Decision Trees

Machine Learning – CSE546
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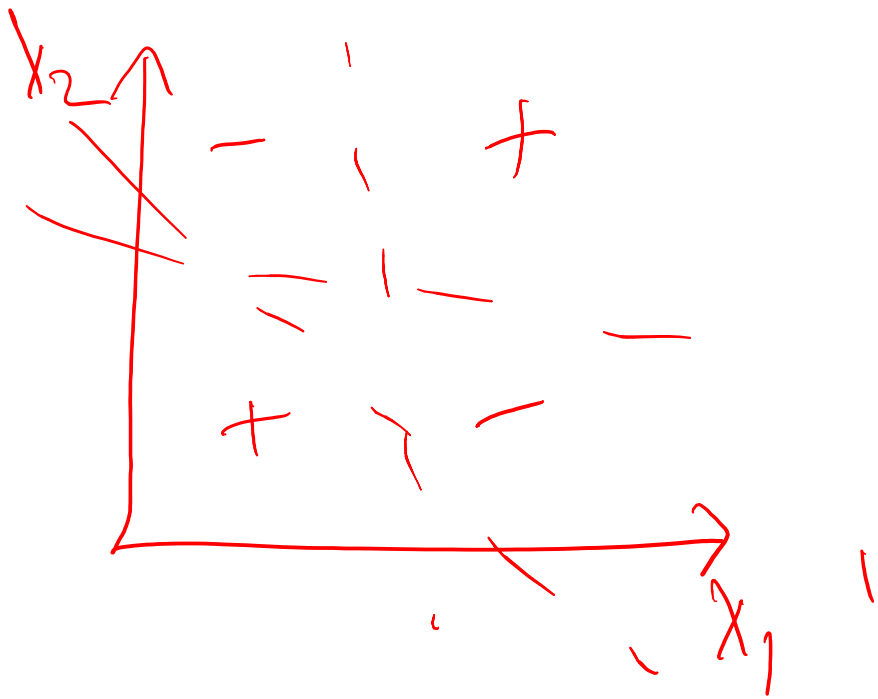
Linear separability

- A dataset is **linearly separable** iff there exists a **separating hyperplane**:
  - Exists **w**, such that:
    - $w_0 + \sum_i w_i x_i > 0$; if $\mathbf{x}=\{x_1,\ldots,x_k\}$ is a positive example
    - $w_0 + \sum_i w_i x_i < 0$; if $\mathbf{x}=\{x_1,\ldots,x_k\}$ is a negative example

Not linearly separable data

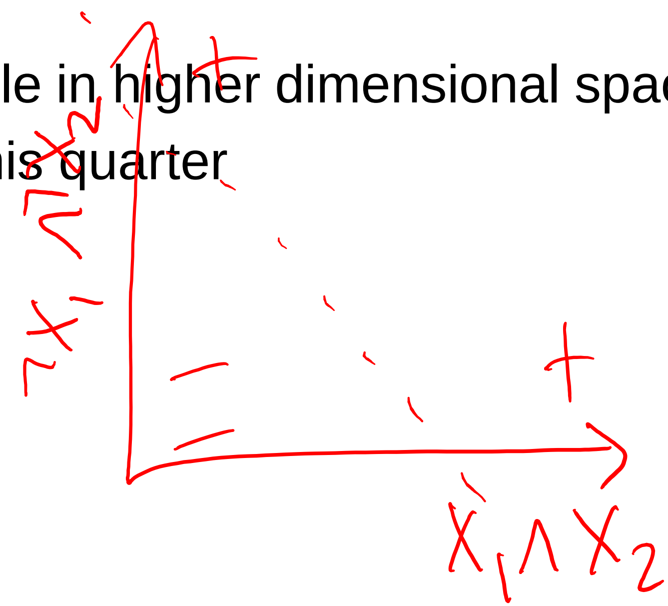
- Some datasets are **not linearly separable!**



X_1	X_2	L
0	0	+
0	1	−
1	0	−
1	1	+

Addressing non-linearly separable data – Option 1, non-linear features

- Choose non-linear features, e.g.,
  - Typical linear features: $w_0 + \sum_i w_i x_i$
  - Example of non-linear features:
    - Degree 2 polynomials, $w_0 + \sum_i w_i x_i + \sum_{ij} w_{ij} x_i x_j$
- Classifier $h_{\mathbf{w}}(\mathbf{x})$ still linear in parameters $\mathbf{w}$
  - As easy to learn
  - Data is linearly separable in higher dimensional spaces
  - More discussion later this quarter



Addressing non-linearly separable data – Option 2, non-linear classifier

- Choose a classifier $h_{\mathbf{w}}(\mathbf{x})$ that is non-linear in parameters **w**, e.g.,
  - Decision trees, boosting, nearest neighbor, neural networks…
- More general than linear classifiers
- But, can often be harder to learn (non-convex/concave optimization required)
- But, but, often very useful
- (BTW. Later this quarter, we'll see that these options are not that different)

A small dataset: Miles Per Gallon

Suppose we want to predict MPG

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
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bad	8	high	high	high	low	70to74	america
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good	4	low	low	low	low	79to83	america
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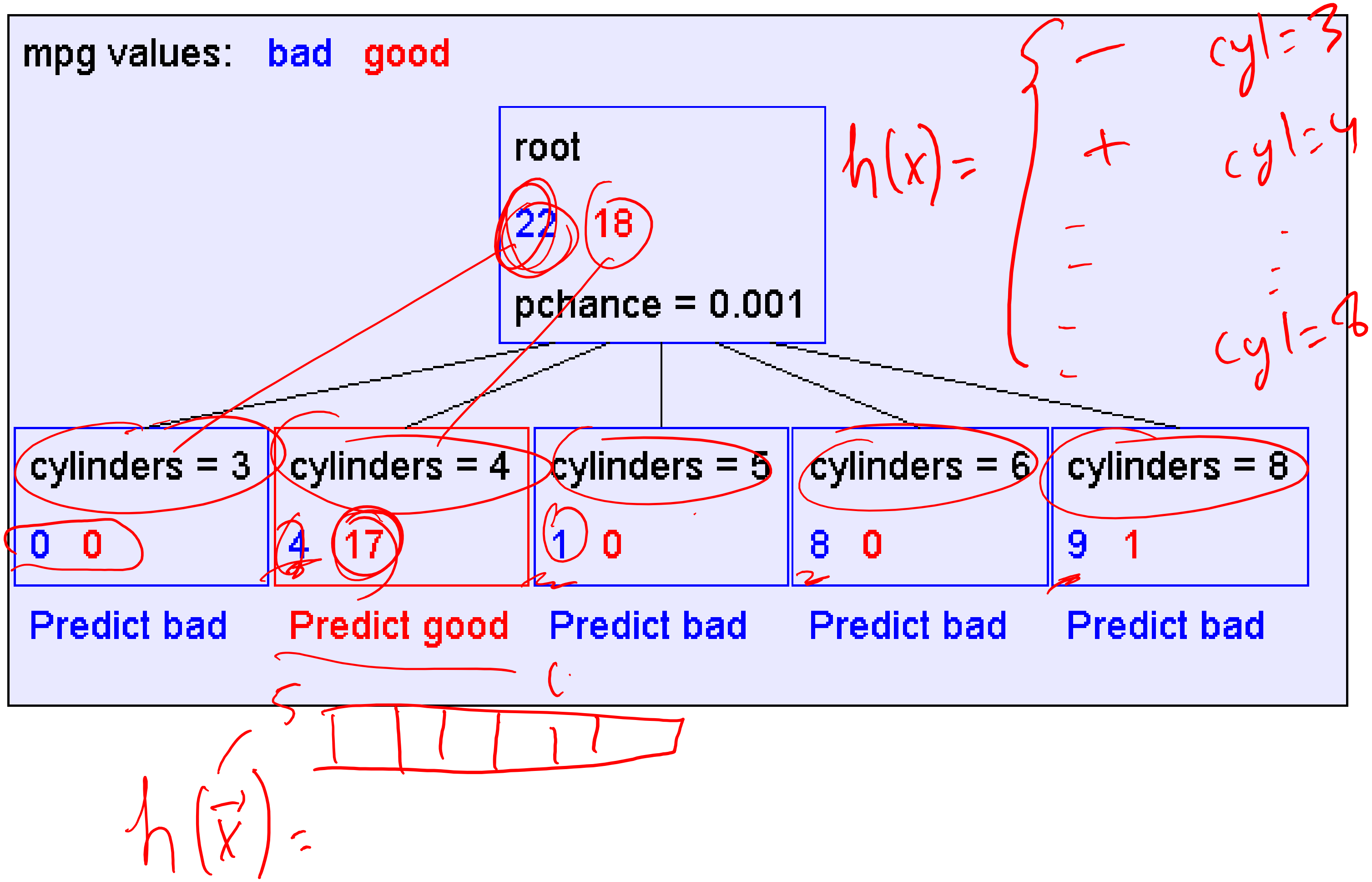
good	4	medium	low	low	low	79to83	america
good	4	low	low	medium	high	79to83	america
bad	8	high	high	high	low	70to74	america
good	4	low	medium	low	medium	75to78	europe
bad	5	medium	medium	medium	medium	75to78	europe

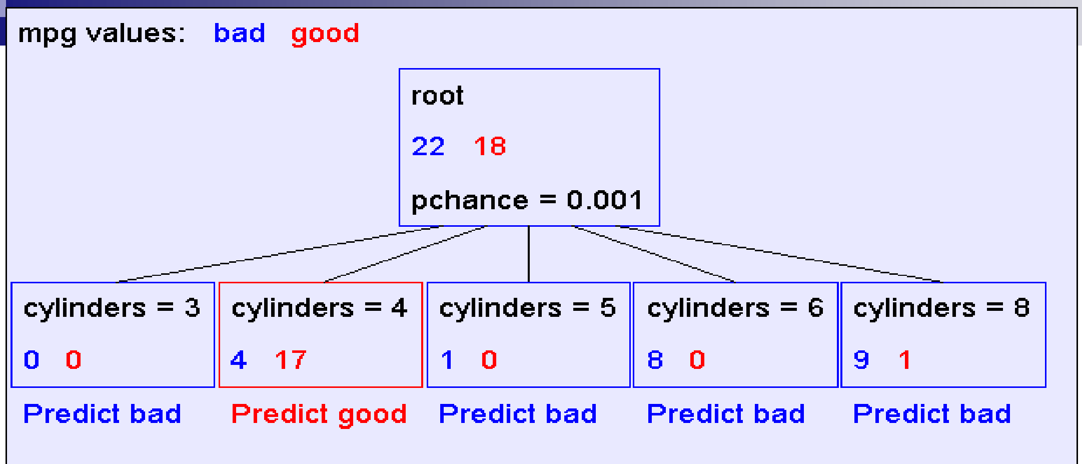
40 training examples

From the UCI repository (thanks to Ross Quinlan)

