Artificial Intelligence
CE-417, Group 2
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).

Classification

(Decision Tree)

$Y = g(X)$

$P(Y|X)$

Discriminative Methods

Sample $P(X|Y)$

Generative

Model - based Classification

more direct

Joint Dist.

Inference

intermediate step is harder than the original problem

A learning problem: predict fuel efficiency

- 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
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
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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

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

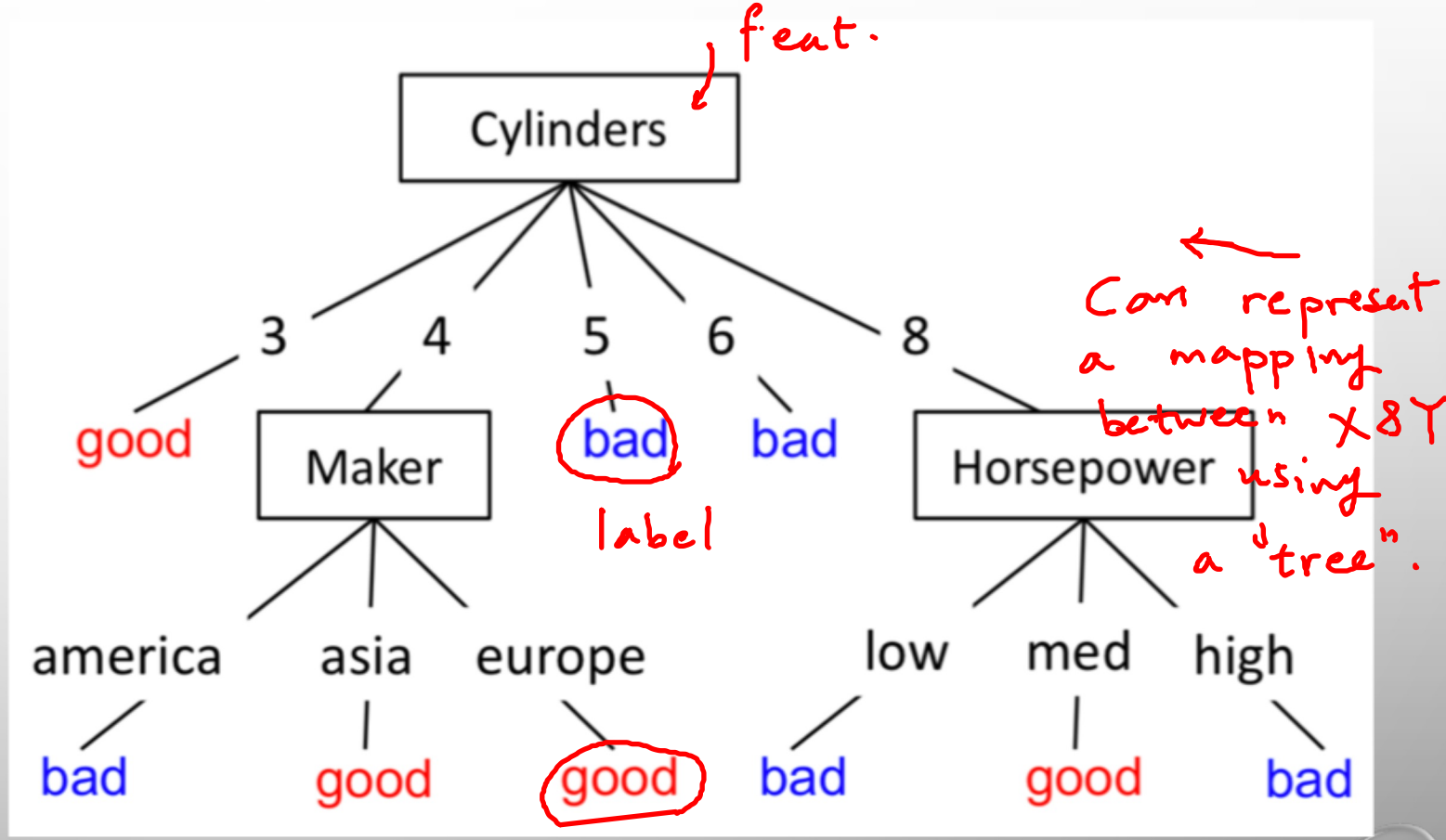
General Propositional Logic?

maker=asia ∨ weight=low

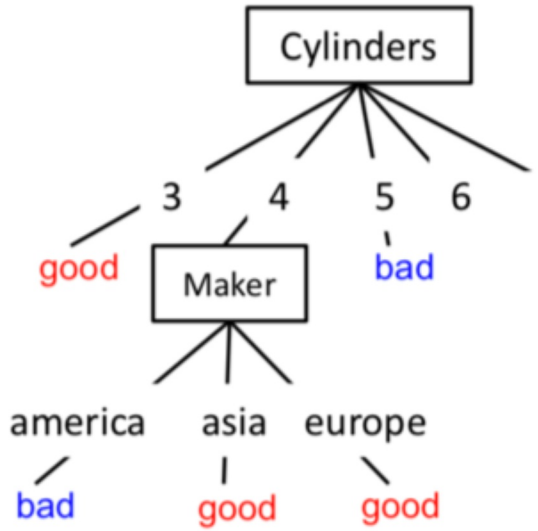
Need to find "Hypothesis": $f : X \rightarrow Y$

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?



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

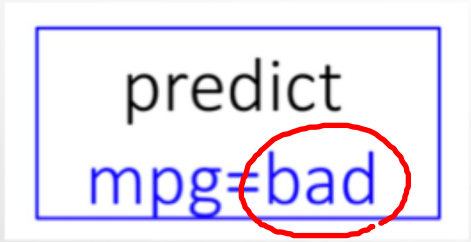
Learning as Search

on all possible DT

- Nodes?
- Operators?
- Start State?
- Goal? Has good acc. on trn. data!
  Search Algorithm?
- Heuristic?

