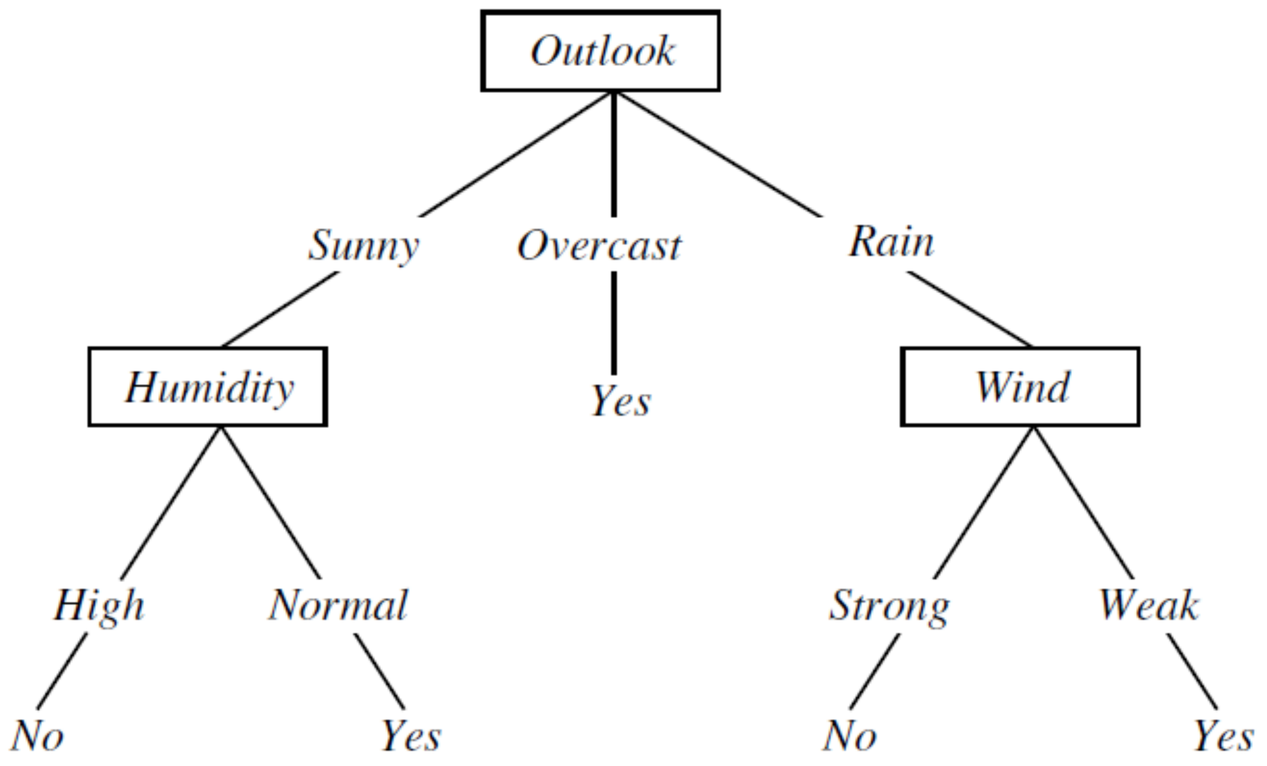
Decision Tree

- Setting:
  - Instances describable by attribute value pair.
  - Target function is discrete valued.
  - Disjunctive hypothesis is required.
  - Training data may contain errors.
  - Training data may contain missing attribute values.

Decision Tree

- Each internal node tests an attribute.
- Each branch corresponds to a value of an attribute.
- Each leaf node assigns a classification.

Decision tree - Example



Decision tree learning

- For a test datapoint:
  - Determine the branches to take at each level based on attribute value.
  - At a leaf level, return the label of current node.
- For training, at each level:
  - Select an attribute split the training dataset on.
  - Examine the purity of data at each splitted node and determine whether it is a leaf node.
  - Determine the label at each node

What attribute to select ?

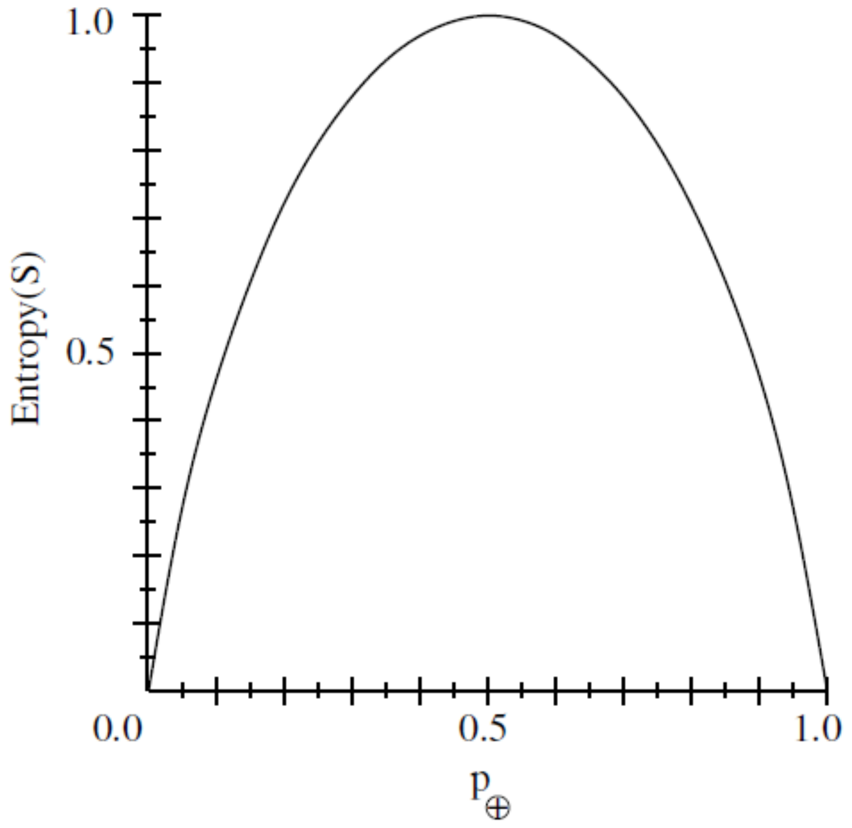
- Entropy:

- S is a sample of training examples
- $p_{\oplus}$ is the proportion of positive examples in S
- $p_{\ominus}$ is the proportion of negative examples in S
- Entropy measures the impurity of S

$$Entropy(S) \equiv -p_{\oplus} \log_2 p_{\oplus} - p_{\ominus} \log_2 p_{\ominus}$$

What attribute to select ?

- Entropy:



What attribute to select ?

$Entropy(S)$ = expected number of bits needed to encode class ($\oplus$ or $\ominus$) of randomly drawn member of S (under the optimal, shortest-length code)

Why?

Information theory: optimal length code assigns $-\log_2 p$ bits to message having probability p.

