Artificial Intelligence CE-417, Group 1 Computer Eng. Department Sharif University of Technology

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Courtesy: Most slides are adopted from CSE-573 (Washington U.), original slides for the textbook, and CS-188 (UC. Berkeley).

Model Based vs. Discriminative

$\underbrace{\mathbb{P}(Y \mid X_1 \dots X_d)}$ vs. $Y = \underline{f}(X_1 \dots X_d)$

tra. acc.

$\max_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left(f(X_1^{(i)} \dots X_d^{(i)}) = Y^{(i)}\right)$

Classification

(Decision Tree)

$\underline{\mathcal{F}}$

Hypothesis Space

Empirical Risk Minimization

A learning problem: predict fuel efficiency

label

features

- From the UCI repository (thanks to Ross Quinlan)

- 40 Records
- Discrete data (for now)
- 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
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
bad	8	high	high	high	low	70to74	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

Y (mpg) X (other columns)

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

How Represent Function?

f (

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

) →

mpg
good

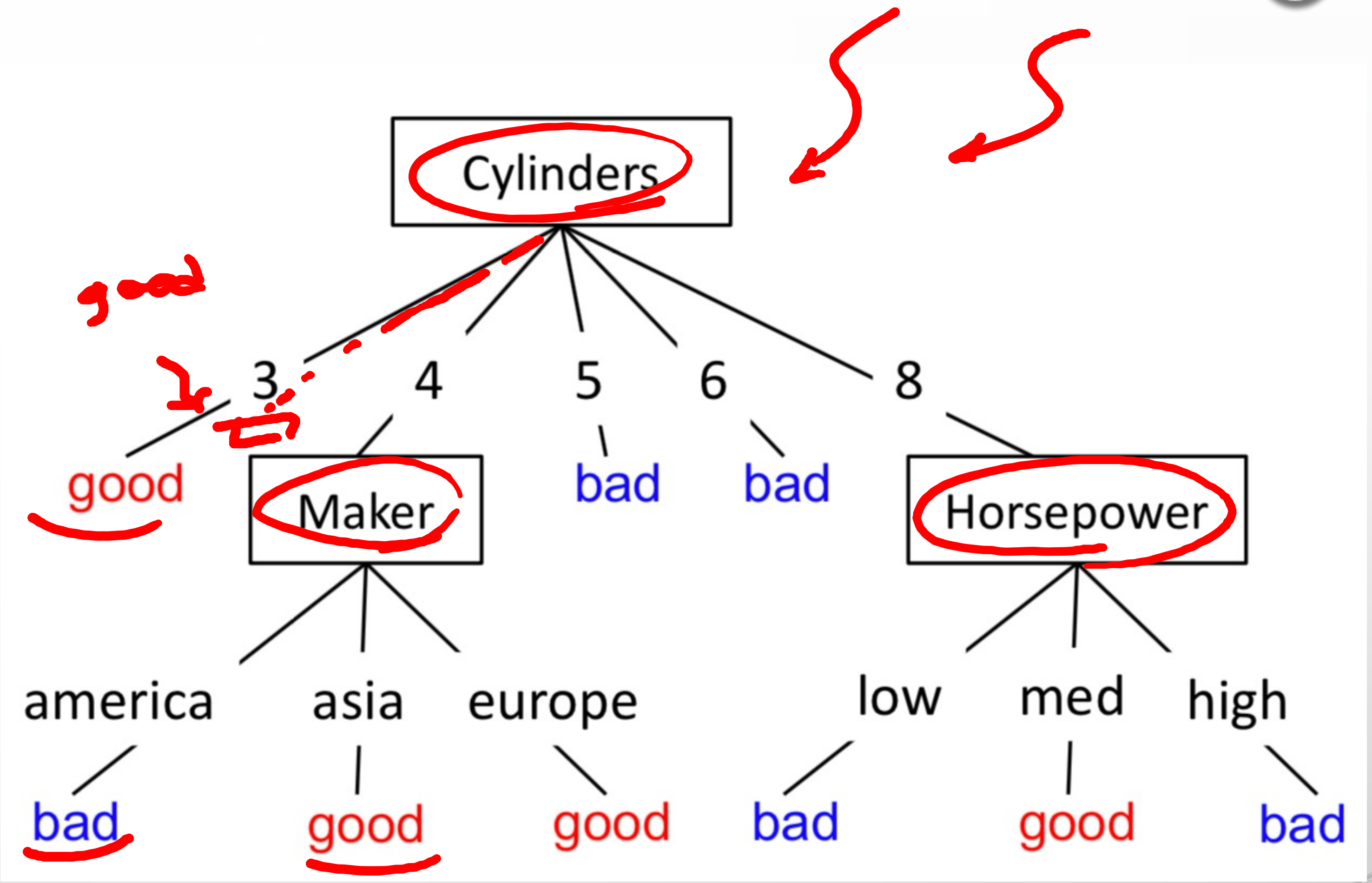
General Propositional Logic?

maker=asia $\vee$ weight=low

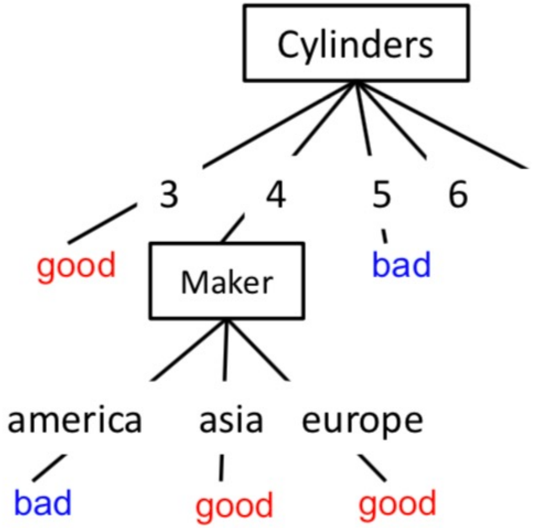
Need to find "Hypothesis": $f : X \rightarrow Y$

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



What functions can be represented?



$$cyl=3 \vee (cyl=4 \wedge (maker=asia \vee maker=europe)) \vee \ldots$$

Learning as Search

- Nodes?
- Operators?
- Start State?
- Goal?
  Search Algorithm?
- Heuristic?

The Starting Node: What is the Simplest Tree?

