CSE446: Decision Trees
Winter 2015

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Slides adapted from Carlos Guestrin and Andrew Moore

A learning problem: predict fuel efficiency

- 40 Records
- Discrete data (for now)
- Predict MPG
- Need to find: $f : X \rightarrow Y$

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
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:	:	:	:	:	:	:	:
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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

Y X

From the UCI repository (thanks to Ross Quinlan)

How to Represent our Function?

f (

cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
4	low	low	low	high	75to78	asia

) →

mpg
good

Conjunctions in Propositional Logic?

maker=asia ∧ weight=low

Need to find "Hypothesis": $f : X \rightarrow Y$

Restricted Hypothesis Space

- Many possible representations
- Natural choice: ***conjunction*** of attribute constraints
- For each attribute:
  - Constrain to a specific value: eg **maker=asia**
  - Don't care: **?**
- For example

maker	***cyl***	***displace***	***weight***	***accel ….***
asia	**?**	**?**	**low**	**?**

Represents **maker=asia** $\wedge$ **weight=low**

Consistency

- Say an "example is consistent with a hypothesis" when the example *logically satisfies* the hypothesis

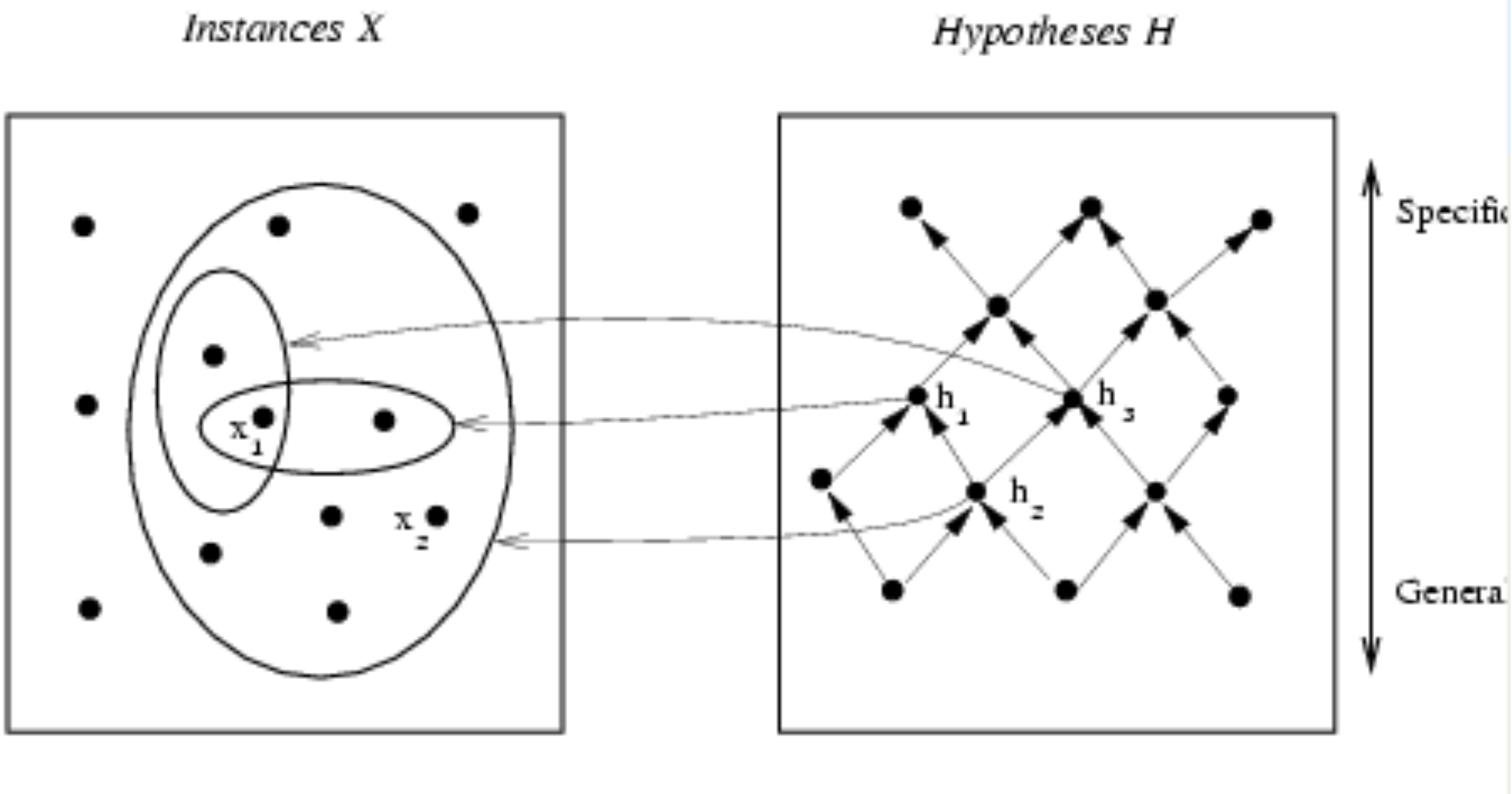
- Hypothesis: **maker=asia ∧ weight=low**

maker	***cyl***	***displace***	***weight***	***accel ….***
asia	**?**	**?**	**low**	**?**

- Examples:

asia	5	low	low	low	…
usa	4	low	low	low	…

Ordering on Hypothesis Space



x_1	asia	5	low	low	low
x_2	usa	4	med	med	med

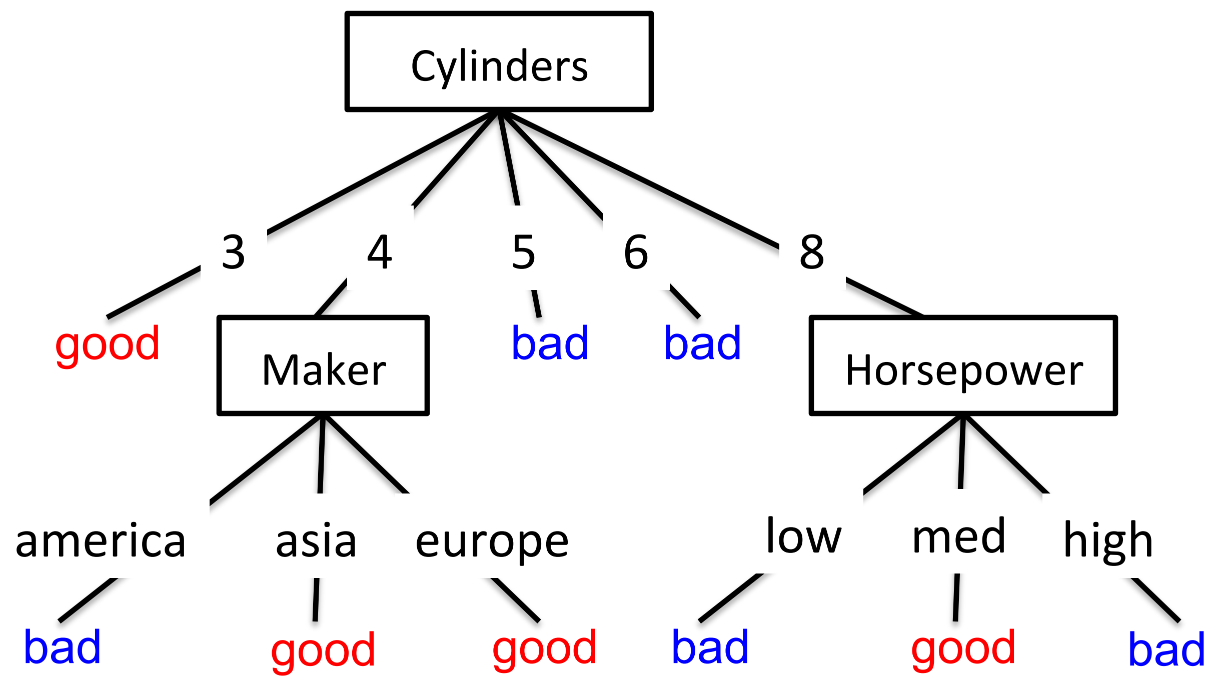
h1: maker=asia ∧ accel=low

h2: maker=asia

h3: maker=asia ∧ weight=low

Hypotheses: decision trees $f : X \rightarrow Y$

- Each internal node tests an attribute x_i
- Each branch assigns an attribute value $x_i = v$
- Each leaf assigns a class y
- To classify input x: traverse the tree from root to leaf, output the labeled y



Hypothesis space

- How many possible hypotheses?
- What functions can be represented?

mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
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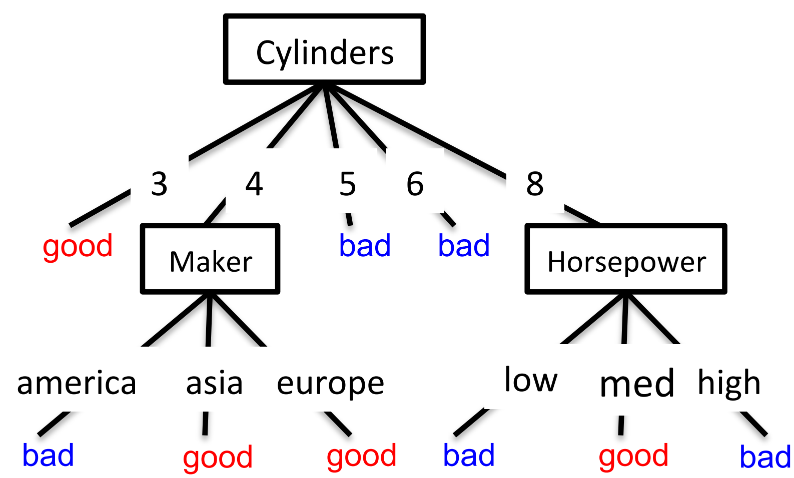
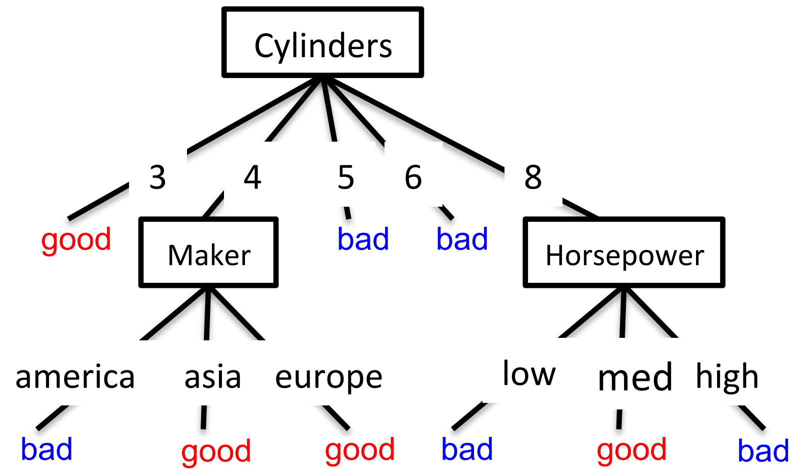


What functions can be represented?