So, expected number of bits to encode $\oplus$ or $\ominus$ of random member of S:

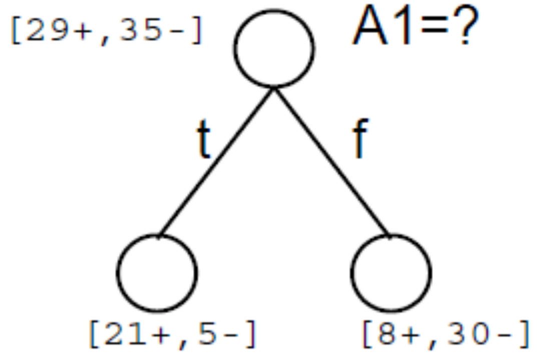
$$p_{\oplus}(-\log_2 p_{\oplus}) + p_{\ominus}(-\log_2 p_{\ominus})$$

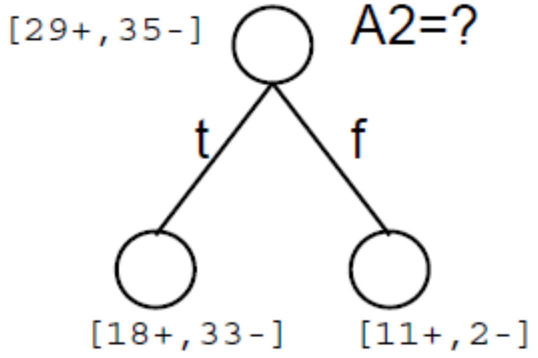
$$Entropy(S) \equiv -p_{\oplus}\log_2 p_{\oplus} - p_{\ominus}\log_2 p_{\ominus}$$

Information Gain

$Gain(S, A)$ = expected reduction in entropy due to sorting on A

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

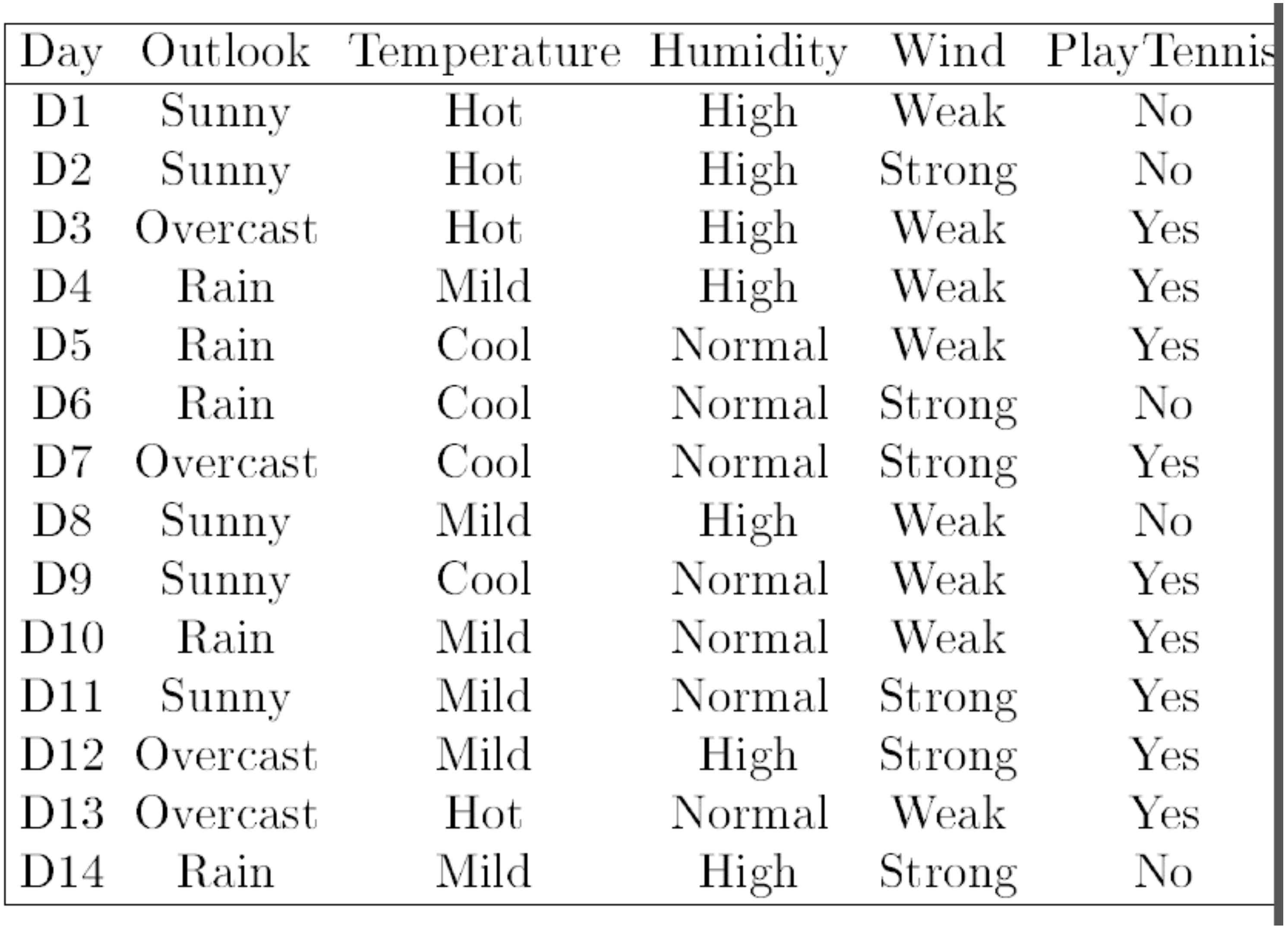




ID3 Algorithm

```
function ID3 (R: attributes, S: a training set, default_value) returns a
    decision tree;
begin
    if S=∅, then return default_value;
    else if S consists of records all with the value v then return
        value v;
    else f R=∅, then return the most frequent value v for records of
        S;
    else
        let A be the attribute with largest Gain(A,S) among attributes in R;
        let {$a_j$| j=1,2, .., m} be the values of attribute A;
        let {$S_j$| j=1,2, .., m} be the subsets of S consisting respectively of
            records with value $a_j$ for A;
        return a tree with root labeled A and arcs labeled $a_1$, $a_2$, .., $a_m$
            going respectively to the trees (ID3(R-{A}, $S_1$), ID3(R-{A}, $S_2$),
            .....,ID3(R-{A}, $S_m$);
```

