Data Mining



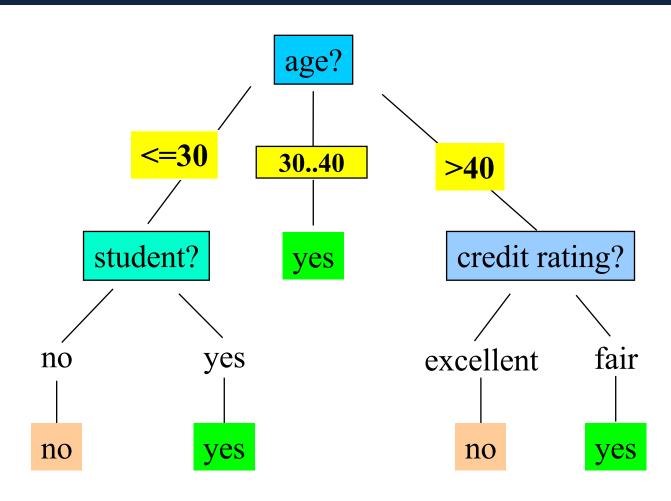
Classification Decision Tree

An Example Dataset

This follows an example from Quinlan's ID3

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
3140	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no

A Decision Tree for "buys_computer"



Classification by Decision Tree Induction

- Decision tree
 - A flow-chart-like tree structure
 - Internal node denotes a test on an attribute
 - Branch represents an outcome of the test
 - Leaf nodes represent class labels or class distribution
- Decision tree generation consists of two phases
 - Tree construction
 - At start, all the training examples are at the root
 - Partition examples recursively based on selected attributes
 - Tree pruning
 - Identify and remove branches that reflect noise or outliers
- Use of decision tree: Classifying an unknown sample
 - Test the attribute values of the Query data against the decision tree

Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
 - Tree is constructed in a top-down recursive divide-and-conquer manner
 - At start, all the training examples are at the root
 - Attributes are categorical (if continuous-valued, they are discretized in advance)
 - Examples are partitioned recursively based on selected attributes
 - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
 - All samples for a given node belong to the same class
 - There are no remaining attributes for further partitioning majority voting is employed for classifying the leaf
 - There are no samples left

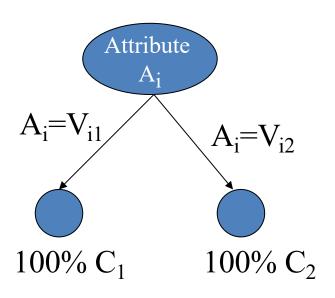
How to select the best attribute?

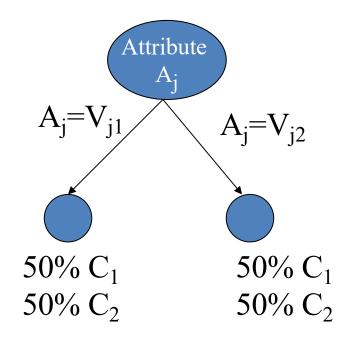
- Random, or Least values or Most values
- Information gain: choose attribute with largest expected information gain, i.e., choose attribute that will result in the smallest expected size of the sub-tree rooted at its children.
 - ID3 (Quinlan 1987)
 - Occam's Razor: The simplest explanation that is consistent with all the observations is the best -> smallest decision tree that correctly classifies all of the training examples is the best

Attribute Selection Measure

- Information gain (ID3)
 - All attributes are assumed to be categorical
 - Can be modified for continuous-valued attributes
 (C4.5 deals with continuous-valued attributes)
- Gini index (IBM IntelligentMiner)
 - All attributes are assumed continuous-valued
 - Assume there exist several possible split values for each attribute
 - May need other tools, such as clustering, to get the possible split values
 - Can be modified for categorical attributes

Attribute Selection





Which attribute is better at splitting up the data?

Information Gain

X = College Major

Y = Likes "Gladiator"

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
History	No
Math	Yes

Definition of Information Gain:

IG(Y|X) = I must transmit Y. How many bits on average would it save me if both ends of the line knew X?

$$IG(Y|X) = H(Y) - H(Y|X)$$

The more predictable Y is given X, the smaller H(Y|X), thus the higher the information gain, IG(Y|X)

Entropy

- Shannon entropy: quantifies the expected value of the information contained in a message.
 - Claude E. Shannon in his 1948 paper "A Mathematical Theory of Communication".
 - The information conveyed by a message (and number of bits required to convey the message) depends on its probability and can be measured in bits as minus the logarithm to base 2 of that probability.

$$-\log_2 p_j$$

 P_i : the probability of a message

Entropy

- Suppose we are to convey the following messages, each has a different probability:
 - High (100%), Medium (50%), Low (25%)
- How much information (in bits) is conveyed by selecting to send the message that has "High" probability?
- What is the expected information conveyed if we are to select any of the three messages to send?
 - → Entropy (H)=

Entropy used in Classification

Suppose attribute X can have one of m values... V_{1} , V_{2} , ... V_{m}

$$P(X=V_1)=p_1$$

$$P(X=V_2)=p_2$$

$$P(X=V_m)=p_m$$

What's the expected number of bits needed to transmit a value randomly drawn from X's distribution?

$$H(X) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 - \dots - p_m \log_2 p_m$$
$$= -\sum_{j=1}^m p_j \log_2 p_j$$

H(X) = The entropy of X

- "High Entropy" means X is from a uniform (boring) distribution
- "Low Entropy" means X is from varied (peaks and valleys) distribution

Attribute Selection

A message may be coded using 4 characters:

C1: 50%

C2: 25%

C3: 12.5%

C4: 12.5%

How about this set?

C1: 50%

C2: 0%

C3: 50%

C4: 0%

Encoding each character requires -log₂ P(C_k) bits of information

C1: $0.5 = 2^{-1}$ \rightarrow 1 bit

C2: $0.25 = 2^{-2}$ \Rightarrow 2 bits

C3: $0.125 = 2^{-3}$ \rightarrow 3 bits

C4: $0.125 = 2^{-3}$ \rightarrow 3 bits

H(C)=(0.5*1+0.25*2+0.125*3+0.125*3) = 1.75

Entropy - General Case

A histogram of the frequency distribution of values of X would be flat

A histogram of the frequency distribution of values of X would have many lows and one or two highs

H(X) = The entropy of X

- "High Entropy" means X is from a uniform (boring) distribution
- "Low Entropy" means X is from varied (peaks and valleys) distribution

Entropy for Attribute Selection

The expected encoding of a class C_k:

$$P(C_k) \cdot (-\log_2 P(C_k))$$

Expected encoding of one child node containing

K classes is:
$$H(\text{node with K classes}) = \sum_{k=1}^{K} P(C_k) \cdot (-\log_2 P(C_k))$$

 For an attribute A_i, having J different values, the expected encoding of all child nodes resulting from selecting this attribute is:

$$H(\text{J child nodes}) = \sum_{j=1}^{J} P(A_i = V_{ij}) \cdot \sum_{k=1}^{K} P(C_k \mid A_i = V_{ij}) (-\log_2 P(C_k \mid A_i = V_{ij}))$$

Maximize information gain

Information Gain=H(parent node) - H(J child nodes)

$$= \sum_{k=1}^{K} P(C_k) \cdot (-\log_2 P(C_k)) - (\sum_{j=1}^{J} P(A_i = V_{ij}) \cdot \sum_{k=1}^{K} P(C_k \mid A_i = V_{ij}) (-\log_2 P(C_k \mid A_i = V_{ij}))$$

- Use Information gain for attribute selection:
 - The reduction in the expected number of encoding for all child nodes formed with the current attribute
 - The larger the reduction, the higher the gain.
 - Select the best attribute by computing the information gain of all attributes that are currently available, pick the one that generates the highest gain

Information Gain for Attribute Selection

Suppose you are trying to predict whether someone is going to live past 80 years. From historical data you might find...