d=0

predict
mpg=bad

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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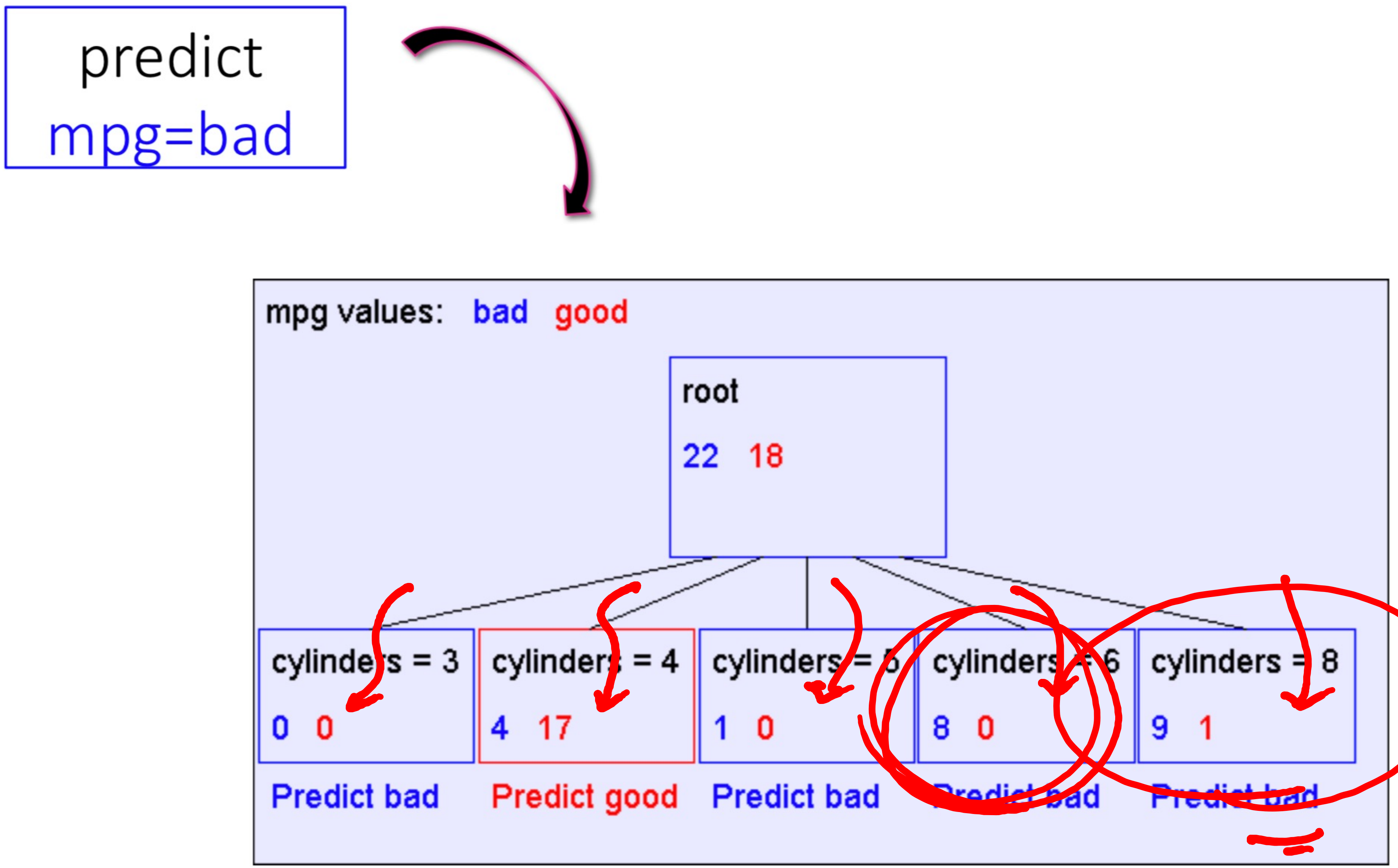
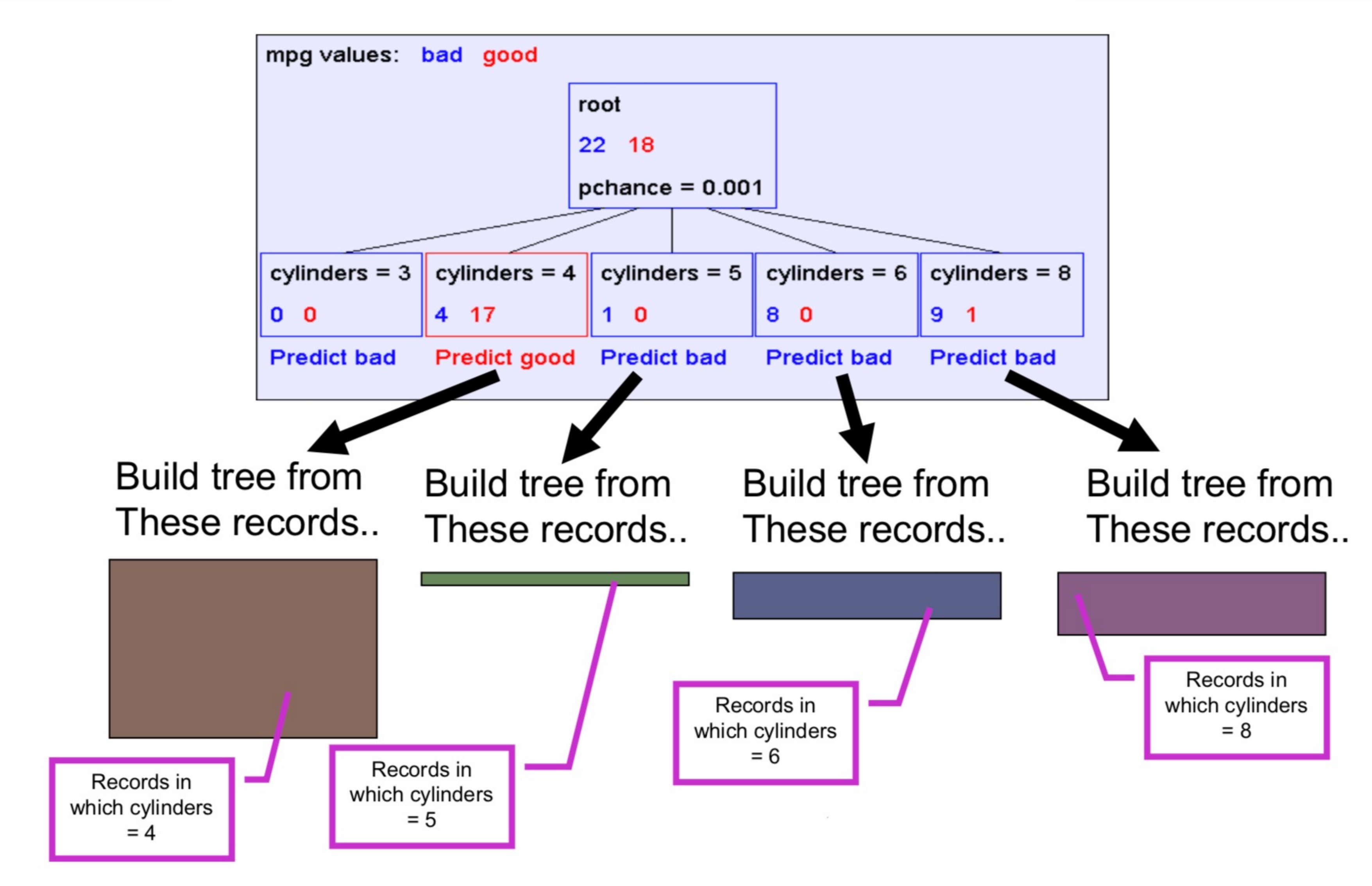
- Is this a good tree?
- [22+, 18-] : Means: correct on 22 examples incorrect on 18 examples.

