Data Mining

Lecture 6: Model Overfitting

Read Sections 4.4 – 4.5

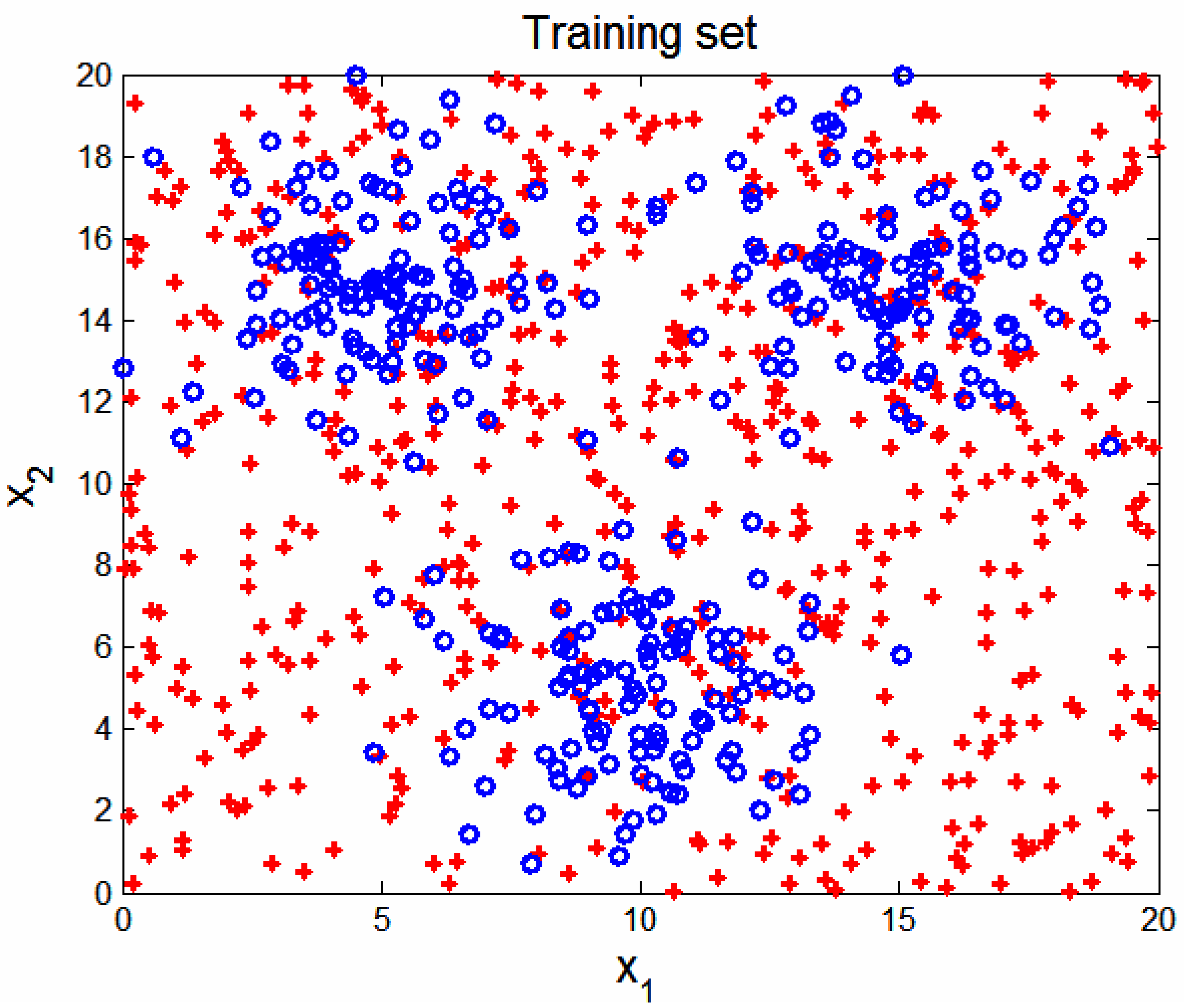
Classification Errors

- Training errors (apparent errors)
  - Errors committed on the training set

- Test errors
  - Errors committed on the test set

- Generalization errors
  - Expected error of a model over random selection of records from same distribution