The Starting Node: What is the Simplest Tree?

initial DT



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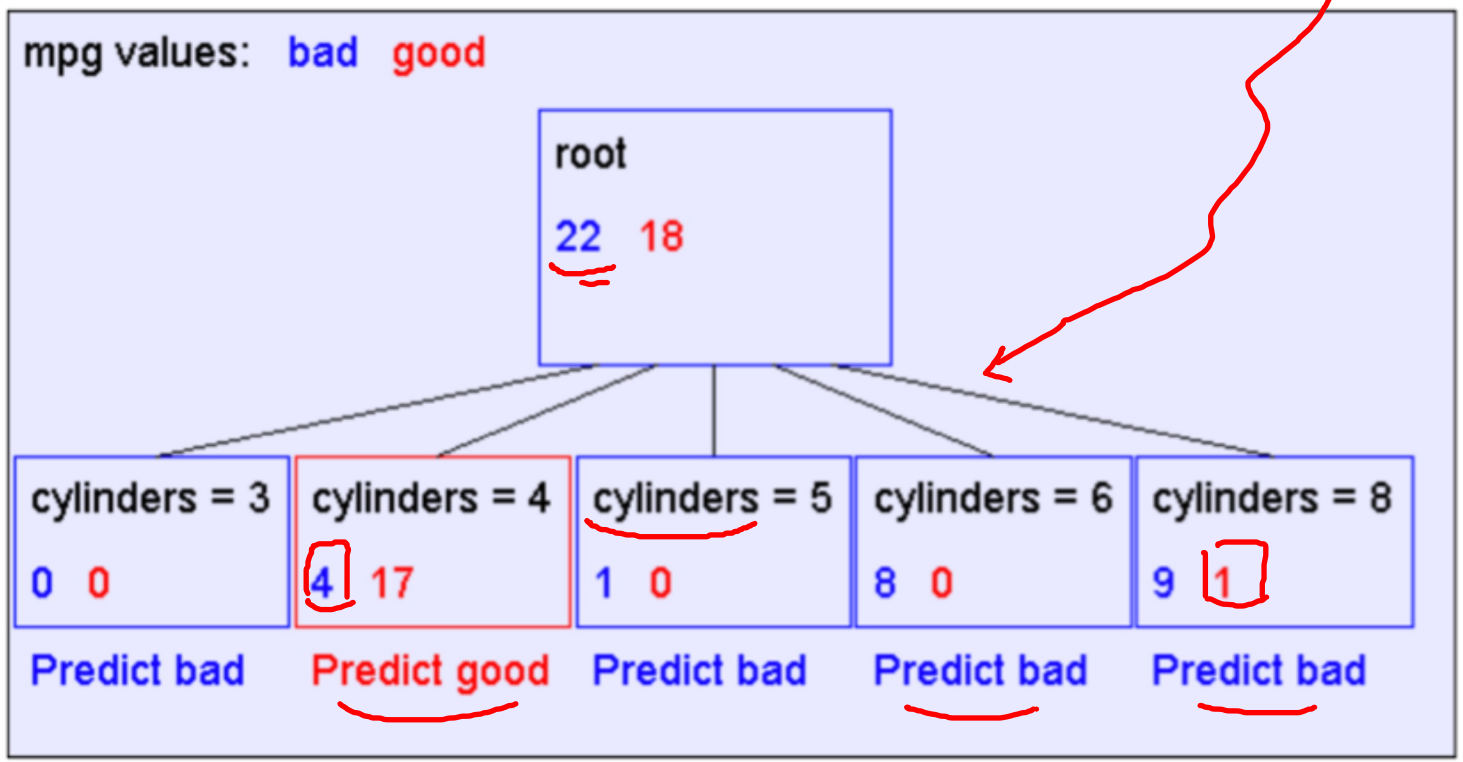
good	4	low	low	medium	high	79to83	america
bad	8	high	high	high	low	70to74	america
good	4	low	medium	low	medium	75to78	europe
bad	5	medium	medium	medium	medium	75to78	europe