- Decision trees can represent any boolean function!
- But, could require exponentially many nodes…



cyl=3 ∨ (cyl=4 ∧ (maker=asia ∨ maker=europe)) ∨ …

Hypothesis space

- How many possible hypotheses?
- What functions can be represented?
- How many will be consistent with a given dataset?
- How will we choose the best one?
  - Lets first look at how to split nodes, then consider how to find the best tree

mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
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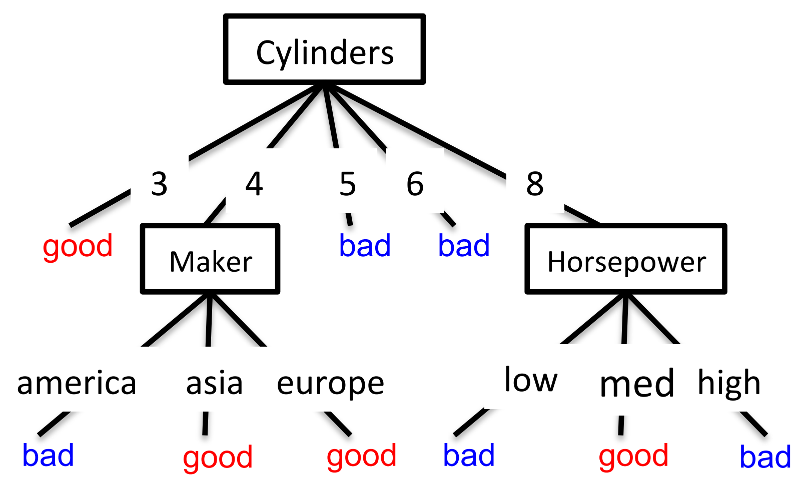

What is the Simplest Tree?

mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
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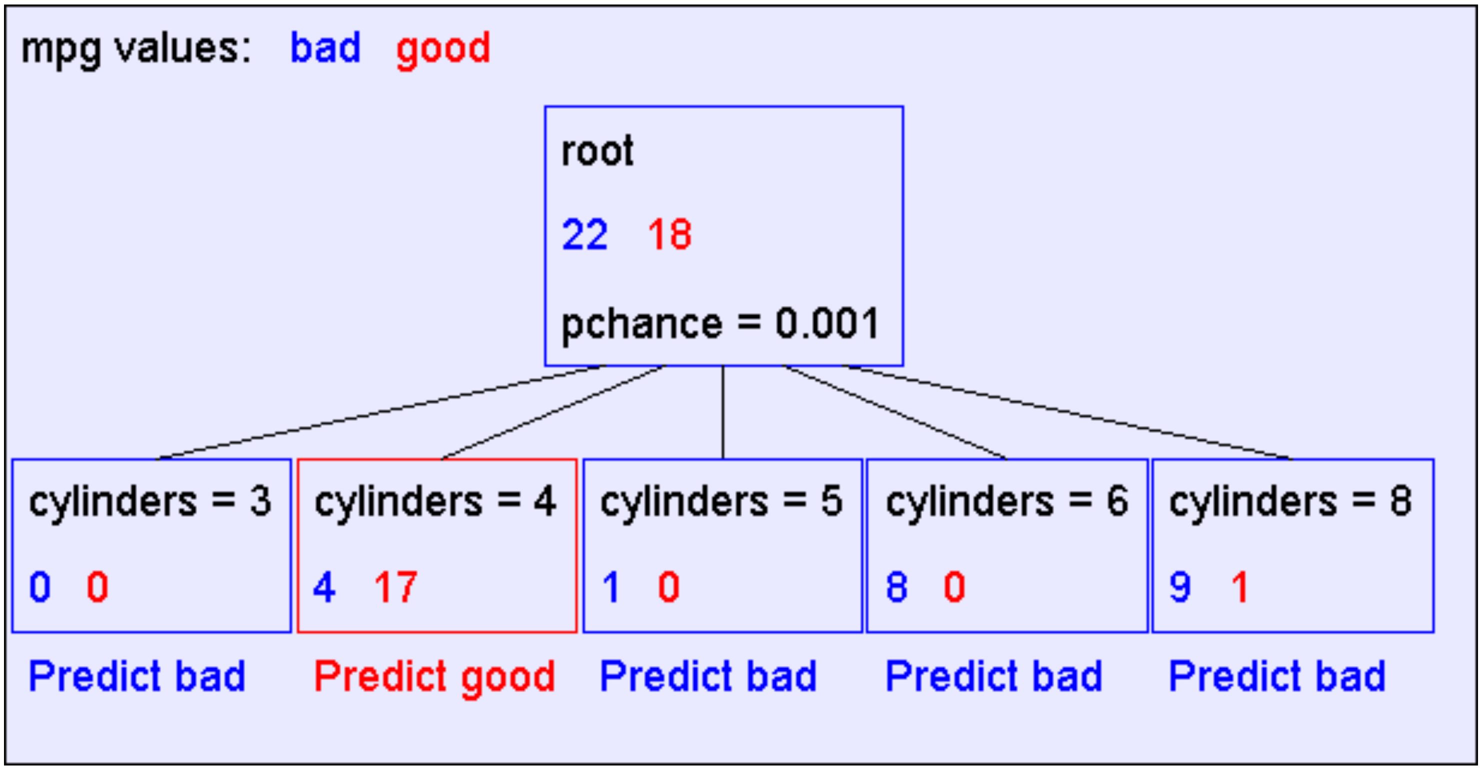
predict
mpg=bad

Is this a good tree?

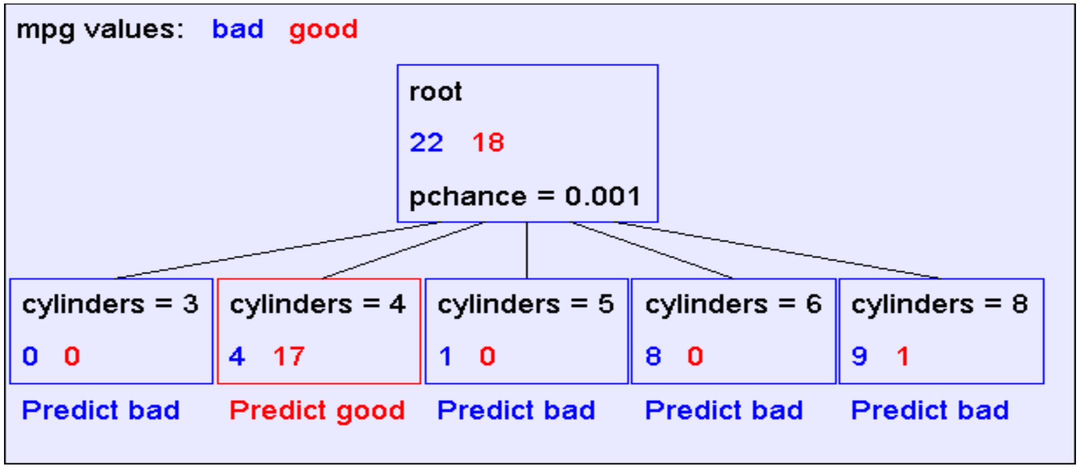
[22+, 18-]

Means:
correct on 22 examples
incorrect on 18 examples

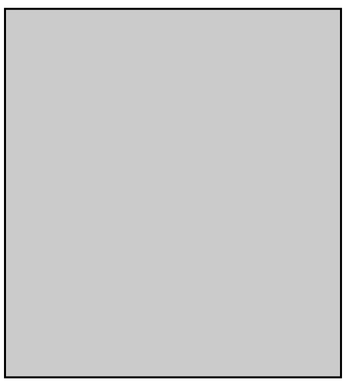
A Decision Stump



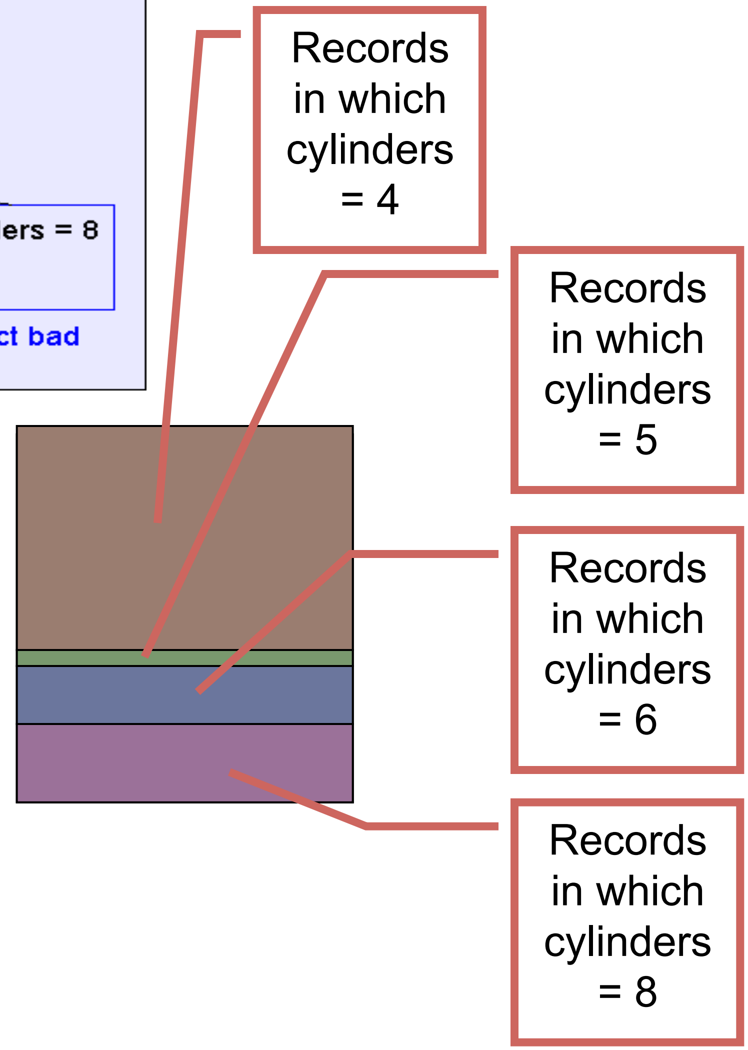
Recursive Step



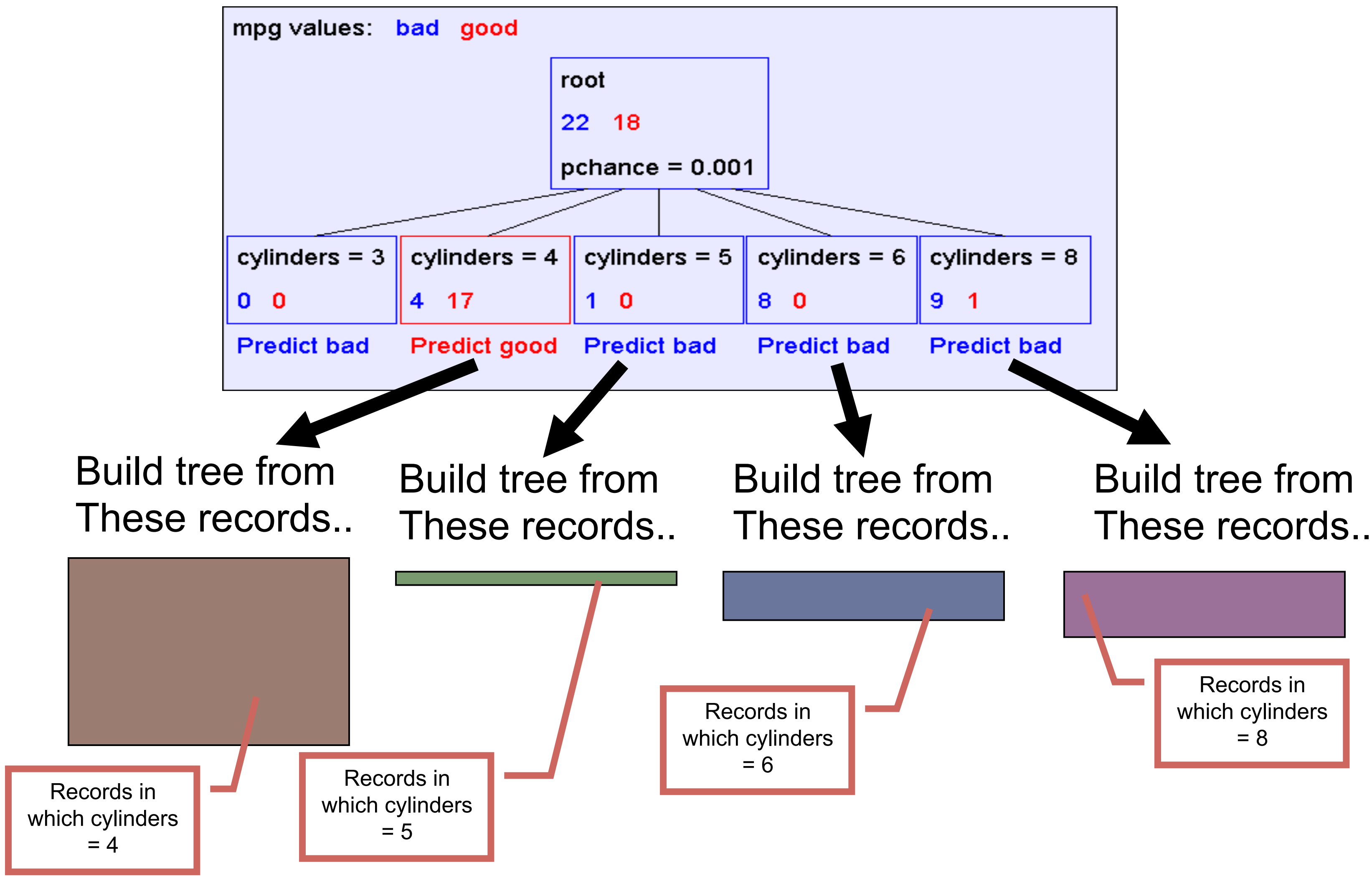
Take the Original Dataset..