ID3 example

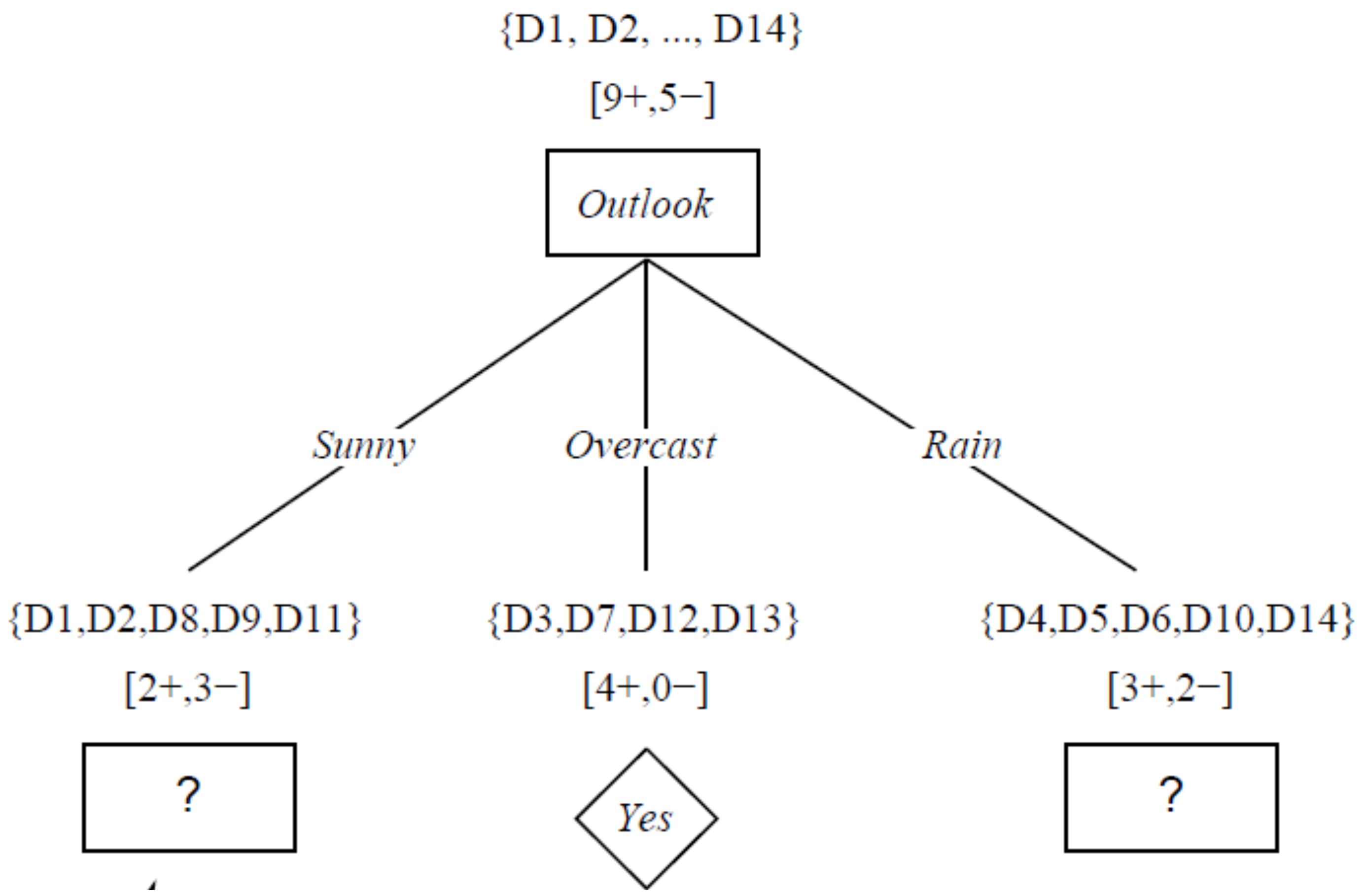


Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

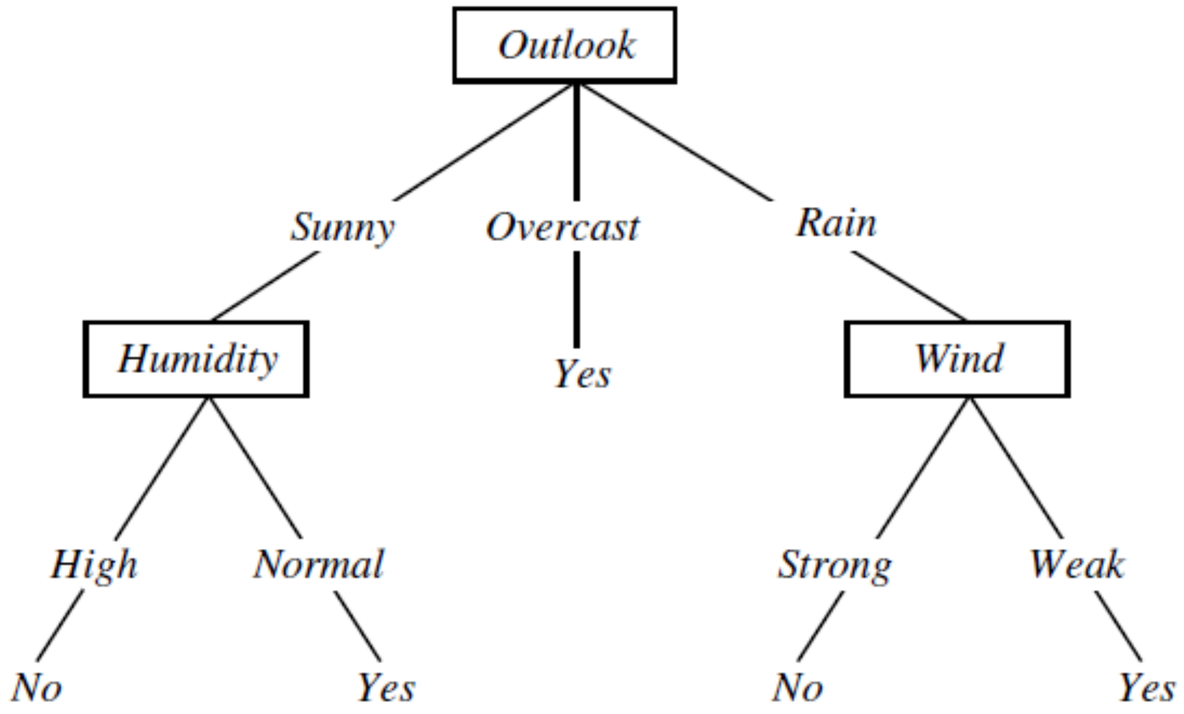
Root level choice

- Gain(S,outlook) = 0.246
- Gain(S, Humidity) = 0.151
- Gain(S, Wind) = 0.048
- Gain(S, Temperature) = 0.029

Root level tree



Tree


Outlook
Sunny
Overcast
Rain
Humidity
Yes
Wind
High
Normal
Strong
Weak
No
Yes
No
Yes

ID3

- Hypothesis space: set of all finite discrete valued functions.
  - The hypothesis space contains all functions.
- ID3 maintains a single hypothesis.
  - Does not enumerate all consistent hypothesis – cannot recommend best training example.
- Utilizes all the data at each stage.
  - Higher computational cost compared to one pass algorithms.
- Performs hill climbing without backtracking
  - Can converge to a local minimum.
- Feature selection criteria robust to errors in data.

Inductive Bias

- Shorter trees are preferred over longer trees.
- Occam’s razor: “Simpler” hypothesis are better than more complex hypothesis.
- Shorter trees are “simpler” because there are less number of them.

- Actually: shorter trees with attributes having more information gain are preferred.

Occam's razor

Why prefer short hypotheses?

Argument in favor:

- Fewer short hyps. than long hyps.

$\rightarrow$ a short hyp that fits data unlikely to be coincidence

$\rightarrow$ a long hyp that fits data might be coincidence

Argument opposed:

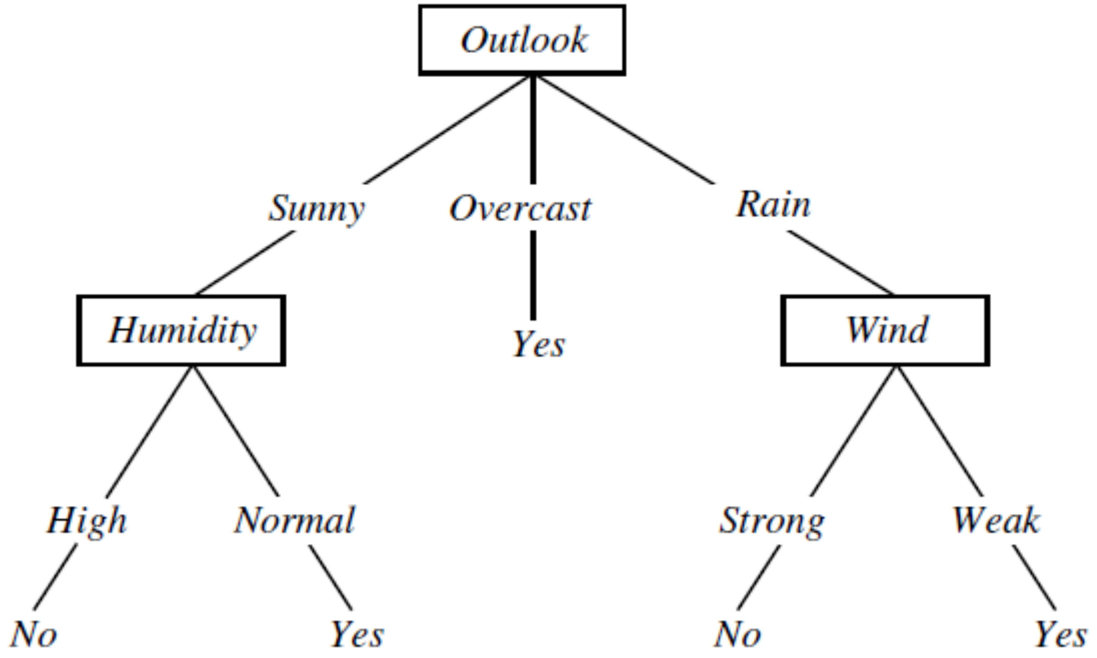
- There are many ways to define small sets of hyps
- e.g., all trees with a prime number of nodes that use attributes beginning with "Z"
- What's so special about small sets based on *size* of hypothesis??

Overfitting

Consider adding noisy training example #15:

$Sunny,\ Hot,\ Normal,\ Strong,\ PlayTennis = No$

What effect on earlier tree?



Overfitting

Consider error of hypothesis h over

- training data: $error_{train}(h)$
- entire distribution $\mathcal{D}$ of data: $error_{\mathcal{D}}(h)$

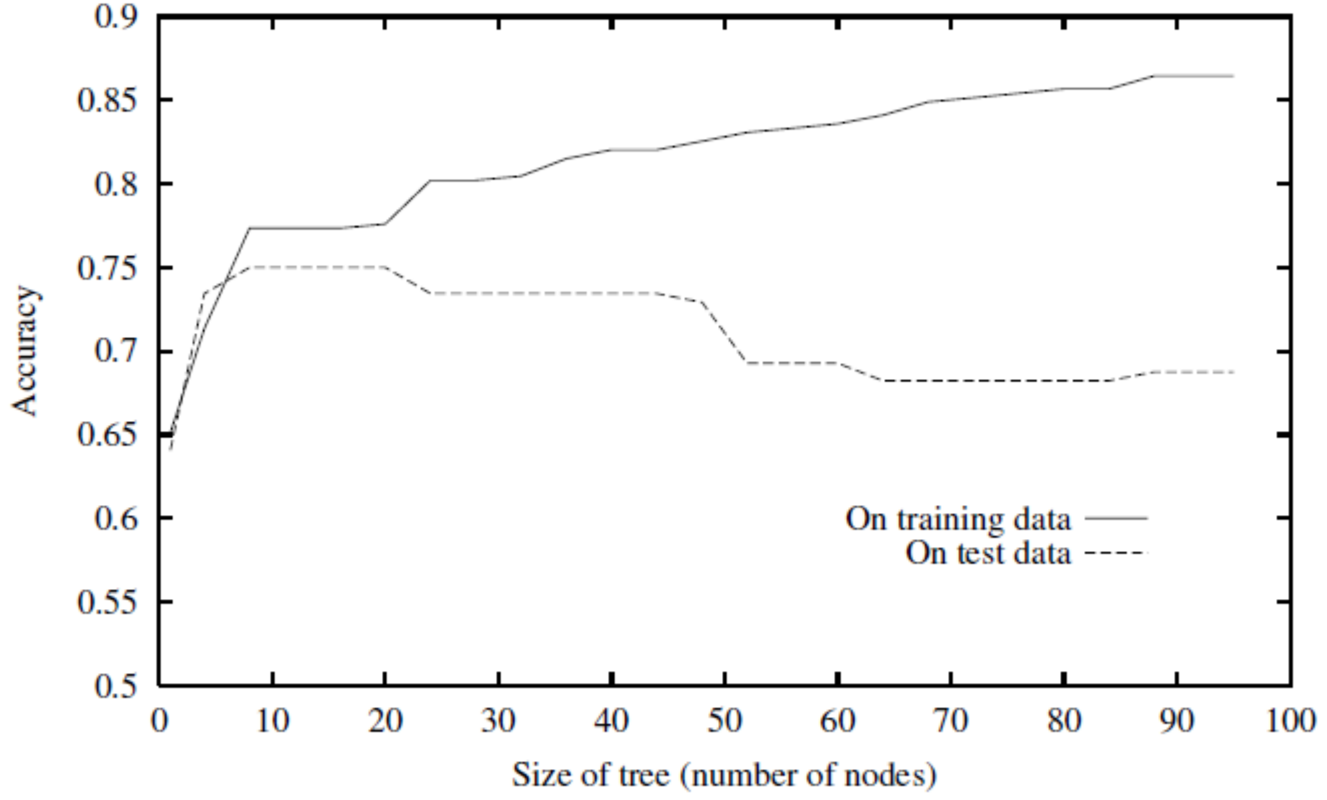
Hypothesis $h \in H$ **overfits** training data if there is an alternative hypothesis $h' \in H$ such that

$$error_{train}(h) < error_{train}(h')$$

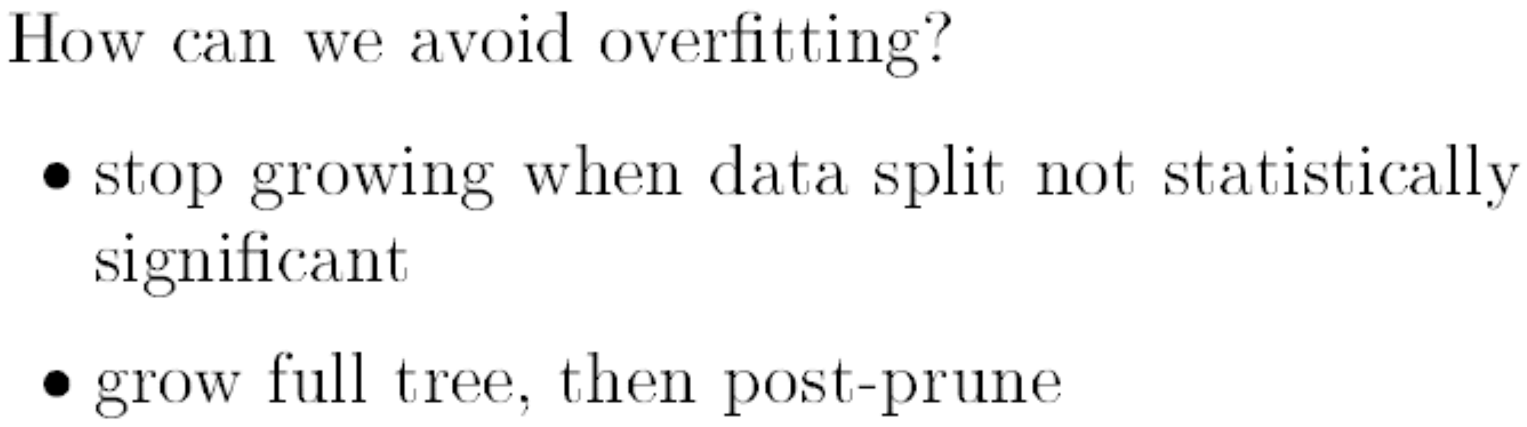
and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

Overfitting



Avoiding overfitting



How can we avoid overfitting?