Operators: Improving the Tree

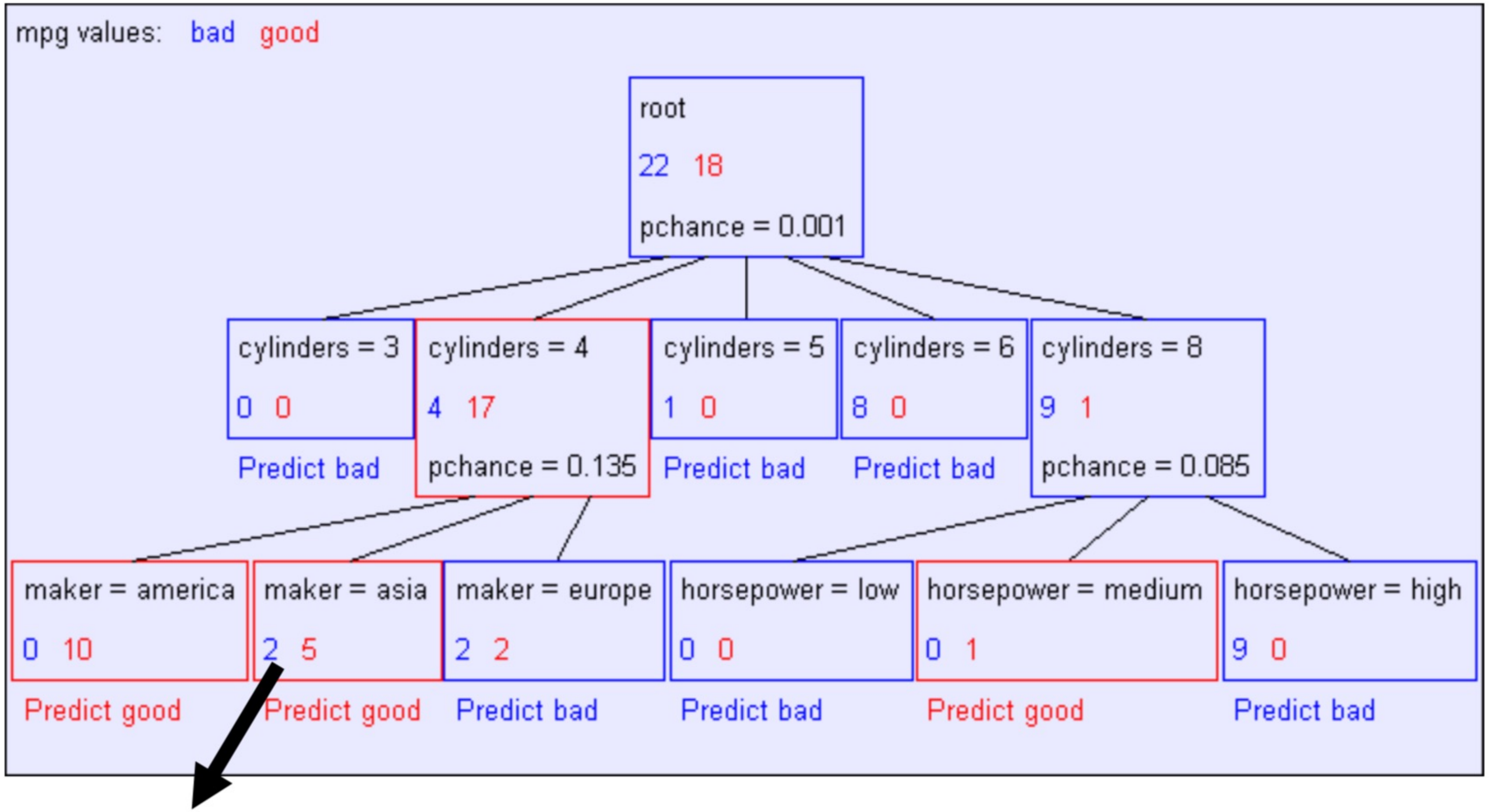


d=1

Recursive Step



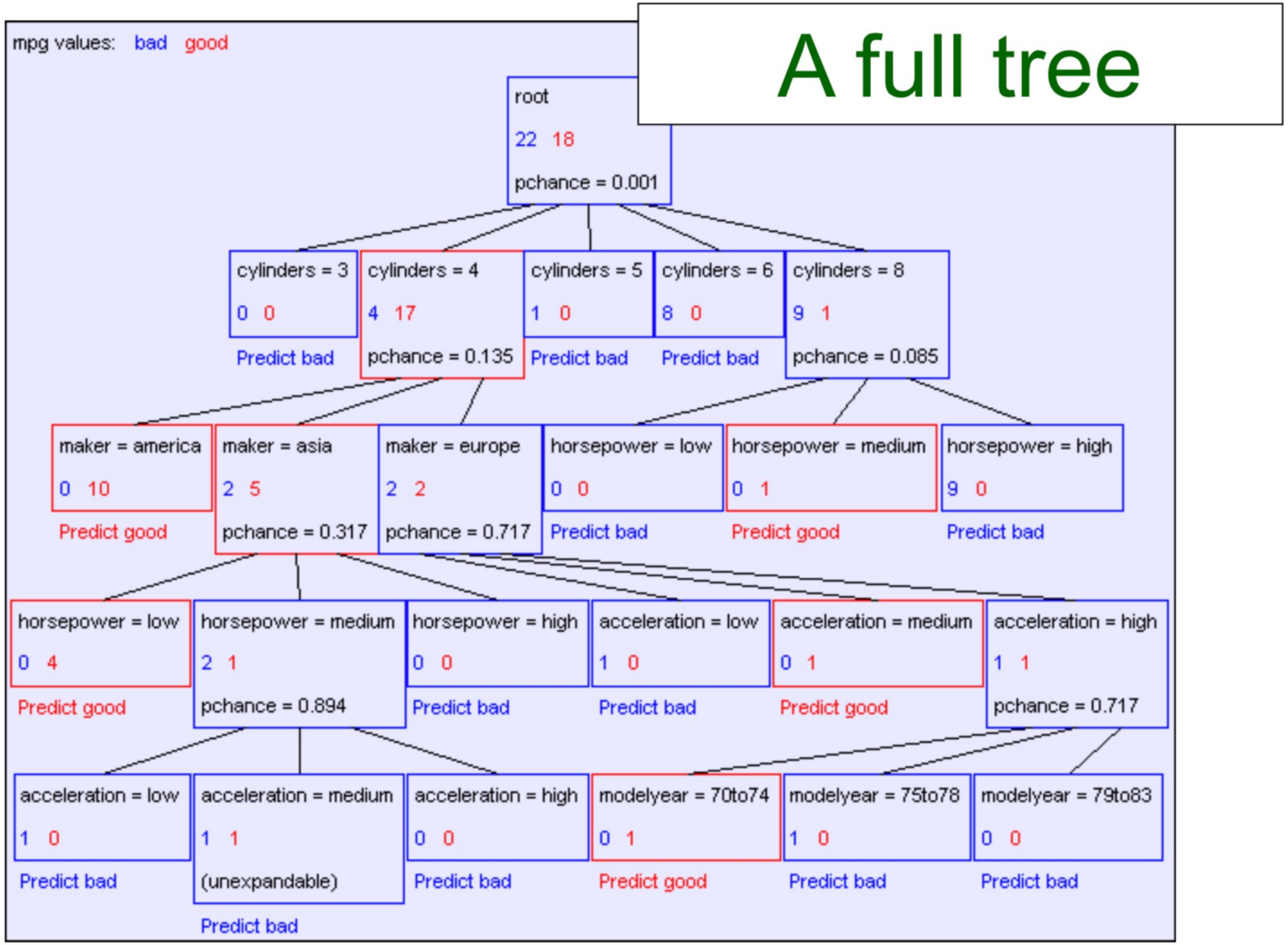
Second level of Tree



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


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

Two Questions

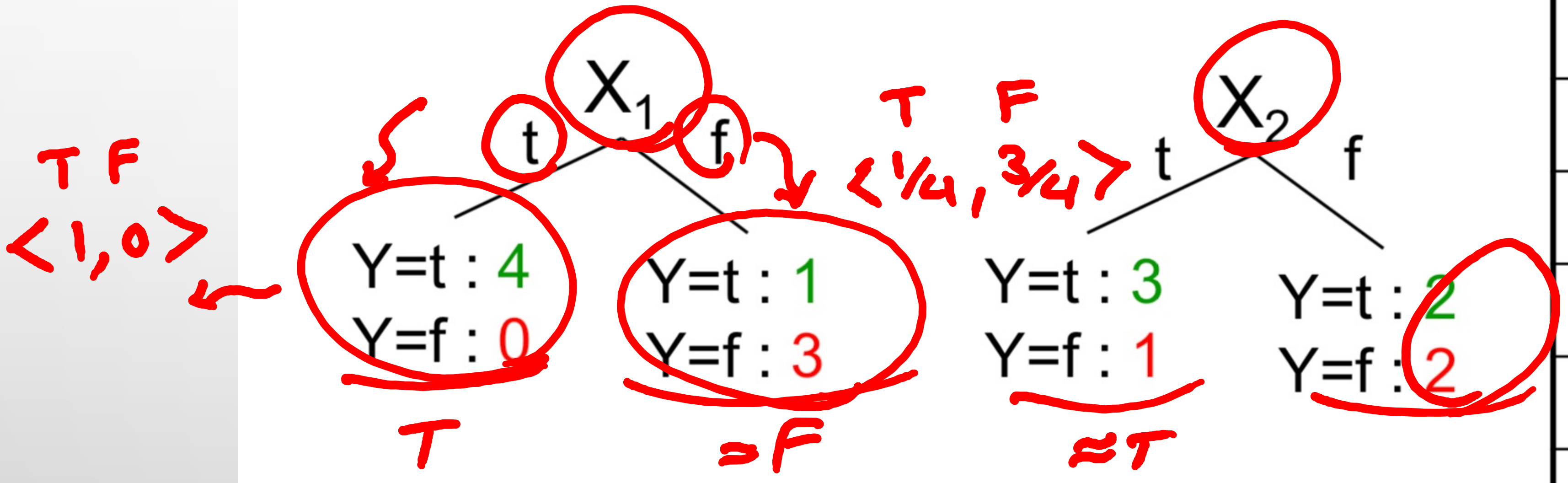
- Hill Climbing Algorithm:
  - Start from empty decision tree
  - Split on the **best attribute (feature)** – Recurse
- Which attribute gives the best split?
- When to stop recursion?

Splitting: choosing a good attribute

$$H(\langle p_1, p_2 \cdots, p_k \rangle) = -\sum_{i=1}^{k} p_i \log p_i$$

Training Set

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

5/8

3/8

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?

$$I(X;Y) = \mathbb{E}_Y \left(D_{KL}\left(P(X|Y) \| P(X)\right)\right)$$

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

P(Y=A) = 1/3	P(Y=B) = 1/4	P(Y=C) = 1/4	P(Y=D) = 1/6

Which attribute gives the best split?

Mutual Information

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

$$\sum_{x_j} P(x_j) \sum_{y_i} -P(y_i|x_j) \log(P(y_i|x_j))$$

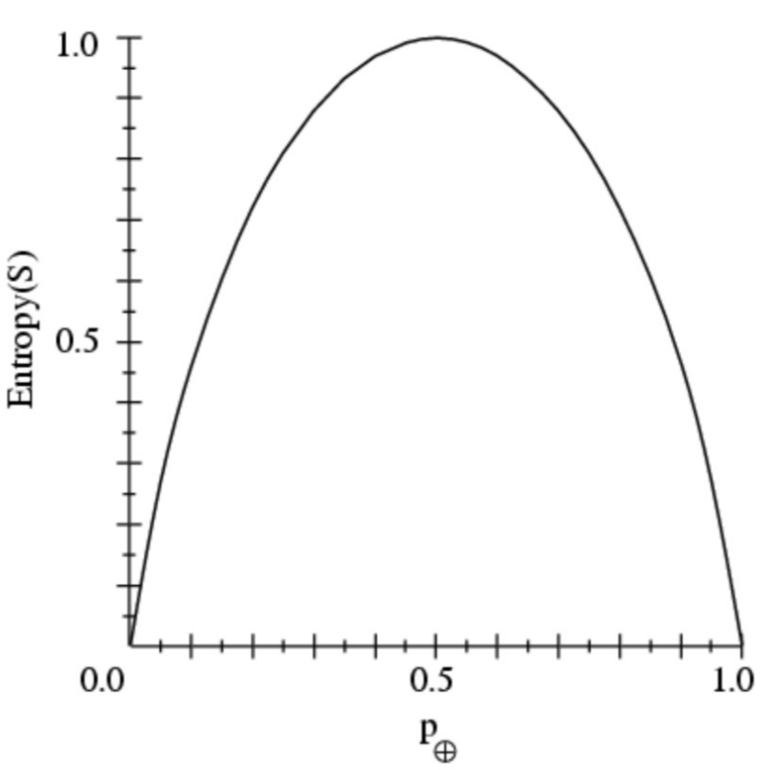
- A1: The one with the highest ***information gain***
  - Defined in terms of ***entropy***
- A2: Actually many alternatives,
  - e.g., ***accuracy***. Seeks to reduce the ***misclassification rate***

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

- P(Y=t) = 5/6, P(Y=f) = 1/6

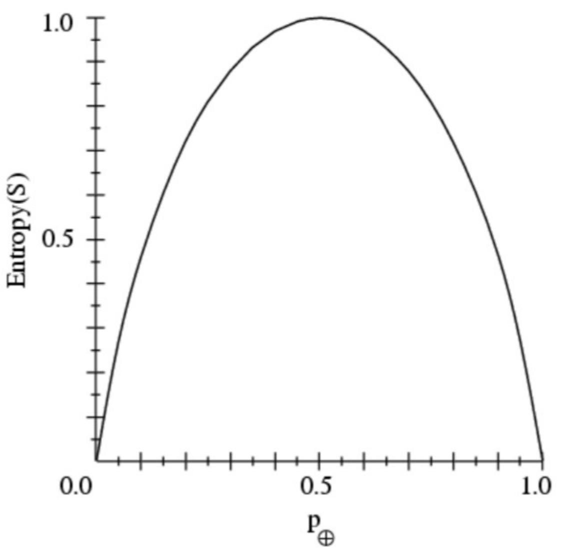
$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