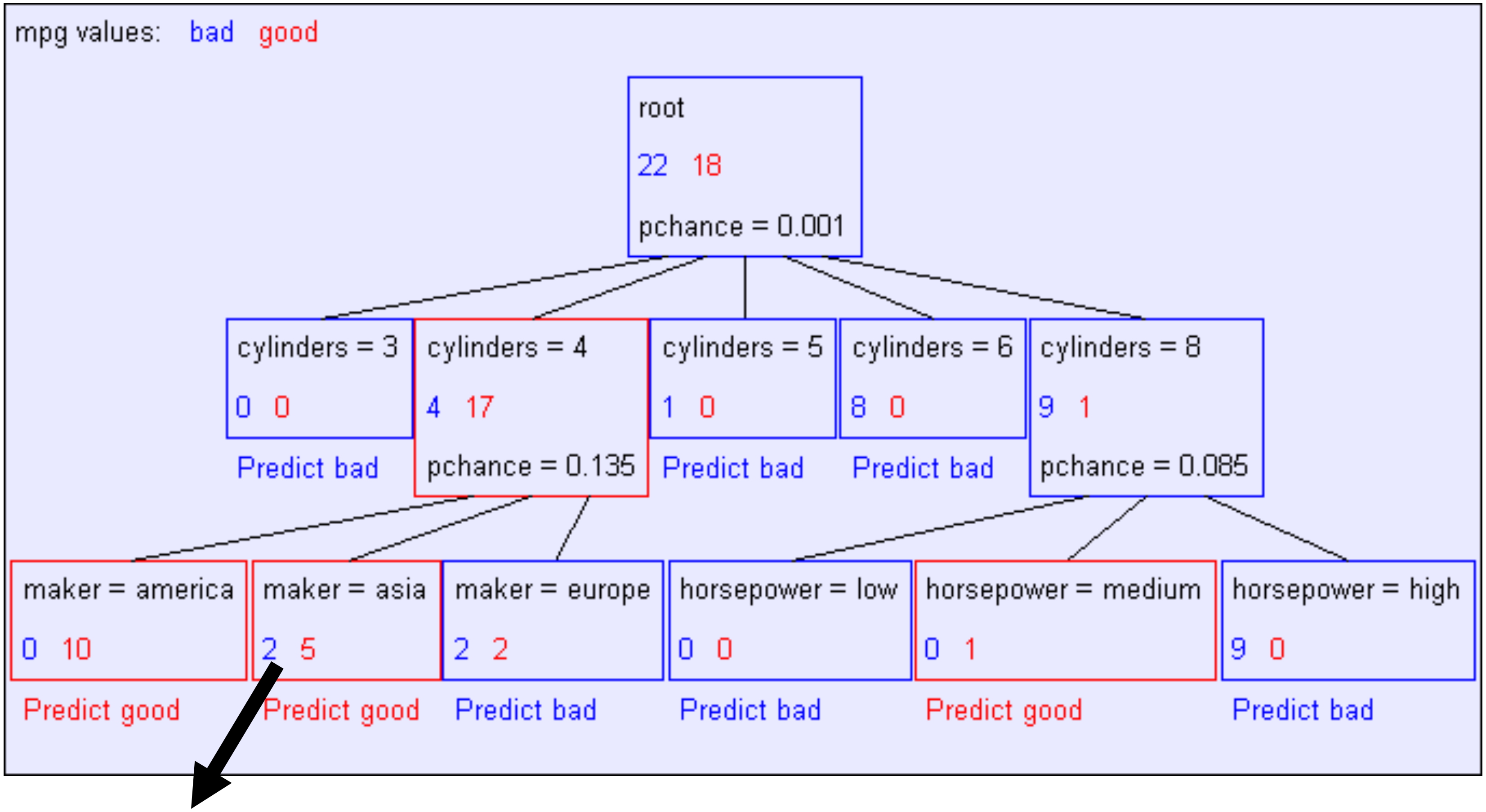
And partition it according to the value of the attribute we split on



Recursive Step



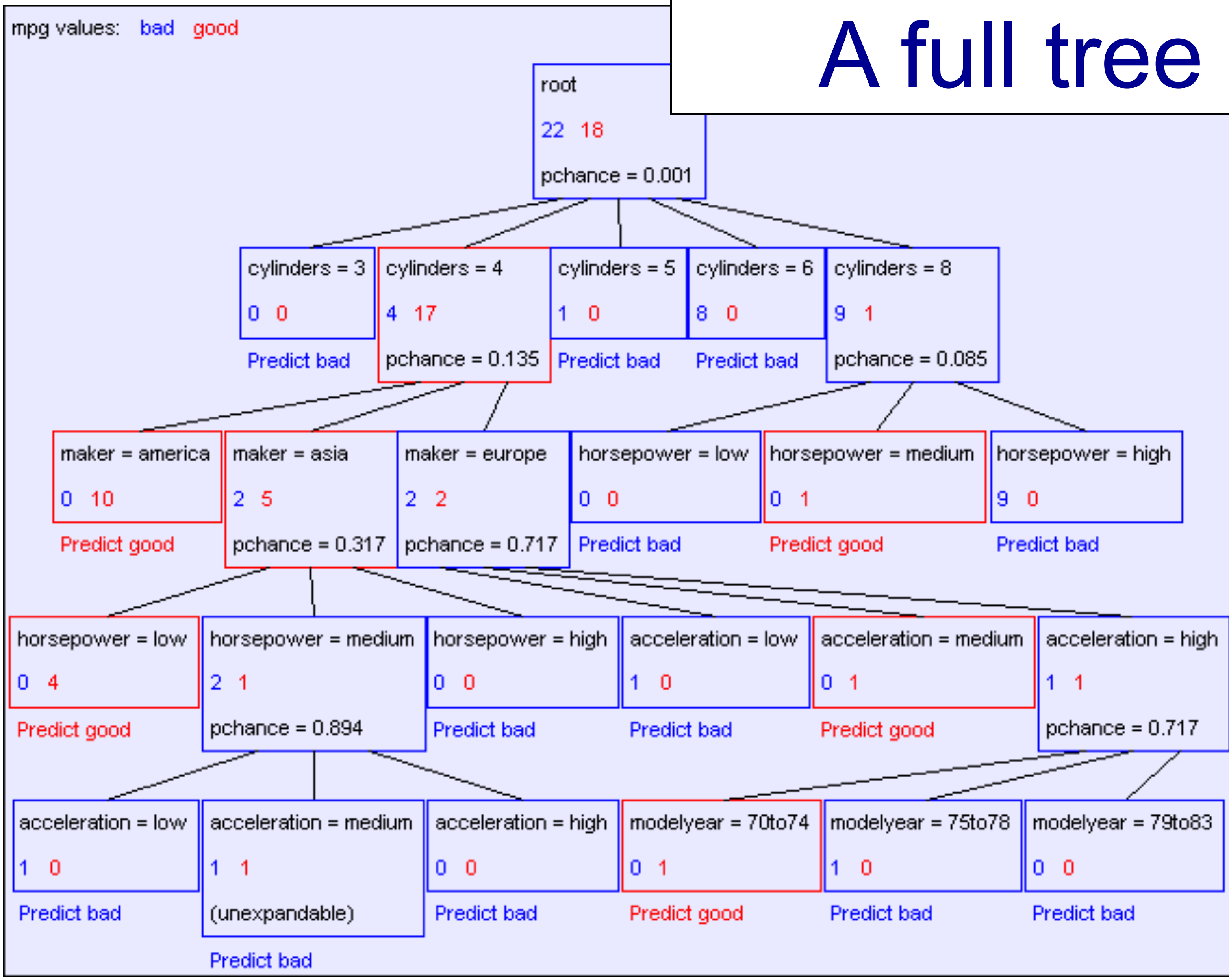
Second level of tree



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

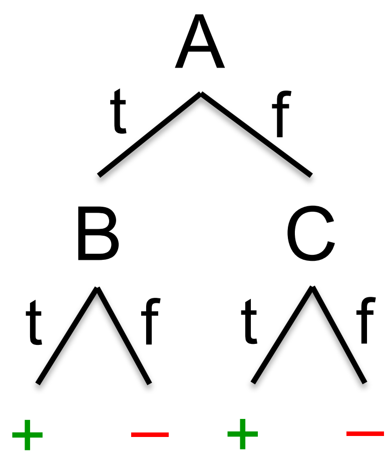
(Similar recursion in the other cases)

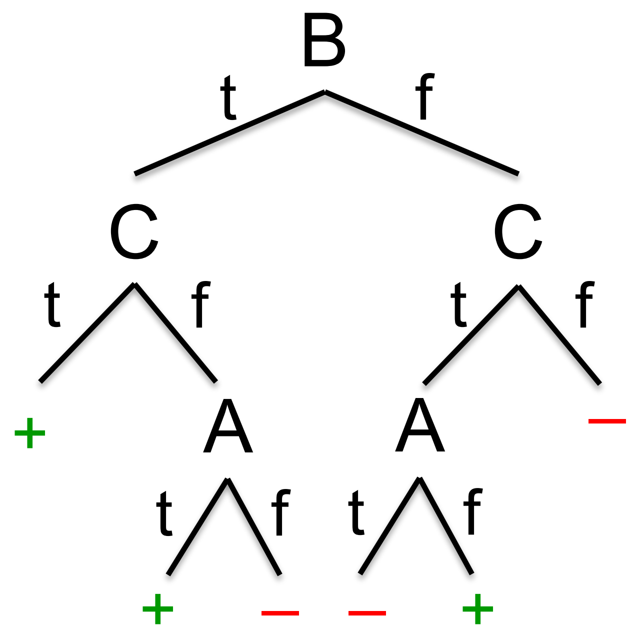
A full tree


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 = low
0 0
Predict bad
horsepower = medium
0 1
Predict good
horsepower = high
9 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

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))





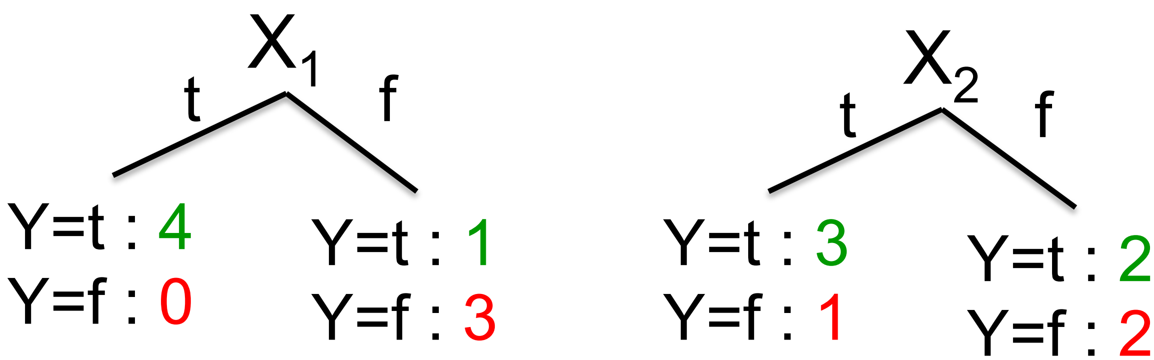
- Which tree do we prefer?
  - Smaller tree has more examples at each leaf!

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

Splitting: choosing a good attribute

Would we prefer to split on X_1 or X_2?



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

Idea: use counts at leaves to define probability distributions, so we can measure uncertainty!