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

correct incorrect

Operators: Improving the Tree

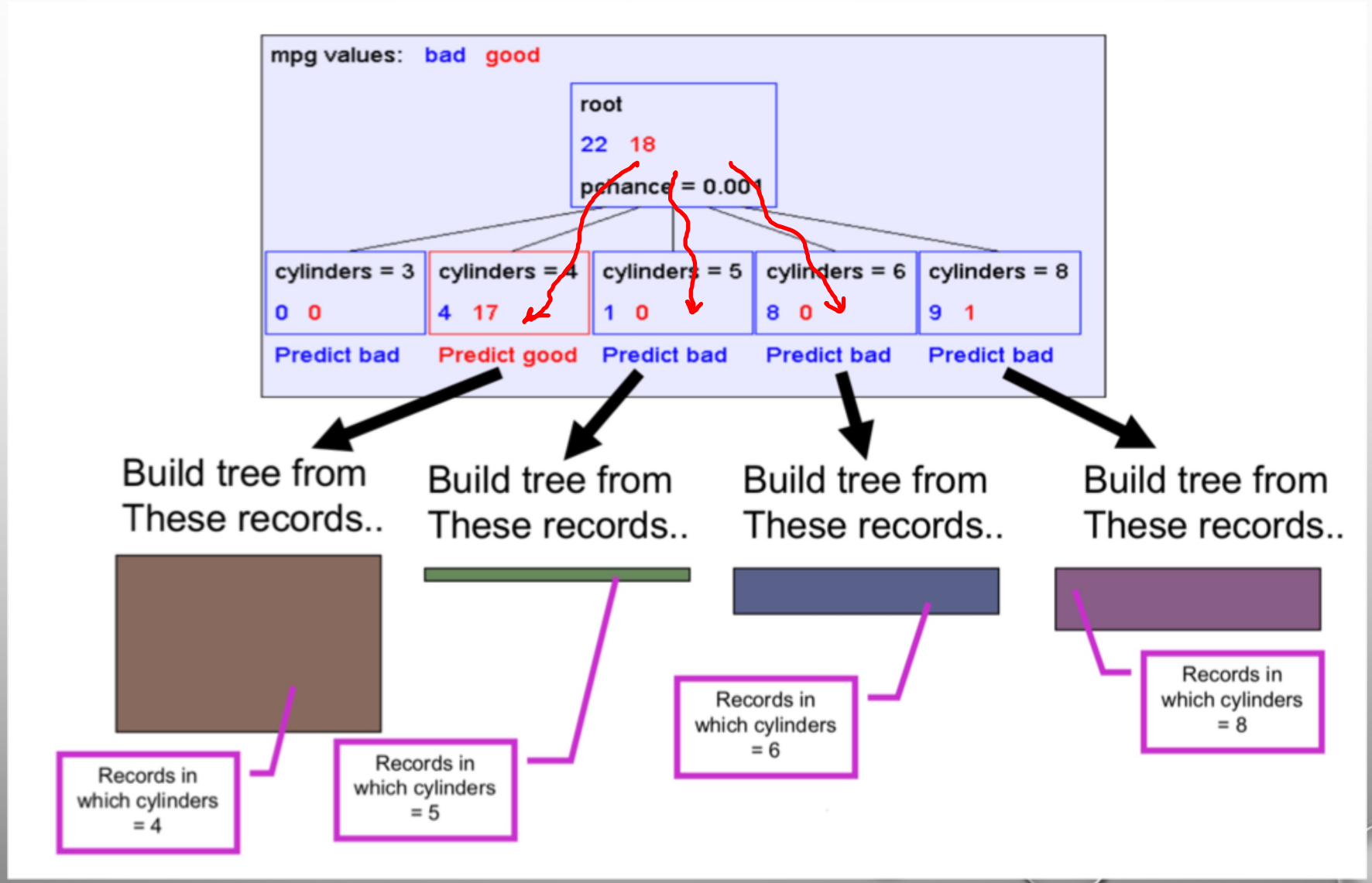
predict
mpg=bad



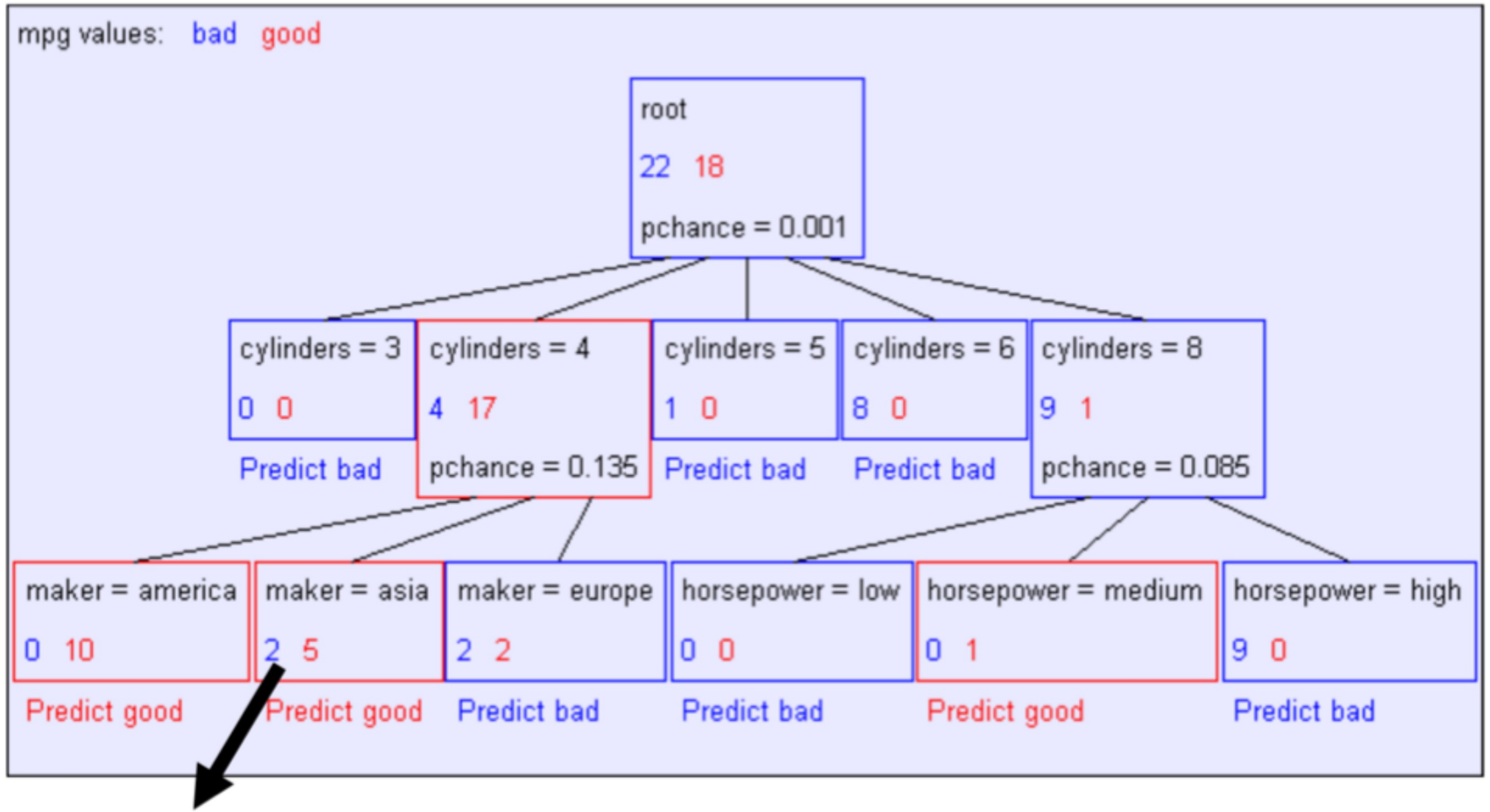
local search

18
→ 5

Recursive Step



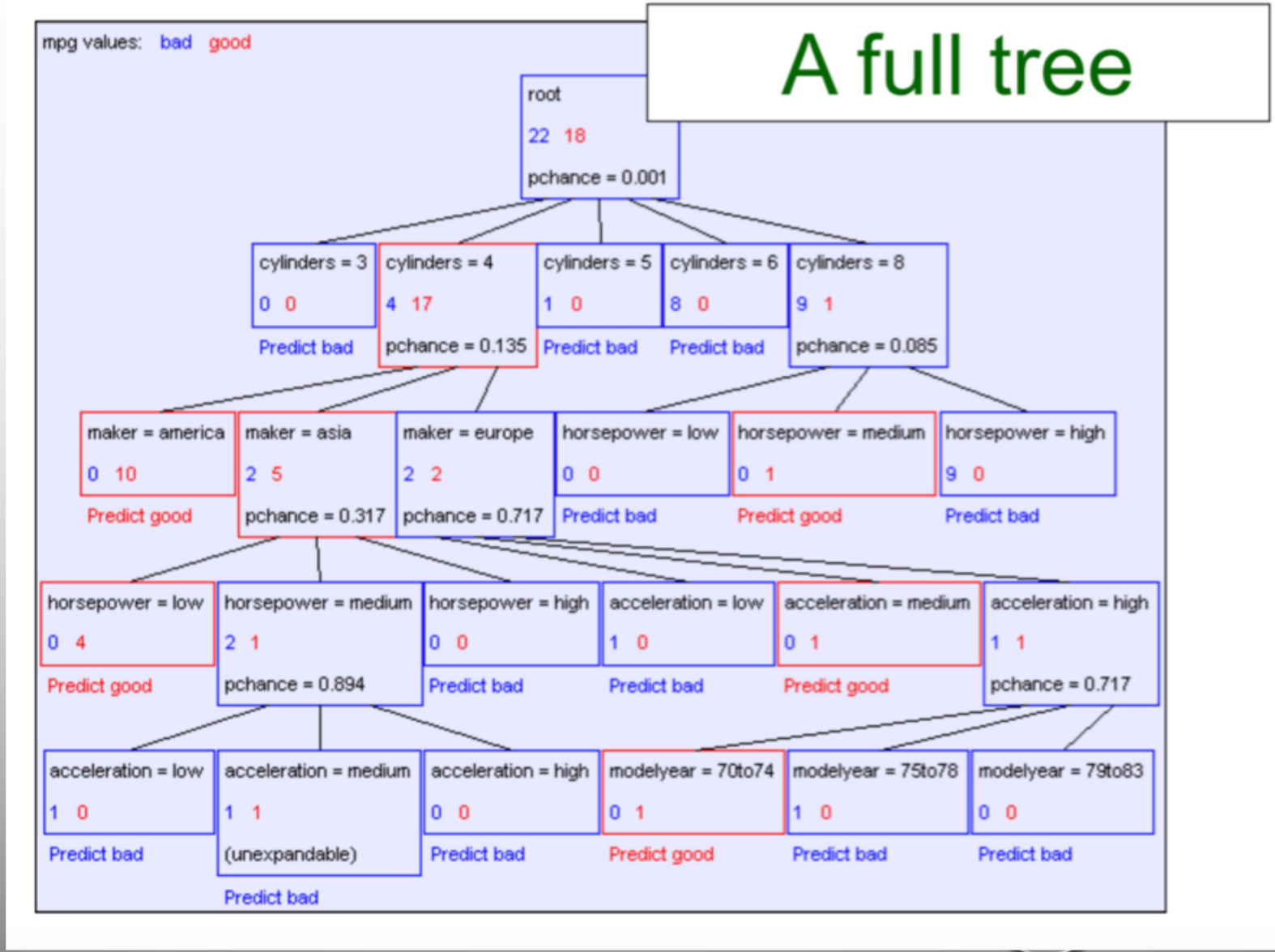