- •IG(LongLife | HairColor) = 0.01
- •IG(LongLife | Smoker) = 0.2
- •IG(LongLife | Gender) = 0.25
- •IG(LongLife | LastDigitOfSSN) = 0.00001

Which attribute best predicts the longevity?

Practice Question

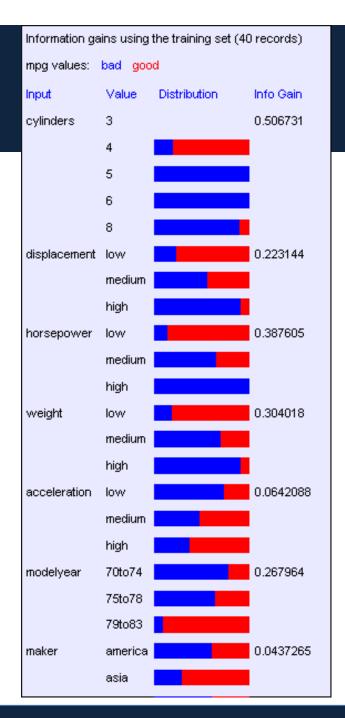
Given the following data, which attribute should be selected to divide the data and build the first level of the decision tree?

Object	Color	Shape	Size	Class
D1	Red	Square	Big	+
D2	Blue	Square	Big	+
D3	Red	Round	Small	
D4	Green	Square	Small	
D5	Red	Round	Big	+
D6	Green	Square	Big	

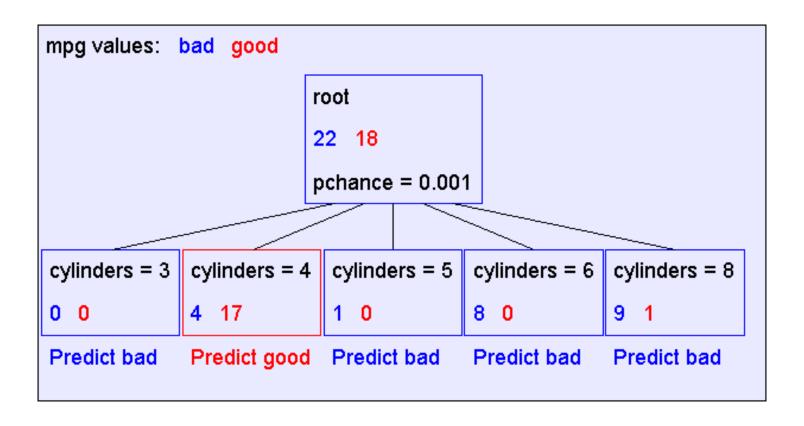
A small dataset: Miles Per Gallon

mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low	medium	low	medium	70to74	asia
bad	4	low	medium	low	low	70to74	asia
bad	8	high	high	high	low	75to78	america
:	:	:	:	:	:	:	:
:	:		:	:	:	:	:
:	:	:	:	:	:	:	:
bad	8	high	high	high	low	70to74	america
good	8	high	medium	high	high	79to83	america
bad	8	high	high	high	low	75to78	america
good	4	low	low	low	low	79to83	america
bad	6	medium	medium	medium	high	75to78	america
good	4	medium	low	low	low	79to83	america
good	4	low	low	medium	high	79to83	america
bad	8	high	high	high	low	70to74	america
good	4	low	medium	low	medium	75to78	europe
bad	5	medium	medium	medium	medium	75to78	europe

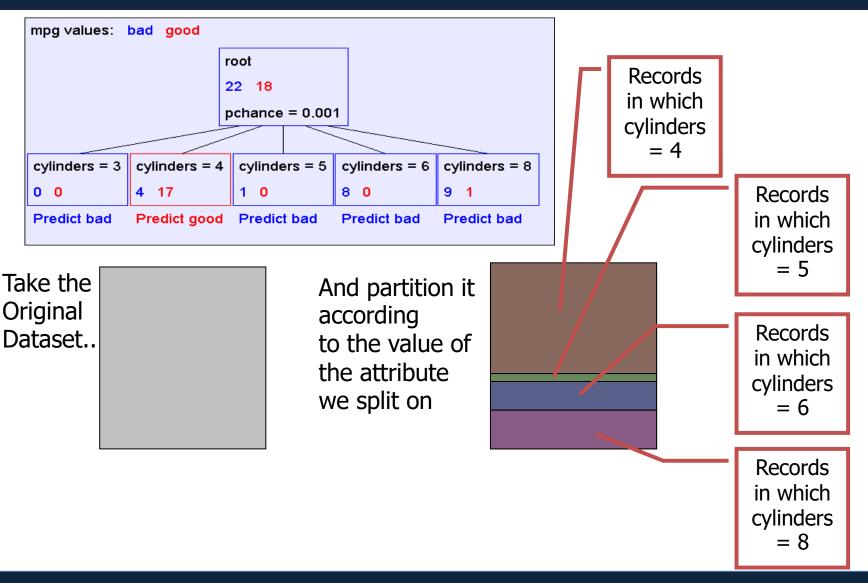
Look at all the information gains...