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

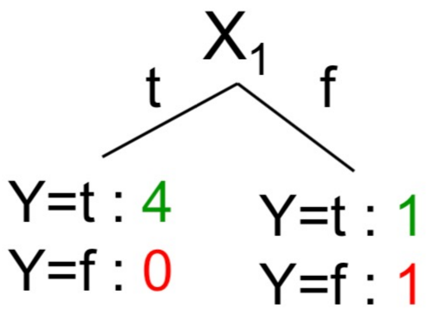
- Conditional Entropy *H(Y|X)* of a random variable *Y* conditioned on a random variable *X*

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

Example:

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

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



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

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

$$= 2/6$$

$$= 0.33$$

Information Gain

- Advantage of attribute – 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

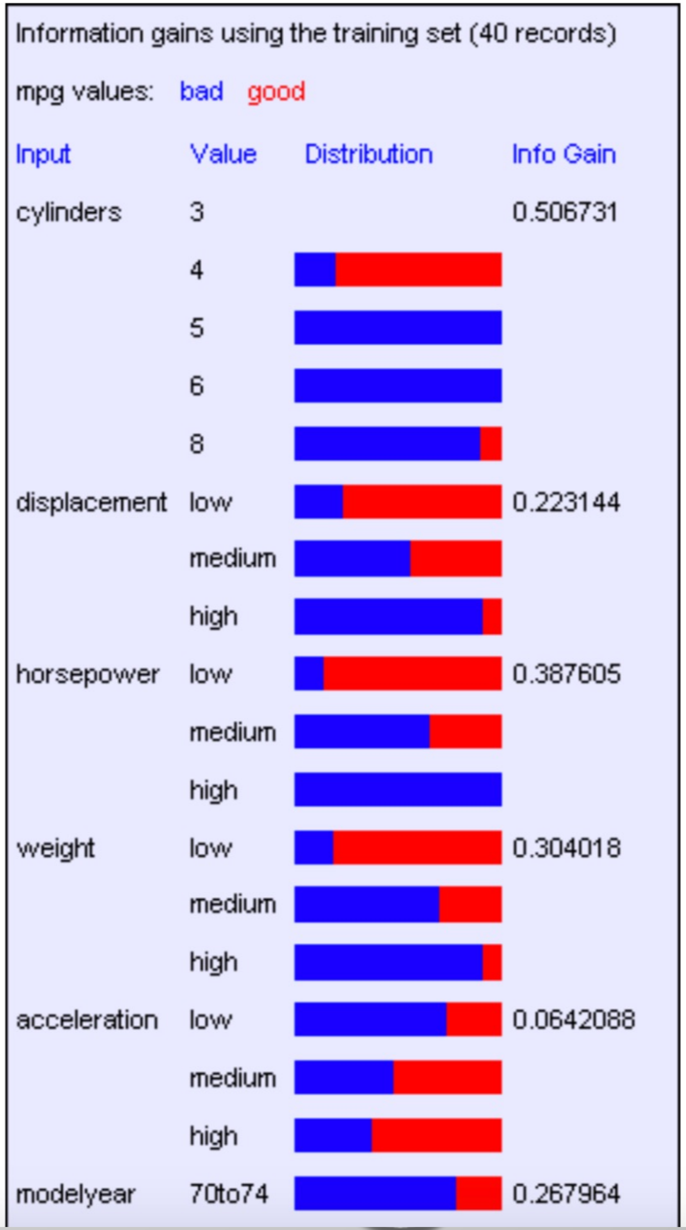
- Start from empty decision tree
- Split on **next best attribute (feature)**
- Use information gain (or...?) to select attribute:

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

- Recurse.

Learning Decision Trees (cont.)

- Suppose we want to predict MPG.
- Now, Look at all the information gains…

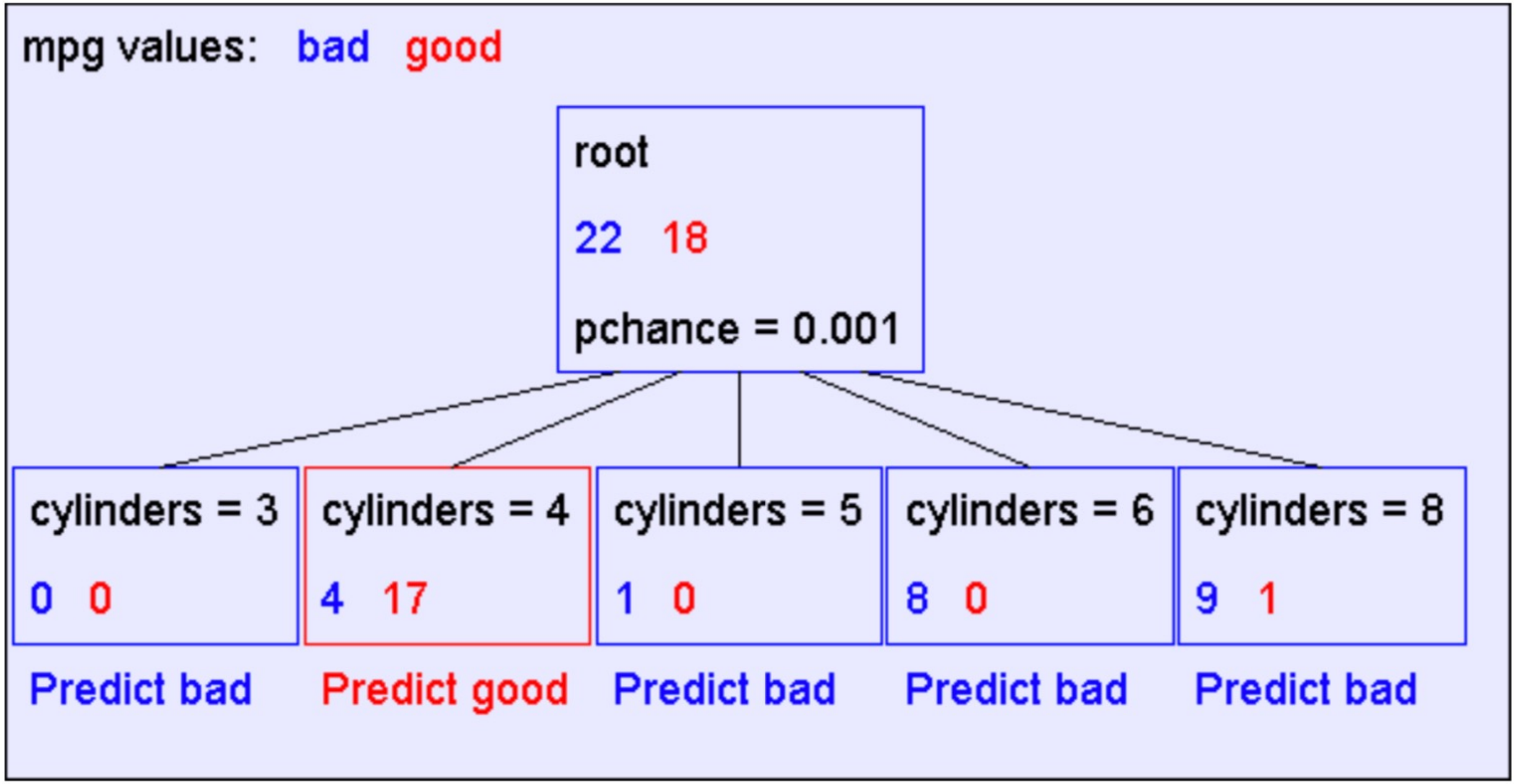


Information gains using the training set (40 records)