Example Data Set



Two class problem:

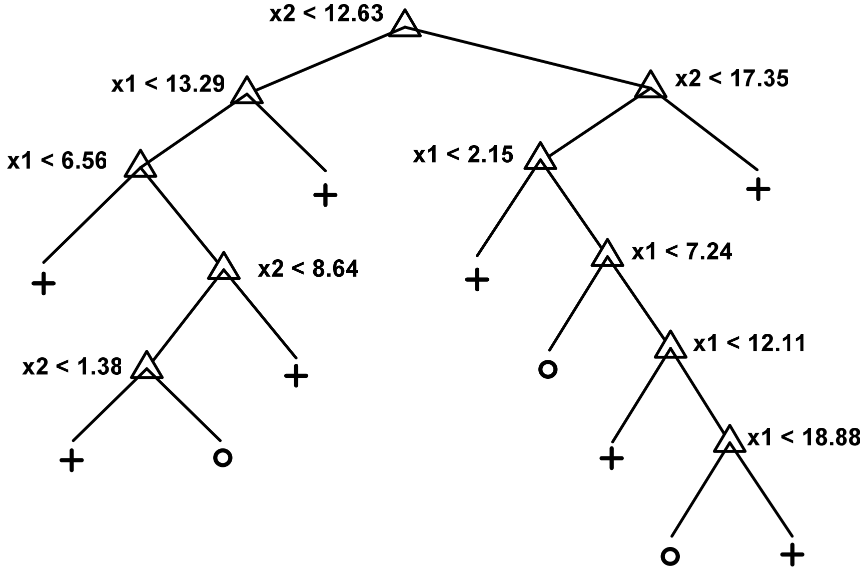
+, o

3000 data points (30% for training, 70% for testing)

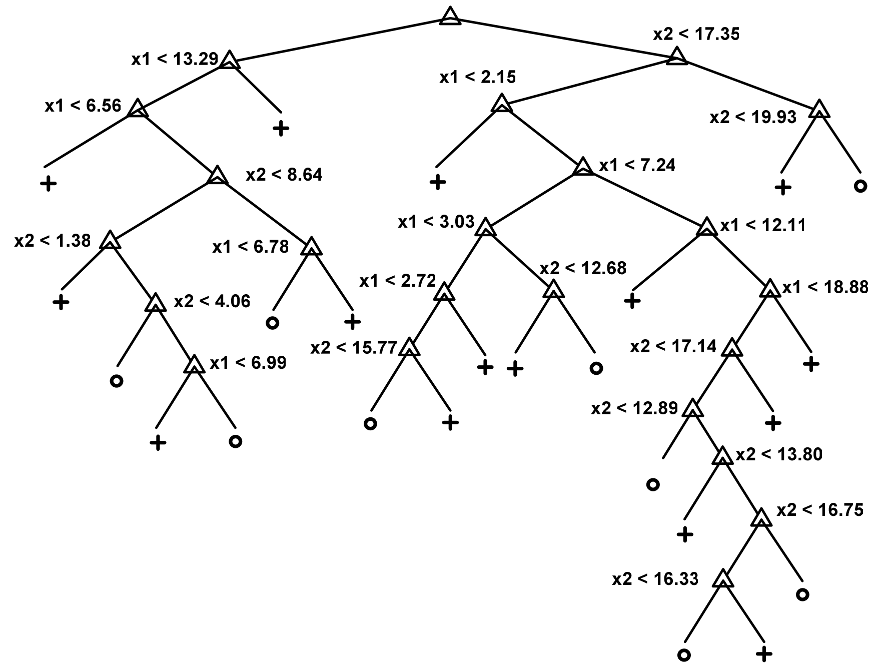
Data set for + class is generated from a uniform distribution

Data set for o class is generated from a mixture of 3 gaussian distributions, centered at (5,15), (10,5), and (15,15)