- stop growing when data split not statistically significant
- grow full tree, then post-prune

- Which is computationally better ?

Avoiding overfitting

Which tree is best ?

- Measure the accuracy over a separate validation set.
- Perform statistical tests over training data, e.g. chi square tests.
- Minimize an explicit performance measure which comprises of training set performance and “complexity” of the model, e.g. MDL.

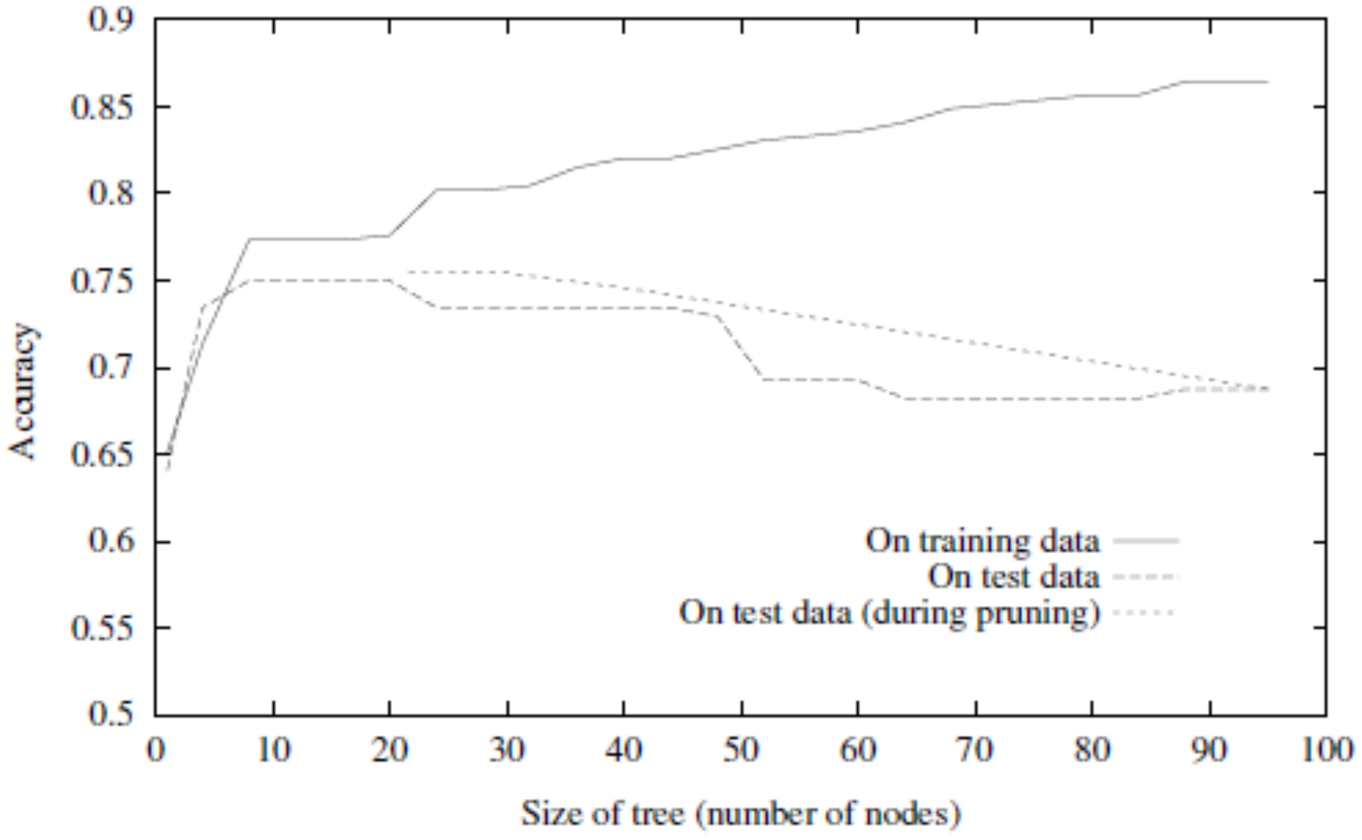
Reduced error pruning

Split data into *training* and *validation* set

Do until further pruning is harmful:

1. Evaluate impact on *validation* set of pruning each possible node (plus those below it)
2. Greedily remove the one that most improves *validation* set accuracy

Reduced error pruning



Rule post pruning

1. Convert tree to equivalent set of rules
2. Prune each rule independently of others
3. Sort final rules into desired sequence for use

Perhaps most frequently used method (e.g., C4.5)

Other issues

- Handling continuous valued attribute.
  - Create a split which produces the highest information gain.
- Handling large number of discrete valued attributes.

$$GainRatio(S, A) \equiv \frac{Gain(S, A)}{SplitInformation(S, A)}$$

$$SplitInformation(S, A) \equiv -\sum_{i=1}^{c} \frac{|S_i|}{|S|} \log_2 \frac{|S_i|}{|S|}$$

Other issues

- Handling missing attributes.
- Training set:
  - Assign a distribution based on exiting values.
  - Default branch for the set of attributed.
- Test set:
  - Default branch which is populated using missing values.

ENSEMBLE METHODS

Rationale for Ensemble Learning

- No Free Lunch thm: There is no algorithm that is always the most accurate
- Generate a group of base-learners which when combined have higher accuracy
- Different learners use different
  - Algorithms
  - Parameters
  - Representations (Modalities)
  - Training sets
  - Subproblems

Voting

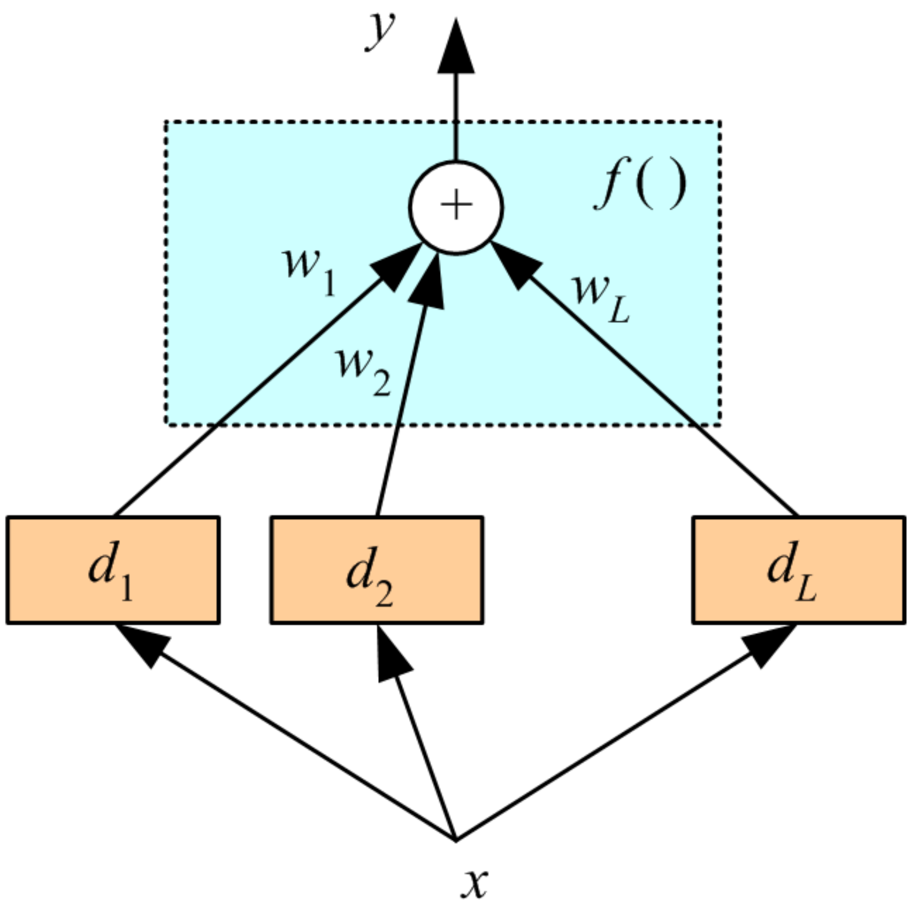
- Linear combination

$$y = \sum_{j=1}^{L} w_j d_j$$

$$w_j \geq 0 \text{ and } \sum_{j=1}^{L} w_j = 1$$

- Classification

$$y_i = \sum_{j=1}^{L} w_j d_{ji}$$



BAGGING

Ensemble methods

- A single decision tree does not perform well
- But, it is super fast
- What if we learn multiple trees?