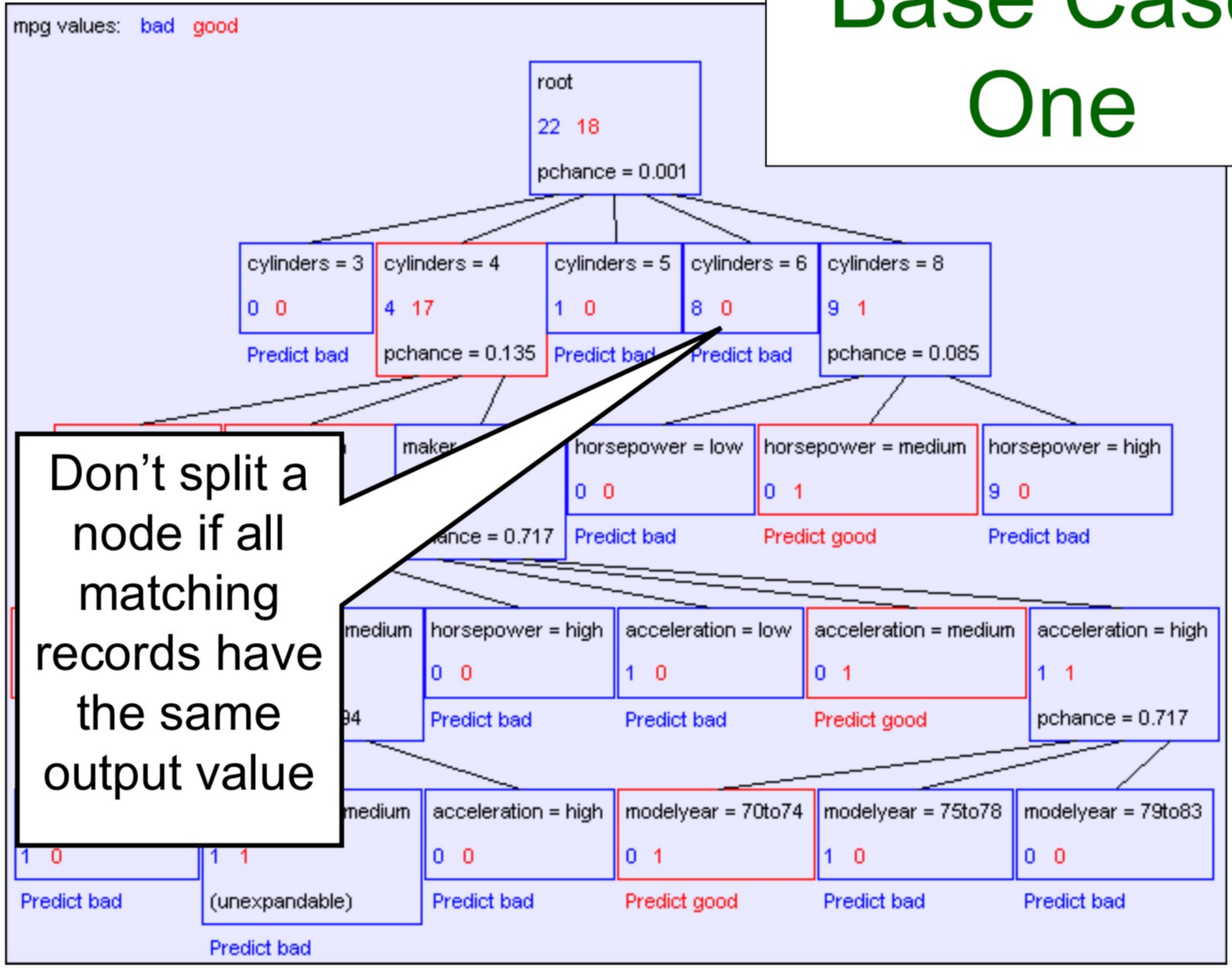
mpg values: bad good

Input	Value	Distribution	Info Gain
cylinders	3		0.506731
	4		
	5		
	6		
	8		
displacement	low		0.223144
	medium		
	high		
horsepower	low		0.387605
	medium		
	high		
weight	low		0.304018
	medium		
	high		
acceleration	low		0.0642088
	medium		
	high		
modelyear	70to74		0.267964

Tree After One Iteration



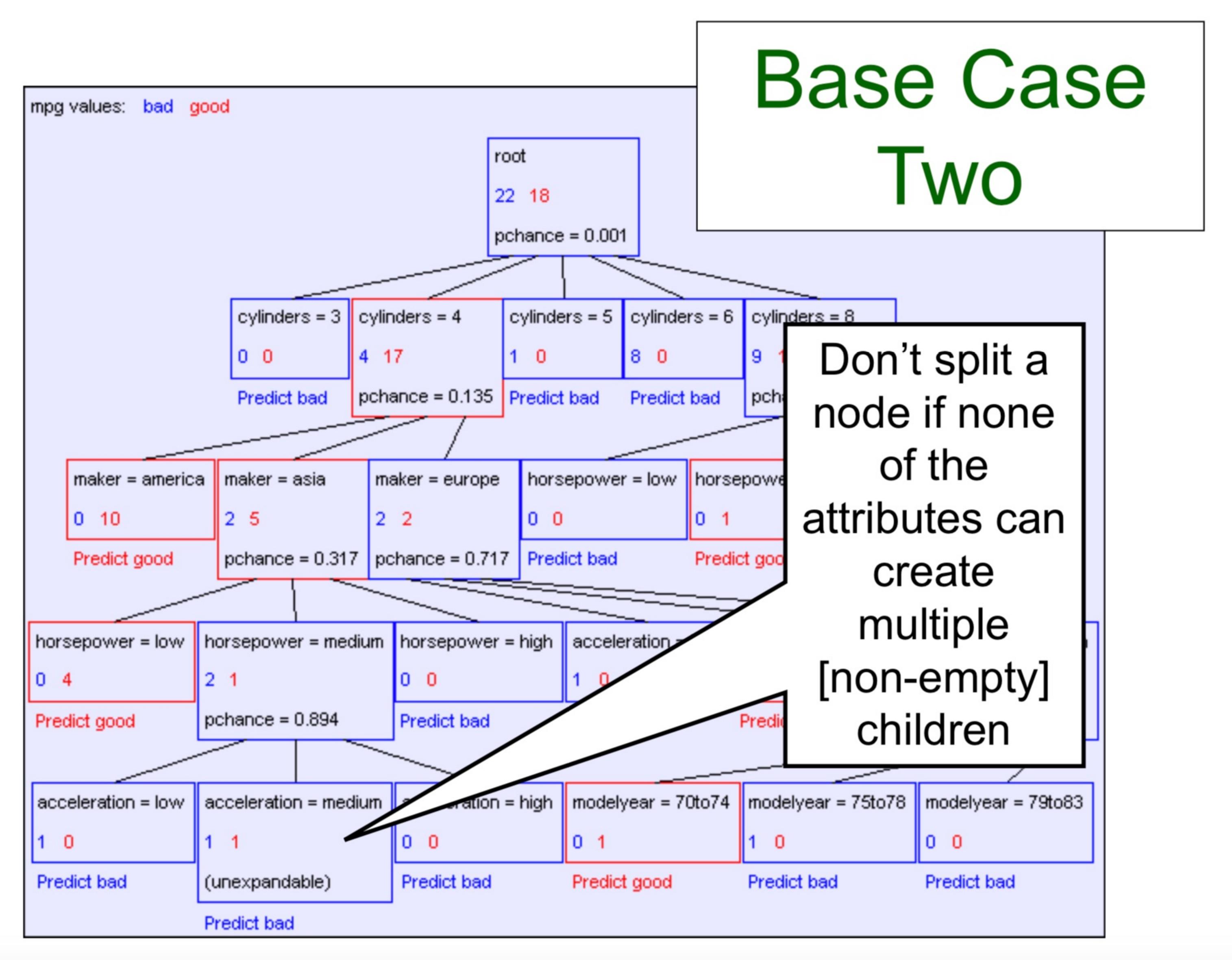
When to Terminate?



Base Case One

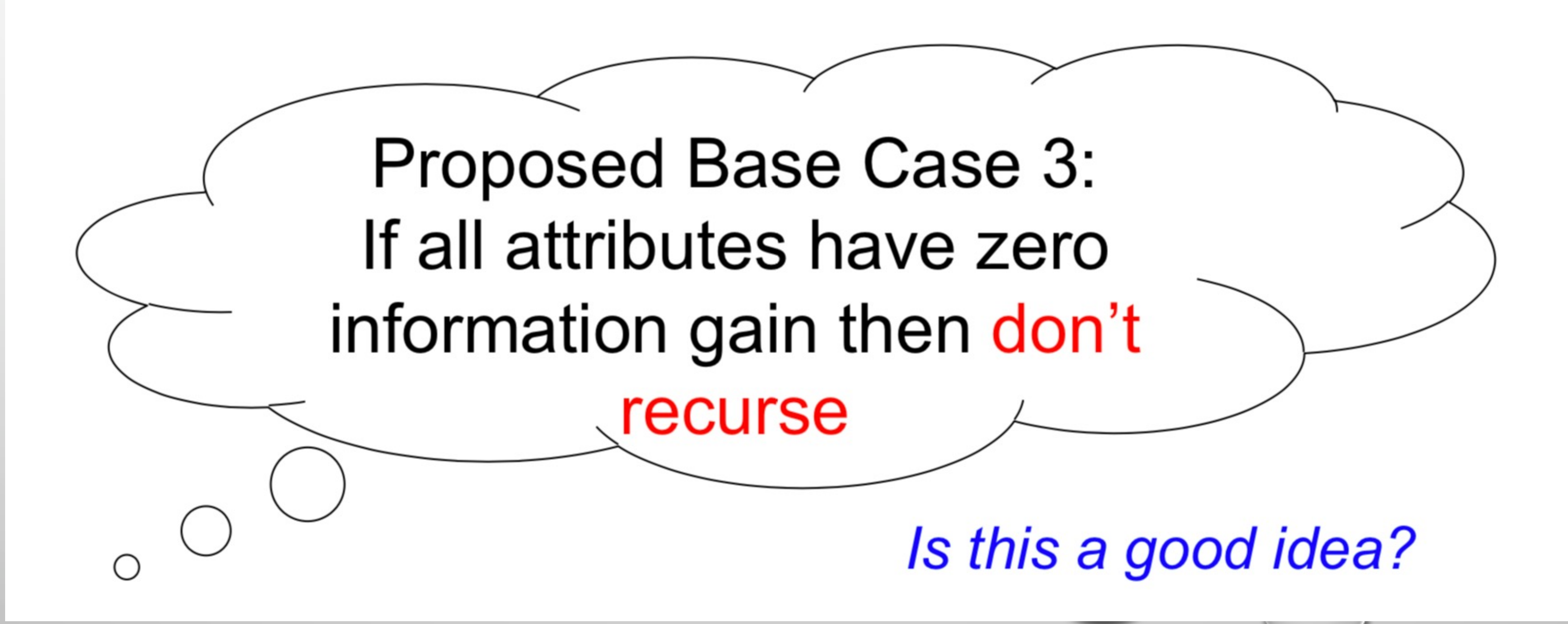
Don't split a node if all matching records have the same output value

When to terminate? (cont.)



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.