Decision Trees



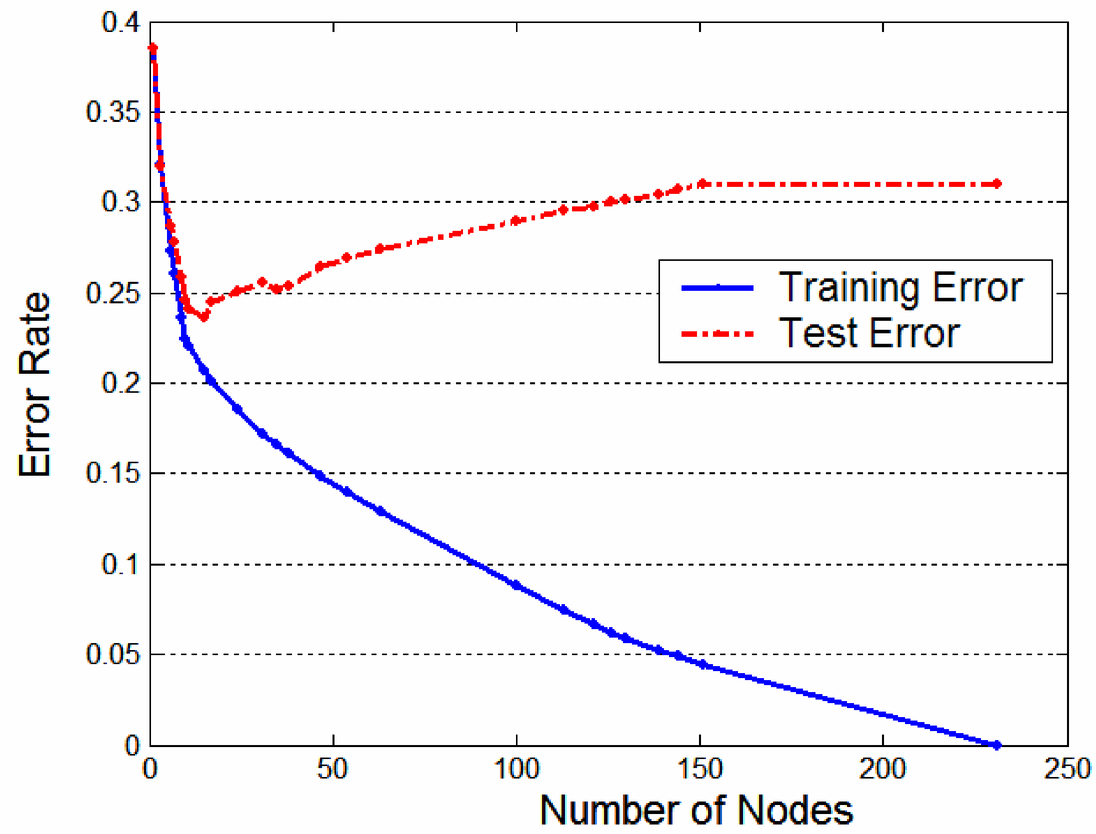
Decision Tree with 11 leaf nodes



Decision Tree with 24 leaf nodes

Which tree is better?

Model Overfitting



Underfitting: when model is too simple, both training and test errors are large

Overfitting: when model is too complex, training error is small but test error is large

Reasons for Model Overfitting

- Presence of Noise

- Lack of Representative Samples

- Multiple Comparison Procedure

Effect of Multiple Comparison Procedure

- Consider the task of predicting whether stock market will rise/fall in the next 10 trading days

- Random guessing:

  $P(correct) = 0.5$

- Make 10 random guesses in a row:

$$P(\# correct \geq 8) = \frac{\binom{10}{8} + \binom{10}{9} + \binom{10}{10}}{2^{10}} = 0.0547$$

Day 1	Up
Day 2	Down
Day 3	Down
Day 4	Up
Day 5	Down
Day 6	Down
Day 7	Up
Day 8	Up
Day 9	Up
Day 10	Down

Effect of Multiple Comparison Procedure

- Approach:
  - Get 50 analysts
  - Each analyst makes 10 random guesses
  - Choose the analyst that makes the most number of correct predictions

- Probability that at least one analyst makes at least 8 correct predictions

$$P(\#\,correct \geq 8) = 1 - (1 - 0.0547)^{50} = 0.9399$$

Effect of Multiple Comparison Procedure

- Many algorithms employ the following greedy strategy:
  - Initial model: M
  - Alternative model: M' = M $\cup$ γ,
    where γ is a component to be added to the model
    (e.g., a test condition of a decision tree)
  - Keep M' if improvement, Δ(M,M') > α