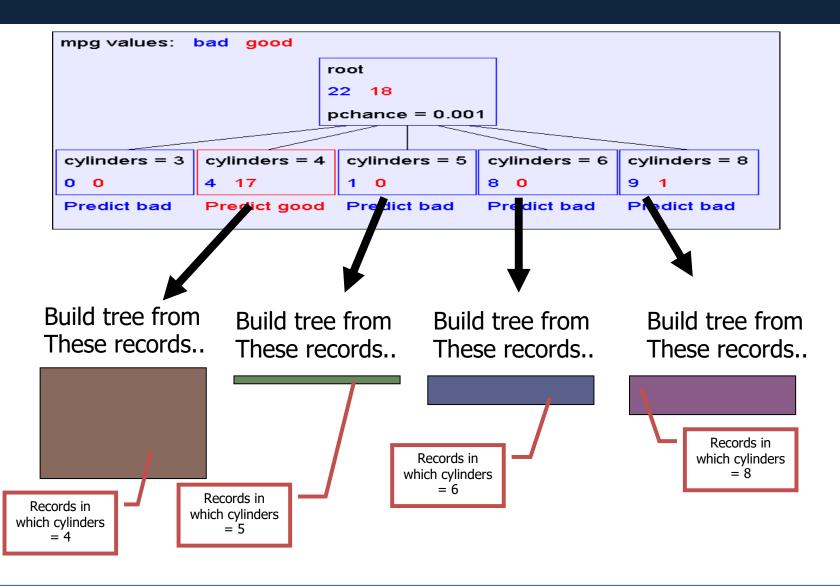
A Decision Stump



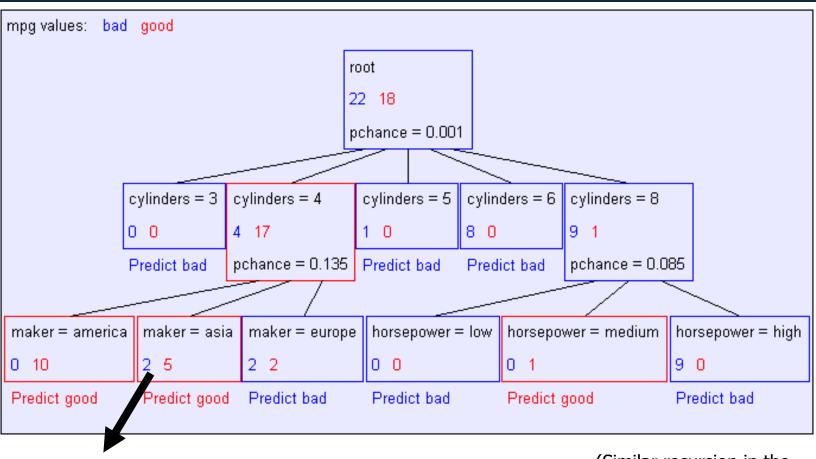
Recursion Step



Recursion Step

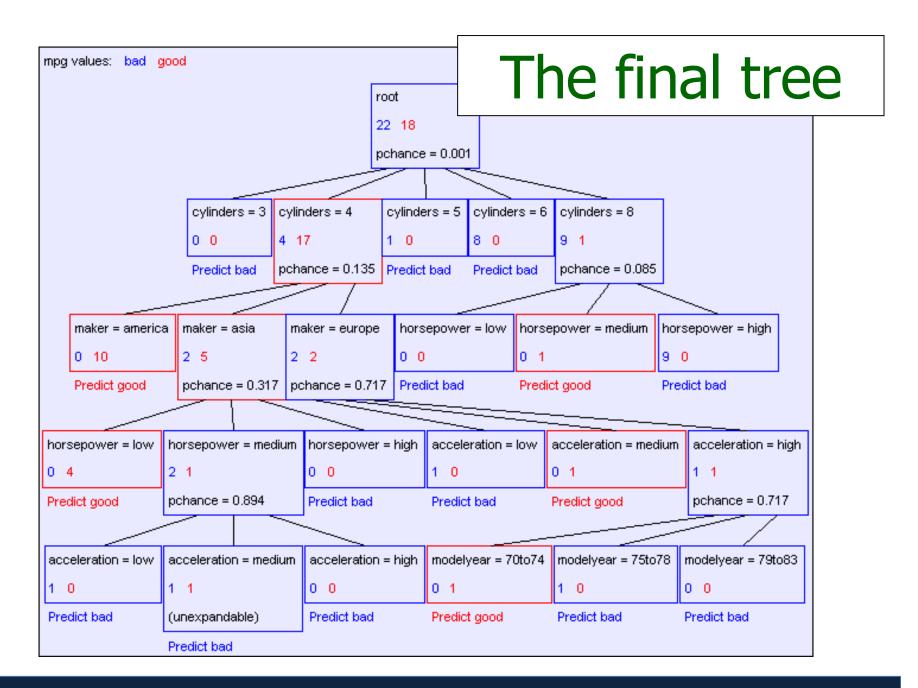


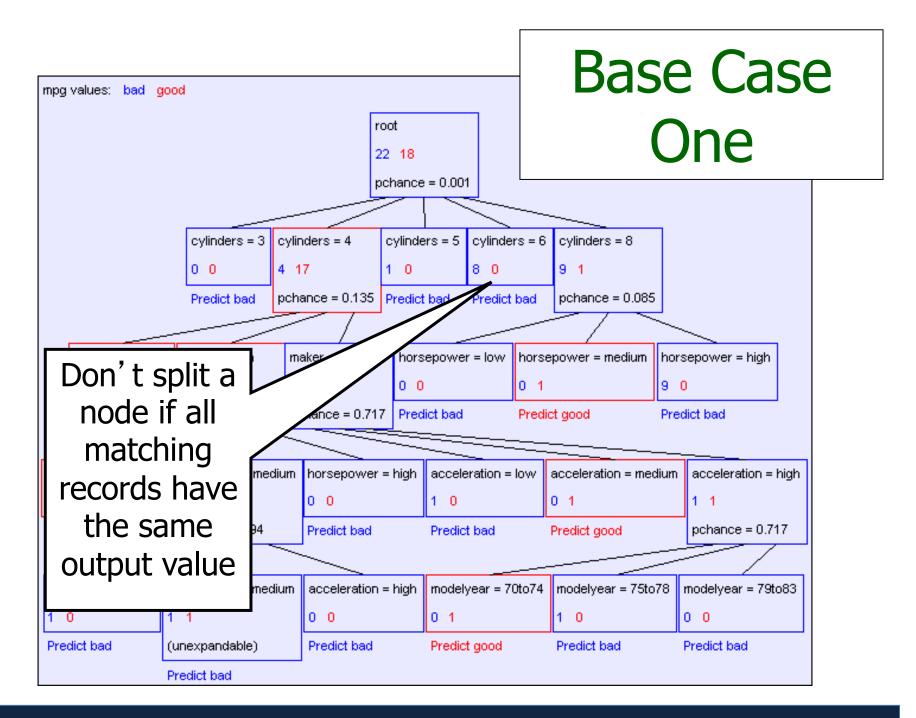
Second level of tree

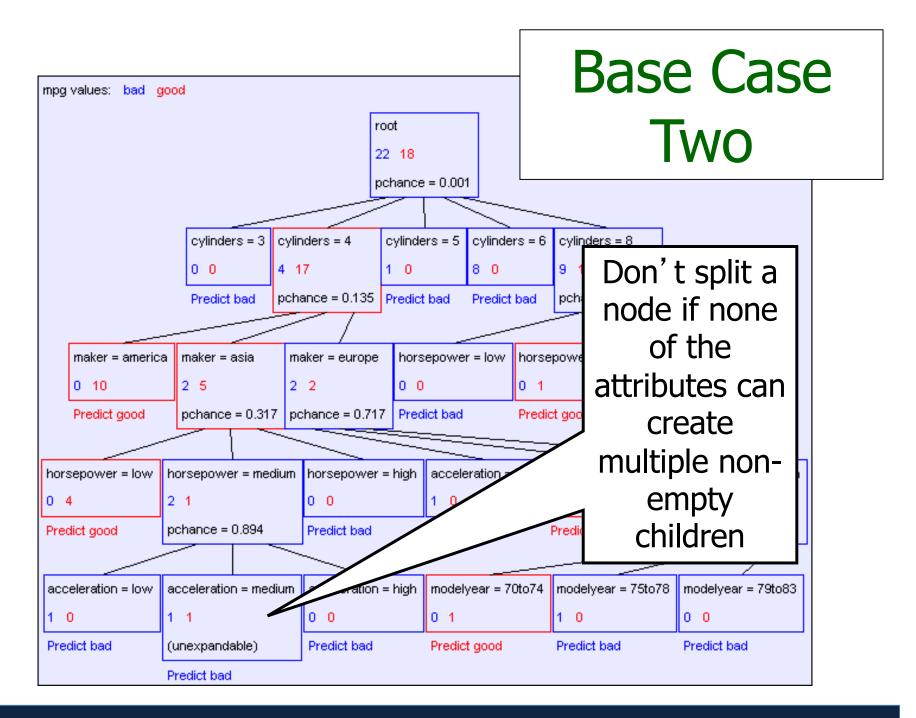


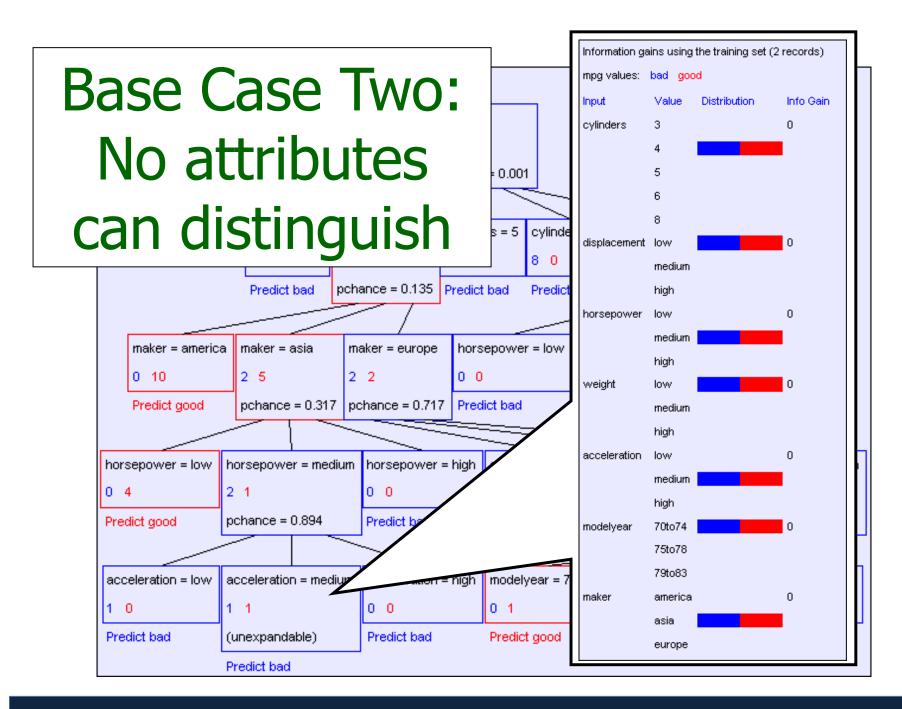
Recursively build a tree from the seven records in which there are four cylinders and the maker was based in Asia