Measuring uncertainty

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

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

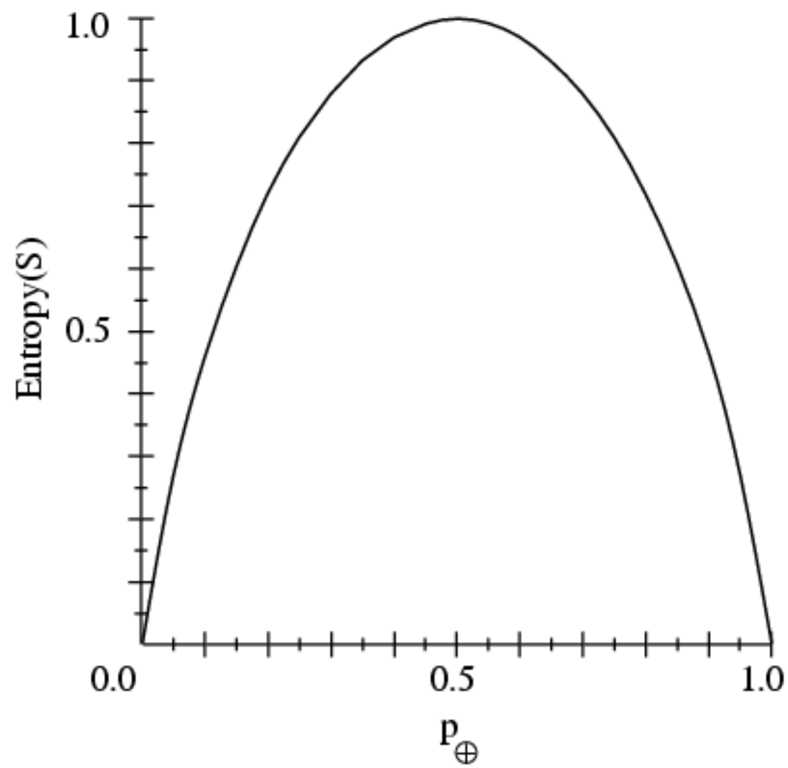
Entropy

Entropy $H(Y)$ of a random variable Y

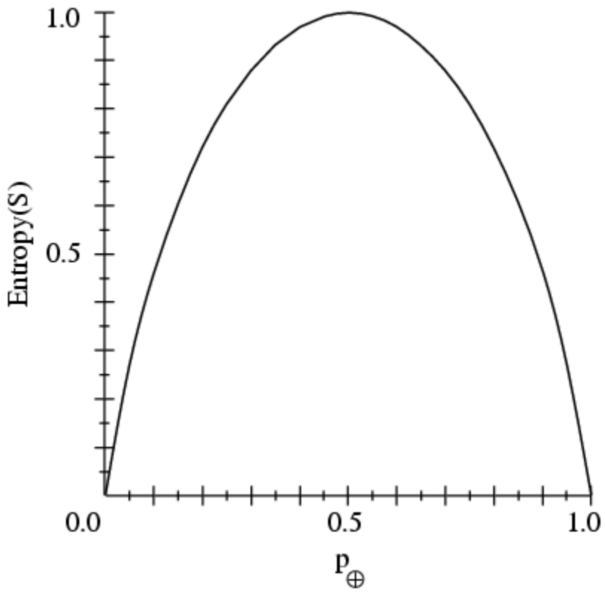
$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

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)



Entropy Example



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

P(Y=t) = 5/6

P(Y=f) = 1/6

H(Y) = - 5/6 $\log_2$ 5/6 - 1/6 $\log_2$ 1/6

= 0.65

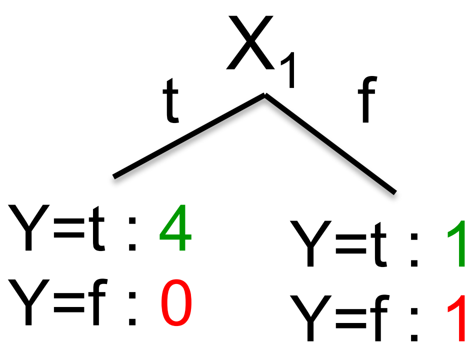
X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

Conditional Entropy

Conditional Entropy $H(Y|X)$ of a random variable Y conditioned on a random variable X

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

Example:



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

$P(X_1=t) = 4/6$

$P(X_1=f) = 2/6$

$$H(Y|X_1) = -\ 4/6\ (1 \log_2 1 + 0 \log_2 0)$$
$$-\ 2/6\ (1/2 \log_2 1/2 + 1/2 \log_2 1/2)$$
$$= 2/6$$

Information gain

- Decrease in entropy (uncertainty) after splitting

$$IG(X) = H(Y) - H(Y \mid X)$$

In our running example:

$IG(X_1) = H(Y) – H(Y|X_1)$
$= 0.65 – 0.33$

$IG(X_1) > 0 \rightarrow$ we prefer the split!

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

Learning decision trees

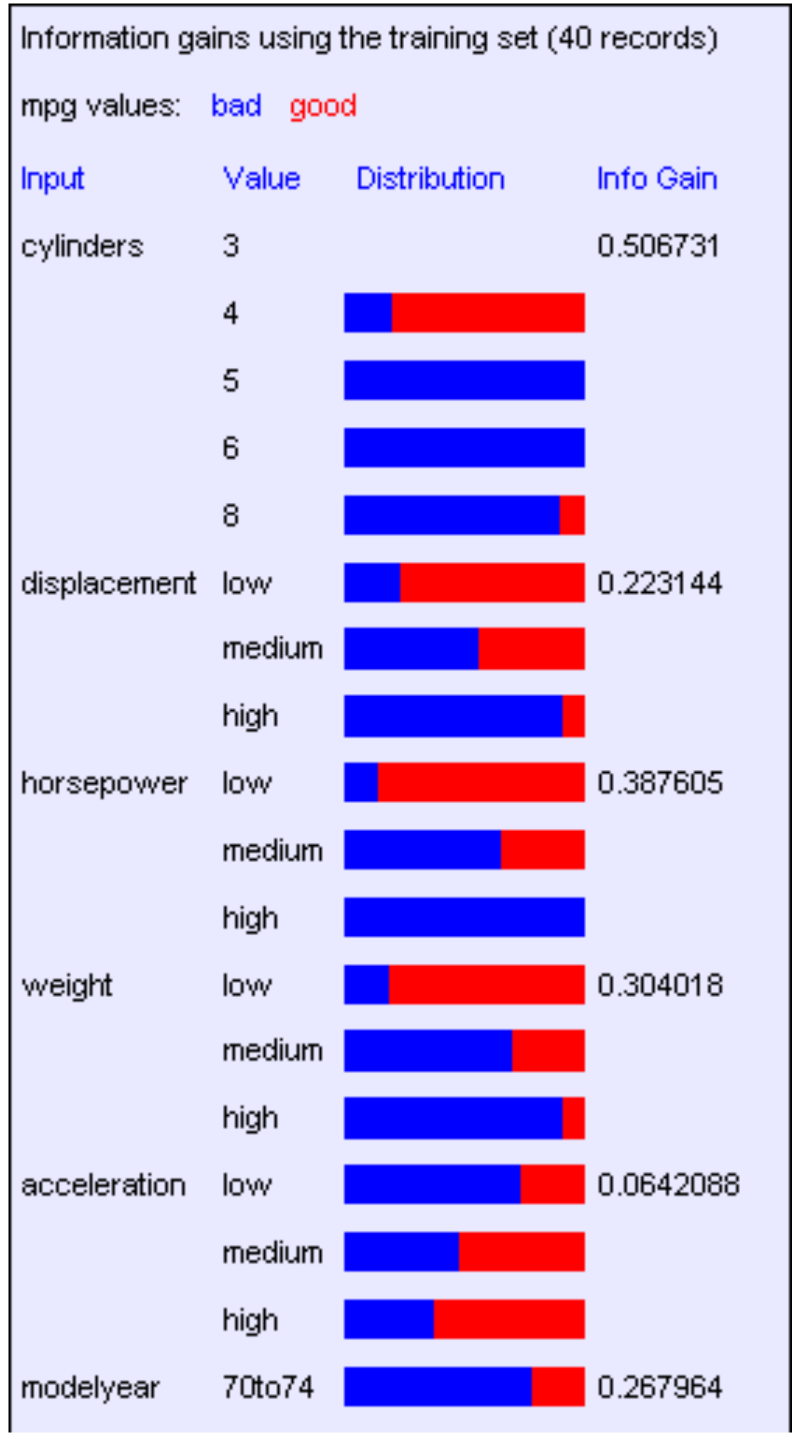
- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