Second level of Tree



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

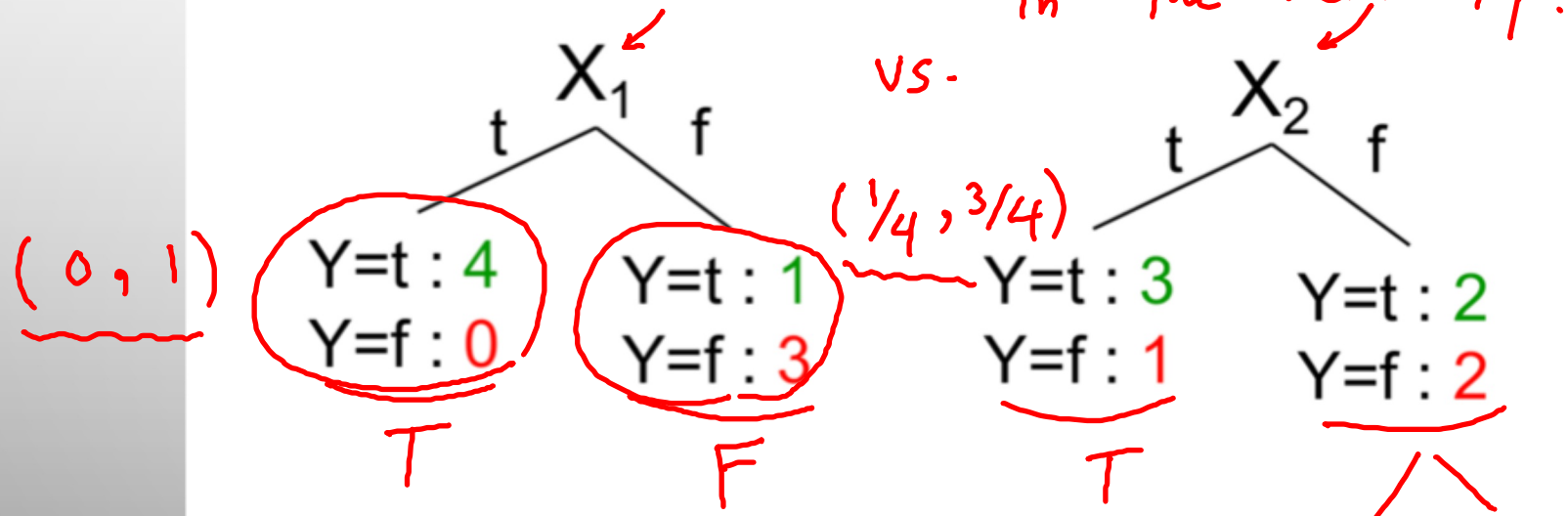
Two Questions

- 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

Would we prefer to split on X_1 or X_2?

purity of the labels in the next step.