(Similar recursion in the other cases)



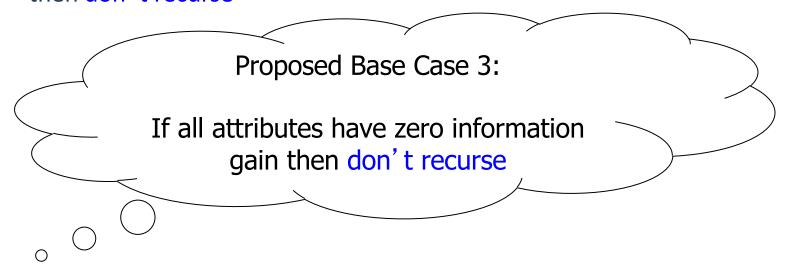






Base Cases: An idea

- Base Case One: If all records in current data subset have the same output then don't recurse
- Base Case Two: If all records have exactly the same set of input attributes then don't recurse



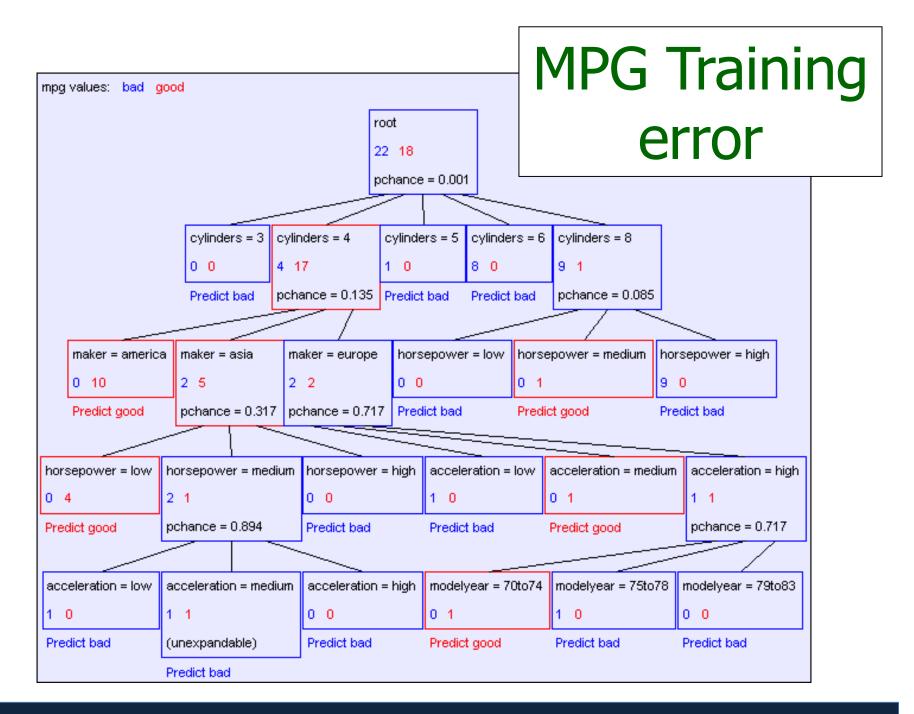
• Is this a good idea?

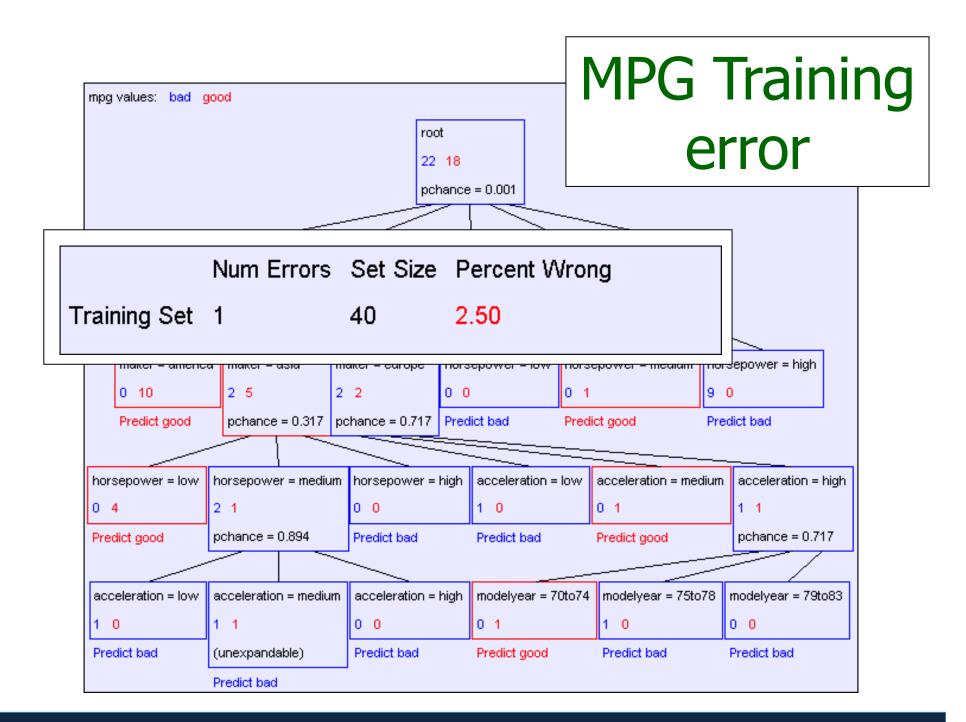
Decision Tree Algorithm

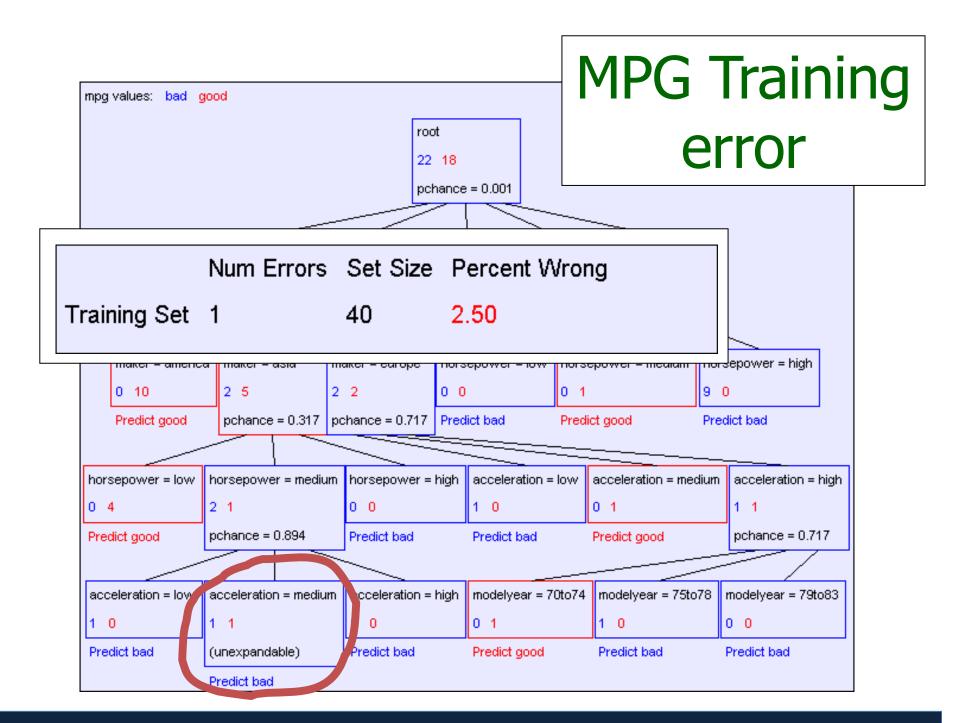
```
function decision-tree-learning (examples, attributes, default)
begin
   if empty(examples) then return (default)
   else if same-classification(example) then return the classification
   else if can not differentiate examples then return majority-classification(examples)
   else
     best ←choose-attribute(attributes, examples)
          tree ← a new decision tree with root test best
     for each value v of attribute best do
     begin
               v-examples \leftarrow subset of examples with best = v
               subtree ← decision-tree-learning (v-examples, attribute-best,
                                                  majority-classification(examples))
               add a branch from tree to subtree with arc labeled v
     end
     return (tree)
end
```

Training Set Error

- For each record, follow the decision tree to see what it would predict
 - For what number of records does the decision tree's prediction disagree with the true value in the database?
- This quantity is called the training set error. The smaller the better.