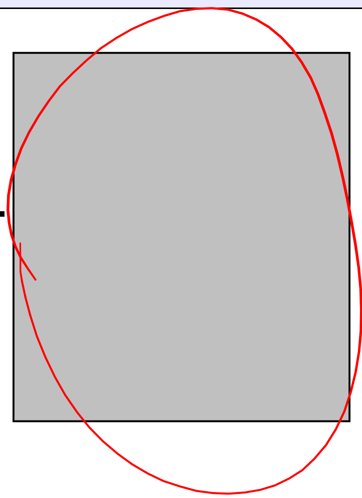
A Decision Stump



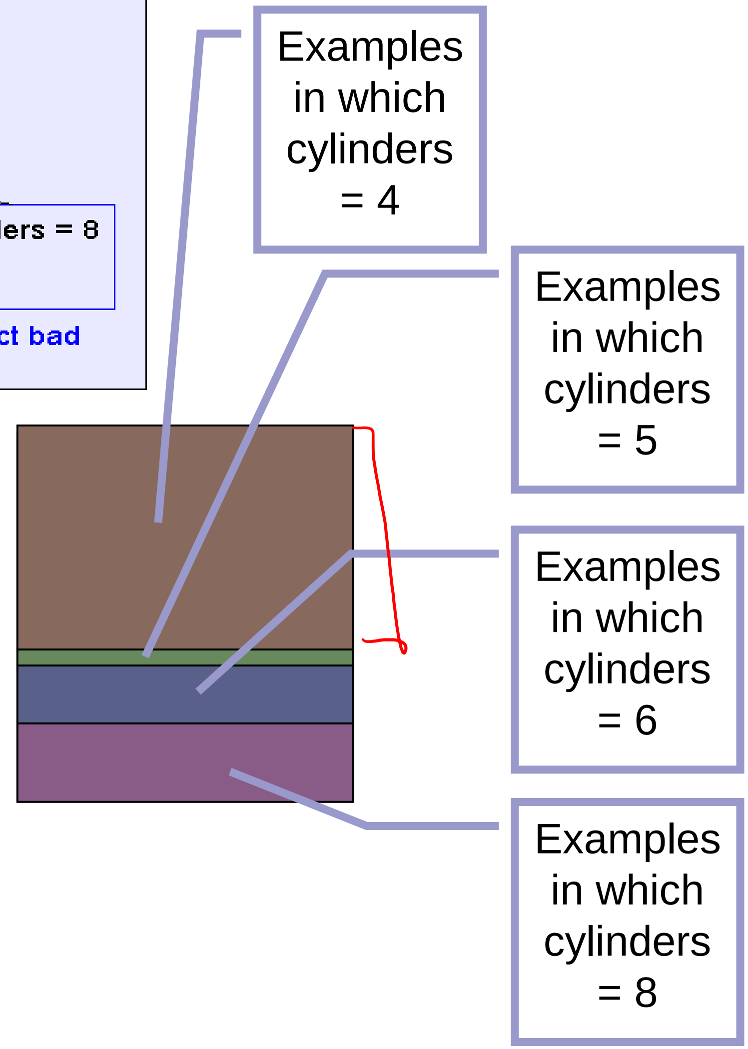
Recursion Step



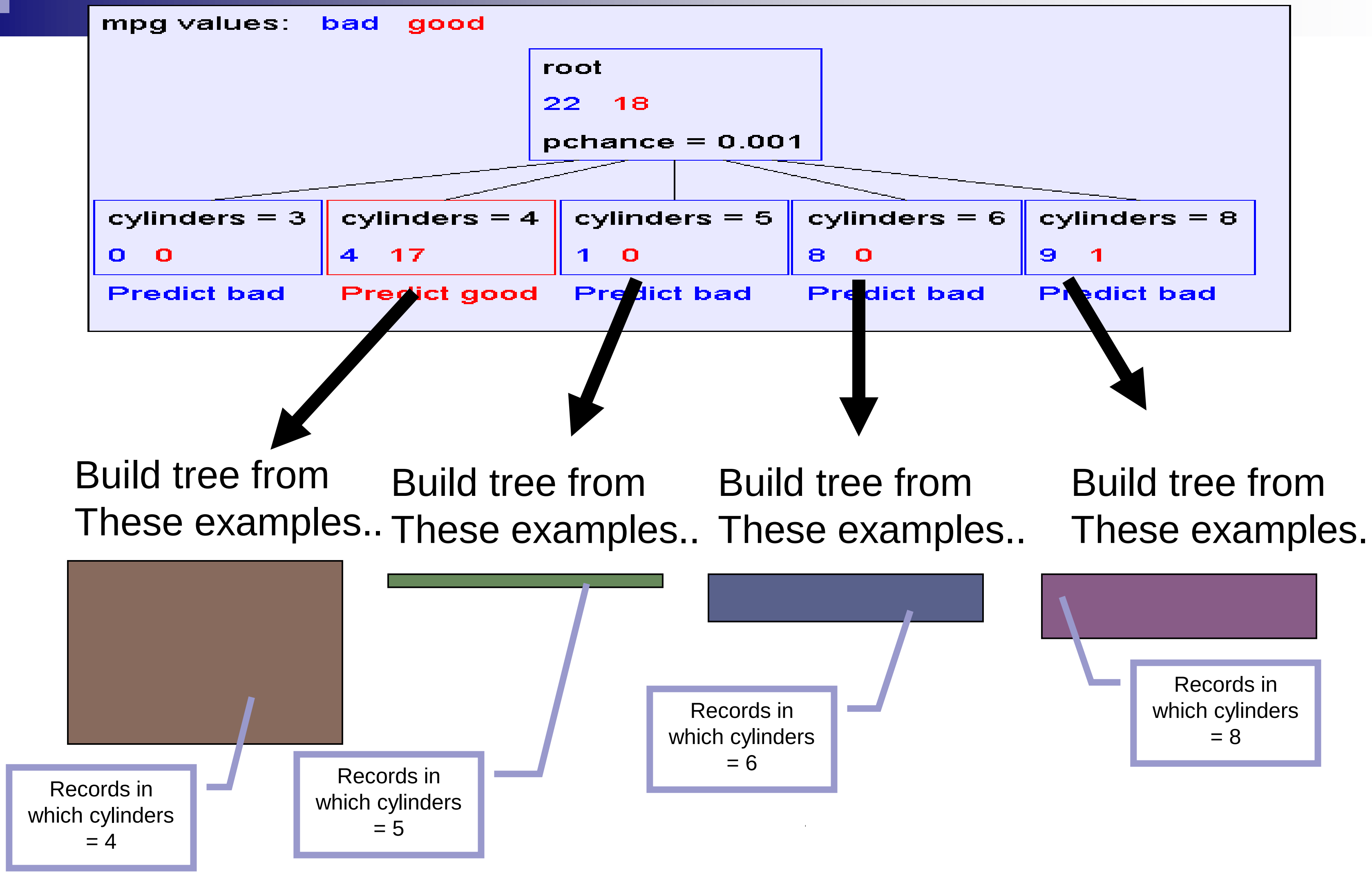
Take the Original Dataset..



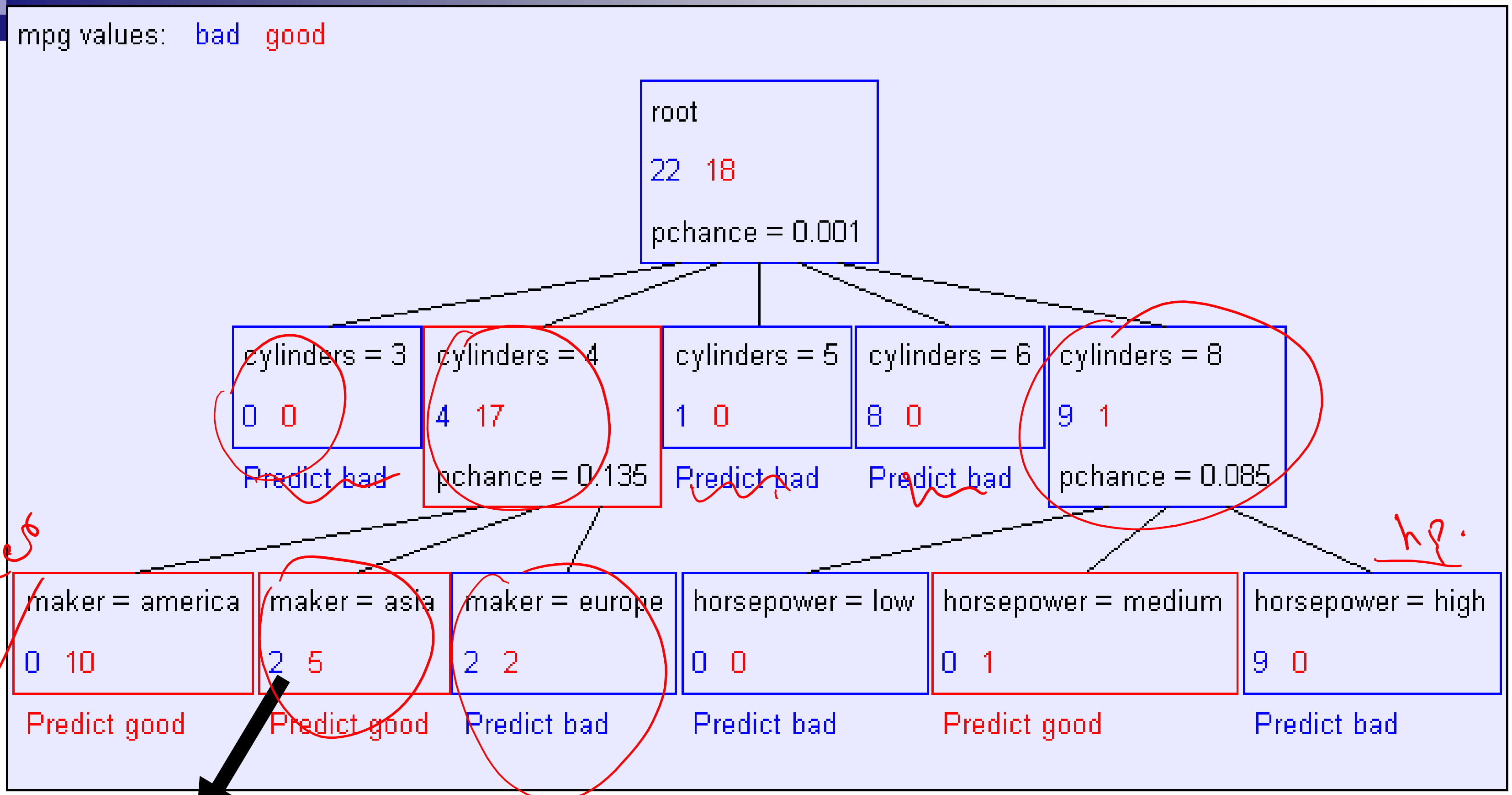
And partition it according to the value of the attribute we split on