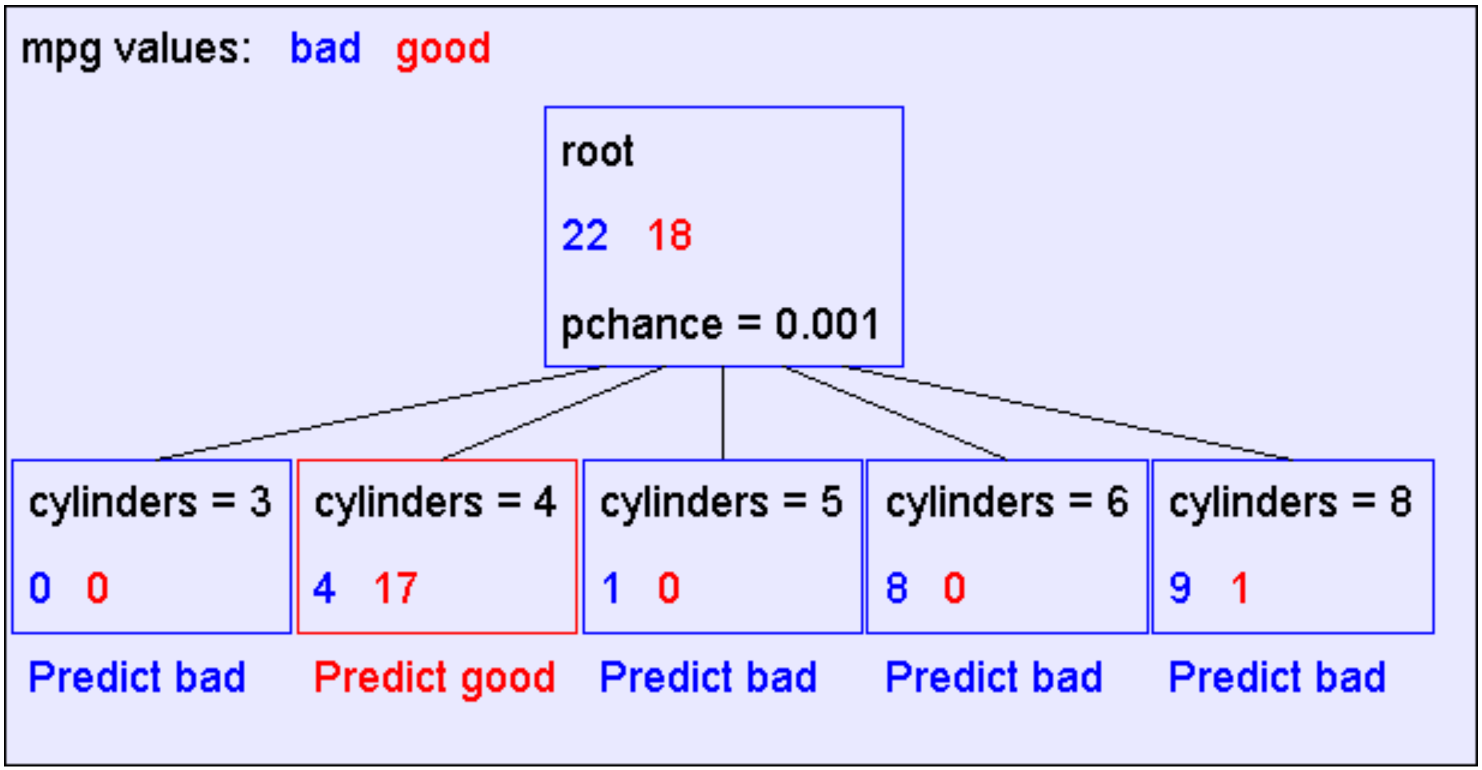
- Recurse

Suppose we want to predict MPG

Look at all the information gains…

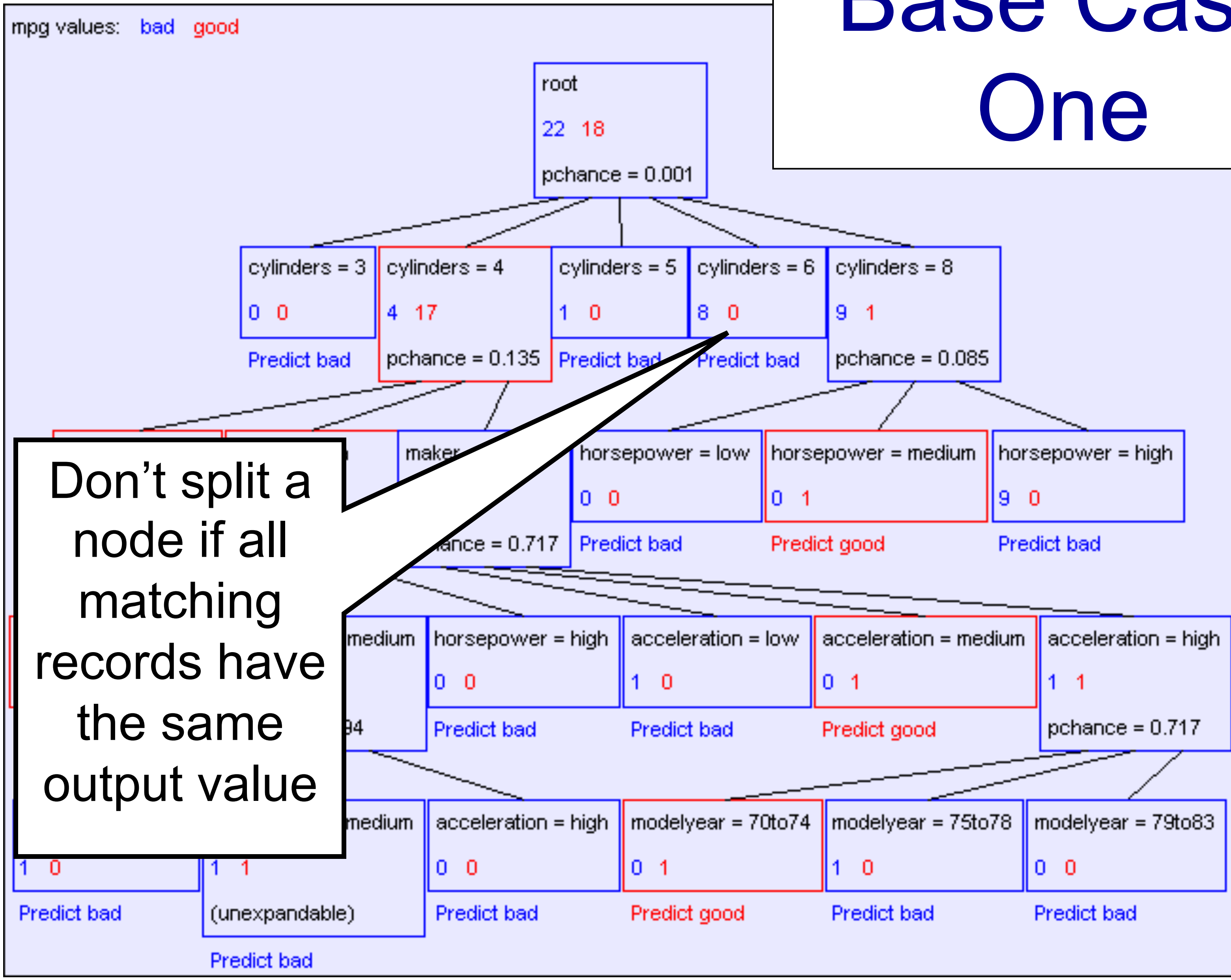


A Decision Stump



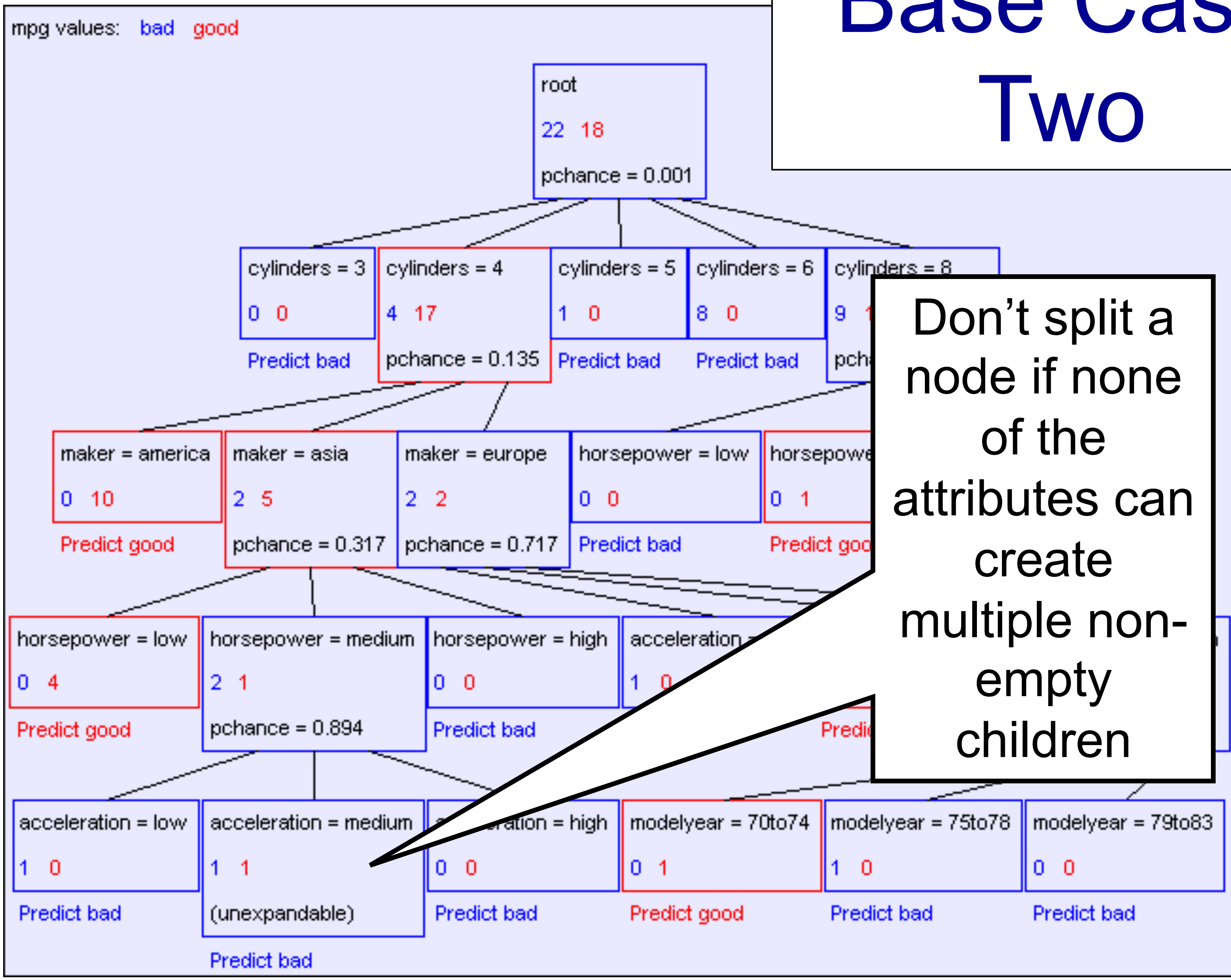
First split looks good! But, when do we stop?

Base Case One

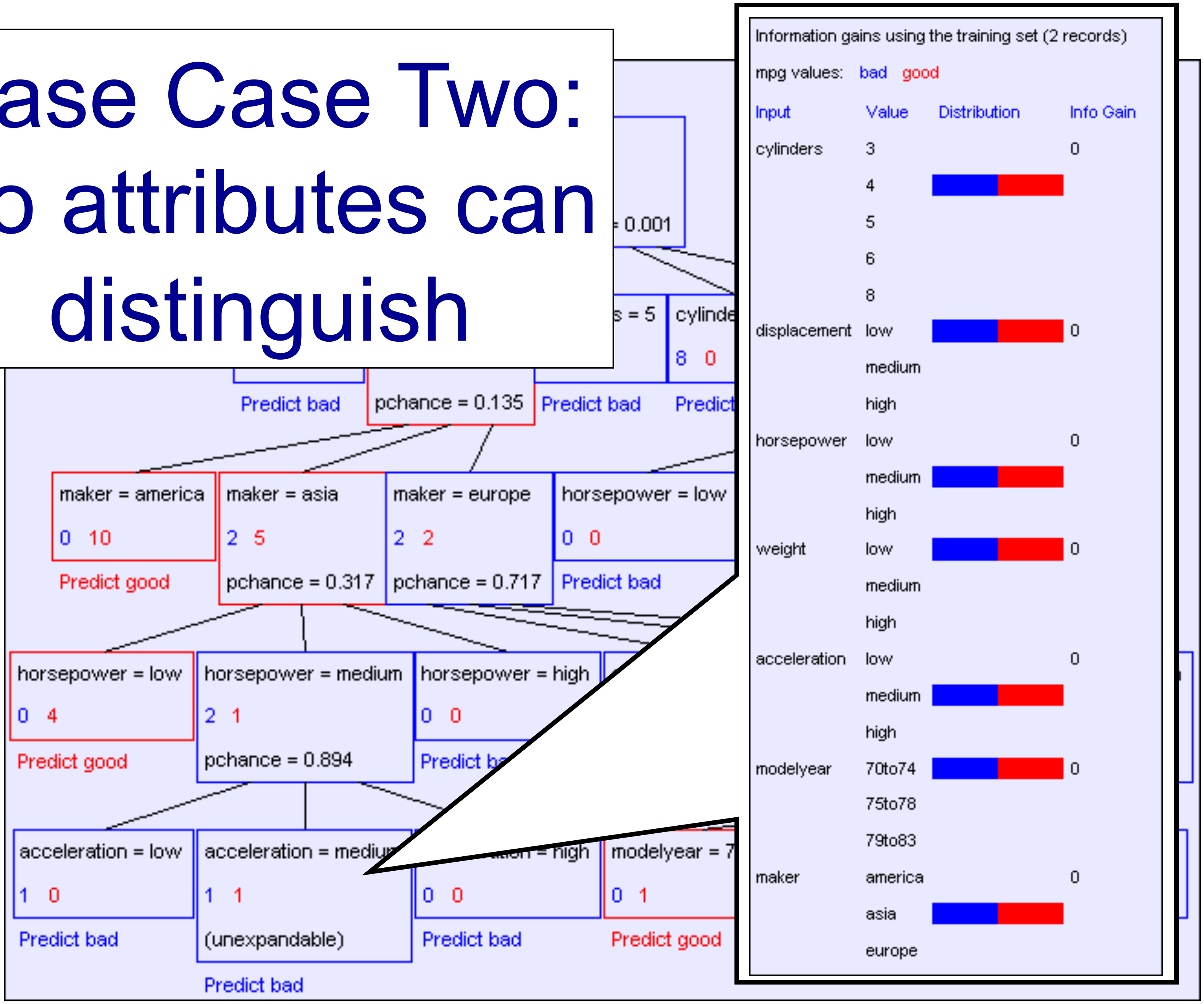


Don't split a node if all matching records have the same output value

Base Case Two



Base Case Two: No attributes can distinguish



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

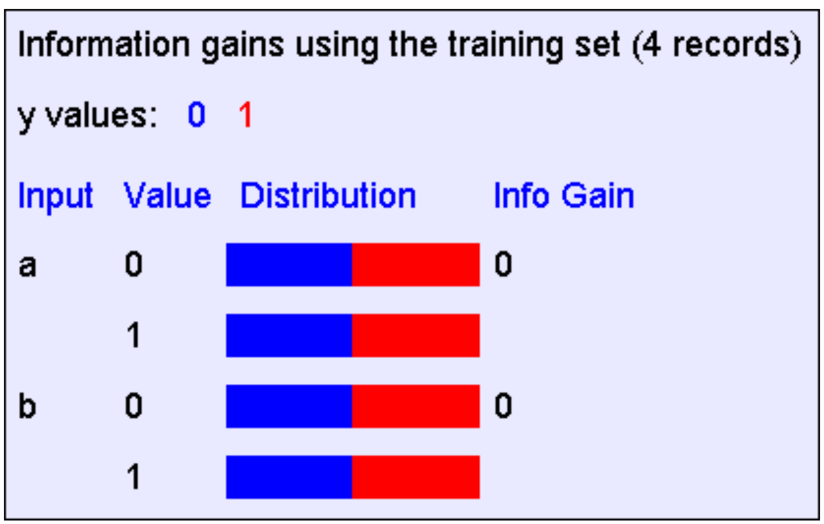
- *Is this a good idea?*

The problem with Base Case 3

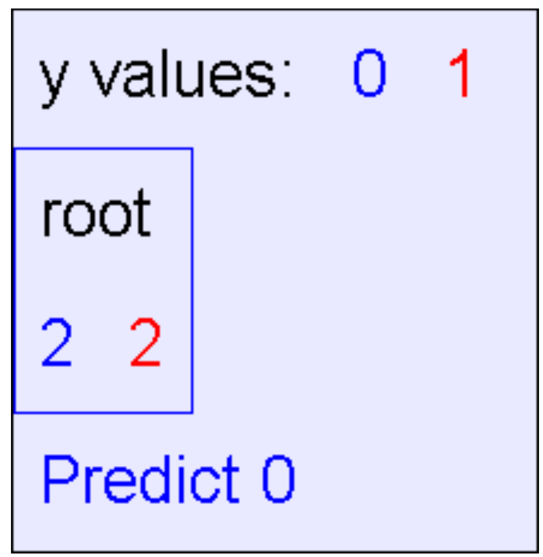
y = a XOR b

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

The information gains:



The resulting decision tree:

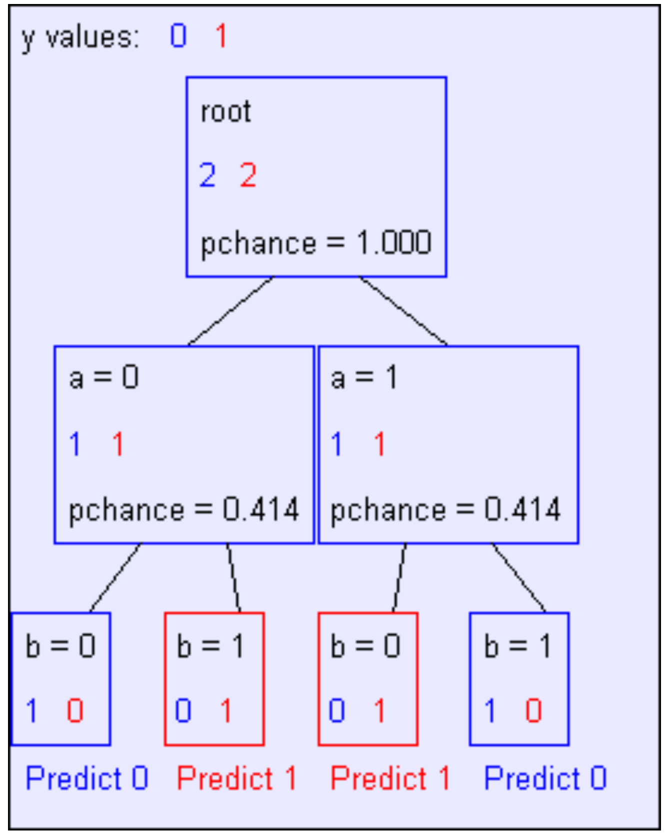


If we omit Base Case 3:

y = a XOR b

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

The resulting decision tree:



Is it OK to omit Base Case 3?

Summary: Building Decision Trees

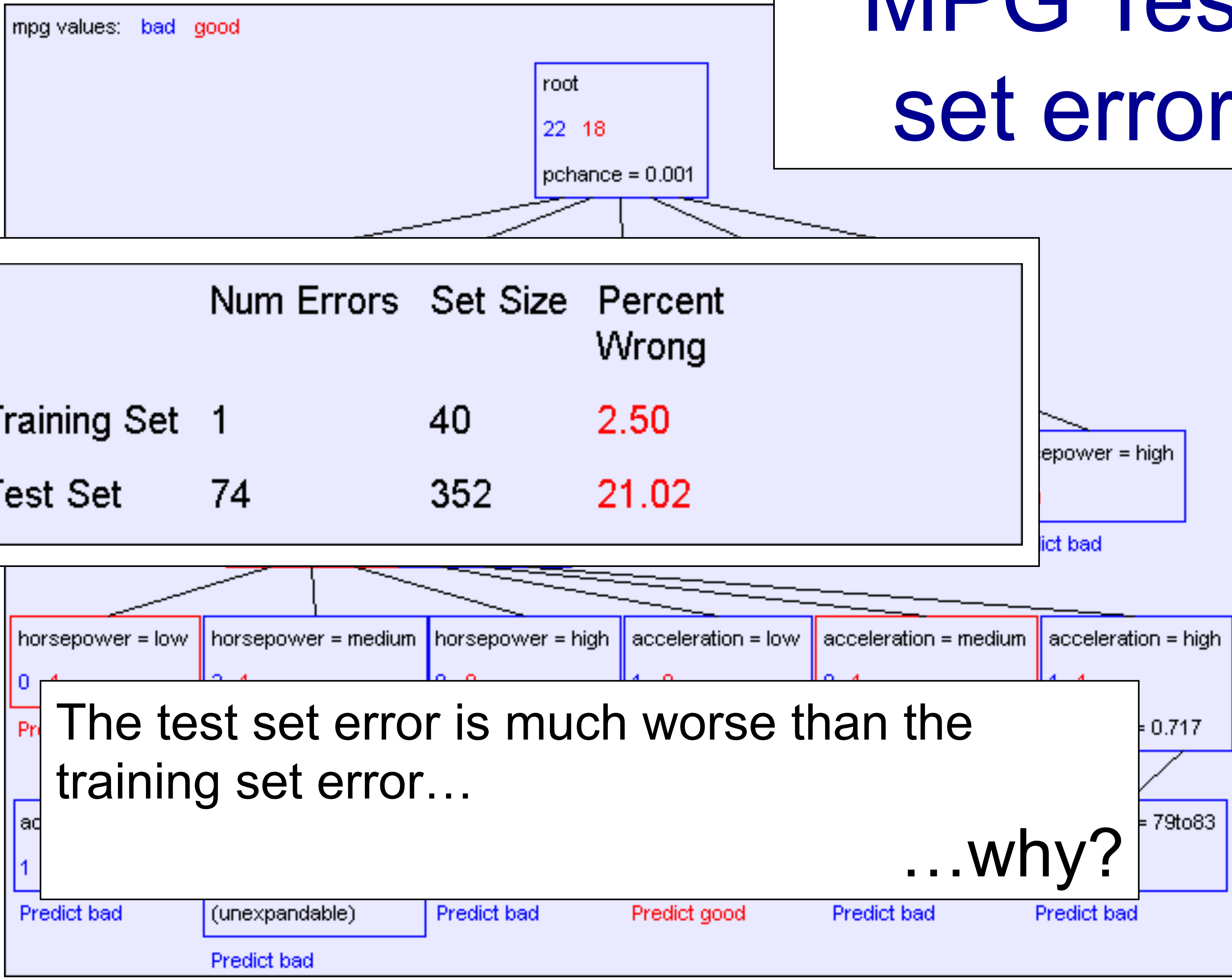
BuildTree(*DataSet,Output*)

- 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 a non-leaf node with n_X children.
  - The *i*'th child should be built by calling

    BuildTree(DS_i,*Output*)

    Where DS_i contains the records in DataSet where X = *i*th 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

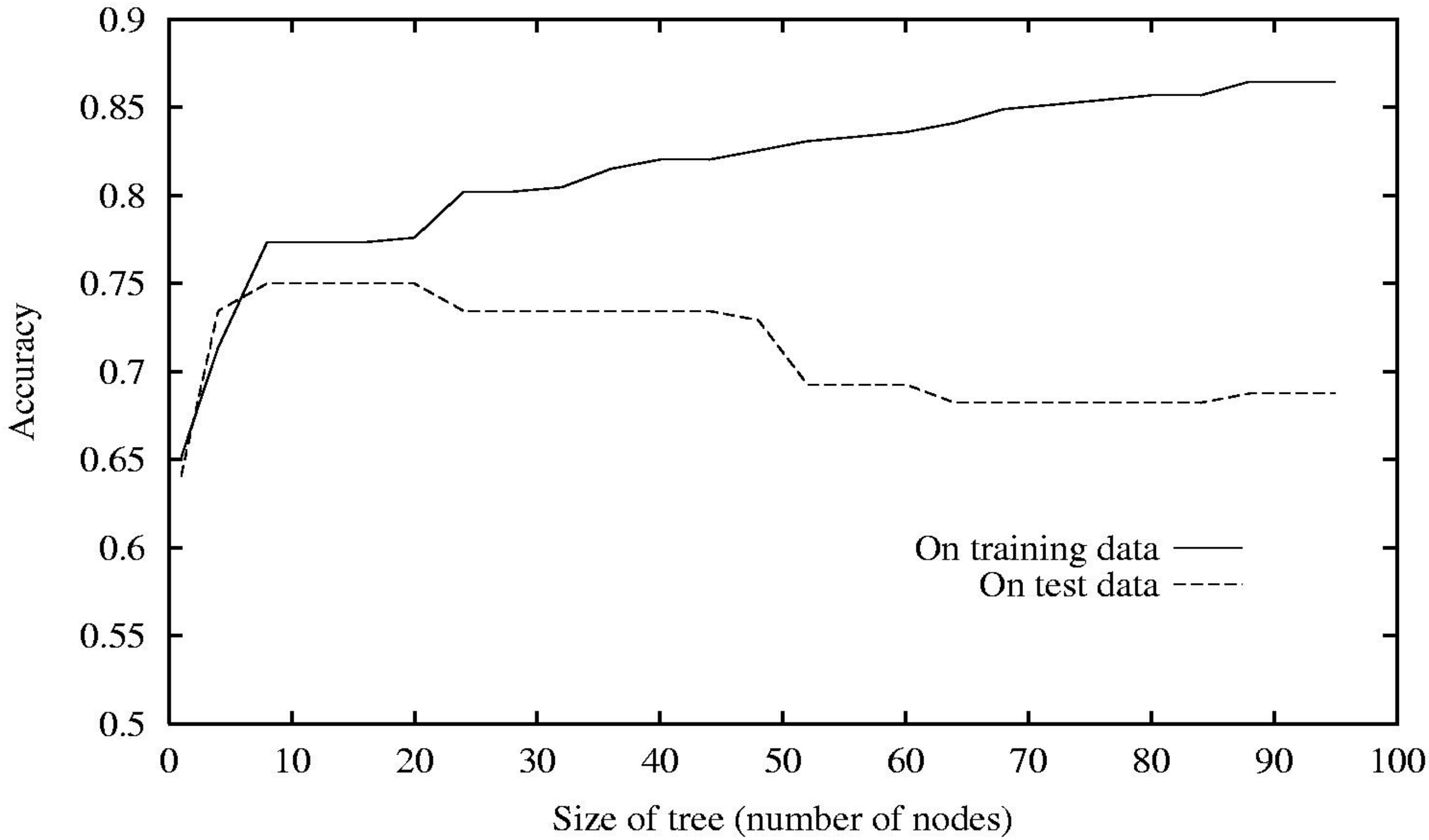
The test set error is much worse than the training set error…

…why?

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
  - Must introduce some bias towards simpler trees
- Many strategies for picking simpler trees
  - Fixed depth
  - Fixed number of leaves
  - Or something smarter…

Decision trees will overfit!!!