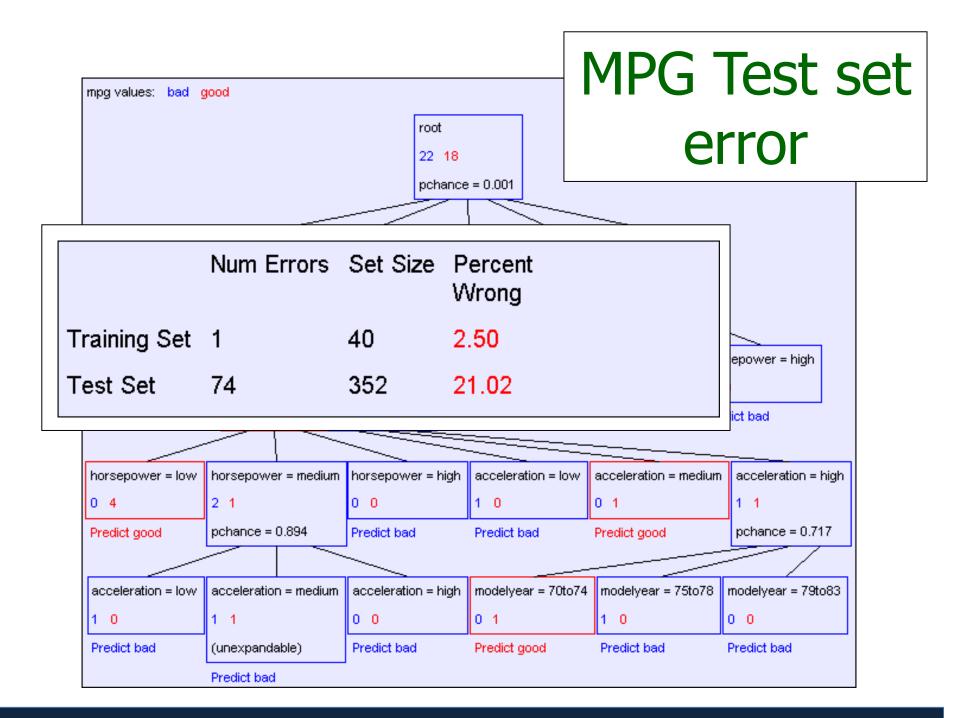


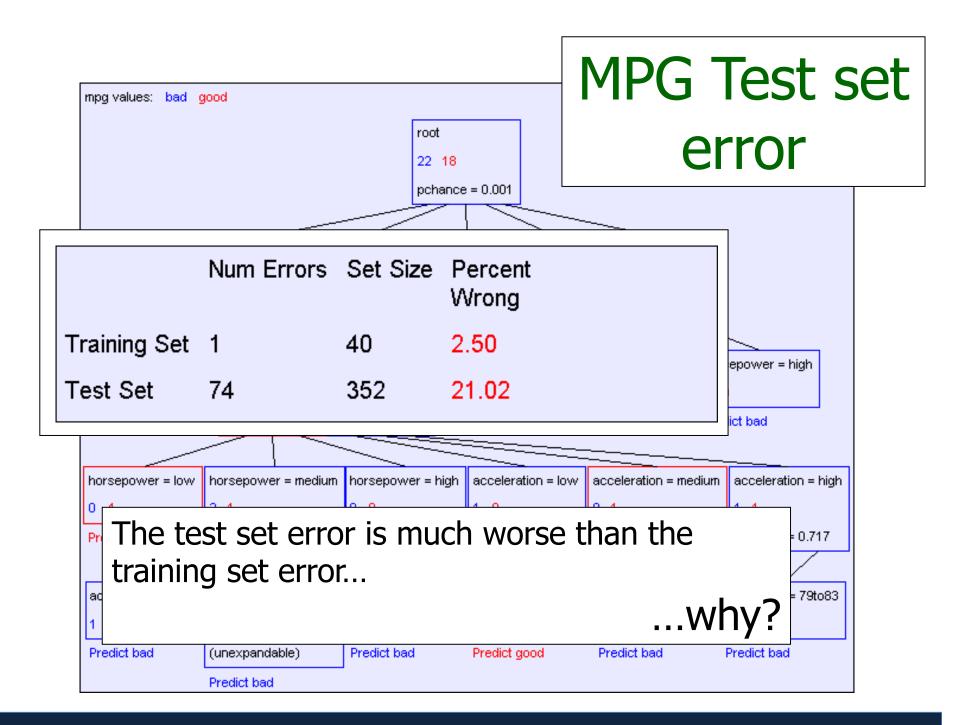
Why are we doing this learning?

- It is not usually in order to predict the training data's output on data we have already seen.
- It is more commonly in order to predict the output value for future data we have not yet seen.

Test Set Error

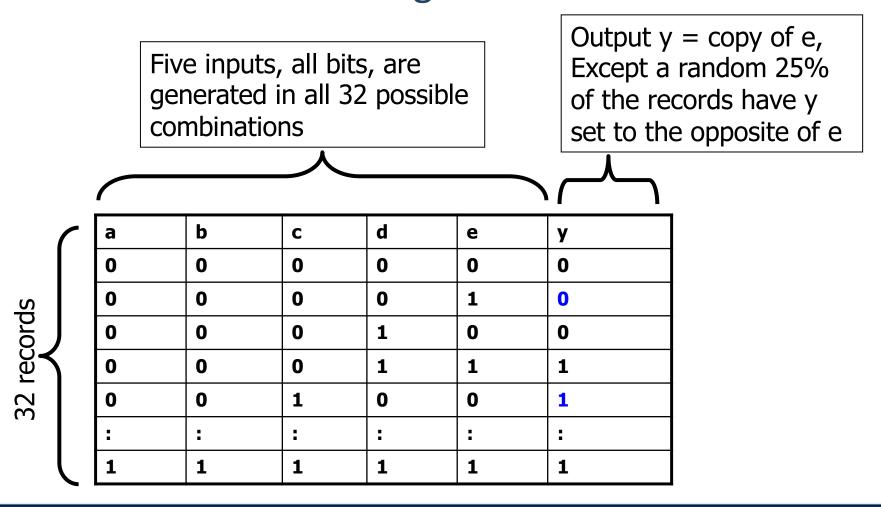
- Suppose we are forward thinking.
- We hide some data away when we learn the decision tree.
- But once learned, we see how well the tree predicts that data.
- This is a good simulation of what happens when we try to predict future data.
- And it is called Test Set Error.