Recursion Step



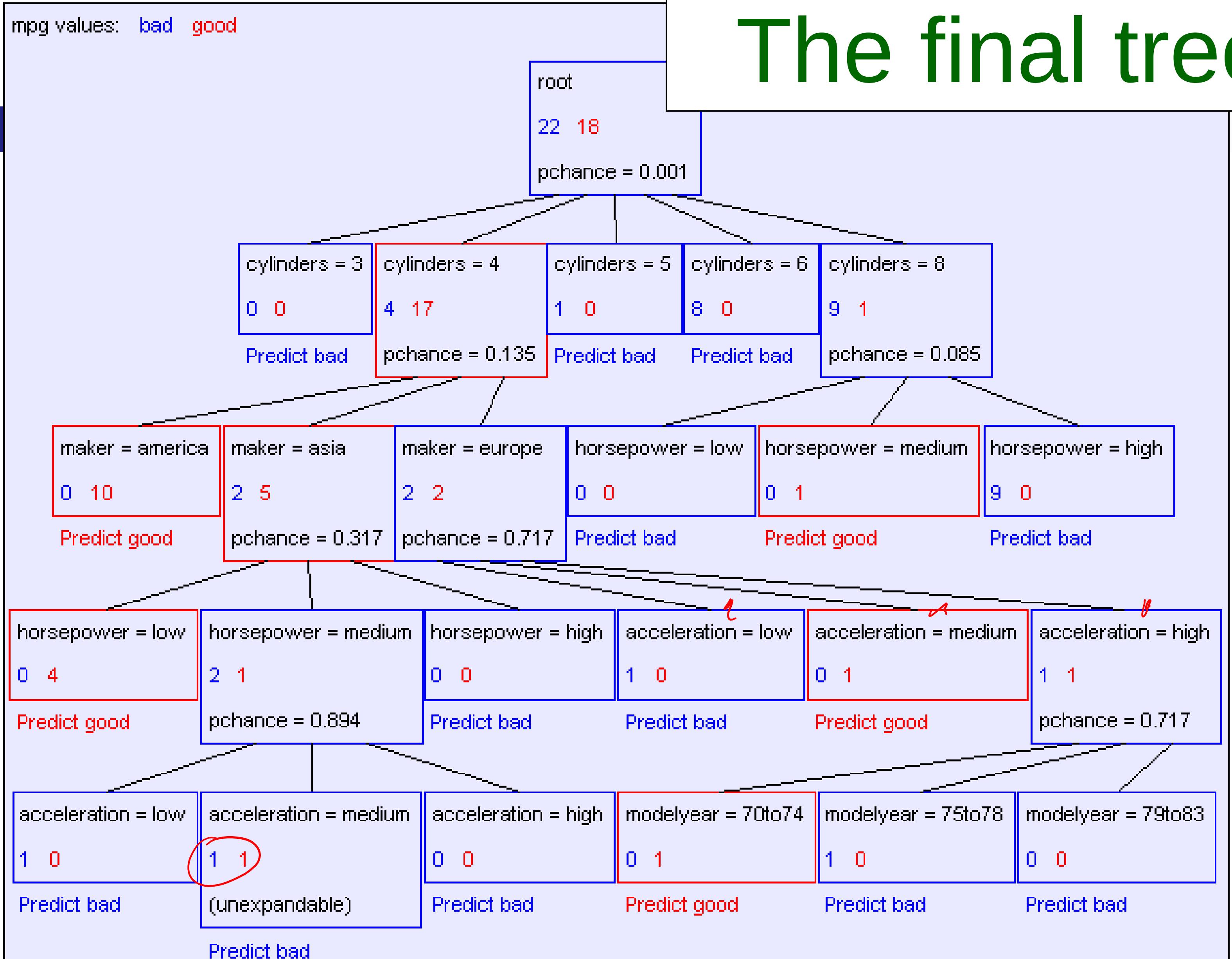
Second level of tree



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

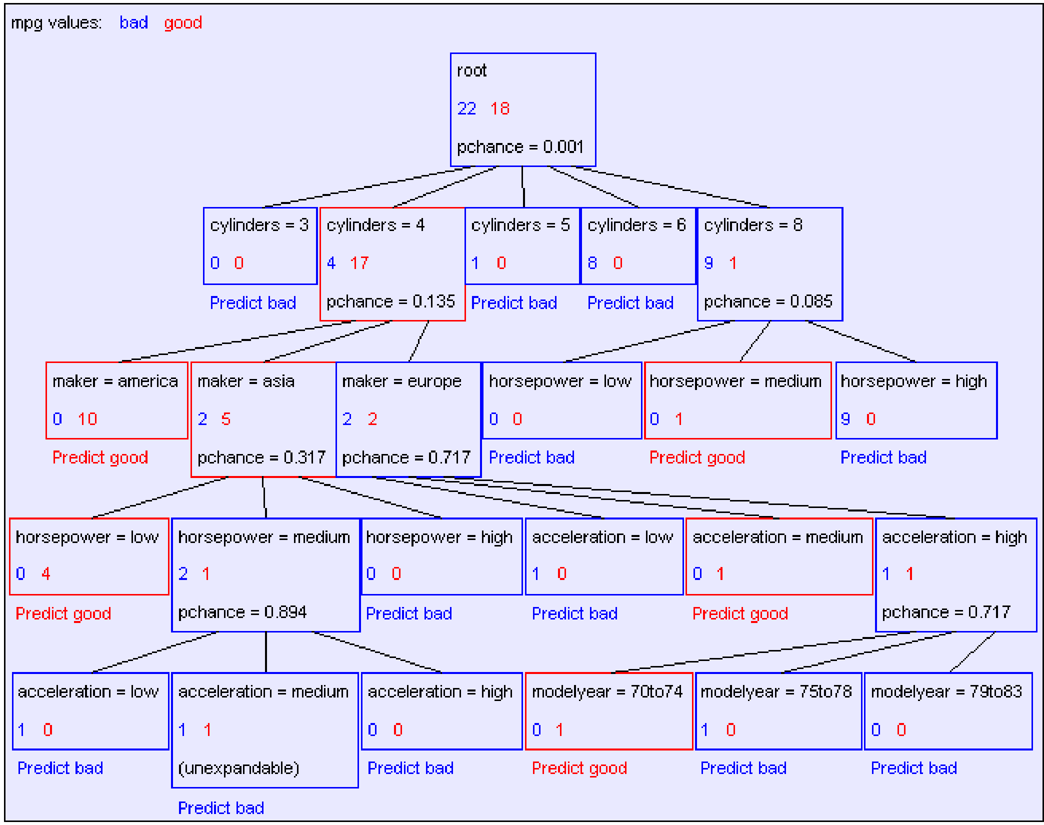
(Similar recursion in the other cases)

The final tree



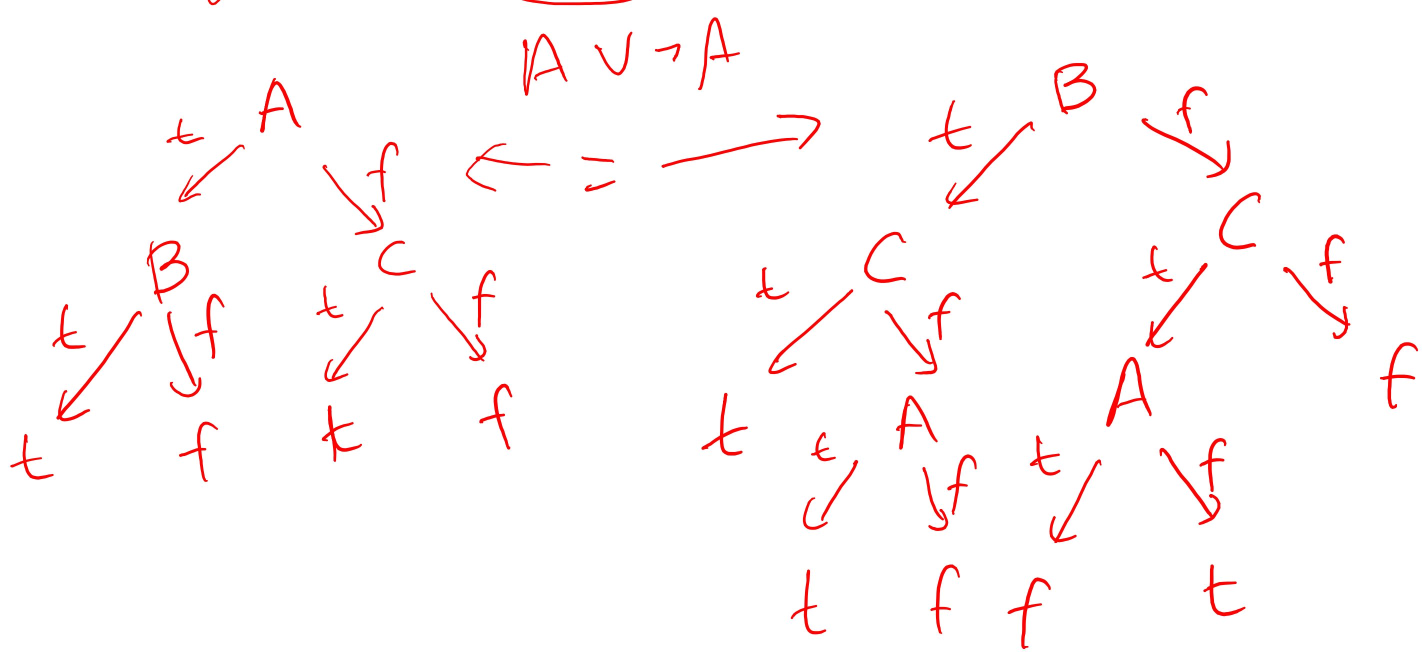
Classification of a new example

- Classifying a test example – traverse tree and report leaf label



Are all decision trees equal?

- Many trees can represent the same concept
- But, not all trees will have the same size!
  - e.g., $\phi = A \wedge B \vee \neg A \wedge C$ ((A and B) or (not A and C))

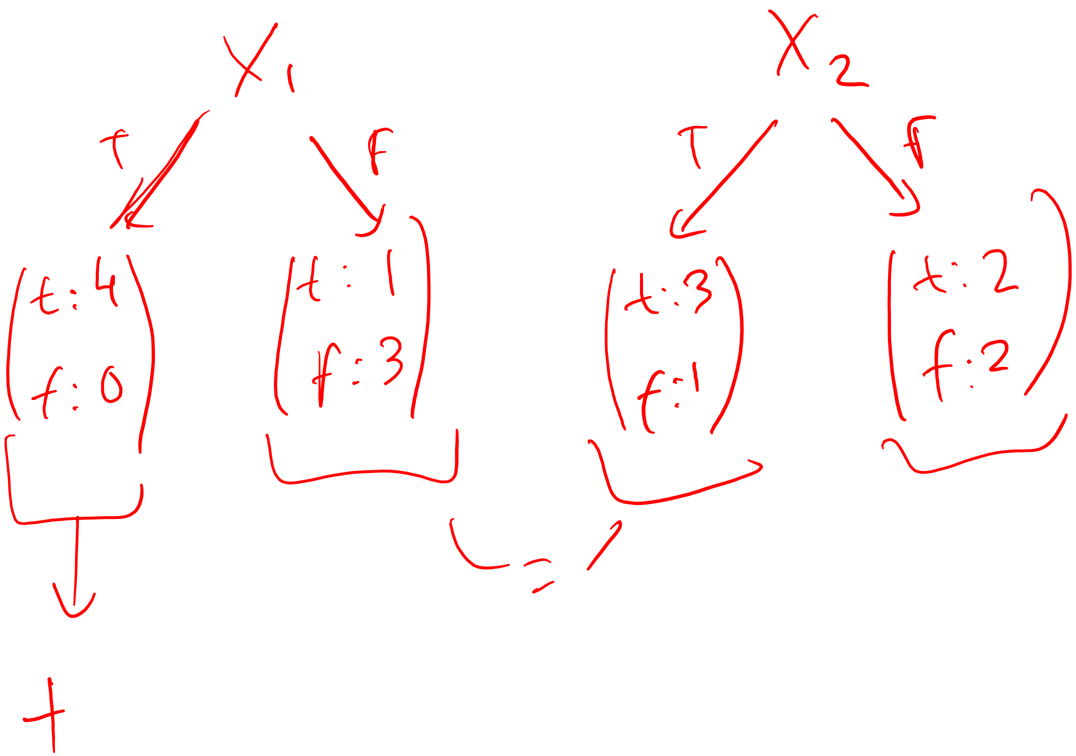


Learning decision trees is hard!!!

- Learning the simplest (smallest) decision tree is an NP-complete problem [Hyafil & Rivest ’76]
- Resort to a greedy heuristic:
  - Start from empty decision tree
  - Split on **next best attribute (feature)**
  - Recurse

Choosing a good attribute

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F
F	T	F
F	F	F

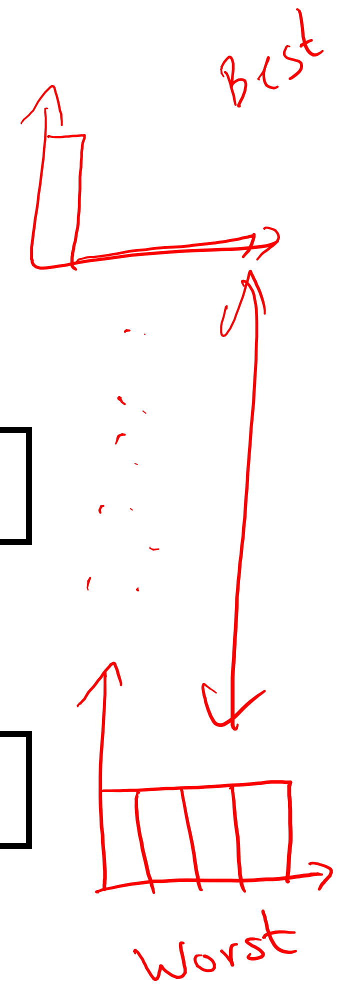


Measuring uncertainty

- Good split if we are more certain about classification after split
  - Deterministic good (all true or all false)
  - Uniform distribution bad

P(Y=A) = 1/2	P(Y=B) = 1/4	P(Y=C) = 1/8	P(Y=D) = 1/8

P(Y=A) = 1/4	P(Y=B) = 1/4	P(Y=C) = 1/4	P(Y=D) = 1/4



Entropy

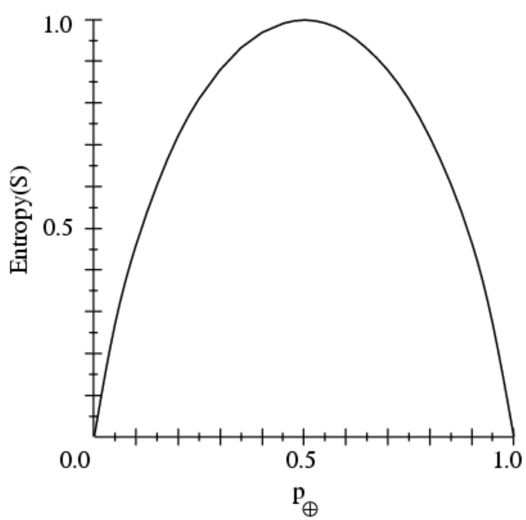
Entropy *H(Y)* of a random variable *Y* $= \{y_1, y_2 \ldots y_k\}$

$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

$-\sum_i p_i \log p_i$

More uncertainty, more entropy!