We need to make sure they do not all just learn the same

Bagging

If we split the data in random different ways, decision trees give different results, **high variance.**

Bagging: Bootstrap **agg**regat**ing** is a method that result in low variance.

If we had multiple realizations of the data (or multiple samples) we could calculate the predictions multiple times and take the average of the fact that averaging multiple onerous estimations produce less uncertain results

Bagging

Say for each sample *b*, we calculate *$f^b(x)$*, then:

$$\hat{f}_{avg}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^b(x)$$

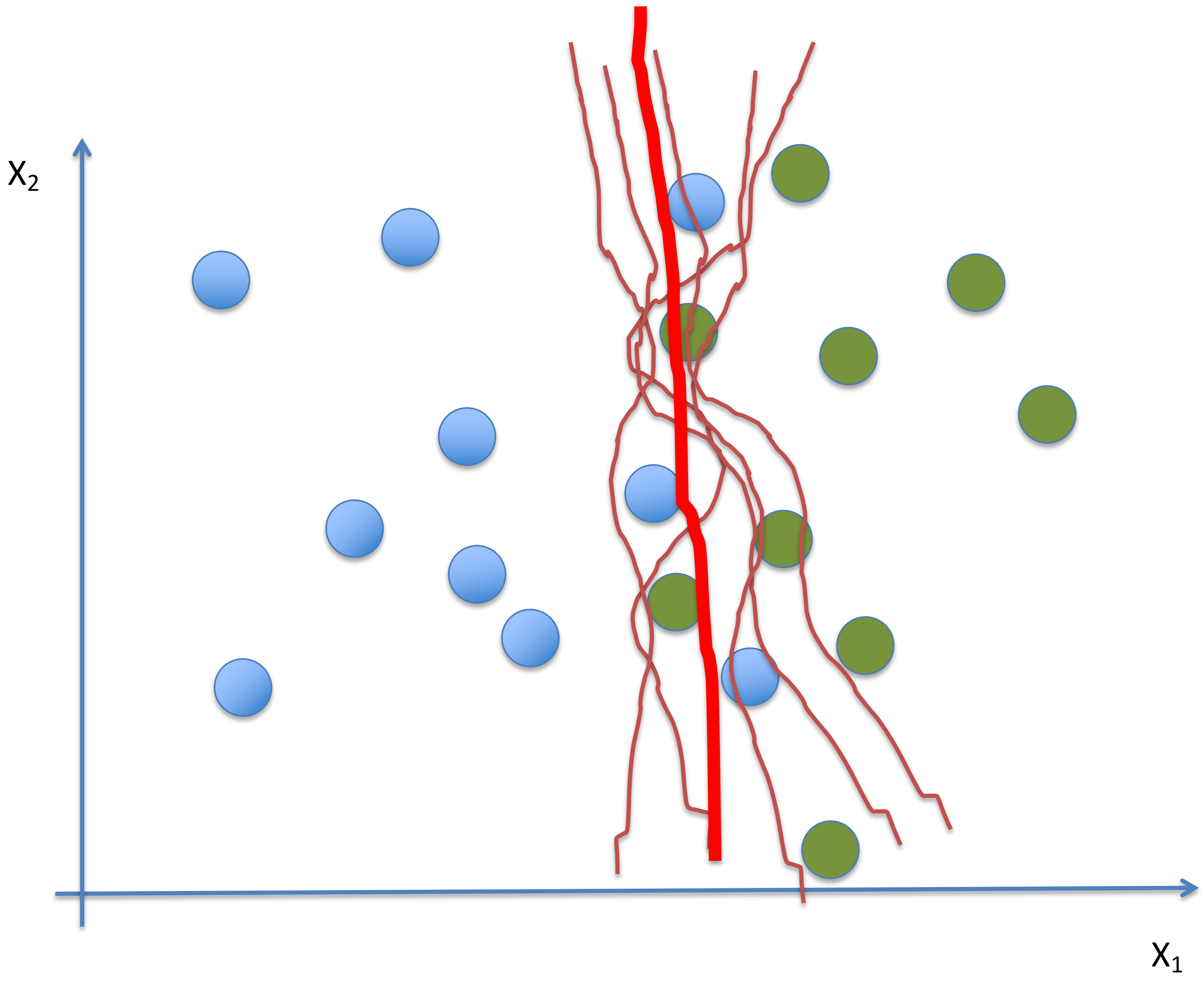
How?

Bootstrap

Construct B (hundreds of) trees (no pruning)