An artificial example

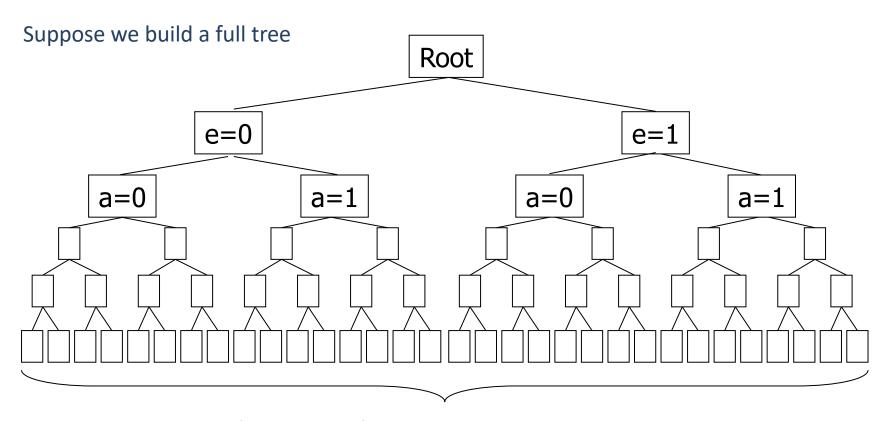
We'll create a training dataset



In our artificial example

- Suppose someone generates a test set according to the same method.
- The test set is identical, except that some of the y's will be different.
 - Some y's that were corrupted in the training set will be uncorrupted in the test set.
 - Some y's that were uncorrupted in the training set will be corrupted in the test set.

Building a tree with the training set



25% of these leaf node labels will be corrupted

Training set error for our artificial tree

All the leaf nodes contain exactly one record and so...

We would have a training set error of zero
 Accuracy 100%

Testing the tree with the test set

	1/4 of the tree nodes are corrupted	3/4 are fine
1/4 of the test set records are corrupted	1/16 of the test set will be correctly predicted for the wrong reasons	3/16 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	3/16 of the test predictions will be wrong because the tree node is corrupted	9/16 of the test predictions will be fine

In total, we expect to be wrong on 3/8 of the test set predictions

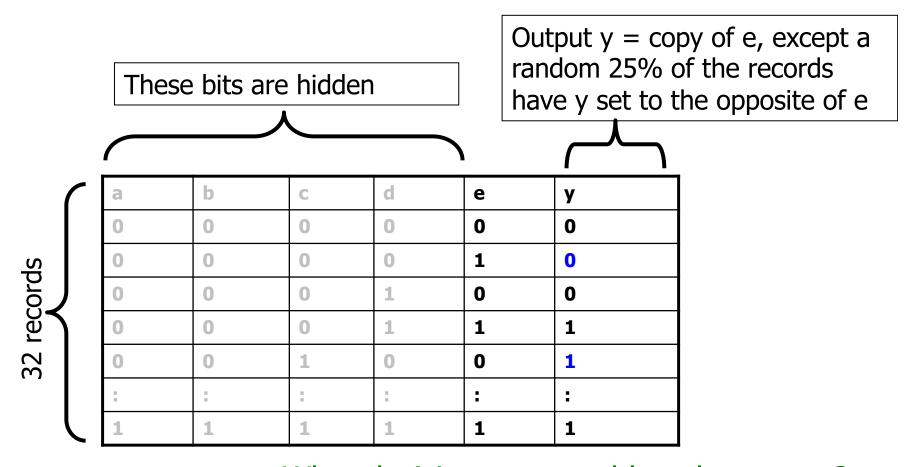
Accuracy: 62.5%

What's this example shown us?

- This explains the discrepancy between training and test set error
- But more importantly... ...it indicates there's something we should do about it if we want to predict well on future data.

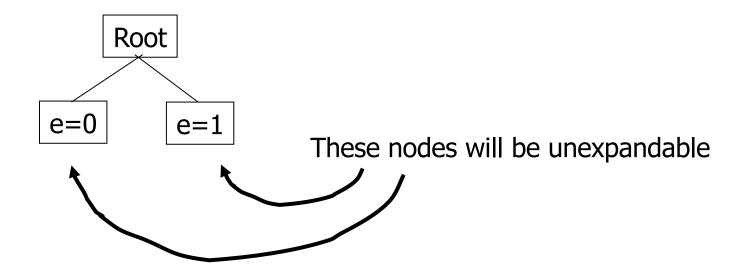
Suppose we had less data

Let's not look at the irrelevant bits

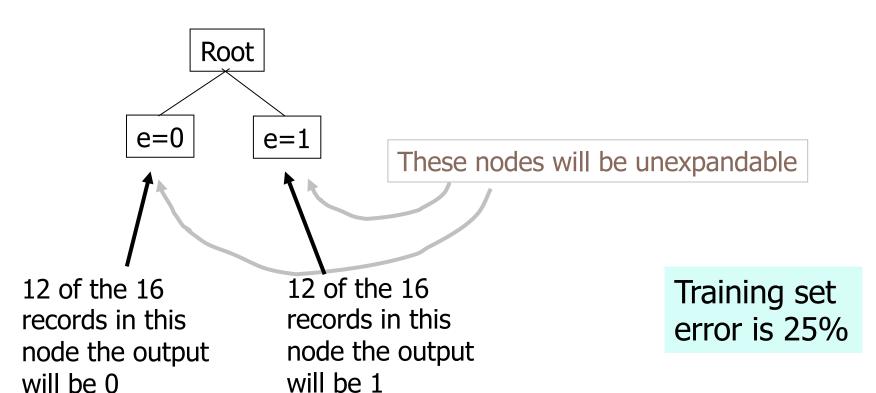


What decision tree would we learn now?

Without access to the irrelevant bits...



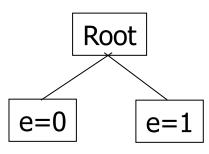
Without access to the irrelevant bits...



So this will almost certainly predict 0

So this will almost certainly predict 1

Without access to the irrelevant bits...



	almost certainly none of the tree nodes are corrupted	almost certainly all are fine
1/4 of the test set records are corrupted	n/a	1/4 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	n/a	3/4 of the test predictions will be fine

In total, we expect to be wrong on only 1/4 of the test set predictions

Training set error is 25%

Overfitting

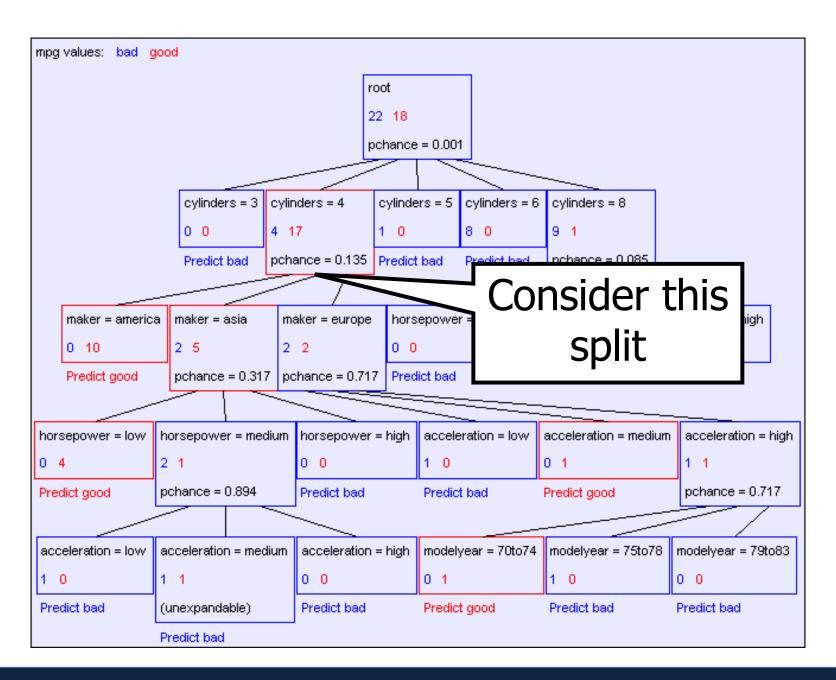
- Definition: If the learning algorithm fits noise (i.e. pays attention to parts of the data that are irrelevant) it is overfitting.
- Fact (theoretical and empirical): If the learning algorithm is overfitting, it often perform less well on test set data.