- Often times, γ is chosen from a set of alternative components, $\Gamma = \{\gamma_1, \gamma_2, \ldots, \gamma_k\}$

- If many alternatives are available, one may inadvertently add irrelevant components to the model, resulting in model overfitting

Notes on Overfitting

- Overfitting results in decision trees that are <u>more complex</u> than necessary

- Training error does not provide a good estimate of how well the tree will perform on previously unseen records

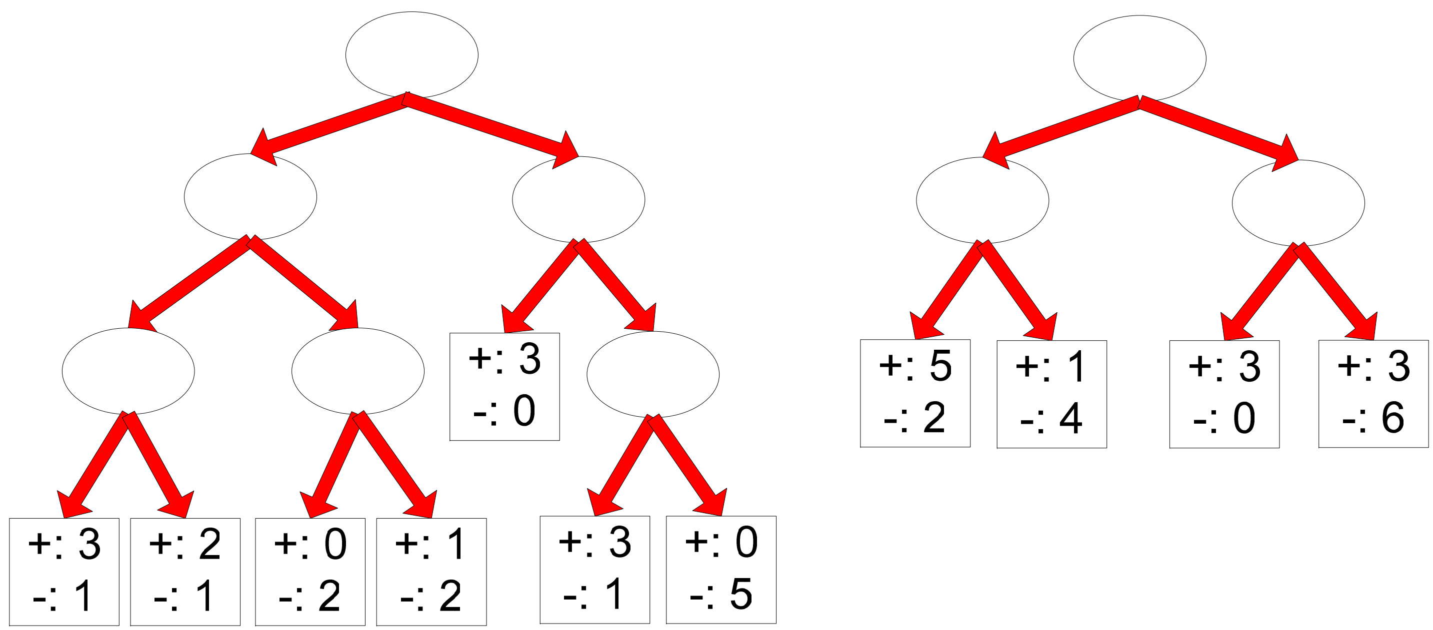
- Need new ways for estimating generalization errors

Estimating Generalization Errors

- Resubstitution Estimate
- Incorporating Model Complexity
- Use Validation Set
- Estimating Statistical Bounds

Resubstitution Estimate

- Using training error as an optimistic estimate of generalization error



Decision Tree, T_L Decision Tree, T_R

$e(T_L) = 4/24$

$e(T_R) = 6/24$

Incorporating Model Complexity

- Rationale: Occam's Razor
  - Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
  - A complex model has a greater chance of being fitted accidentally by errors in data
  - Therefore, one should include model complexity when evaluating a model