One Definition of Overfitting

- Assume:
  - Data generated from distribution $D(X,Y)$
  - A hypothesis space H
- Define errors for hypothesis $h \in H$
  - Training error: $error_{train}(h)$
  - Data (true) error: $error_D(h)$

- We say h ***overfits*** the training data if there exists an $h' \in H$ such that:

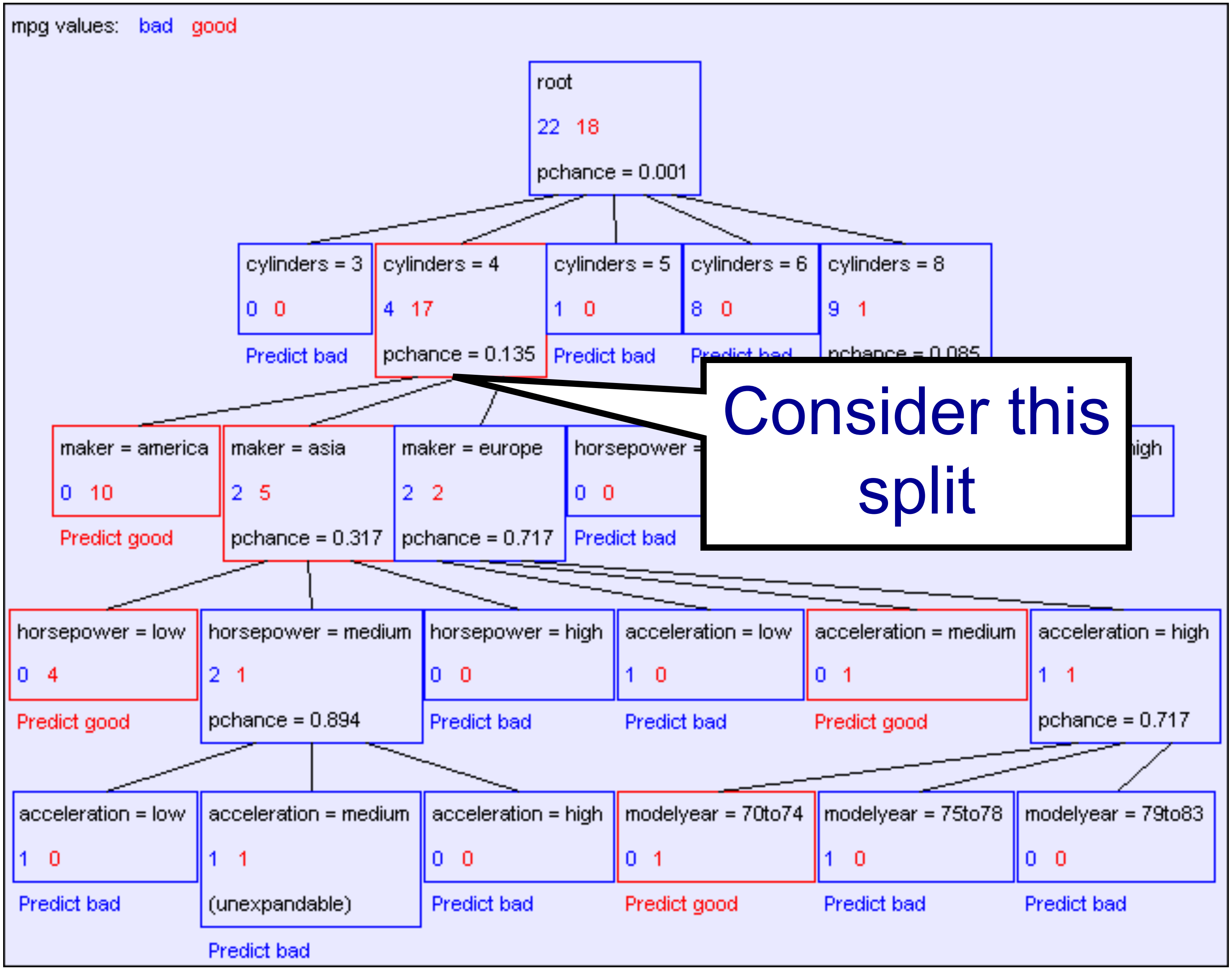
$$error_{train}(h) < error_{train}(h')$$

and

$$error_D(h) > error_D(h')$$

Occam's Razor

- Why Favor Short Hypotheses?
- Arguments for:
  - Fewer short hypotheses than long ones
    - →A short hyp. less likely to fit data by coincidence
    - →Longer hyp. that fit data may might be coincidence
- Arguments against:
  - Argument above really uses the fact that hypothesis space is small!!!
  - What is so special about small sets based on the size of each hypothesis?

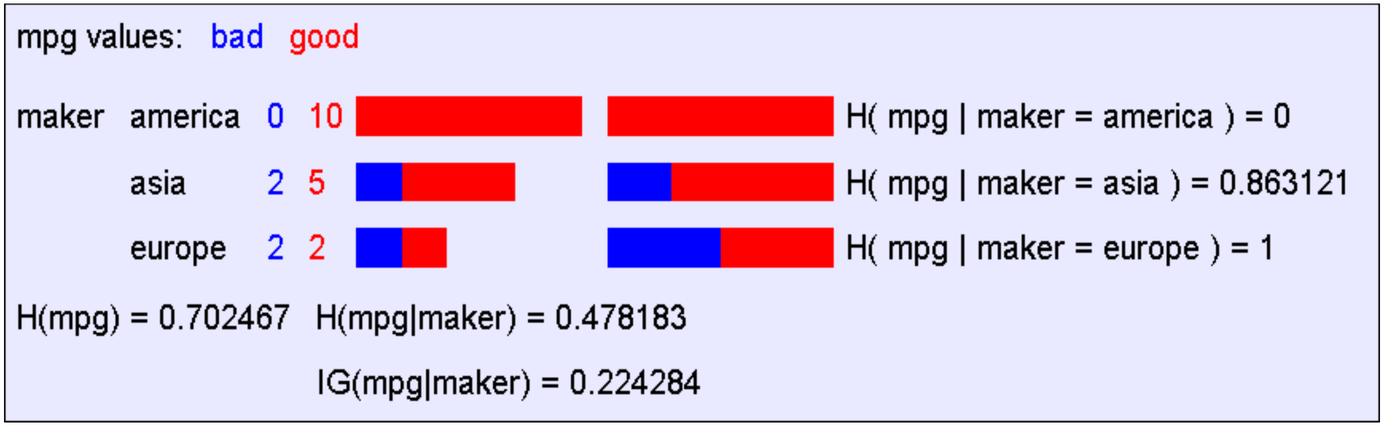

mpg values: bad good
root
22 18
pchance = 0.001
cylinders = 3
0 0
Predict bad
cylinders = 4
4 17
pchance = 0.135
cylinders = 5
1 0
Predict bad
cylinders = 6
8 0
Predict bad
cylinders = 8
9 1
pchance = 0.085
maker = america
0 10
Predict good
maker = asia
2 5
pchance = 0.317
maker = europe
2 2
pchance = 0.717
horsepower =
0 0
Predict bad
high
Consider this split
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

How to Build Small Trees

Two reasonable approaches:

- Optimize on the held-out (development) set
  - If growing the tree larger hurts performance, then stop growing!!!
  - Requires a larger amount of data…
- Use statistical significance testing
  - Test if the improvement for any split it likely due to noise
  - If so, don't do the 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?

By using a particular kind of chi-square test, the answer is 13.5%

We will not cover Chi Square tests in class. See page 93 of the original ID3 paper [Quinlan, 86], linked from the course web site.

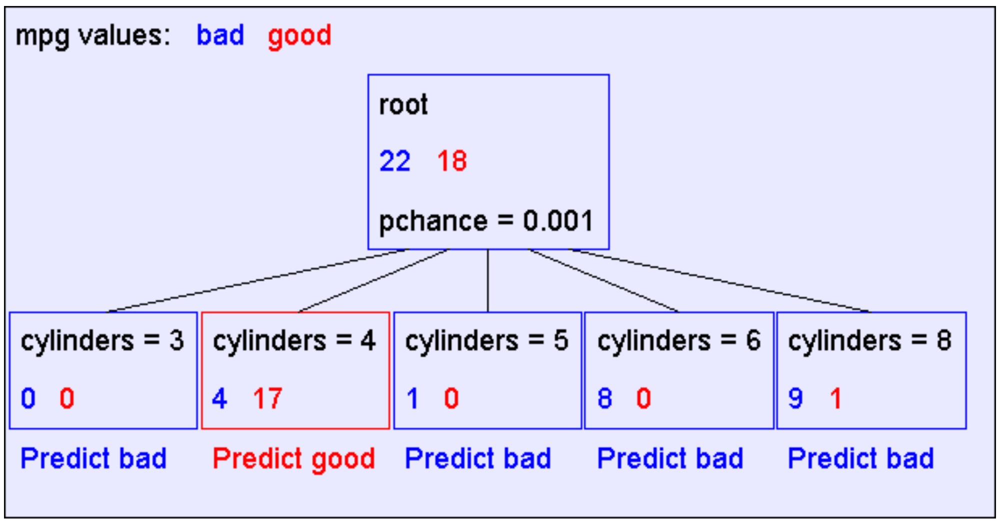
Using Chi-squared to avoid overfitting

- 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 = 0.05, you will see the following MPG decision tree:

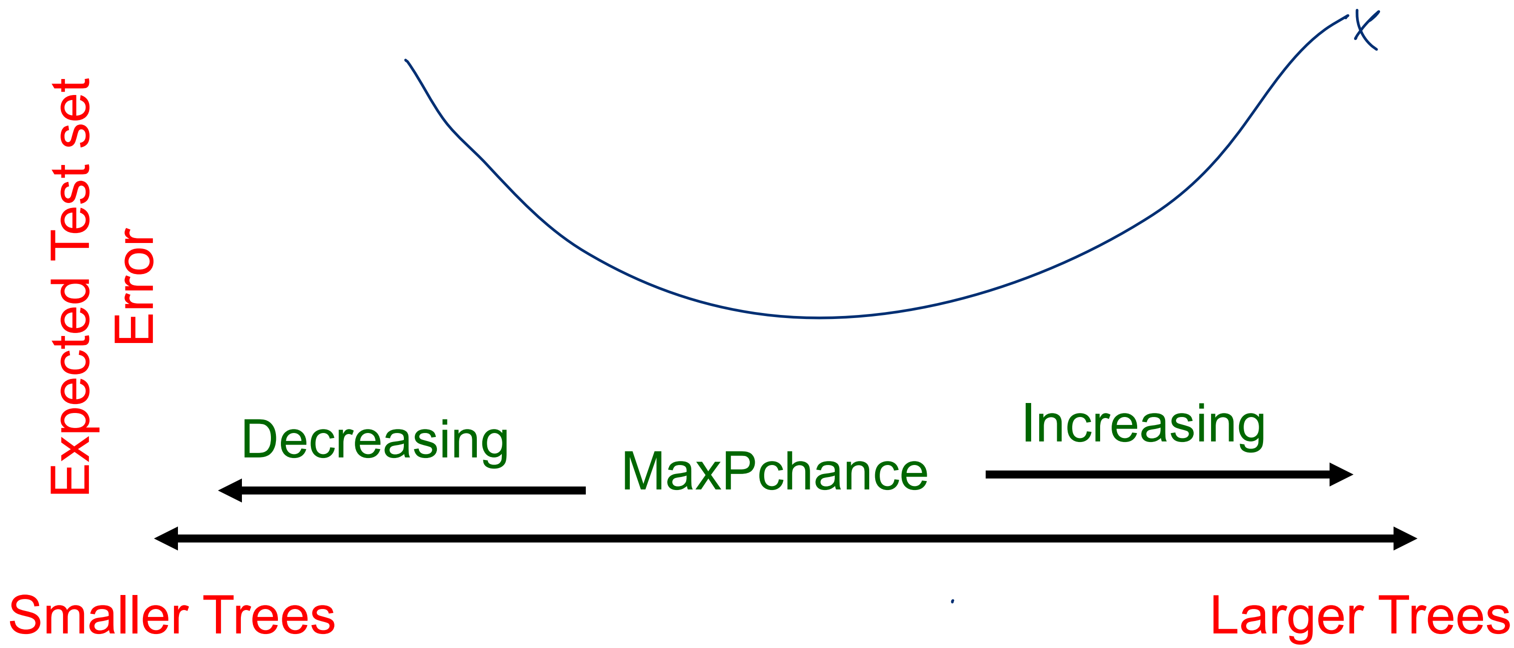


When compared to the unpruned tree
- improved test set accuracy
- worse training accuracy

	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



We'll learn to choose the value of magic parameters like this one later!