Information Theory interpretation: H(Y) is the expected number of bits needed to encode a randomly drawn value of *Y* (under most efficient code)



$P_0 = 0$, $P_1 = 1$: $-0 - 0 = 0$

$P_0 = \frac{1}{2}$, $P_1 = \frac{1}{2}$: $-\frac{1}{2}\log\frac{1}{2} - \frac{1}{2}\log\frac{1}{2} = 1$

$P_1 = 0$, $P_0 = 1$: $-0 - 0 = 0$

Information gain

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

- Advantage of attribute – decrease in uncertainty
  - Entropy of Y before you split
  - Entropy after split
    - Weight by probability of following each branch, i.e., normalized number of records

$$H(Y \mid X) = -\sum_{j=1}^{v} P(X = x_j) \sum_{i=1}^{k} P(Y = y_i \mid X = x_j) \log_2 P(Y = y_i \mid X = x_j)$$

- Information gain is difference $IG(X) = H(Y) - H(Y \mid X)$

Learning decision trees

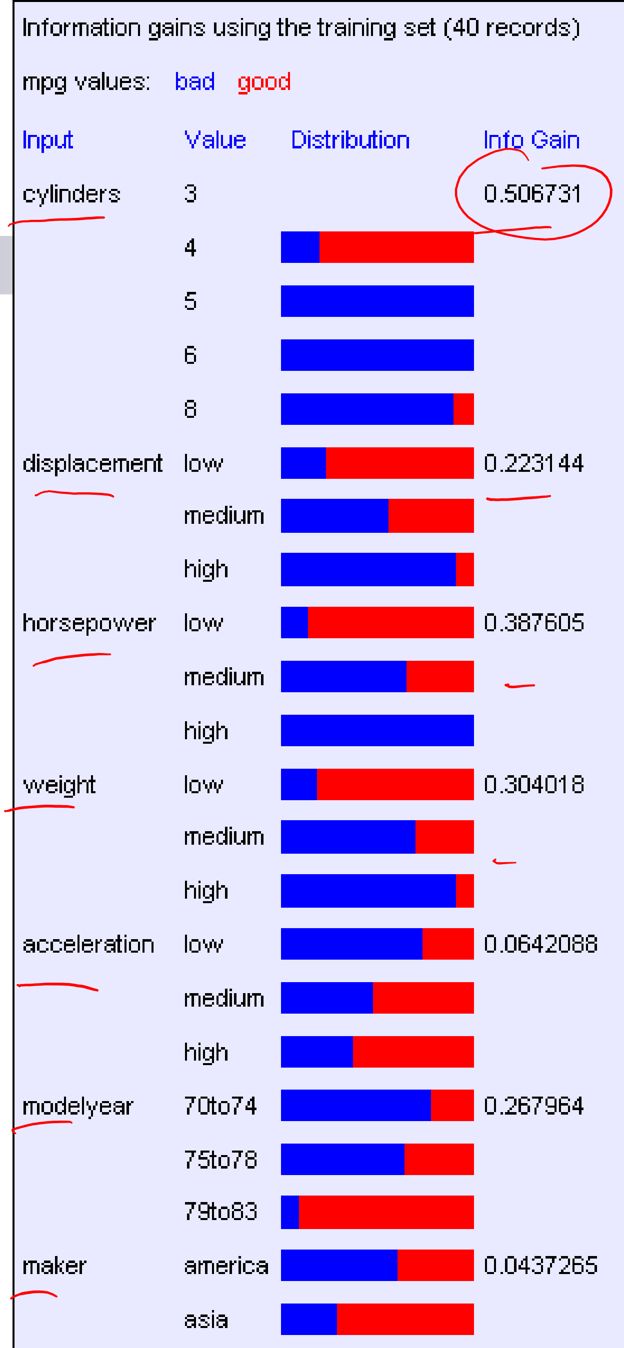
- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute
  - Split on $\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$
- Recurse

When do I stop?

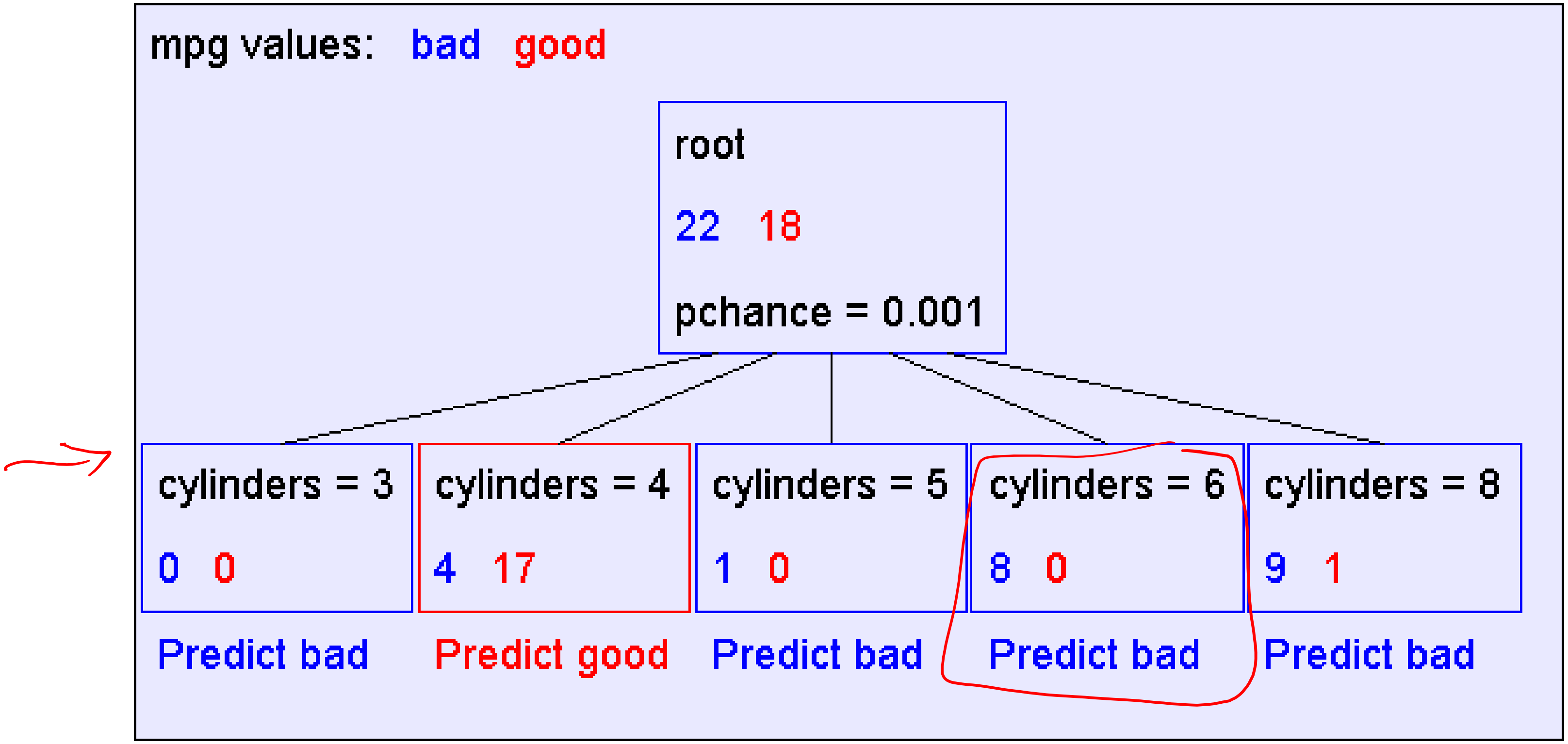
1) Entropy is 0 → predict the label
2) Cannot split → all feats used
   → no feats helping
3) .... info gain is 0 (small)