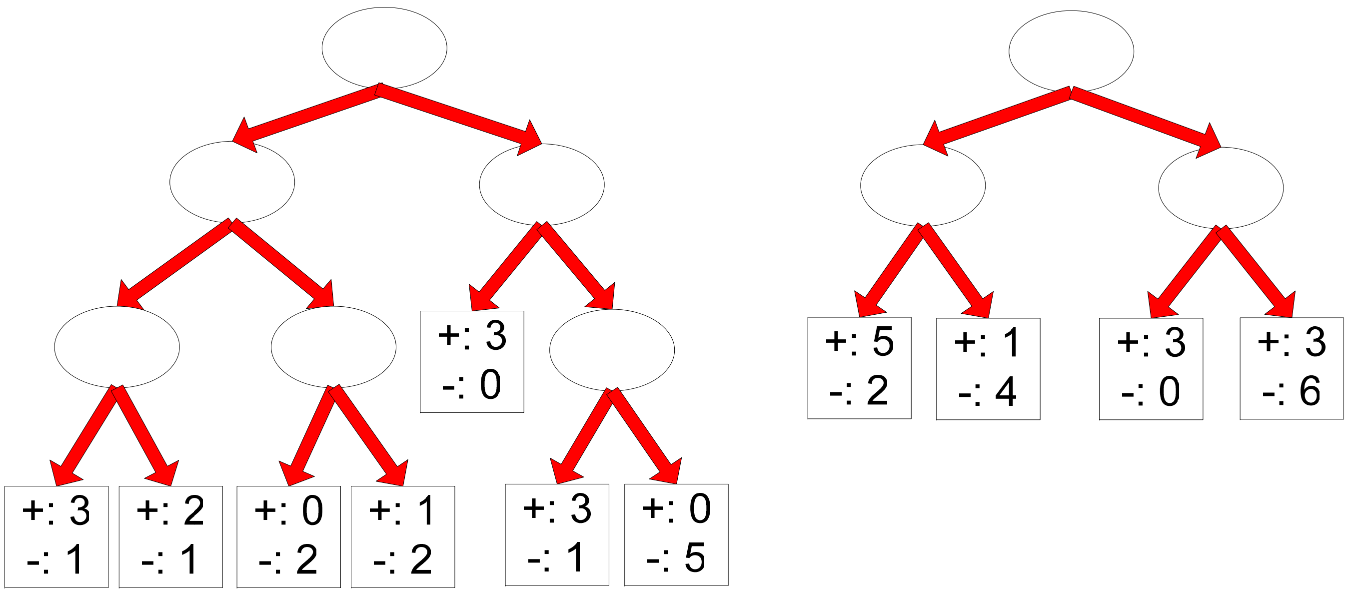
Pessimistic Estimate

- Given a decision tree node t
  - $n(t)$: number of training records classified by t
  - $e(t)$: misclassification error of node t
  - Training error of tree T:

$$e'(T) = \frac{\sum_i \left[e(t_i) + \Omega(t_i) \right]}{\sum_i n(t_i)} = \frac{e(T) + \Omega(T)}{N}$$