Avoiding overfitting

- Usually we do not know in advance which are the irrelevant variables
- ...and it may depend on the context

For example, if y = a AND b then b is an irrelevant variable only in the portion of the tree in which a=0

But we can use simple statistics to warn us that we might be overfitting.



Test for significance

- Suppose that mpg was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?
 - Is the association really significant or by chance?

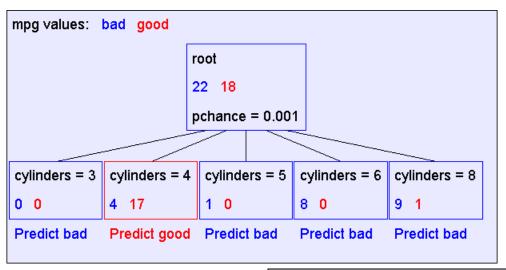
Pruning to avoid overfitting

- Build the full decision tree as before.
- But when you can grow it no more, start to prune:
 - Beginning at the bottom of the tree, delete splits in which $p_{chance} > MaxPchance$.
 - Continue working you way up until there are no more prunable nodes.

MaxPchance is a magic parameter you must specify to the decision tree, indicating your willingness to risk fitting noise.

Pruning example

• With MaxPchance = 0.1, you will see the following MPG decision tree:



Note the improved test set accuracy compared with the unpruned tree

	Num Errors	Set Size	Percent Wrong
Training Set	5	40	12.50
Test Set	56	352	15.91

MaxPchance

- Good news: The decision tree can automatically adjust its pruning decisions according to the amount of apparent noise and data.
- Bad news: The user must come up with a good value of MaxPchance.
- Good news: But with extra work, the best MaxPchance value can be estimated automatically by a technique called cross-validation.

Pruning using Chi Square Test

- Assume: the samples are a good random sample of the population it represents
- Is "Gender" what you can use to predict an undergrad's preference of his/her footwear?
- Null hypothesis "Gender and Footwear Preference have no relationship"

	Sandals	Sneakers	Leather shoes	Boots	Other	Total
Male	6	17	13	9	5	50
Female	13	5	7	16	9	50
Total	19	22	20	25	14	100

Chi Square Test – Compute Expected values

	Sandals	Sneaker s	Leather shoes	Boots	Other	Total
Male Observed	6	17	13	9	5	50
Male Expected						
Female Observed	13	5	7	16	9	50
Female Expected						
Total	19	22	20	25	14	100

Chi square value =
$$\sum_{i=1}^{rowsize} \sum_{j=1}^{colsize} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$$

Chi Square Test – Compute Expected values

Male/Sandals: $((19 \times 50)/100) = 9.5$

Male/Sneakers: $((22 \times 50)/100) = 11$

Male/Leather Shoes: $((20 \times 50)/100) = 10$

Male/Boots: $((25 \times 50)/100) = 12.5$

Male/Other: $((14 \times 50)/100) = 7$

Female/Sandals: $((19 \times 50)/100) = 9.5$

Female/Sneakers: $((22 \times 50)/100) = 11$

Female/Leather Shoes: $((20 \times 50)/100) = 10$

Female/Boots: $((25 \times 50)/100) = 12.5$

Female/Other: $((14 \times 50)/100) = 7$

	Sandals	Sneaker s	Leather shoes	Boots	Other	Total
Male Observed	6	17	13	9	5	50
Male Expected	9.5	11	10	12.5	7	
Female Observed	13	5	7	16	9	50
Female Expected	9.5	11	10	12.5	7	
Total	19	22	20	25	14	100

Compute Chi Square Value

$$\sum_{i=1}^{rowsize} \sum_{j=1}^{colsize} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$$

Total = 14.026

Male/Sandals: $((6 - 9.5)^2/9.5) = 1.289$

Male/Sneakers: $((17 - 11)^2/11) = 3.273$

Male/Leather Shoes: $((13 - 10)^2/10) = 0.900$

Male/Boots: ((9-12.5)²/12.5)=0.980

Male/Other: $((5 - 7)^2/7) = 0.571$

Female/Sandals: $((13-9.5)^2/9.5)=1.289$

Female/Sneakers: $((5 - 11)^2/11) = 3.273$

Female/Leather Shoes: $((7-10)^2/10)=0.900$

Female/Boots: $((16 - 12.5)^2/12.5) = 0.980$

Female/Other: $((9 - 7)^2/7) = 0.571$

	Sandals	Sneakers	Leather shoes	Boots	Other	Total
Male Observed	6	17	13	9	5	50
Male Expected	9.5	11	10	12.5	7	
Female Observed	13	5	7	16	9	50
Female Expected	9.5	11	10	12.5	7	
Total	19	22	20	25	14	100

Chi Square Test Computation

- What odds are we willing to accept that we are wrong in generalizing from the results in our sample to the population it represents? → confidence 5%
- Degree of Freedom of this problem
 = (# of rows 1)(# of cols 1) = (2-1)(5-1)=4
- From Chi Square table of statistics book, with p=0.05, r=4, critical value is 9.49,
 - if Chi square value is less than 9.49, accept the null hypothesis that there is no statistically significant relationship between gender and shoe preference
- In this case, Chi square value is 14.026 > 9.49, so we can reject the null hypothesis and conclude: male and female undergraduates of the Univ. differ significantly in their footwear preferences.

Cross-validation

- To minimize the effect of dependency on choice of training and test data, measure performance of algorithm using K-fold cross-validation
- Method:

```
Partition data into K disjoint sets S = \{S_1, S_2, ... S_K\}

i = 1

loop K times:

Let training set be (S - S_i), and

test set be S_i,

Learn the classifier based on the current training set,

Test the performance of the classifier on the current test set

Record the predication accuracy

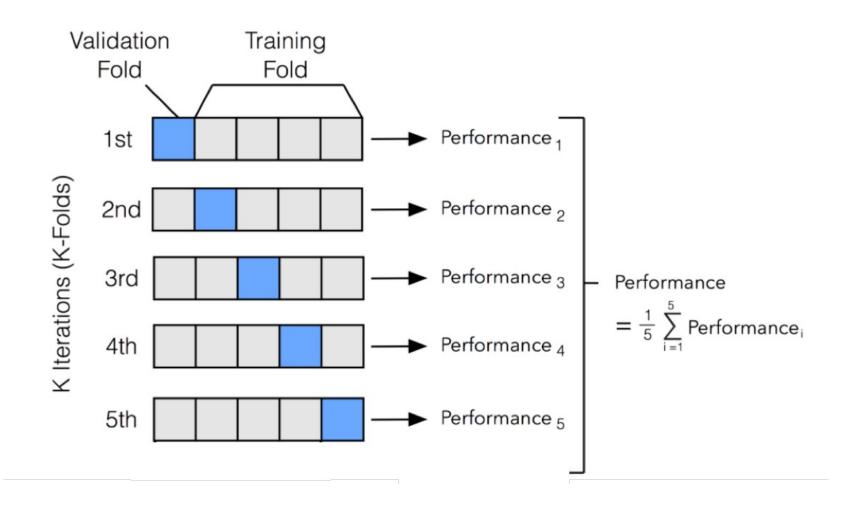
i = i + 1;

end loop

Compute the average predication accuracy for the K runs
```

Ten fold cross validation (K=10)

K-fold Cross-validation



Cross Validation for Parameter Tuning

```
depth = [x for x in range(3,15)]
cv_scores = []
for k in depth:
    decision_tree = DecisionTreeClassifier(random_state=0, max_depth=2)
    scores = cross_val_score(decision_tree, X, y, cv=10, scoring='accuracy')
    cv_scores.append(scores.mean())
```

```
neighbors = [x for x in range(1,50) if x % 2 != 0]
cv_scores = []
for k in neighbors:
    knn = KNeighborsClassifier(n_neighbors=k)
    scores = cross_val_score(knn, X, y, cv=10, scoring='accuracy')
    cv_scores.append(scores.mean())
```