Suppose we want to predict MPG

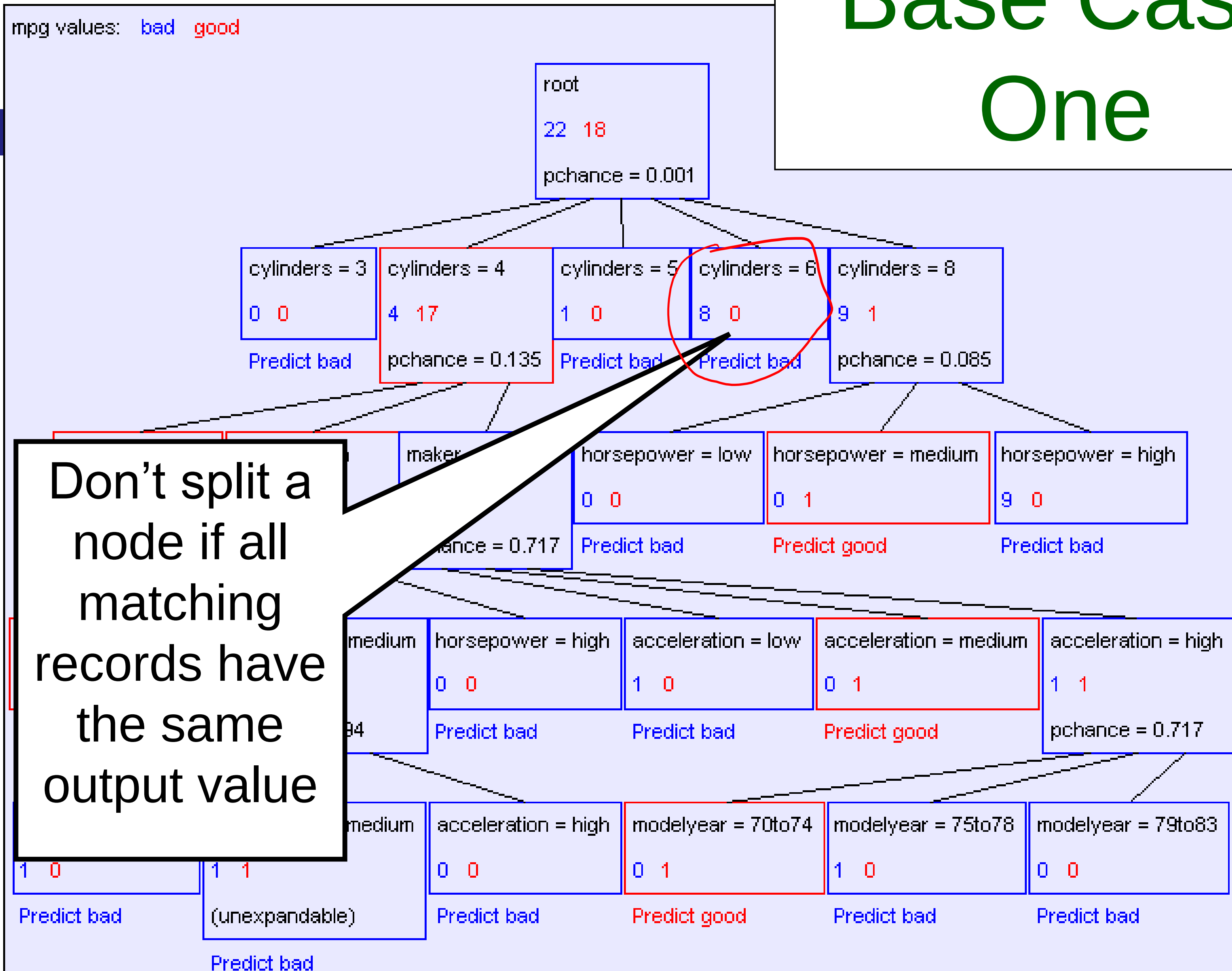
Look at all the information gains…



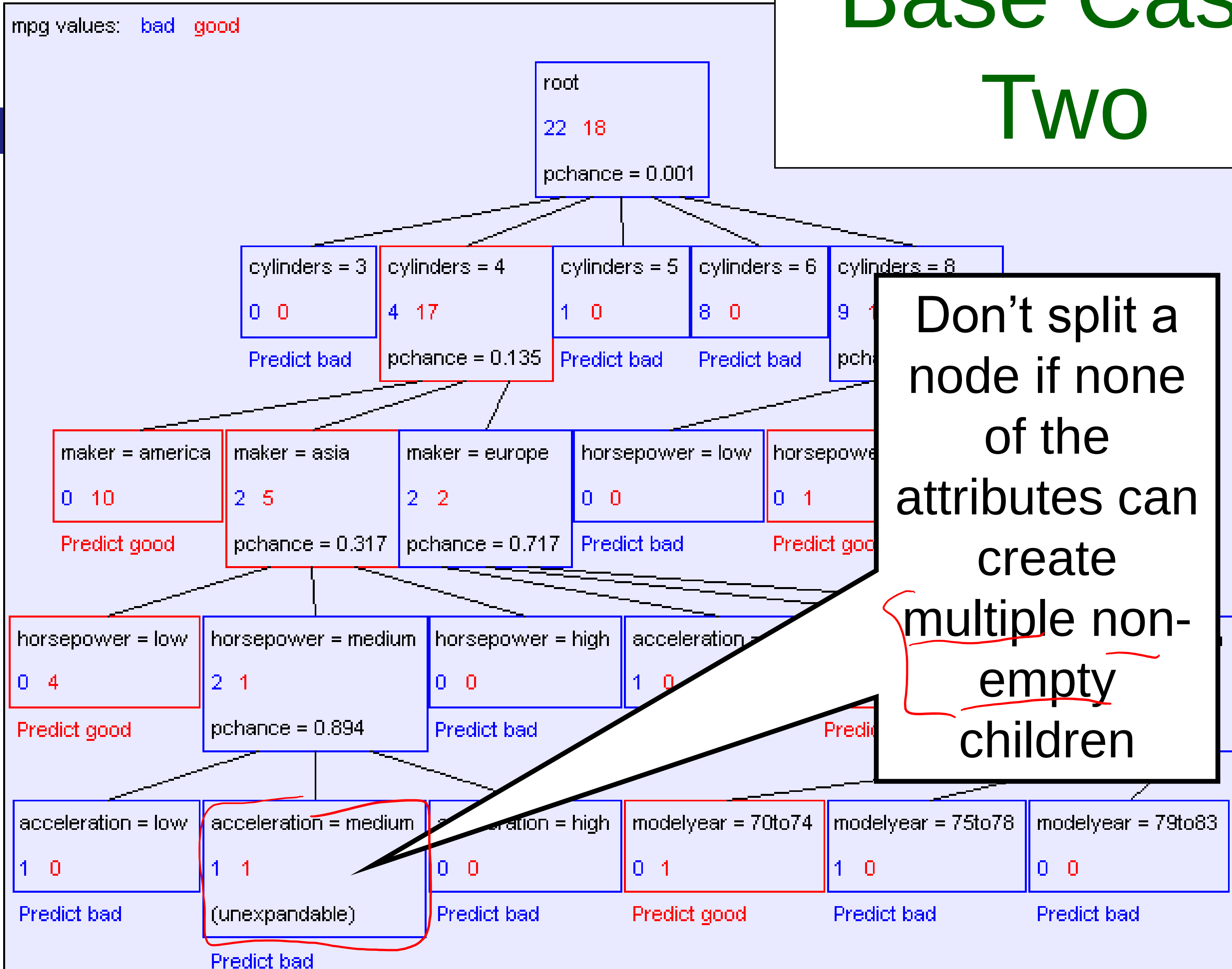
A Decision Stump



Base Case One

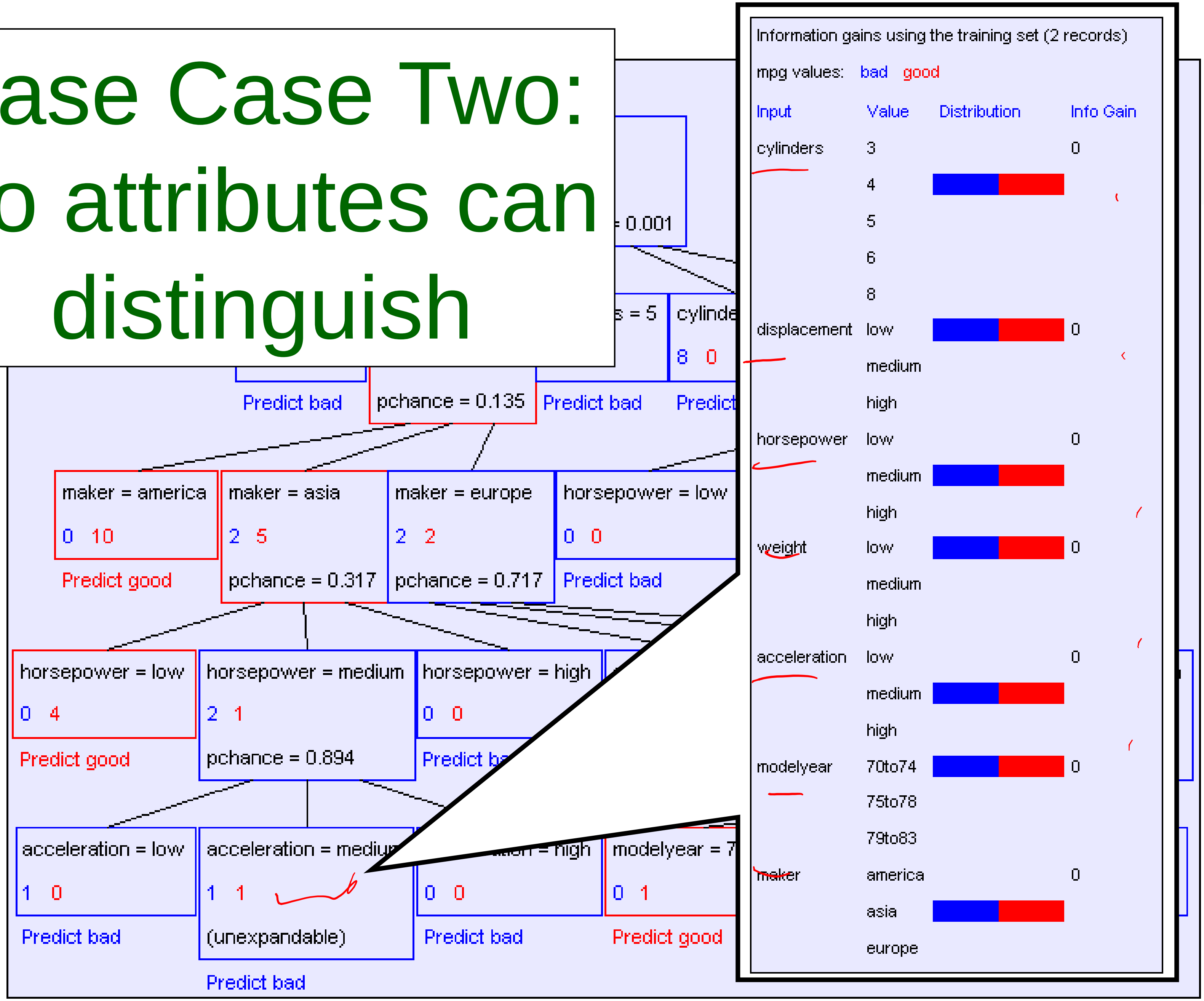


Base Case Two



Don't split a node if none of the attributes can create multiple non-empty children

Base Case Two: No attributes can distinguish



Base Cases

- 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

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

Proposed Base Case 3:

If all attributes have zero information gain then don't recurse

•*Is this a good idea?*

No.

The problem with Base Case 3

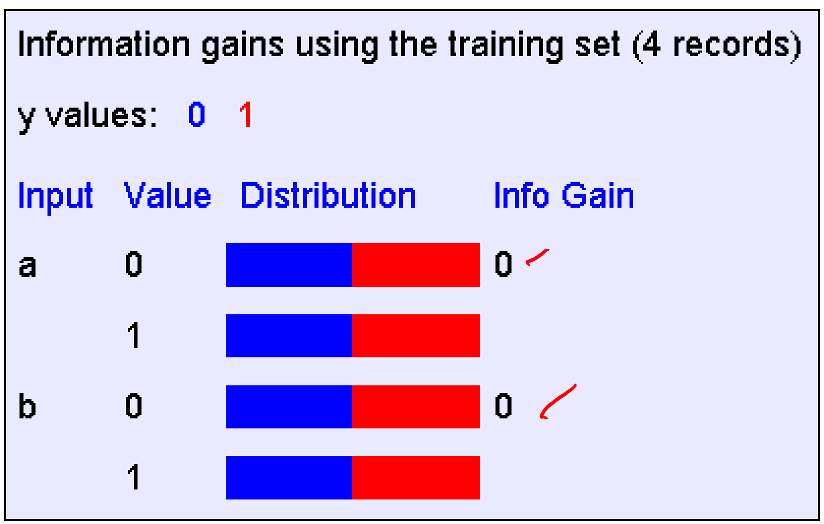
a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

Y = A XOR B

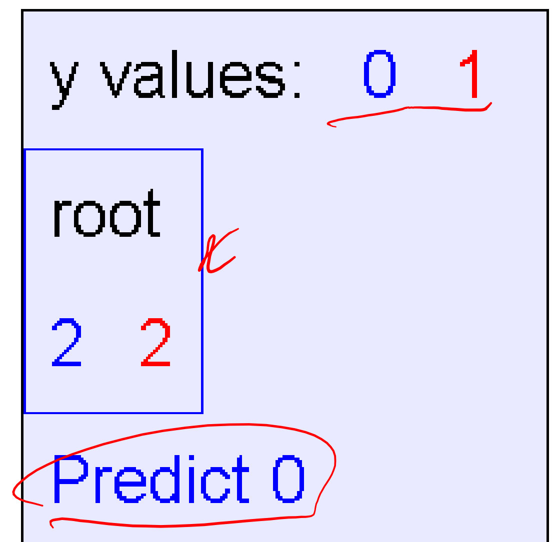
$H(Y|a) = -\frac{1}{2}(1) - \frac{1}{2}(1) = 1$

$H(Y) = 1 \quad IG(a) = 0$

The information gains:



The resulting bad decision tree:

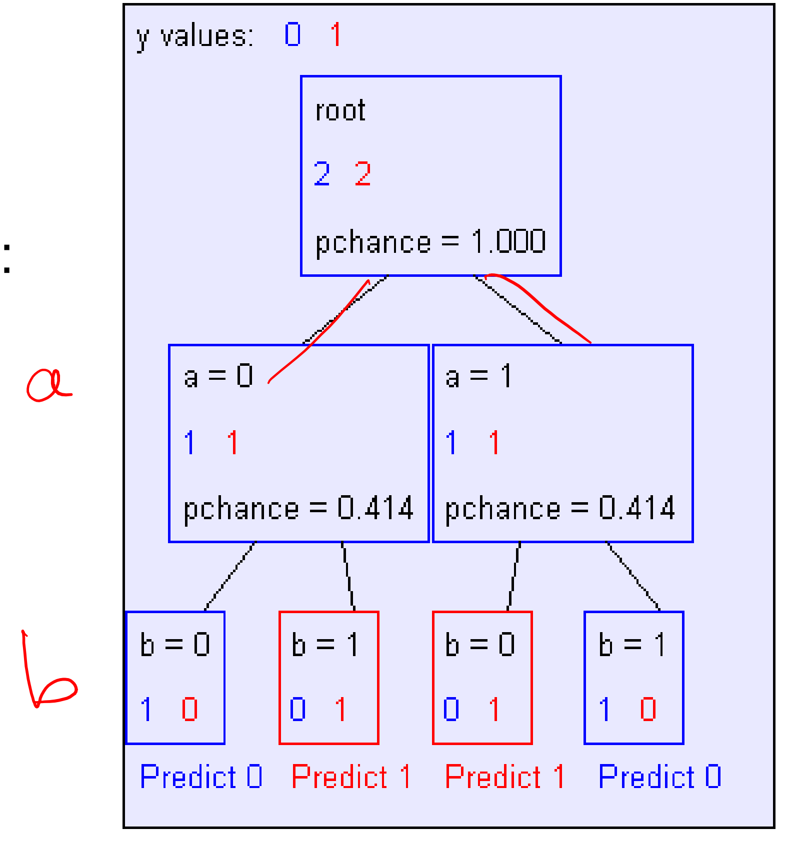


If we omit Base Case 3:

a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

y = a XOR b

The resulting decision tree:



Basic Decision Tree Building Summarized

BuildTree(*DataSet*,*Output*)

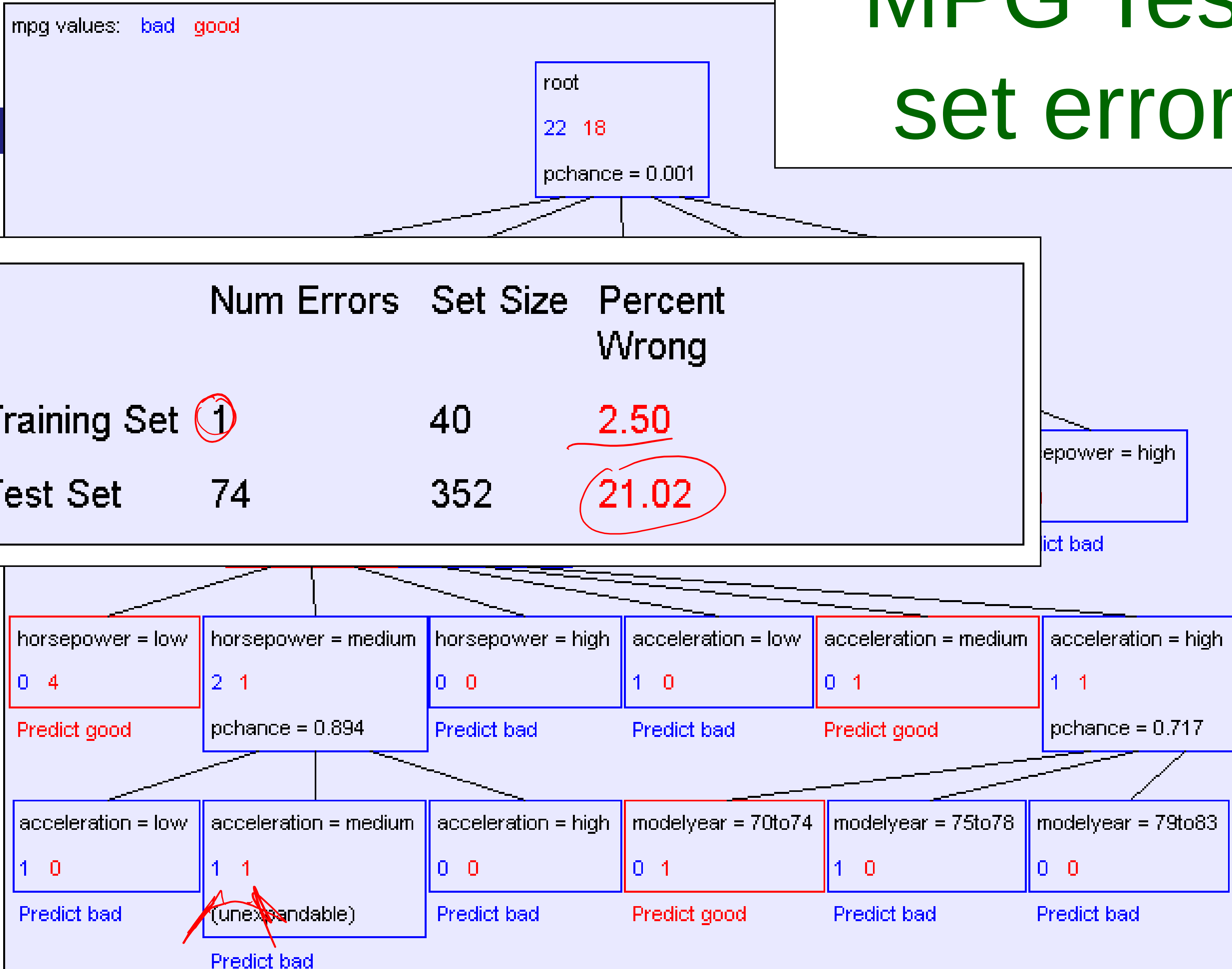
- If all output values are the same in *DataSet*, return a leaf node that says "predict this unique output"
- If all input values are the same, return a leaf node that says "predict the majority output"
- Else find attribute *X* with highest Info Gain
- Suppose *X* has n_X distinct values (i.e. X has arity n_X).
  - Create and return a non-leaf node with n_X children.
  - The *i*'th child should be built by calling

    BuildTree(DS_i,*Output*)

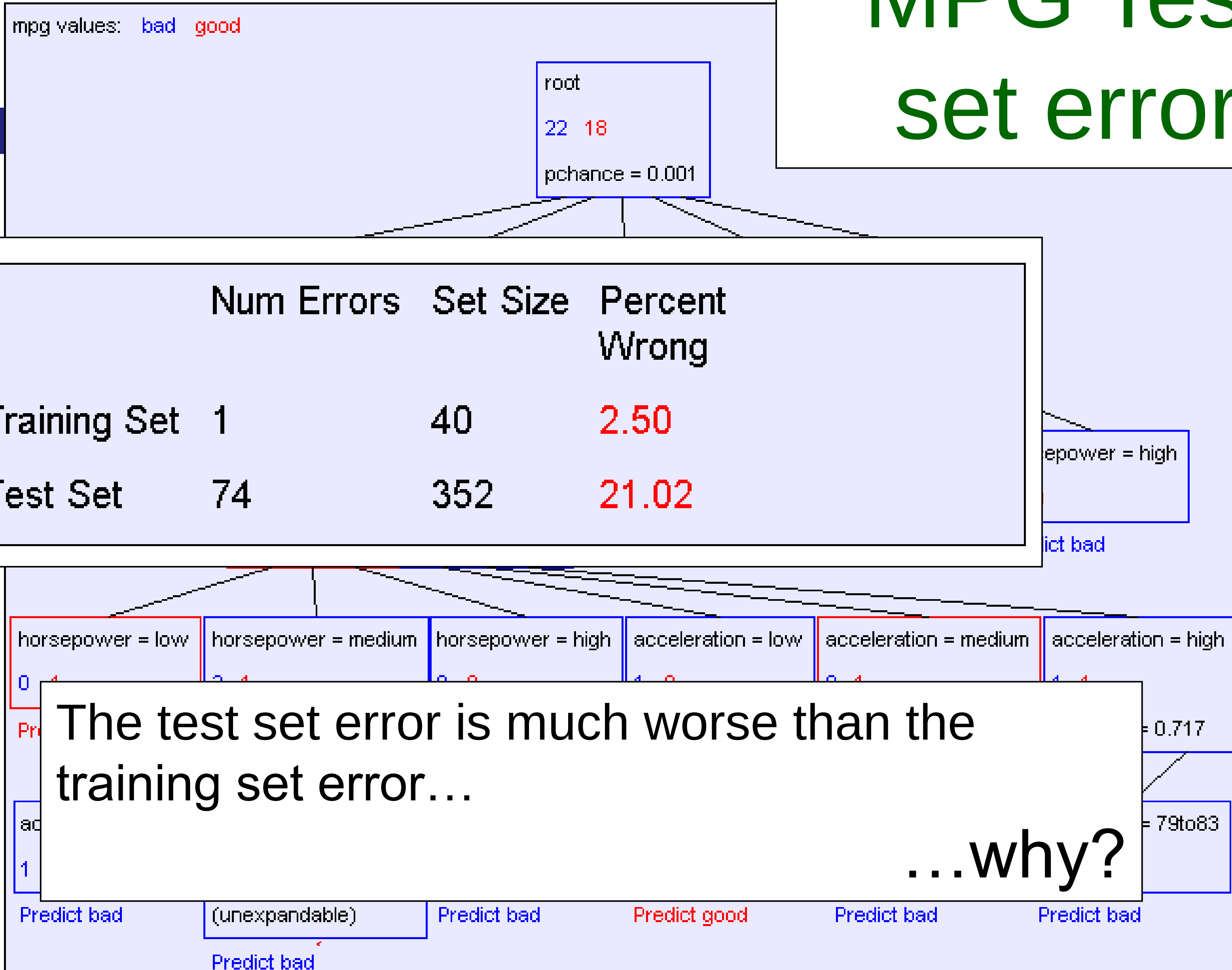
    Where DS_i built consists of all those records in DataSet for which X = *i*th distinct value of X.

MPG Test set error

	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02



MPG Test set error



	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

The test set error is much worse than the training set error…

…why?

Decision trees & Learning Bias

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
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bad	4	low	medium	low	medium	70to74	asia
bad	4	low	medium	low	low	70to74	asia
bad	8	high	high	high	low	75to78	america
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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

No label noise

$\nexists\, x_1, x_2, y_1, y_2$ s.t.