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

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

label

F T
(3/8, 5/8)

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

Which attribute gives the best split?

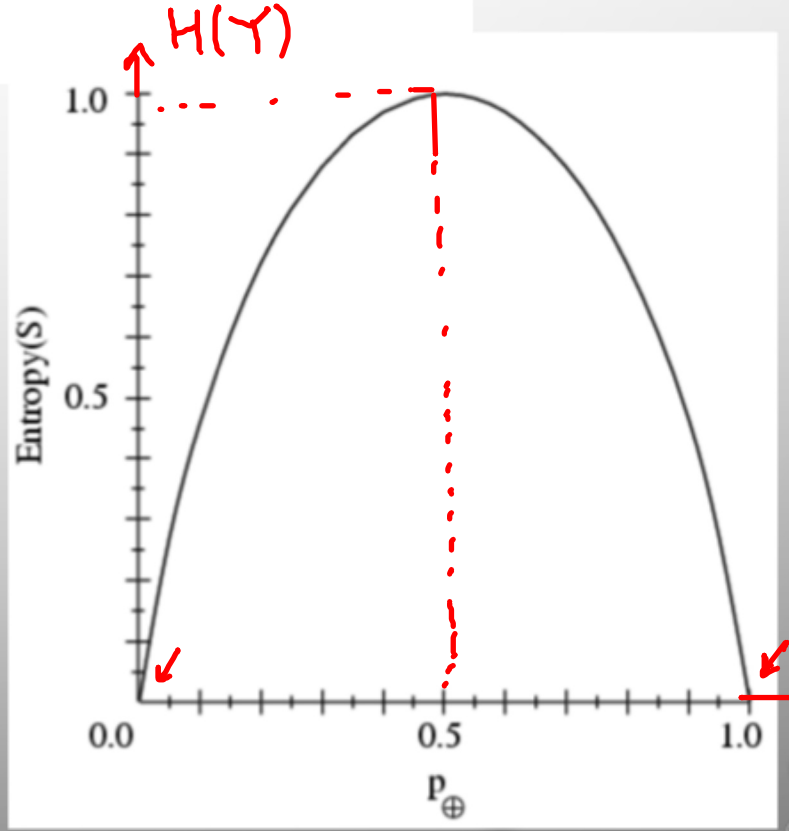
- A1: The one with the highest ***information gain***
  - Defined in terms of ***entropy***
- A2: Actually many alternatives,
  - e.g., ***accuracy***. Seeks to reduce the ***misclassification rate***

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

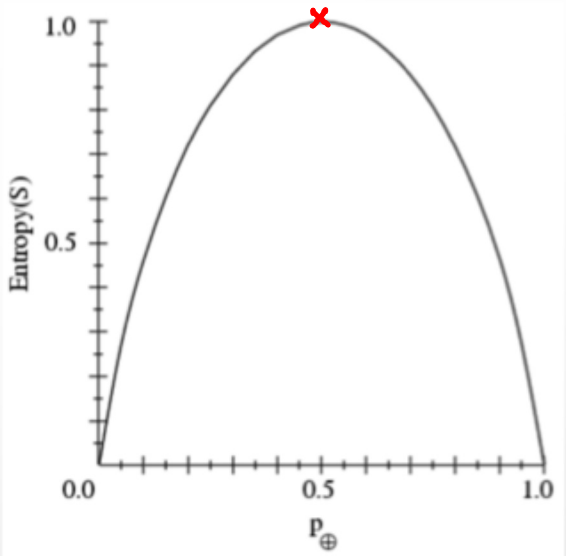
$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

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:

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

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

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

$-\ 2/6\ (1/2 \log_2 1/2 + 1/2 \log_2 1/2)$

$= 2/6$

$= 0.33$

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

Information Gain

- Advantage of attribute – decrease in entropy (uncertainty) after splitting

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

IG = 0

X indep. of Y

H(Y|X) = H(Y)

In our running example:

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

$IG(X_1) > 0$ → 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:

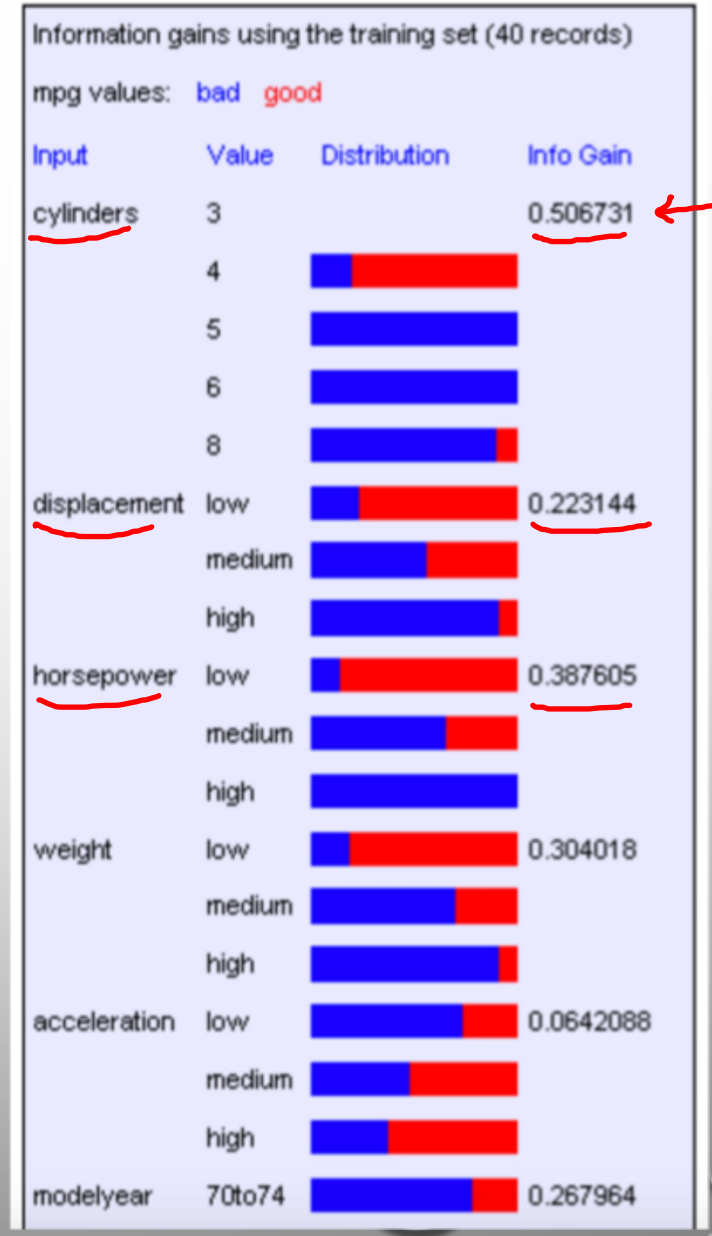
$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

Which attribute for the split

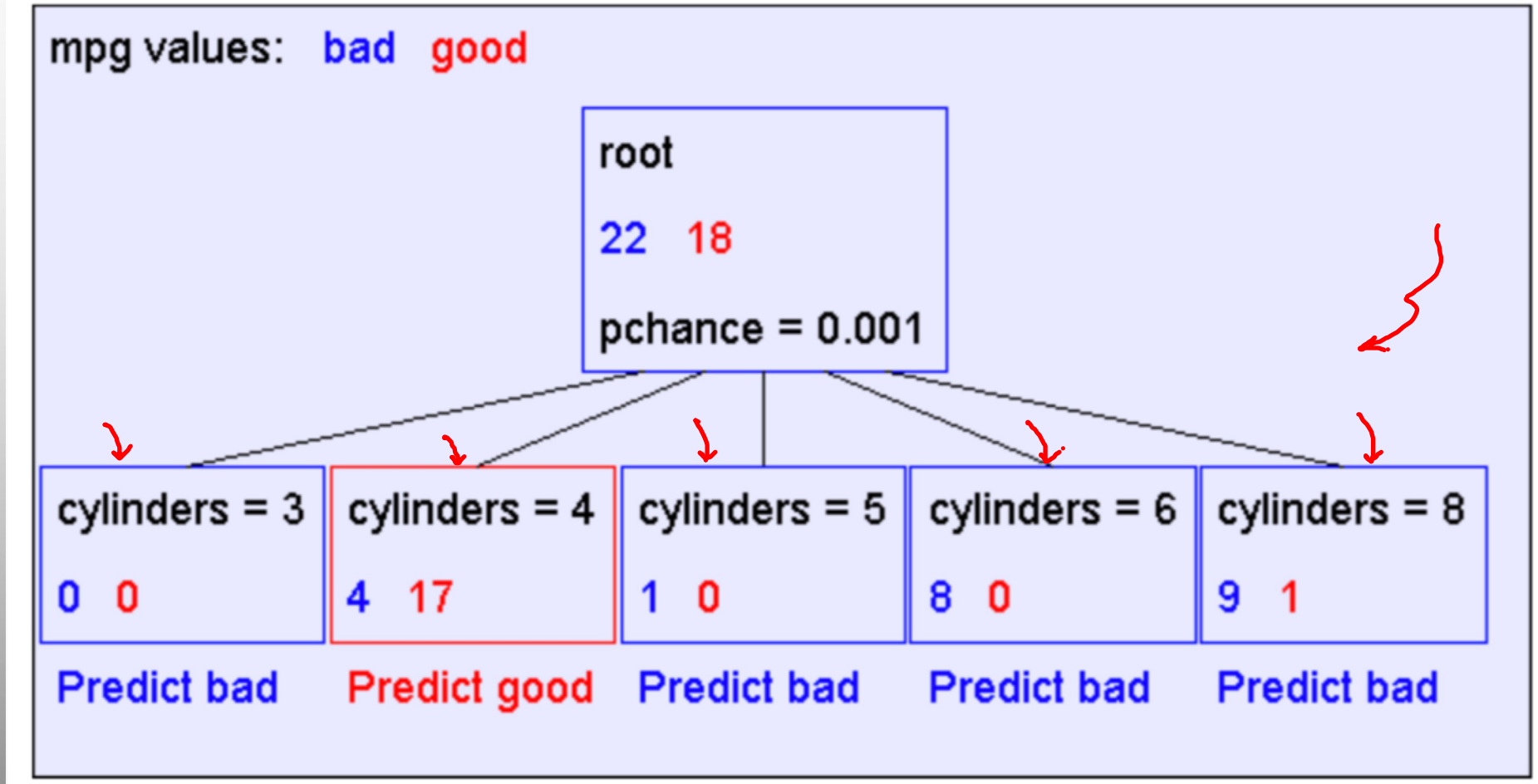
- Recurse.

Learning Decision Trees (cont.)