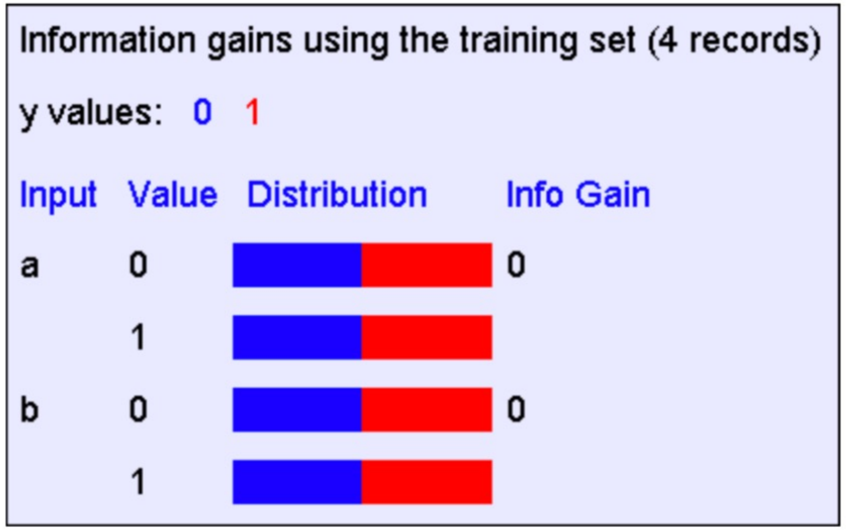


The problem with Base Case 3

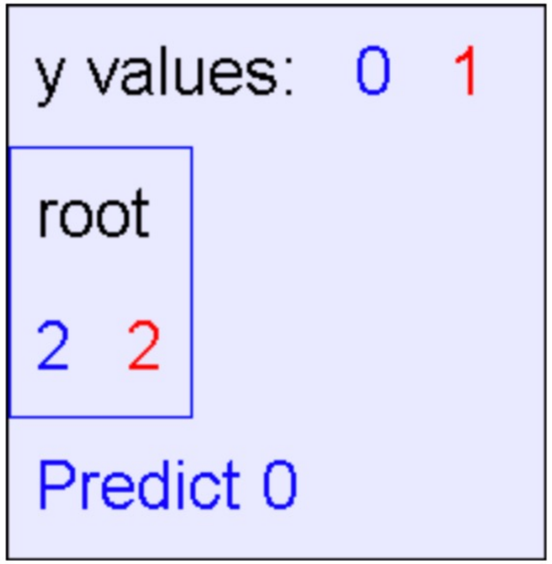
y = a XOR b

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

The information gains:



The resulting decision tree:

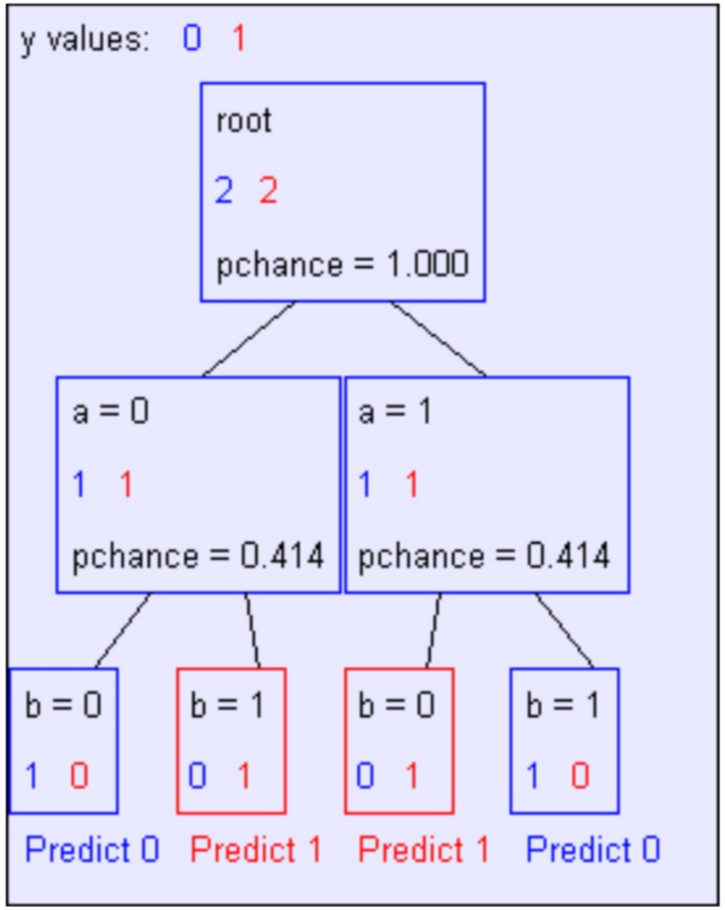


But *Without* Base Case 3:

y = a XOR b

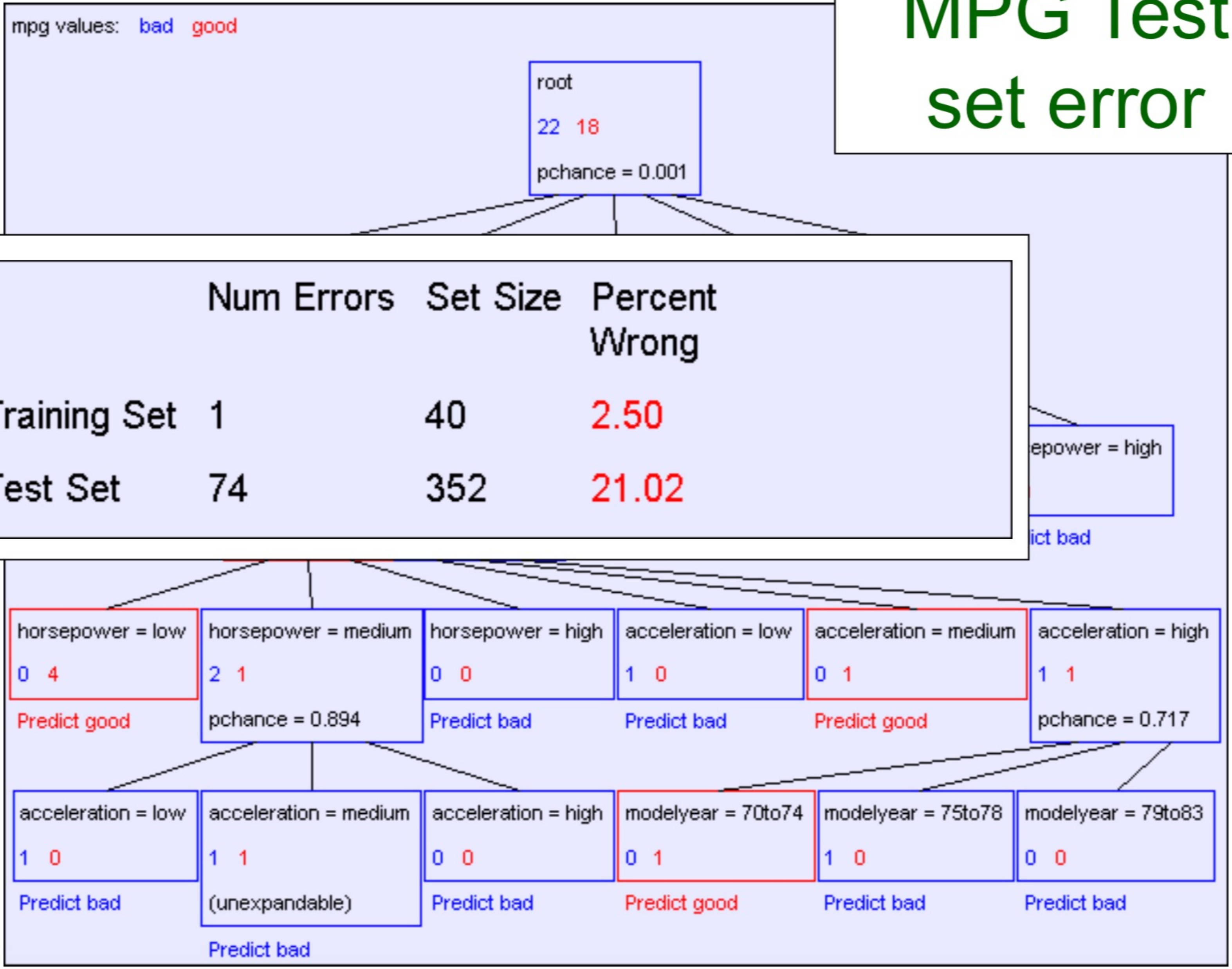
a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

The resulting decision tree:



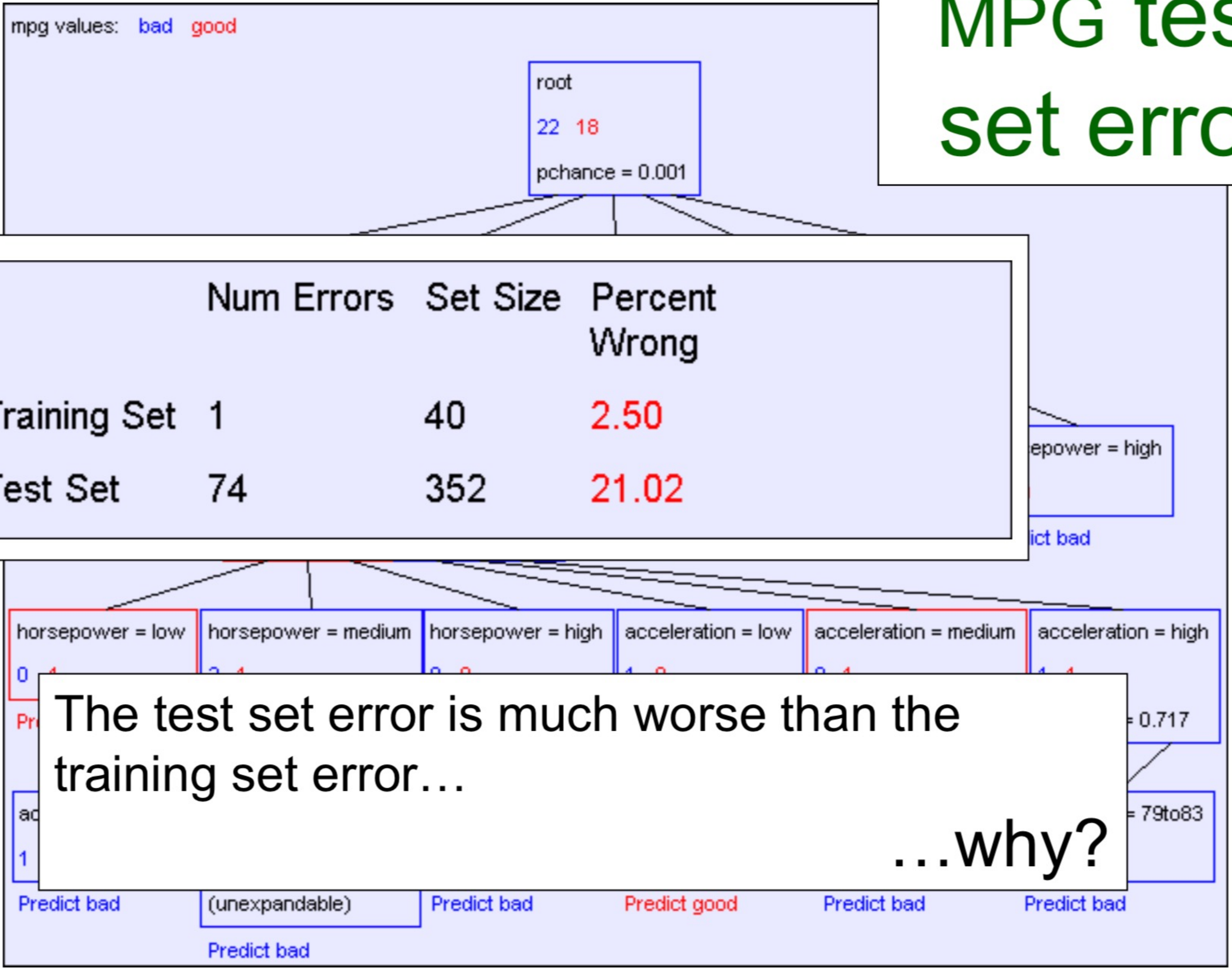
So: Base Case 3? Include or Omit?

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 will overfit

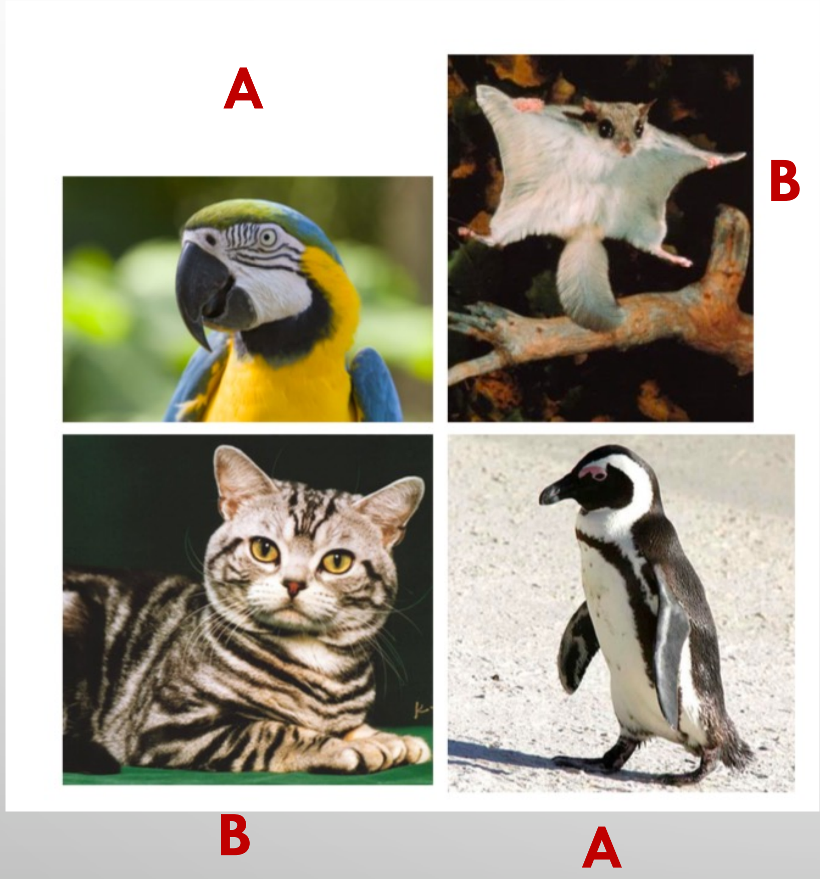
- Our decision trees have no learning bias
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Will definitely overfit!!!
  - Must introduce some bias towards *simpler* trees
- Why might one pick simpler trees?

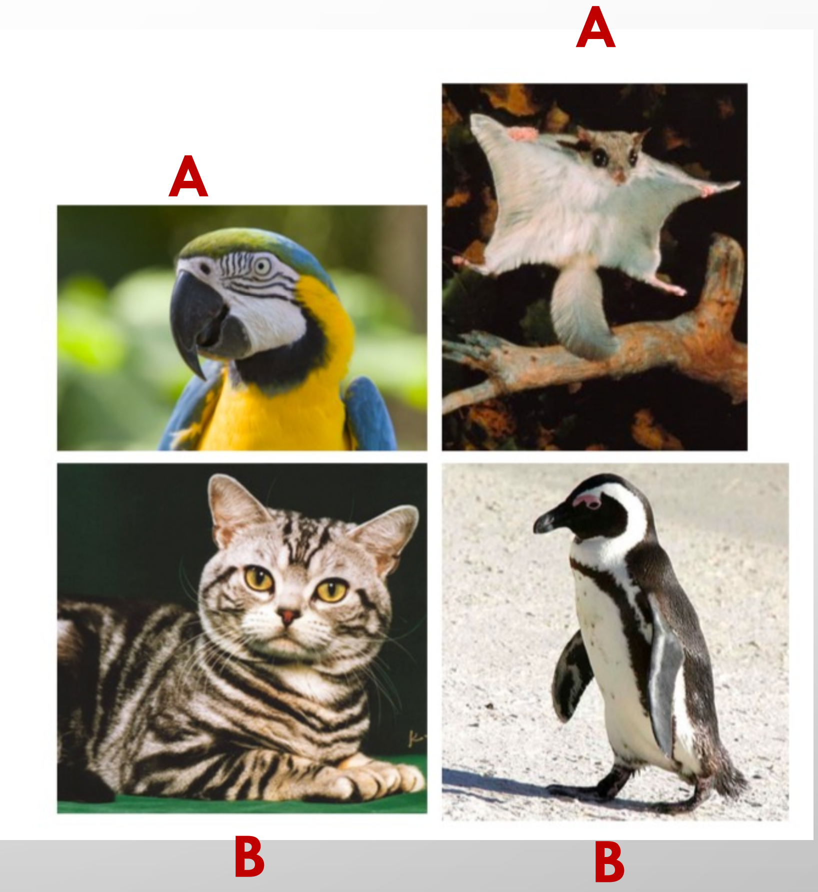
Inductive bias

- Suppose that you are given 8 training samples for two classes A and B.

Inductive bias (cont.)

- What is your guess on the classes of the following test data?



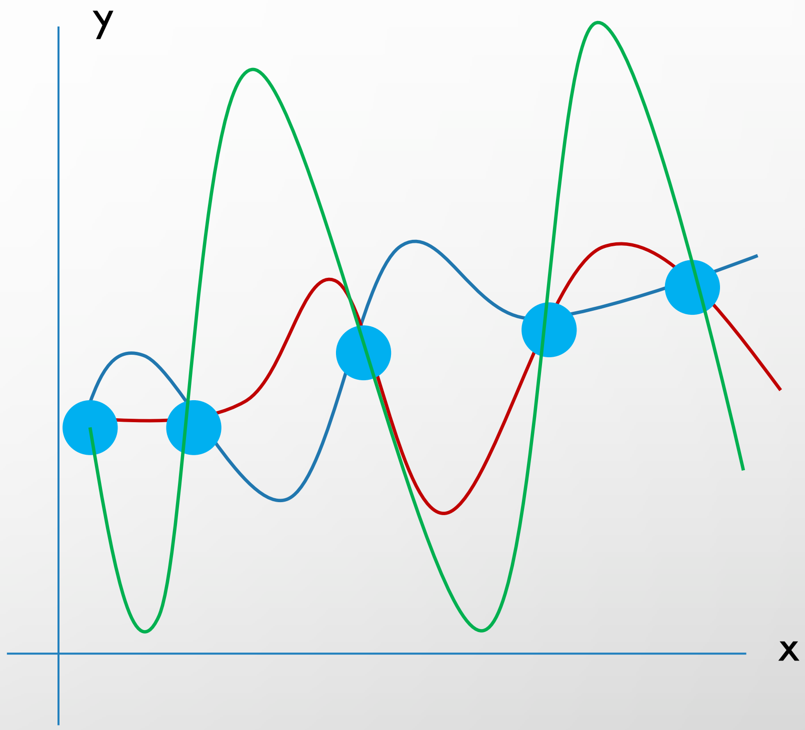


Inductive bias (cont.)