$x_1 = x_2 \wedge y_1 \neq y_2$

then

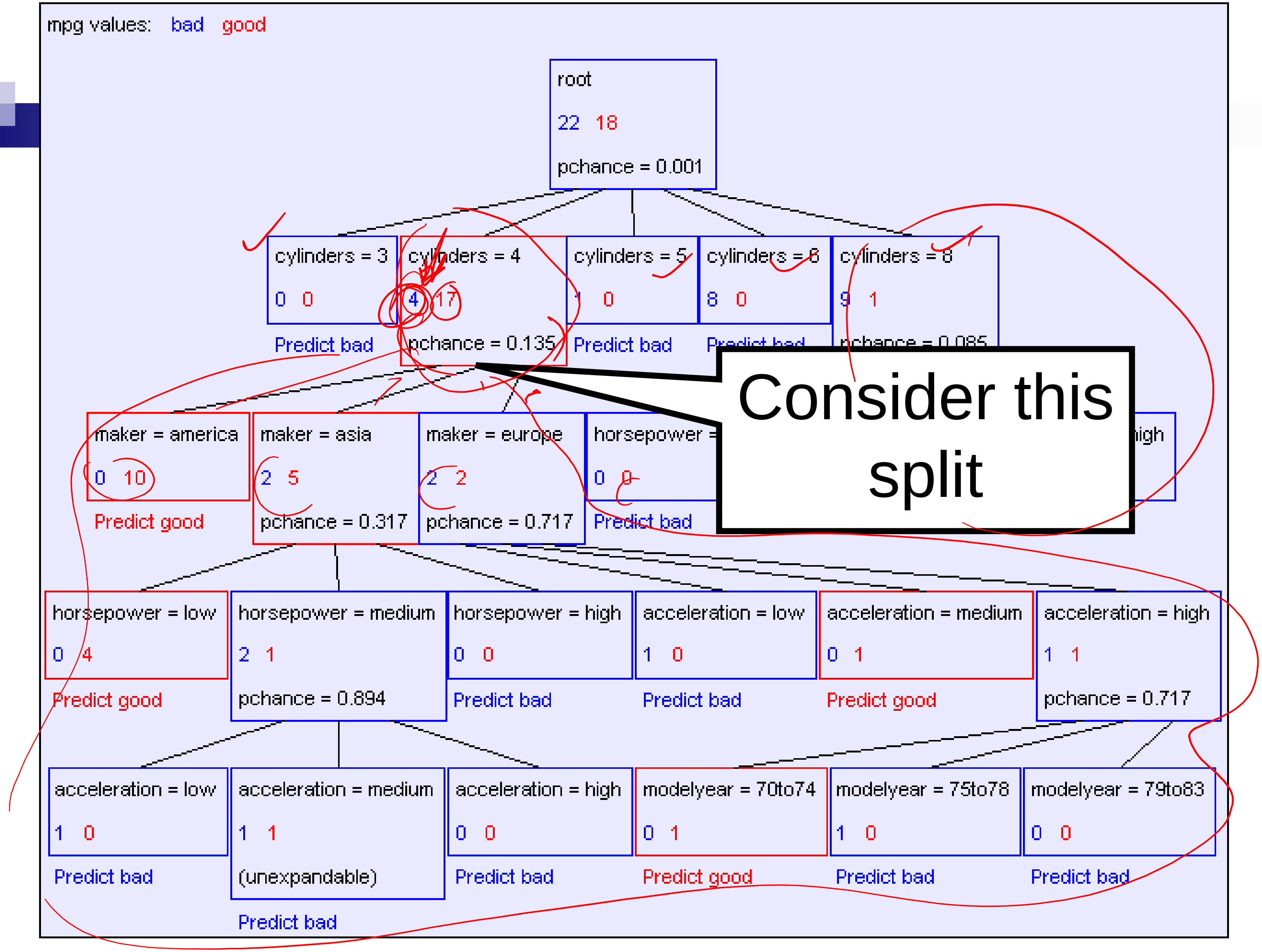
Decision Trees obtain 0 training error

+ fits the bias

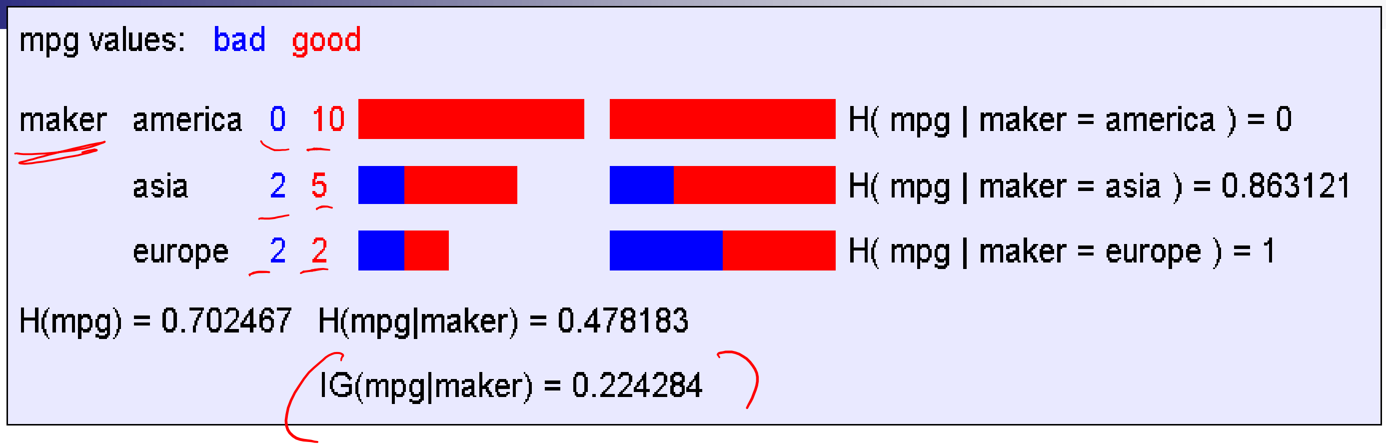
− high variance

Decision trees will overfit

- Standard decision trees have no learning bias
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Will definitely overfit!!!
  - Must bias towards simpler trees
- Many strategies for picking simpler trees:
  - Fixed depth $d = 3, 4 \ldots$
  - Fixed number of leaves $W = 10, 20$
  - Or something smarter…


mpg values: bad good
root
22 18
pchance = 0.001
cylinders = 3
0 0
Predict bad
cylinders = 4
4 17
pchance = 0.135
cylinders = 5
1 0
Predict bad
cylinders = 6
8 0
Predict bad
cylinders = 8
9 1
pchance = 0.085
maker = america
0 10
Predict good
maker = asia
2 5
pchance = 0.317
maker = europe
2 2
pchance = 0.717
horsepower =
0 0
Predict bad
horsepower = low
0 4
Predict good
horsepower = medium
2 1
pchance = 0.894
horsepower = high
0 0
Predict bad
acceleration = low
1 0
Predict bad
acceleration = medium
0 1
Predict good
acceleration = high
1 1
pchance = 0.717
acceleration = low
1 0
Predict bad
acceleration = medium
1 1
(unexpandable)
Predict bad
acceleration = high
0 0
Predict bad
modelyear = 70to74
0 1
Predict good
modelyear = 75to78
1 0
Predict bad
modelyear = 79to83
0 0
Predict bad
Consider this split

A chi-square test

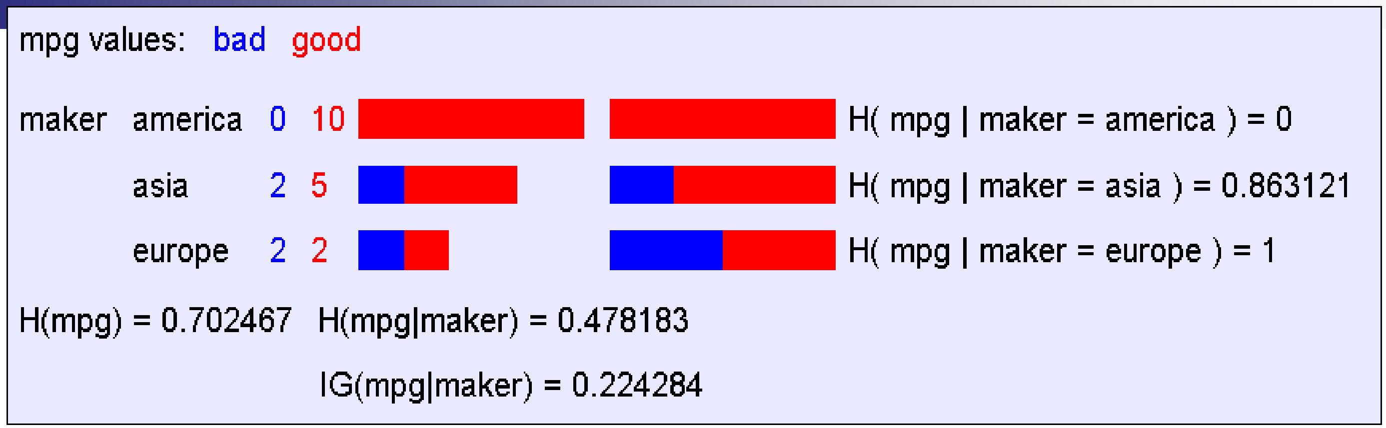


- Suppose that MPG was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

Hypothesis Testing

- Null: no correlation
- Hypothesis: MPG is related to maker

A chi-square test



- 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?

By using a particular kind of chi-square test, the answer is 7.2%

(Such simple hypothesis tests are very easy to compute, unfortunately, not enough time to cover in the lecture, but see readings…)

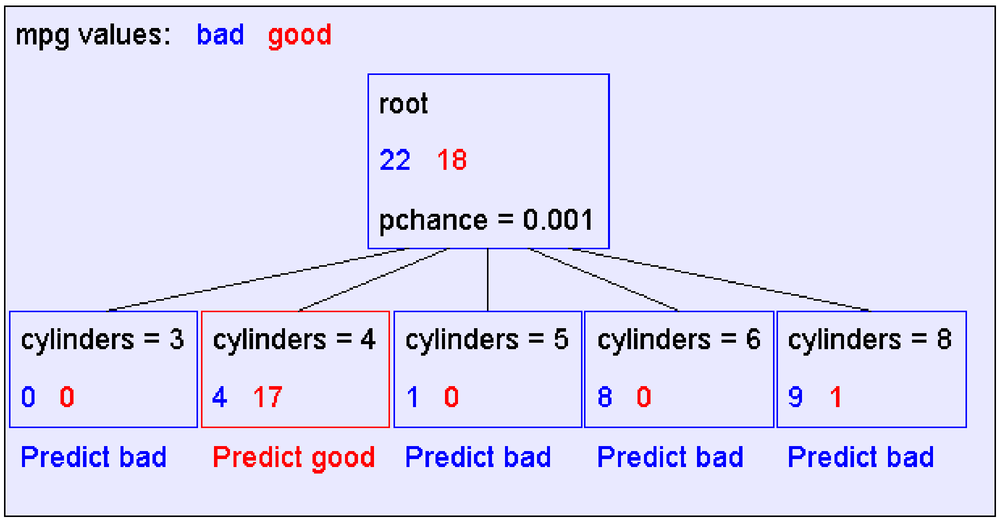
Using Chi-squared to avoid overfitting

- 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:

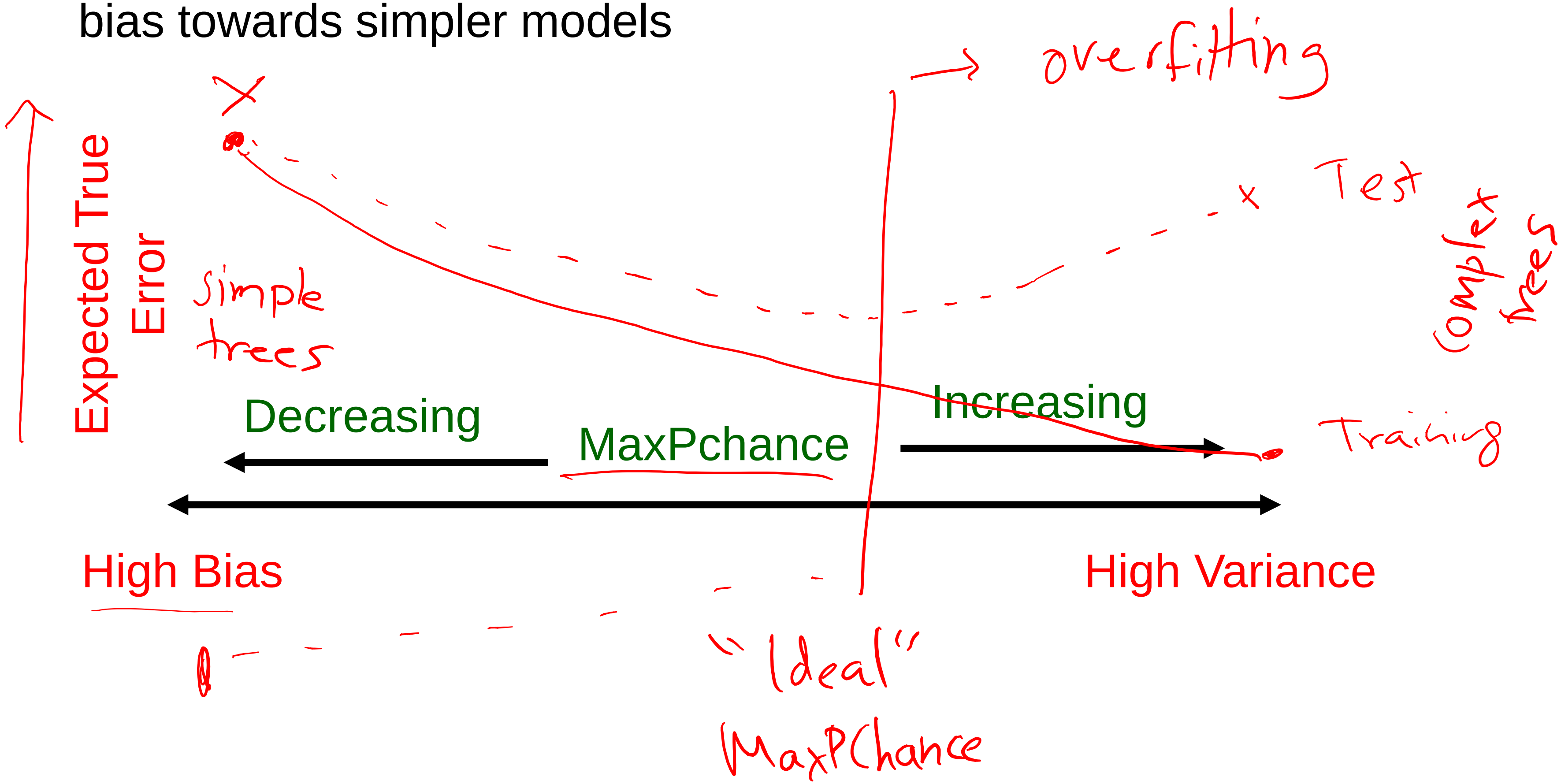


Note the improved test set accuracy compared with the unpruned tree

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

MaxPchance

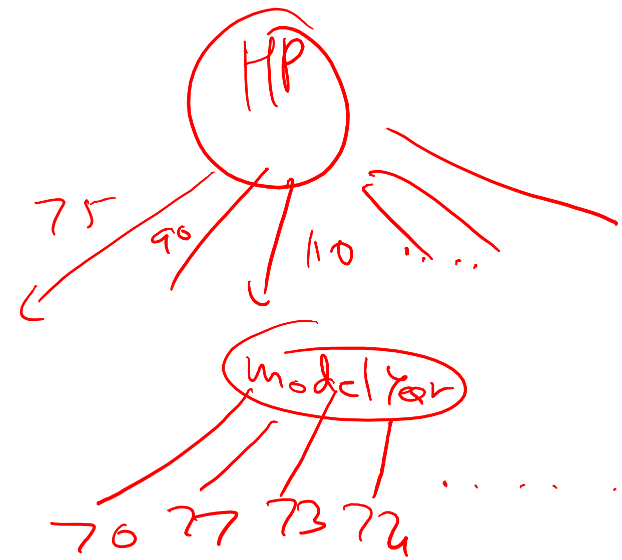
- Technical note MaxPchance is a regularization parameter that helps us bias towards simpler models