    - Ω: is the cost of adding a node
    - N: total number of training records

Pessimistic Estimate



Decision Tree, T_L

Decision Tree, T_R

$e(T_L) = 4/24$

$e(T_R) = 6/24$

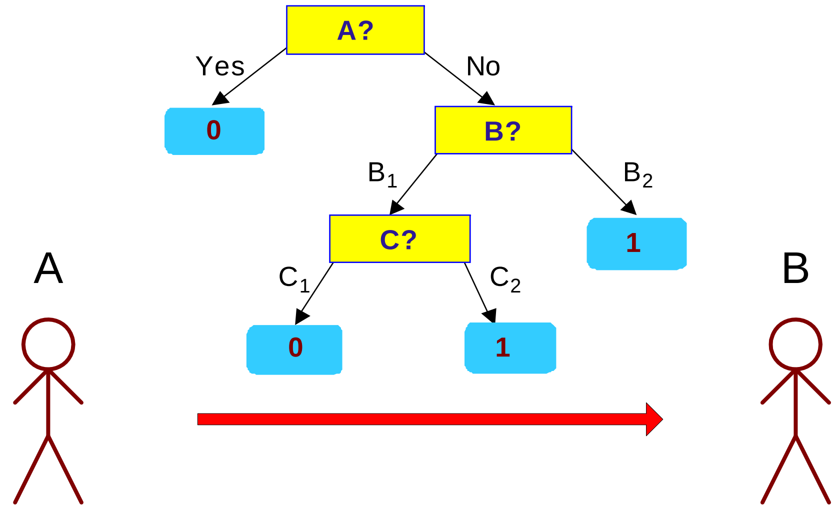
$\Omega = 1$

$e'(T_L) = (4 + 7 \times 1)/24 = 11/24 = 0.458$

$e'(T_R) = (6 + 4 \times 1)/24 = 10/24 = 0.417$

Minimum Description Length (MDL)

X	y
X_1	1
X_2	0
X_3	0
X_4	1
…	…
X_n	1



X	y
X_1	?
X_2	?
X_3	?
X_4	?
…	…
X_n	?

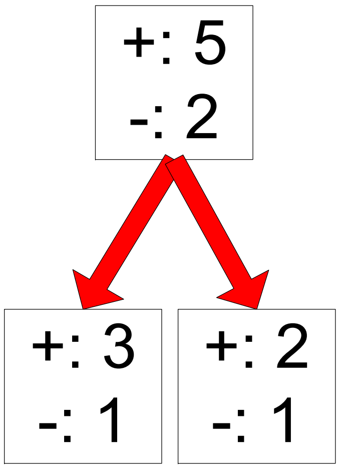
- Cost(Model,Data) = Cost(Data|Model) + Cost(Model)
  - Cost is the number of bits needed for encoding.
  - Search for the least costly model.
- Cost(Data|Model) encodes the misclassification errors.
- Cost(Model) uses node encoding (number of children) plus splitting condition encoding.

Using Validation Set

- Divide <u>training</u> data into two parts:
  - Training set:
    - use for model building
  - Validation set:
    - use for estimating generalization error
    - Note: validation set is not the same as test set

- Drawback:
  - Less data available for training

Estimating Statistical Bounds



$$e'(N,e,\alpha) = \frac{e + \frac{z_{\alpha/2}^2}{2N} + z_{\alpha/2}\sqrt{\frac{e(1-e)}{N} + \frac{z_{\alpha/2}^2}{4N^2}}}{1 + \frac{z_{\alpha/2}^2}{N}}$$

Before splitting: e = 2/7, e'(7, 2/7, 0.25) = 0.503

e'(T) = 7 $\times$ 0.503 = 3.521

After splitting:

e(T_L) = 1/4, e'(4, 1/4, 0.25) = 0.537

e(T_R) = 1/3, e'(3, 1/3, 0.25) = 0.650

e'(T) = 4 $\times$ 0.537 + 3 $\times$ 0.650 = 4.098

Therefore, do not split

Handling Overfitting in Decision Tree

- Pre-Pruning (Early Stopping Rule)
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of instances is less than some user-specified threshold
    - Stop if class distribution of instances are independent of the available features (e.g., using χ^2 test)
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).
    - Stop if estimated generalization error falls below certain threshold

Handling Overfitting in Decision Tree

- Post-pruning
  - Grow decision tree to its entirety
  - Subtree replacement
    - Trim the nodes of the decision tree in a bottom-up fashion
    - If generalization error improves after trimming, replace sub-tree by a leaf node
    - Class label of leaf node is determined from majority class of instances in the sub-tree
  - Subtree raising
    - Replace subtree with most frequently used branch