- Each person has a bias in learning (bird vs. Non-bird or flying vs. Non-flying).
- In the **absence** of data that narrows down the relevant concept, what type of solutions are we more likely to prefer?
- Different approaches that we introduce in this course are different types of biases.
- Suppose that we restrict depth of a decision tree. What would be the inductive bias?
- **Correct inductive bias is necessary for a problem to be learnable.**

"No free lunch" theorem

- Suppose that all the functions that are consistent with any given training data are **equally likely a solution to our induction**.
- Then all learning algorithms would have the same average true error on out-of-training-sample (D_o), where average is taken across different problems.
- This includes random guessing!
  - So in absence of any sense on what functions are more likely, learning is impossible!



Occam's Razor

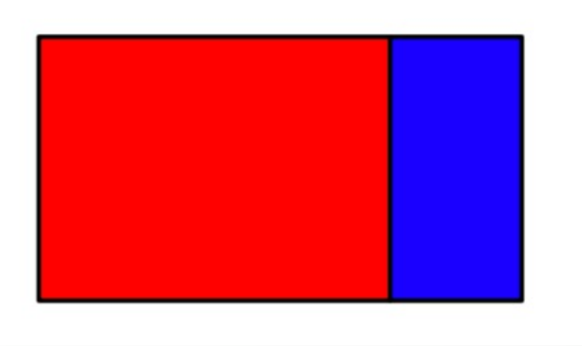
- Why Favor Short Hypotheses?
- Arguments for:
  - Fewer short hypotheses than long ones
  - → A short hyp. less likely to fit data by coincidence
  - → Longer hyp. that fit data might be coincidence

How to Build Small Trees

- Several reasonable approaches:
- **Stop growing tree before overfit**
  - Bound depth or # leaves
  - Base Case 3
  - *Doesn't work well in practice*
- **Grow full tree; then prune**
  - **Optimize on a held-out (development set)**
    - If growing the tree hurts performance, then cut back
    - Con: Requires a larger amount of data…
  - **Use statistical significance testing**
    - Test if the improvement for any split is likely due to noise
    - If so, then prune the split!

Reduced Error Pruning

- Split data into ***training*** & ***validation*** sets (10-33%)



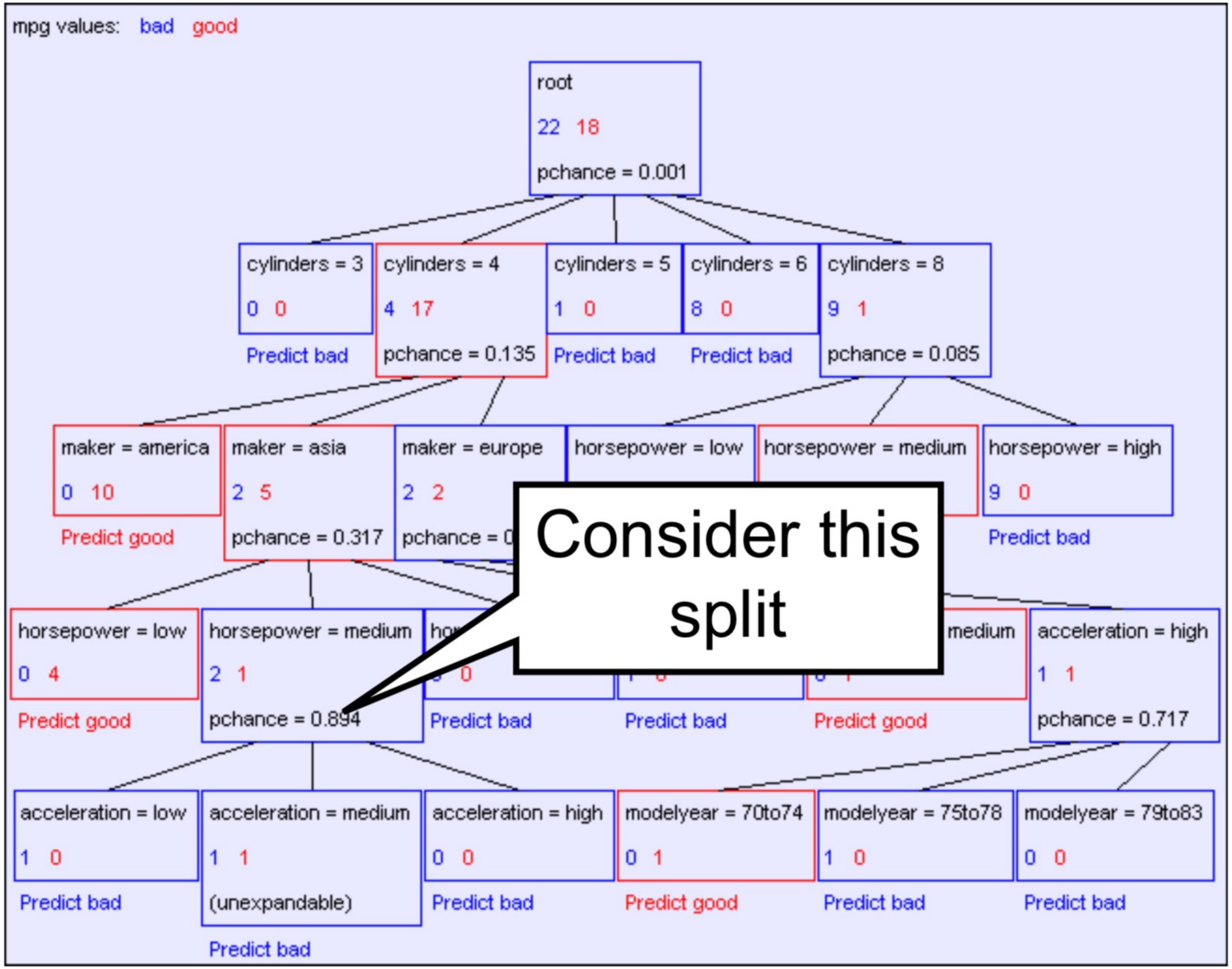
- Train on training set (overfitting)
- Do until further pruning is harmful:

  1) Evaluate effect on validation set of pruning ***each*** possible node (and tree below it)

  2) Greedily remove the node that ***most improves accuracy of validation set***

Alternatively

- Chi-squared pruning
  - Grow tree fully
  - Consider leaves in turn
    - Is parent split worth it?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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
horsepower = low
horsepower = medium
horsepower = high
9 0
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horsepower = low
0 4
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horsepower = medium
2 1
pchance = 0.894
Predict bad
Predict bad
medium
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acceleration = medium
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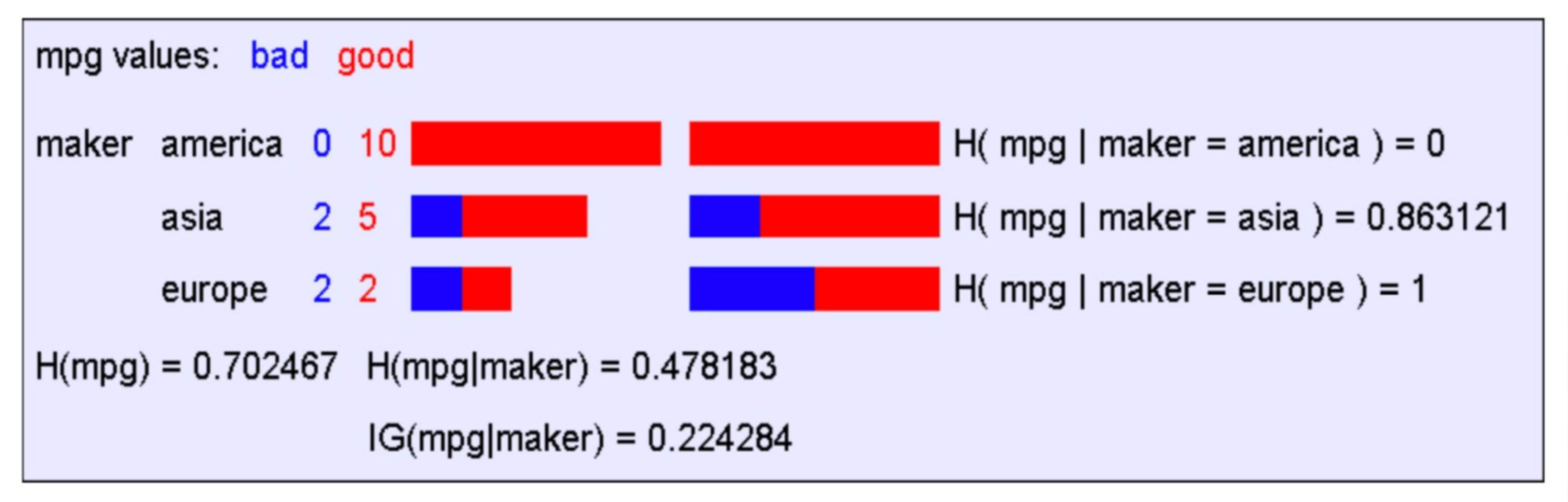
(unexpandable)
Predict bad
acceleration = high
0 0
Predict bad
modelyear = 70to74
0 1
Predict good
modelyear = 75to78
1 0
Predict bad
modelyear = 79to83
0 0
Predict bad
Consider this split

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?
- By using a particular kind of chi-square test, the answer is 13.5%. Such hypothesis tests are relatively easy to compute, but involved

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

Regularization