Real-Valued inputs

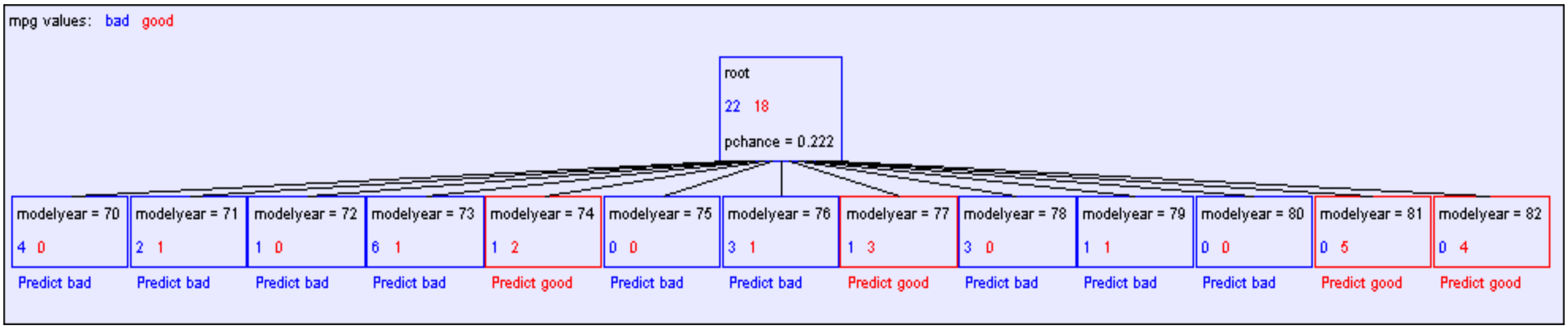
What should we do if some of the inputs are real-valued?

Infinite number of possible split values!!!

Finite dataset, only finite number of relevant splits!

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

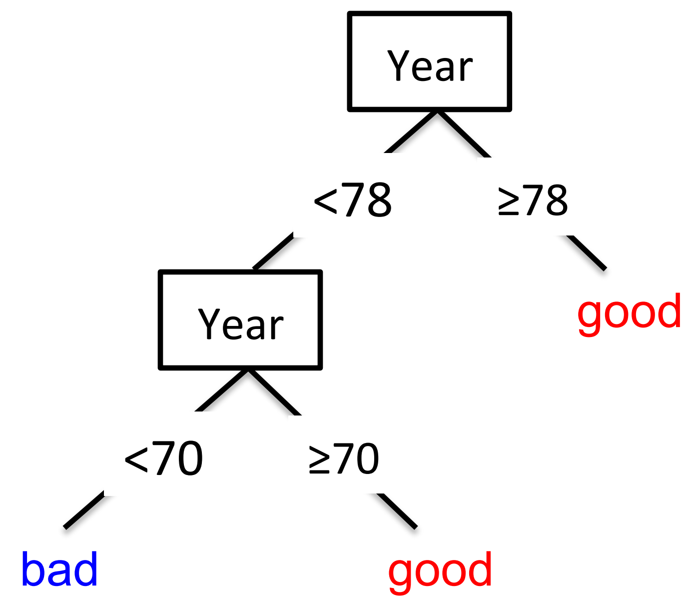
"One branch for each numeric value" idea:



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

Threshold splits

- Binary tree: split on attribute X at value t
  - One branch: X < t
  - Other branch: X ≥ t
- Requires small change
  - Allow repeated splits on same variable
  - How does this compare to "branch on each value" approach?



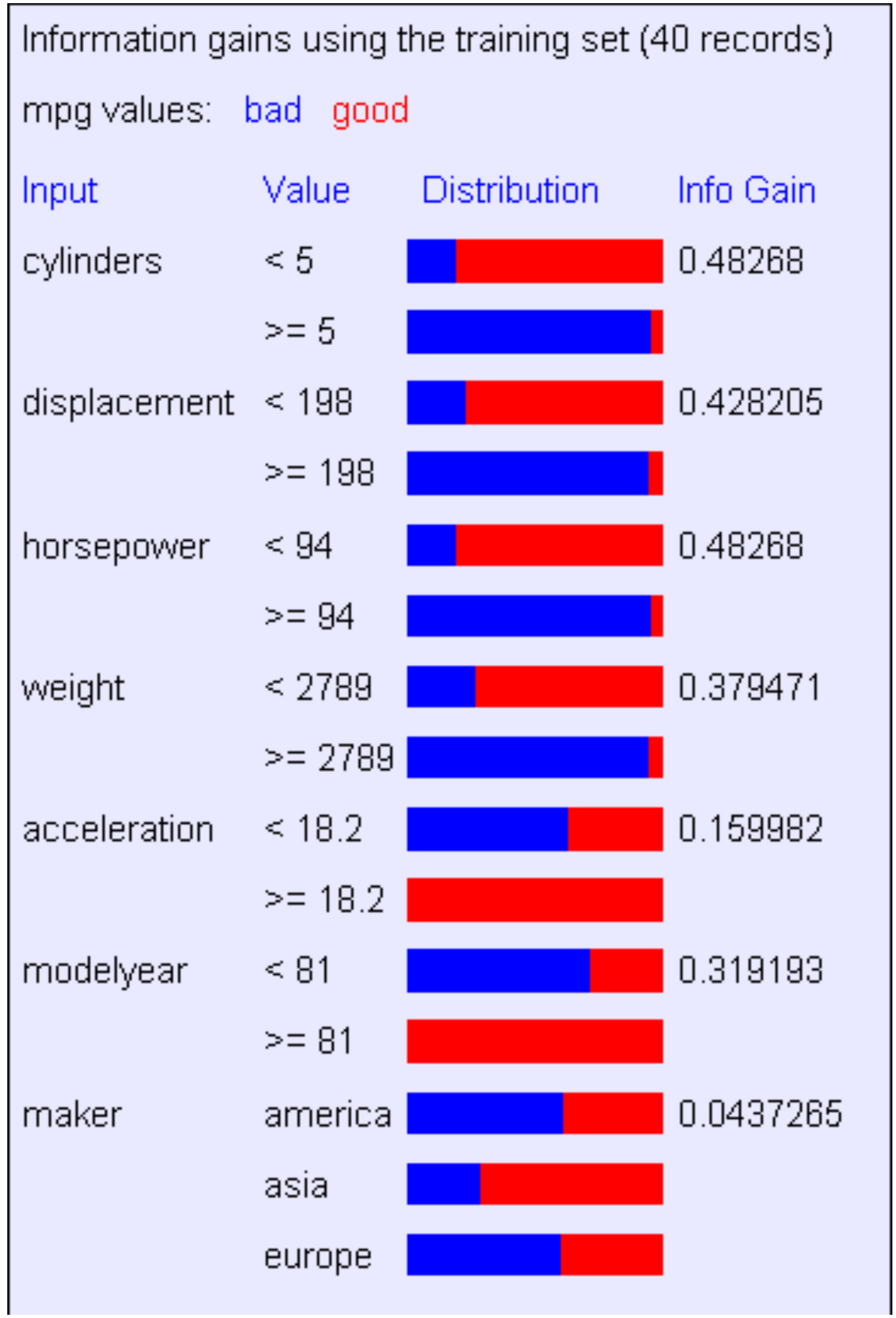
The set of possible thresholds

- Binary tree, split on attribute X
  - One branch: $X < t$
  - Other branch: $X \geq t$
- Search through possible values of *t*
  - Seems hard!!!
- But only finite number of *t*'s are important
  - Sort data according to X into $\{x_1,\ldots,x_m\}$
  - Consider split points of the form $x_i + (x_{i+1} - x_i)/2$

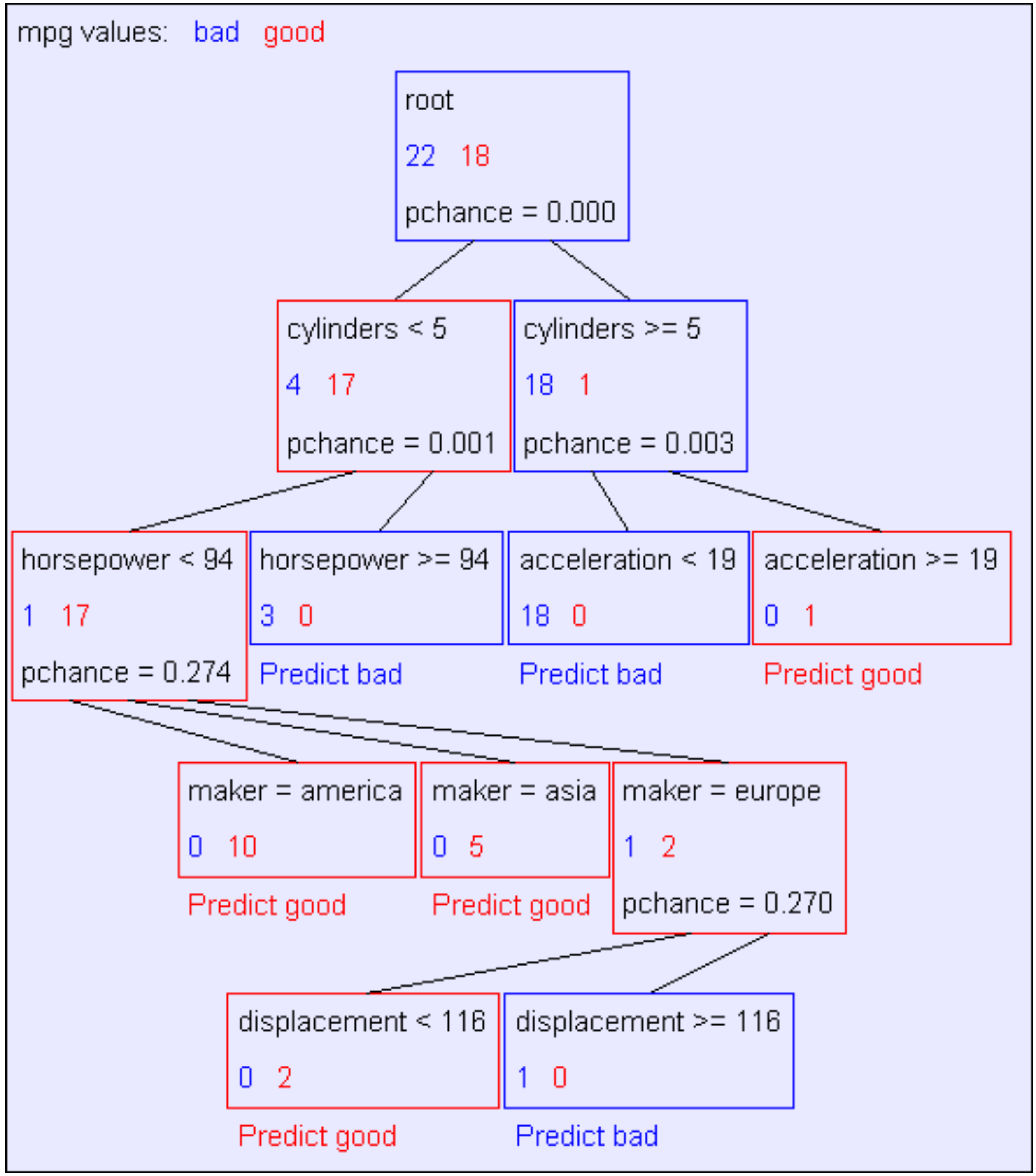
Picking the best threshold

- Suppose X is real valued with threshold t
- Want $IG(Y|X:t)$: the information gain for Y when testing if X is greater than or less than t
- Define:
  - $H(Y|X:t) =$
    $$H(Y|X < t)\ P(X < t) + H(Y|X >= t)\ P(X >= t)$$
  - $IG(Y|X:t) = H(Y) - H(Y|X:t)$
  - $IG^*(Y|X) = max_t\ IG(Y|X:t)$
- Use: $IG^*(Y|X)$ for continuous variables

Example with MPG



Example tree for our continuous dataset



What you need to know about decision trees

- Decision trees are one of the most popular ML tools
  - Easy to understand, implement, and 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!!!
  - 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