Learn a classifier for each bootstrap sample and average them

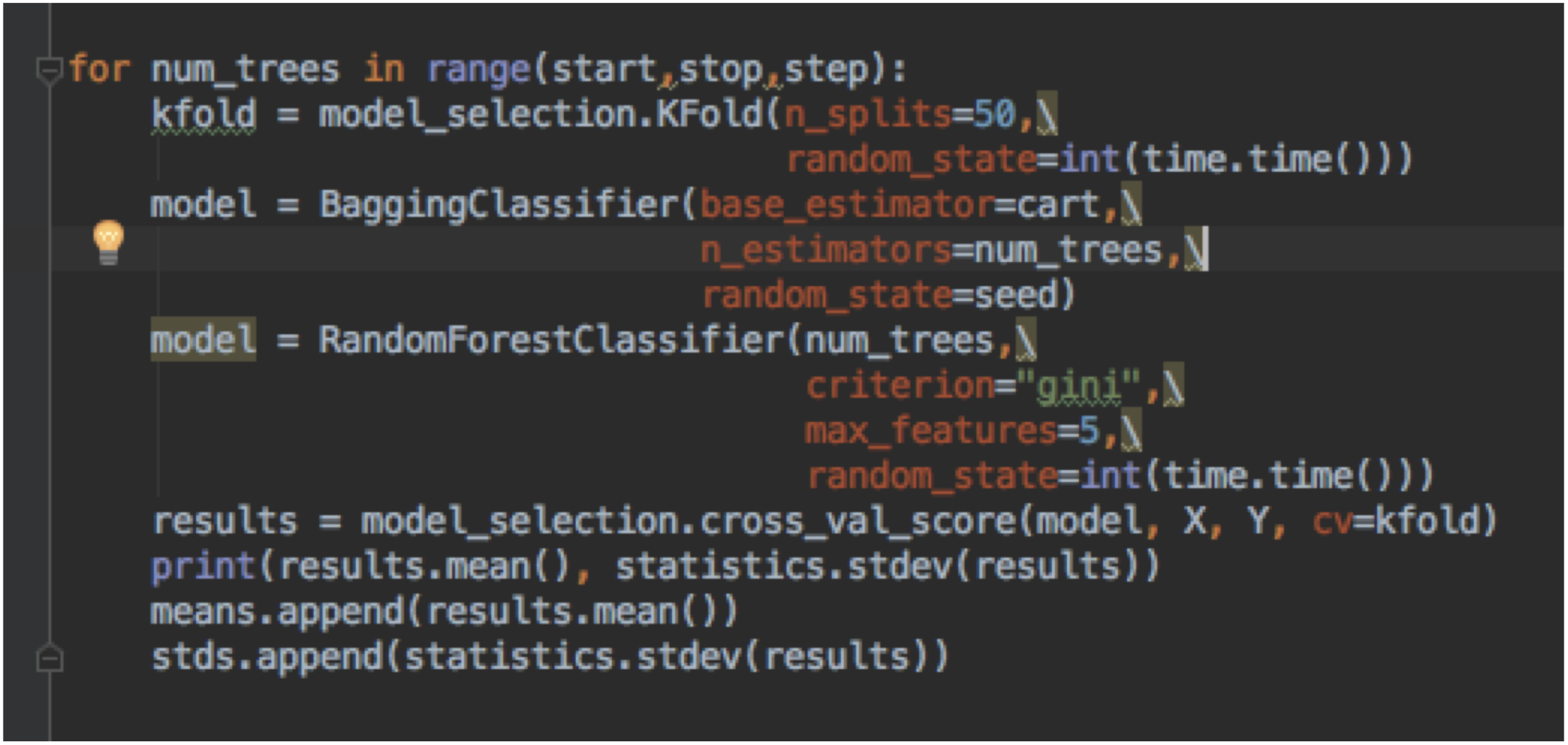
Very effective


X_2
X_1

Example

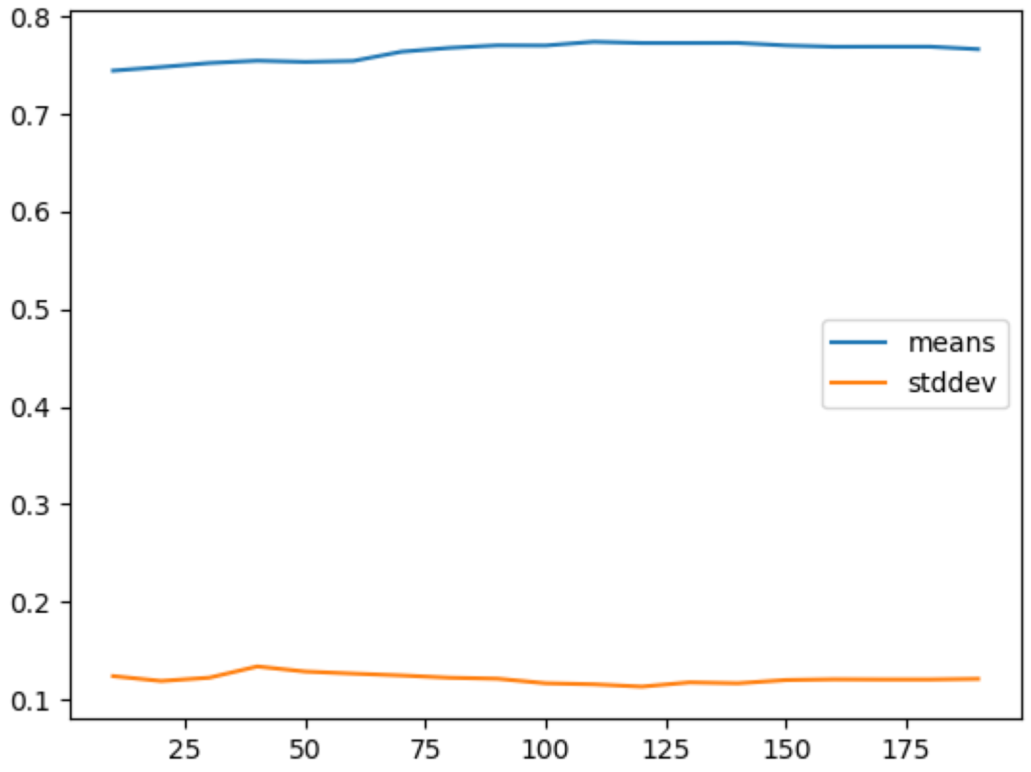
- Pima Indians Diabetes data:
- 768 examples, 8 features
- Features: 'preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age'

Example



```
for num_trees in range(start,stop,step):
    kfold = model_selection.KFold(n_splits=50,\
                                  random_state=int(time.time()))
    model = BaggingClassifier(base_estimator=cart,\
                              n_estimators=num_trees,\
                              random_state=seed)
    model = RandomForestClassifier(num_trees,\
                                   criterion="gini",\
                                   max_features=5,\
                                   random_state=int(time.time()))
    results = model_selection.cross_val_score(model, X, Y, cv=kfold)
    print(results.mean(), statistics.stdev(results))
    means.append(results.mean())
    stds.append(statistics.stdev(results))
```

Example



# trees

Out-of-Bag Error Estimation

- No cross validation?
- Remember, in bootstrapping we sample with replacement, and therefore **not all observations are used for each bootstrap sample**. On average 1/3 of them are not used!
- We call them out-of-bag samples (OOB)
- We can predict the response for the *i-th* observation using each of the trees in which that observation was OOB and do this for *n* observations
- Calculate overall OOB MSE or classification error

Bagging

- Reduces overfitting (variance)
- Normally uses one type of classifier
- Decision trees are popular
- Easy to parallelize

Bagging - issues

Each tree is identically distributed (i.d.)

➔ the expectation of the average of *B* such trees is the same as the expectation of any one of them

➔the bias of bagged trees is the same as that of the individual trees

i.d. and not i.i.d

Bagging - issues

An average of *B* i.i.d. random variables, each with variance σ^2, has variance*:* σ^2/B

If i.d. (identical but not independent) and pair correlation ρ is present, then the variance is:

$$\rho\,\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

As *B* increases the second term disappears but the first term remains

Why does bagging generate correlated trees?

Bagging - issues

Suppose that there is one very strong predictor in the data set, along with a number of other moderately strong predictors.

Then all bagged trees will select the strong predictor at the top of the tree and therefore all trees will look similar.

How do we avoid this?

RANDOM FORESTS

Random Forests

As in bagging, we build a number of decision trees on bootstrapped training samples each time a split in a tree is considered, a random sample of *m* predictors is chosen as split candidates from the full set of p predictors.

Note that if $m = p$, then this is bagging.