Gain Ratio

- Problem with Information Gain
 - Favors smaller partitions formed by attribute with many unique values
- Gain Ratio takes into account the number of branches generated from the split test:

split info (X) =
$$-\sum_{i=1}^{n} \frac{|T_i|}{|T|} \times \log_2(\frac{|T_i|}{|T|})$$

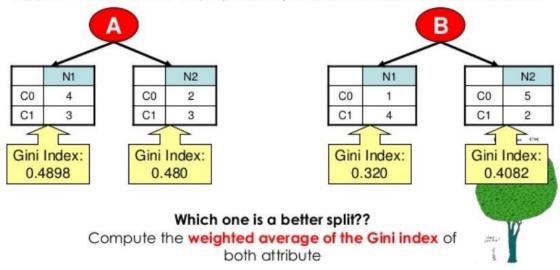
$$Gain \ Ratio(X) = \frac{gain(X)}{\text{split info}(X)}$$

Gini Index

 Another impurity criterion favoring larger partitions:

$$Gini = 1 - \sum_{j} p_j^2$$

Suppose there are two ways (A and B) to split the data into smaller subset.



The smaller the G value, the purer the node

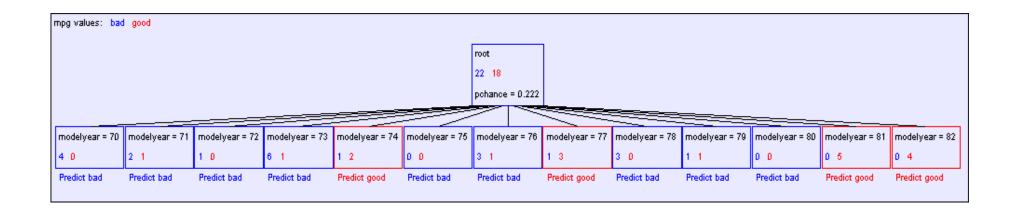
Real-Valued inputs

 What should we do if some of the inputs are real-valued?

mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	97	75	2265	18.2	77	asia
bad	6	199	90	2648	15	70	america
bad	4	121	110	2600	12.8	77	europe
bad	8	350	175	4100	13	73	america
bad	6	198	95	3102	16.5	74	america
bad	4	108	94	2379	16.5	73	asia
bad	4	113	95	2228	14	71	asia
bad	8	302	139	3570	12.8	78	america
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
good	4	120	79	2625	18.6	82	america
bad	8	455	225	4425	10	70	america
good	4	107	86	2464	15.5	76	europe
bad	5	131	103	2830	15.9	78	europe

Idea One: Branch on each possible real value

"One branch for each numeric value"



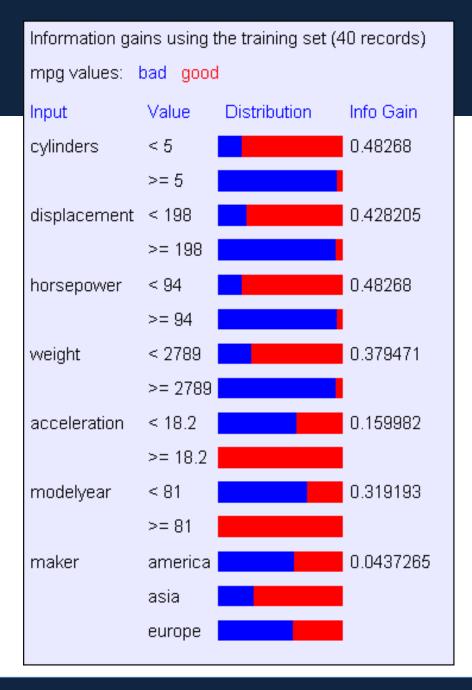
Hopeless: with such high branching factor will shatter the dataset and over fit

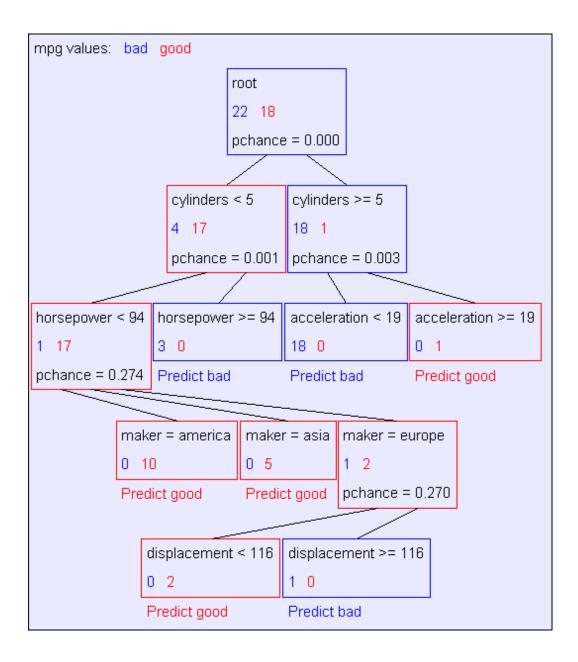
Note pchance is 0.222 in the above...if MaxPchance was 0.05 that would end up pruning away to a single root node.

A better idea: thresholded splits

- Suppose X is real valued.
- Define *IG(Y|X:t)* as *H(Y) H(Y|X:t)*
- Define H(Y|X:t) = H(Y|X < t) P(X < t) + H(Y|X >= t) P(X >= t)
 - *IG(Y|X:t)* is the information gain for predicting Y if all you know is whether X is greater than or less than t
- Then define $IG^*(Y|X) = \max_t IG(Y|X:t)$
- For each real-valued attribute, use IG*(Y|X) for assessing its suitability as a split

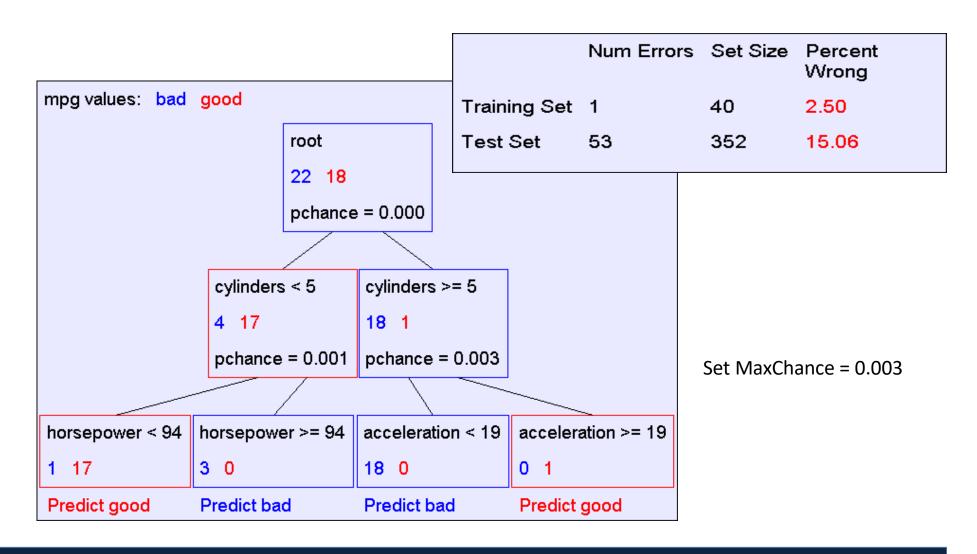
Example with MPG





Unpruned tree using reals

Pruned tree using reals



Additional Considerations

- How to deal with Missing Data?
- Other tree pruning methods
 - Cost-complexity pruning
 - Reduced-error pruning

In Summary

- Decision trees has been a popular data mining tool
 - Easy to understand
 - Easy to implement
 - Easy to use
 - Computationally cheap
- It's possible to get in trouble with overfitting
- They do classification: predict a categorical output from categorical and/or real inputs