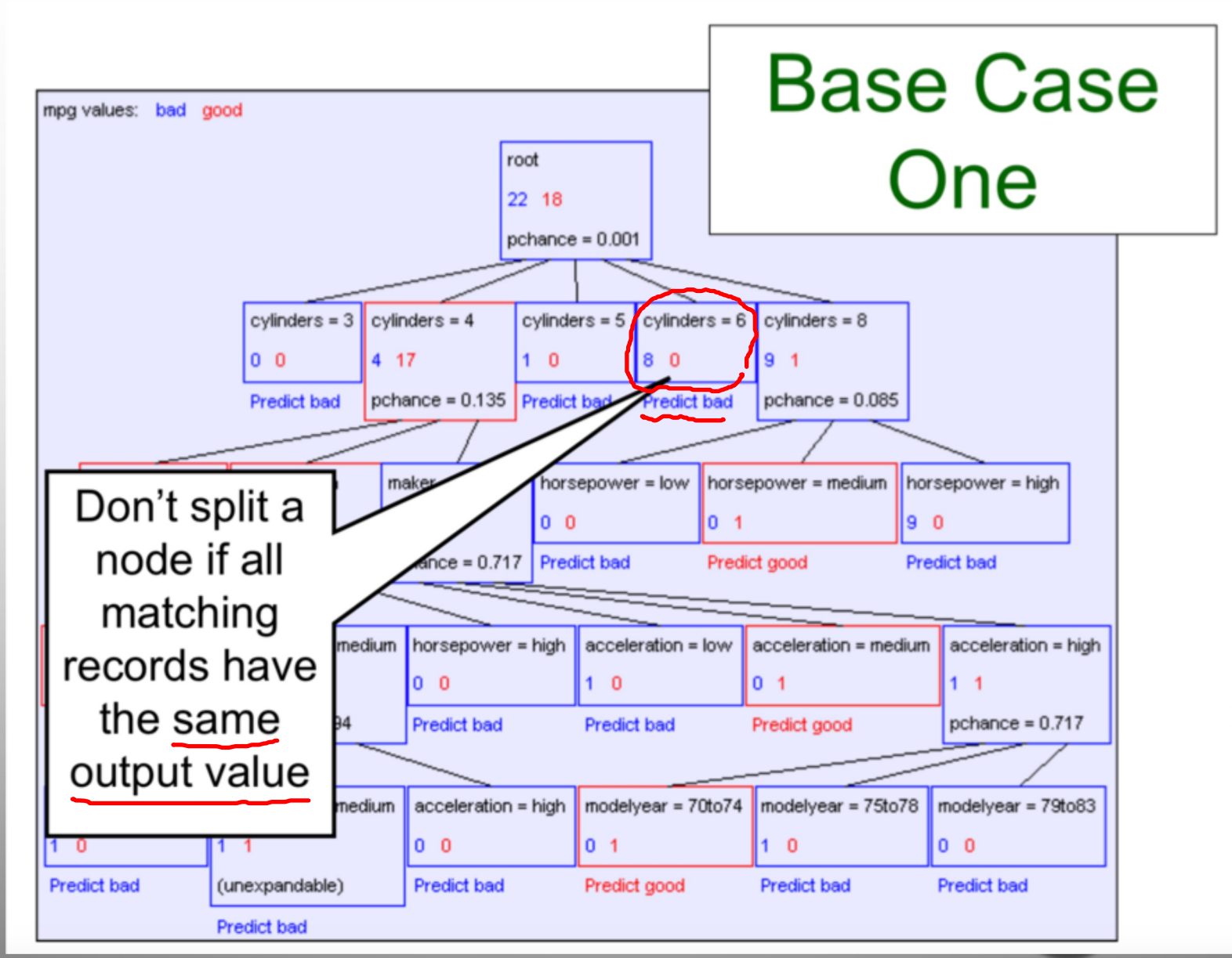
- Suppose we want to predict MPG.
- Now, Look at all the information gains...