Example of Post-Pruning

Class = Yes	20
Class = No	10
Error = 10/30	

Training Error (Before splitting) = 10/30

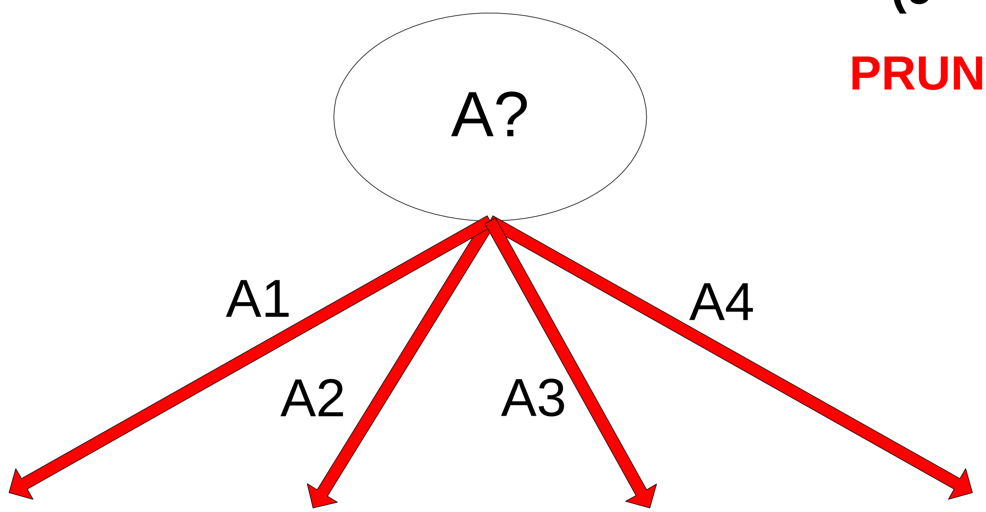
Pessimistic error = (10 + 0.5)/30 = 10.5/30

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

= (9 + 4 $\times$ 0.5)/30 = 11/30

PRUNE!



A1		A2		A3		A4	
Class = Yes	8	Class = Yes	3	Class = Yes	4	Class = Yes	5
Class = No	4	Class = No	4	Class = No	1	Class = No	1

Examples of Post-pruning

Decision Tree:

```
depth = 1 :
|  breadth > 7 : class 1
|  breadth <= 7 :
|  |  breadth <= 3 :
|  |  |  ImagePages > 0.375 : class 0
|  |  |  ImagePages <= 0.375 :
|  |  |  |  totalPages <= 6 : class 1
|  |  |  |  totalPages > 6 :
|  |  |  |  |  breadth <= 1 : class 1
|  |  |  |  |  breadth > 1 : class 0
|  |  width > 3 :
|  |  |  MultiIP = 0:
|  |  |  |  ImagePages <= 0.1333 : class 1
|  |  |  |  ImagePages > 0.1333 :
|  |  |  |  |  breadth <= 6 : class 0
|  |  |  |  |  breadth > 6 : class 1
|  |  |  MultiIP = 1:
|  |  |  |  TotalTime <= 361 : class 0
|  |  |  |  TotalTime > 361 : class 1
depth > 1 :
|  MultiAgent = 0:
|  |  depth > 2 : class 0
|  |  depth <= 2 :
|  |  |  MultiIP = 1: class 0
|  |  |  MultiIP = 0:
|  |  |  |  breadth <= 6 : class 0
|  |  |  |  breadth > 6 :
|  |  |  |  |  RepeatedAccess <= 0.0322 : class 0
|  |  |  |  |  RepeatedAccess > 0.0322 : class 1
|  MultiAgent = 1:
|  |  totalPages <= 81 : class 0
|  |  totalPages > 81 : class 1
```

Subtree Raising

Subtree Replacement

Simplified Decision Tree:

```
depth = 1 :
|  ImagePages <= 0.1333 : class 1
|  ImagePages > 0.1333 :
|  |  breadth <= 6 : class 0
|  |  breadth > 6 : class 1
depth > 1 :
|  MultiAgent = 0: class 0
|  MultiAgent = 1:
|  |  totalPages <= 81 : class 0
|  |  totalPages > 81 : class 1
```

Evaluating Performance of Classifier

- Model Selection
  - Performed during model building
  - Purpose is to ensure that model is not overly complex (to avoid overfitting)
  - Need to estimate generalization error

- Model Evaluation
  - Performed after model has been constructed
  - Purpose is to estimate performance of classifier on previously unseen data (e.g., test set)

Methods for Classifier Evaluation

- Holdout
  - Reserve k% for training and (100-k)% for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n
- Bootstrap
  - Sampling with replacement
  - .632 bootstrap:

$$acc_{boot} = \frac{1}{b}\sum_{i=1}^{b}\left(0.632 \times acc_i + 0.368 \times acc_s\right)$$