Real-Valued inputs

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

mpg	cylinders	displacemen	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

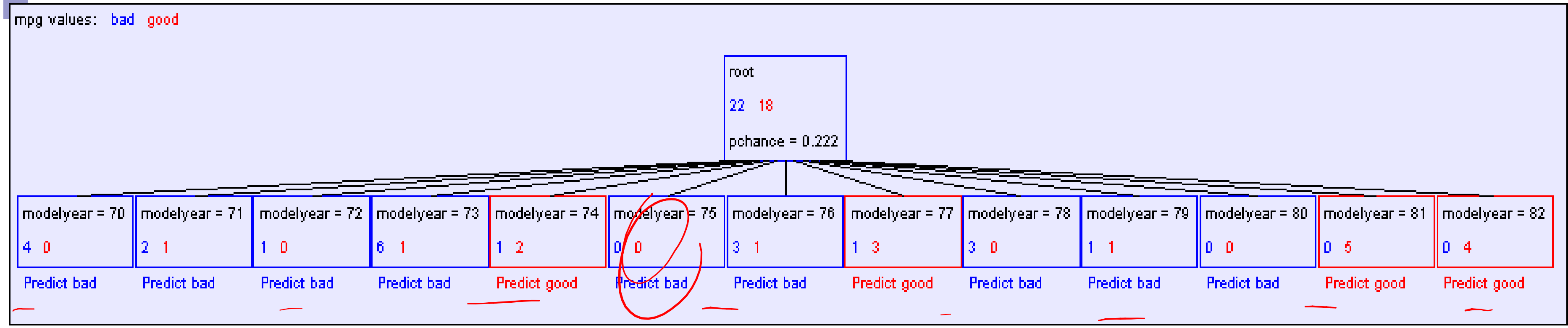


Infinite number of possible split values!!!

Finite dataset, only finite number of relevant splits!

Idea One: Branch on each possible real value

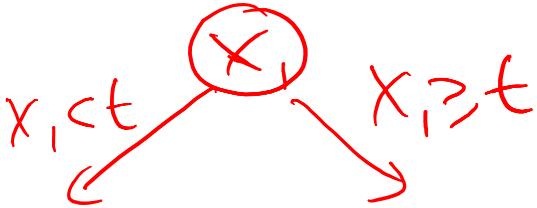
"One branch for each numeric value" idea:



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

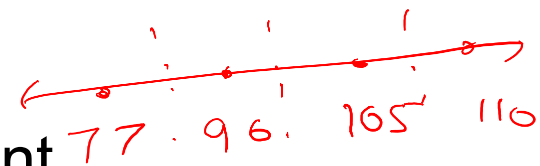
Threshold splits

- Binary tree, split on attribute X_i
  - One branch: $X_i < t$
  - Other branch: $X_i \geq t$

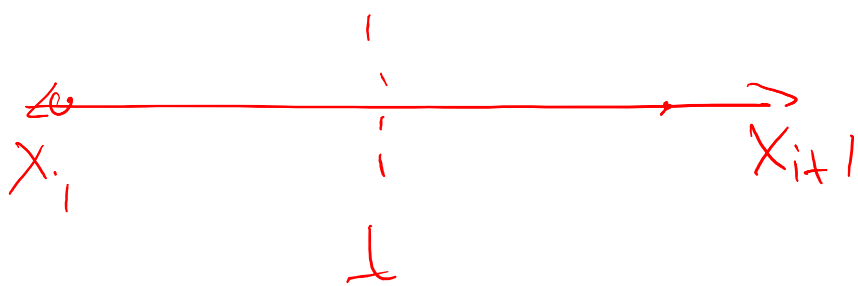


Choosing threshold split

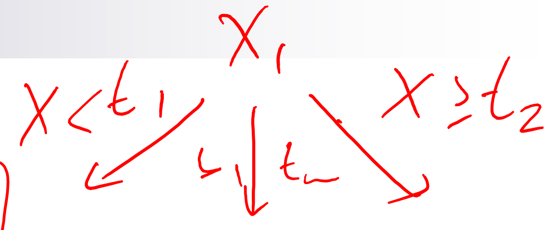
- Binary tree, split on attribute X_i
  - One branch: $X_i < t$
  - Other branch: $X_i \geq t$
- Search through possible values of *t*
  - Seems hard!!!



- But only finite number of *t*'s are important
  - Sort data according to X_i into $\{x_1,\ldots,x_m\}$
  - Consider split points of the form $x_a + (x_{a+1} - x_a)/2$



A better idea: thresholded splits



- Suppose X_i is real valued
- Define $IG(Y|X_i{:}t)$ as $H(Y) - H(Y|X_i{:}t)$
- Define $H(Y|X_i{:}t) =$

  $$H(Y|X_i < t)\, P(X_i < t) + H(Y|X_i >= t)\, P(X_i >= t)$$

  - $IG(Y|X_i{:}t)$ is the information gain for predicting Y if all you know is whether X_i is greater than or less than t
- Then define $IG^*(Y|X_i) = \max_t IG(Y|X_i{:}t)$
- For each real-valued attribute, use $IG^*(Y|X_i)$ for assessing its suitability as a split

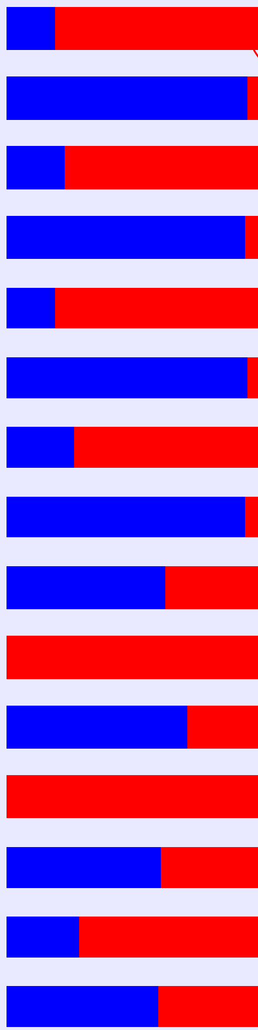
- Note, may split on an attribute multiple times, with different thresholds

Example with MPG

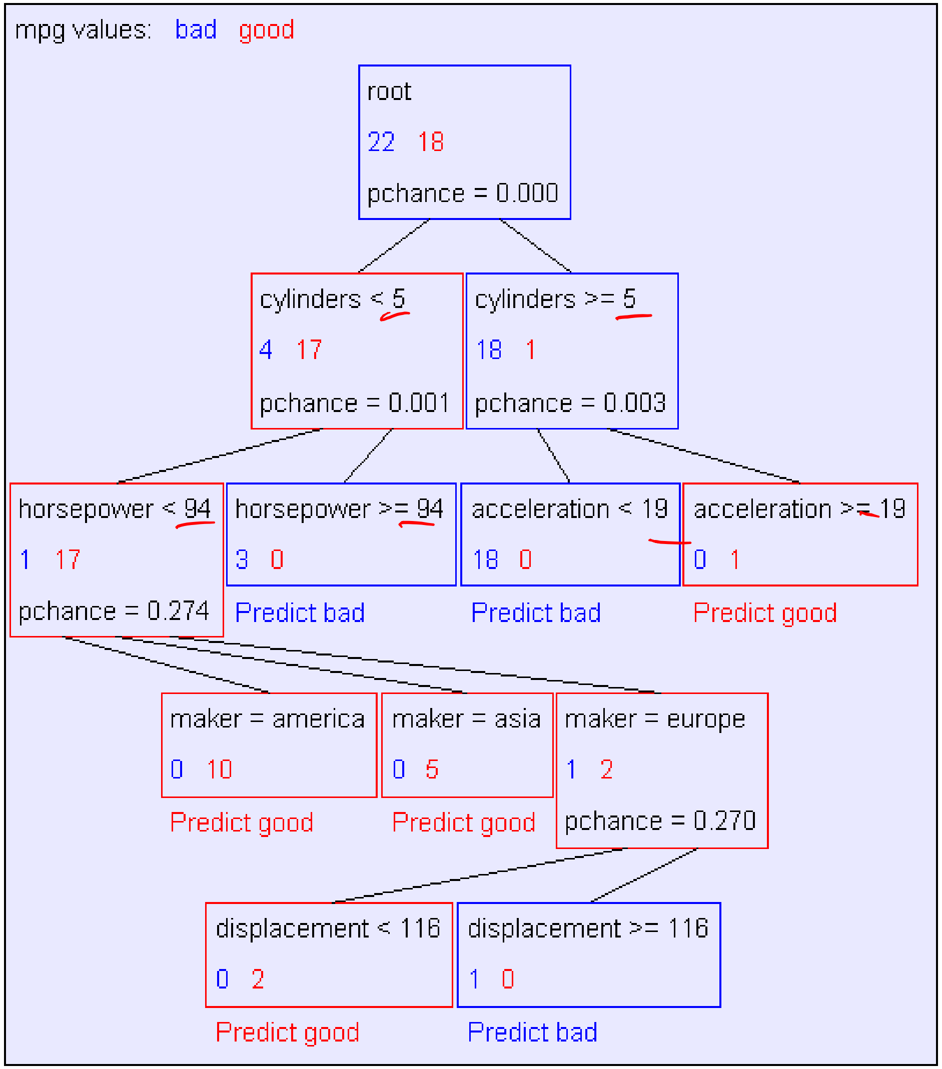
Information gains using the training set (40 records)

mpg values: bad good

Input	Value	Distribution	Info Gain
cylinders	< 5		0.48268
	>= 5		
displacement	< 198		0.428205
	>= 198		
horsepower	< 94		0.48268
	>= 94		
weight	< 2789		0.379471
	>= 2789		
acceleration	< 18.2		0.159982
	>= 18.2		
modelyear	< 81		0.319193
	>= 81		
maker	america		0.0437265
	asia		
	europe		



Example tree using reals



What you need to know about decision trees

- Decision trees are one of the most popular data mining tools
  - Easy to understand
  - Easy to implement
  - Easy to use
  - Computationally cheap (to solve heuristically)
- Information gain to select attributes (ID3, C4.5,…)
- Presented for classification, can be used for regression and density estimation too
- Decision trees will overfit!!!
  - Zero bias classifier $\rightarrow$ Lots of variance
  - Must use tricks to find "simple trees", e.g.,
    - Fixed depth/Early stopping
    - Pruning
    - Hypothesis testing

Acknowledgements

- Some of the material in the decision trees presentation is courtesy of Andrew Moore, from his excellent collection of ML tutorials:
  - http://www.cs.cmu.edu/~awm/tutorials