Random Forests

Random forests are popular. Leo Breiman’s and Adele Cutler maintains a random forest website where the software is freely available, and of course it is included in every ML/STAT package

http://www.stat.berkeley.edu/~breiman/RandomForests/

Random Forests Algorithm

```
For b = 1 to B:
    (a) Draw a bootstrap sample Z∗ of size $N$ from the training data.
    (b) Grow a random-forest tree to the bootstrapped data, by
recursively repeating the following steps for each terminal node of the
tree, until the minimum node size $n_{min}$ is reached.
        i. Select $m$ variables at random from the $p$ variables.
        ii. Pick the best variable/split-point among the $m$.
        iii. Split the node into two daughter nodes.
Output the ensemble of trees.
```

To make a prediction at a new point *x* we do:

For regression: average the results

For classification: majority vote

Random Forests Tuning

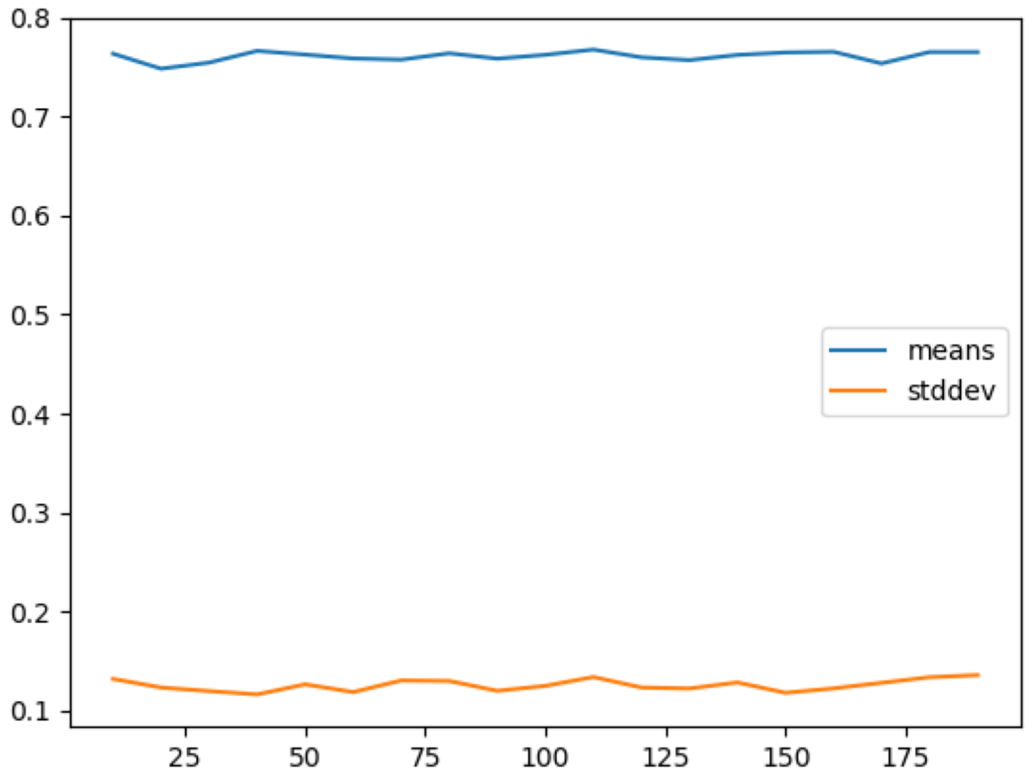
The inventors make the following recommendations:

- For classification, the default value for *m* is $\sqrt{p}$ and the minimum node size is one.
- For regression, the default value for m is *p/3* and the minimum node size is five.

In practice the best values for these parameters will depend on the problem, and they should be treated as tuning parameters.

Like with Bagging, we can use OOB and therefore RF can be fit in one sequence, with cross-validation being performed along the way. Once the OOB error stabilizes, the training can be terminated.

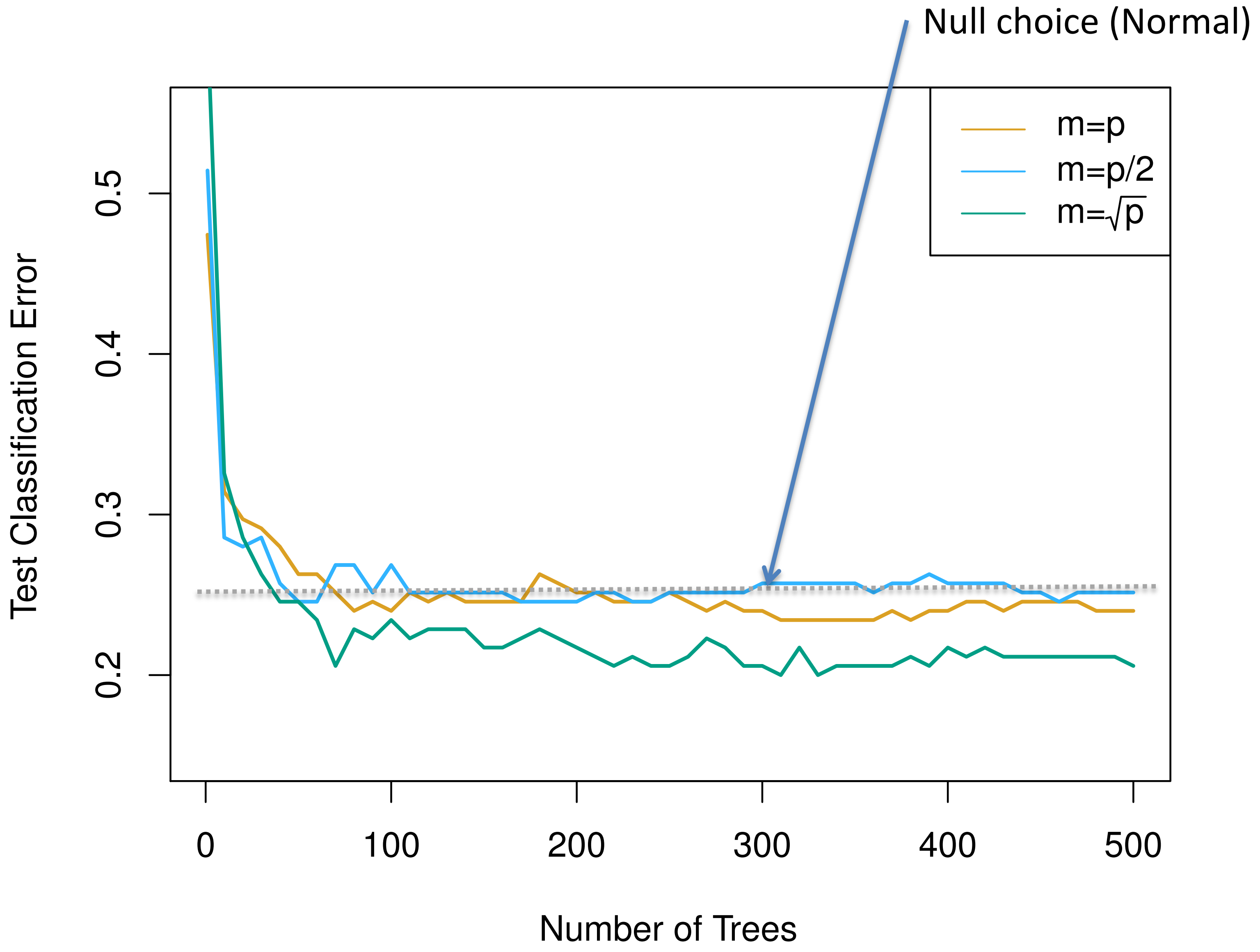
Example



Example

- 4,718 genes measured on tissue samples from 349 patients.
- Each gene has different expression
- Each of the patient samples has a qualitative label with 15 different levels: either normal or 1 of 14 different types of cancer.

Use random forests to predict cancer type based on the 500 genes that have the largest variance in the training set.


Null choice (Normal)
m=p
m=p/2
m=√p
Test Classification Error
0.2
0.3
0.4
0.5
Number of Trees
0
100
200
300
400
500

Random Forests Issues

When the number of variables is large, but the fraction of relevant variables is small, random forests are likely to perform poorly when *m* is small

Why?

Because:

At each split the chance can be small that the relevant variables will be selected

For example, with 3 relevant and 100 not so relevant variables the probability of any of the relevant variables being selected at any split is ~0.25

Can RF overfit?

Random forests “cannot overfit” the data wrt to number of trees.

Why?

The number of trees, *B* does not mean increase in the flexibility of the model