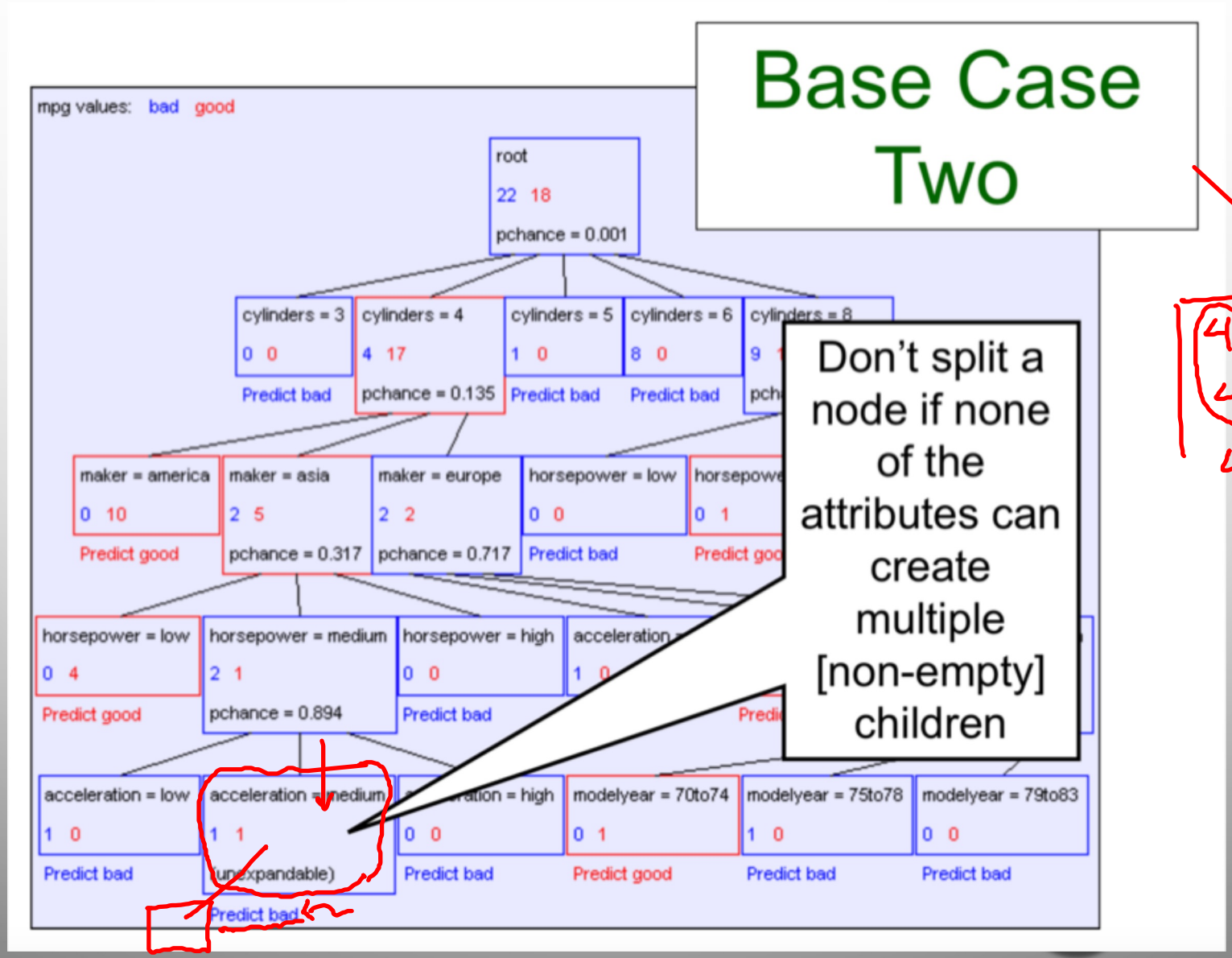
Tree After One Iteration



When to Terminate?

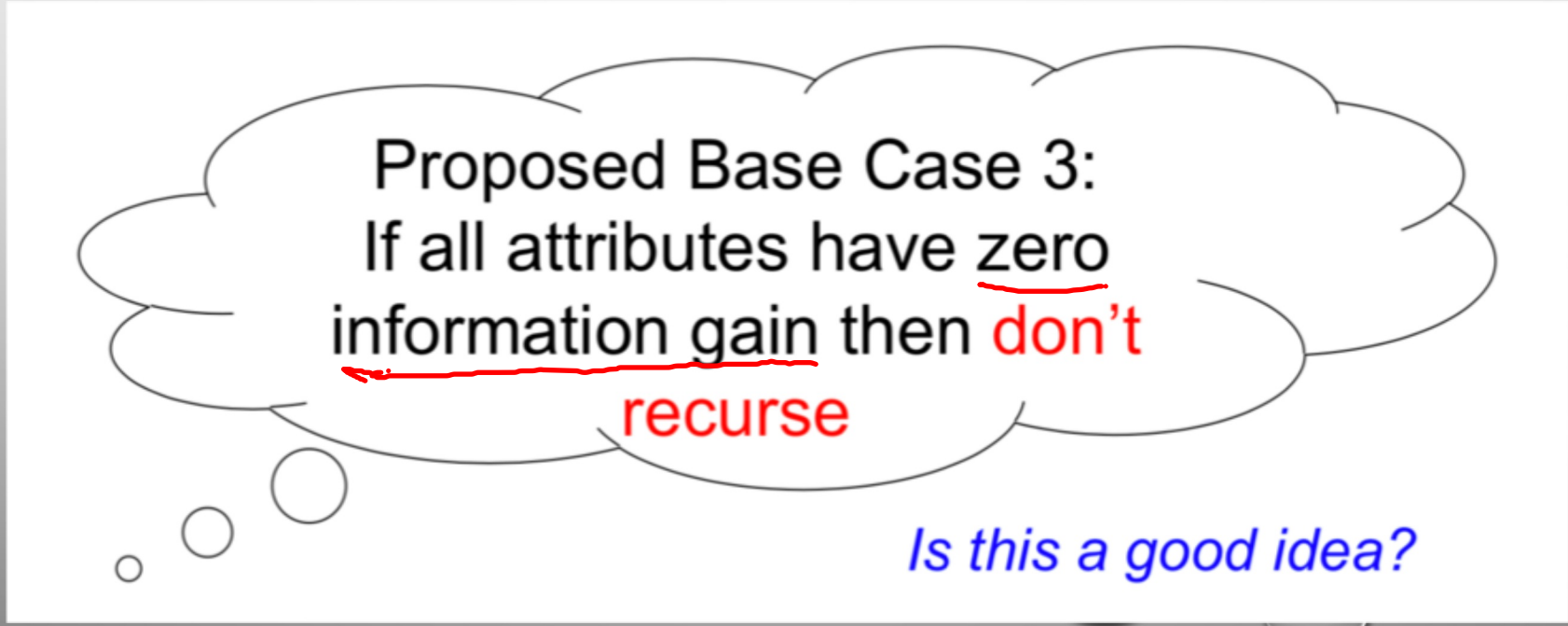


When to terminate? (cont.)



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

$$y = a \text{ XOR } b$$

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

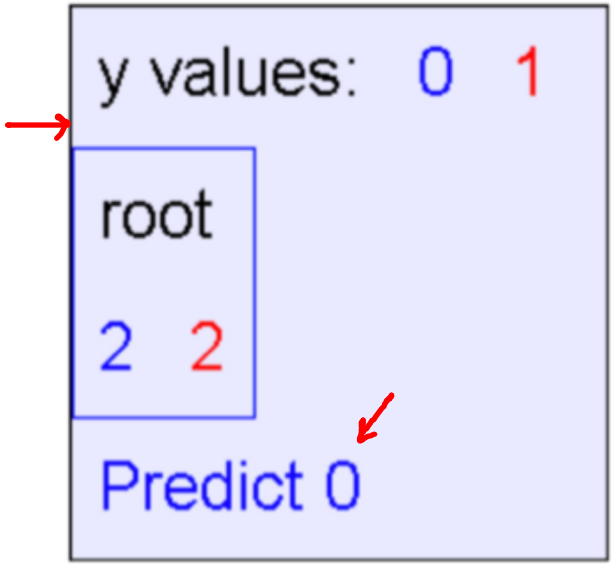
The information gains:

Information gains using the training set (4 records)

y values: 0 1

Input	Value	Distribution	Info Gain
a	0		0
	1		
b	0		0
	1		

The resulting decision tree:



50%

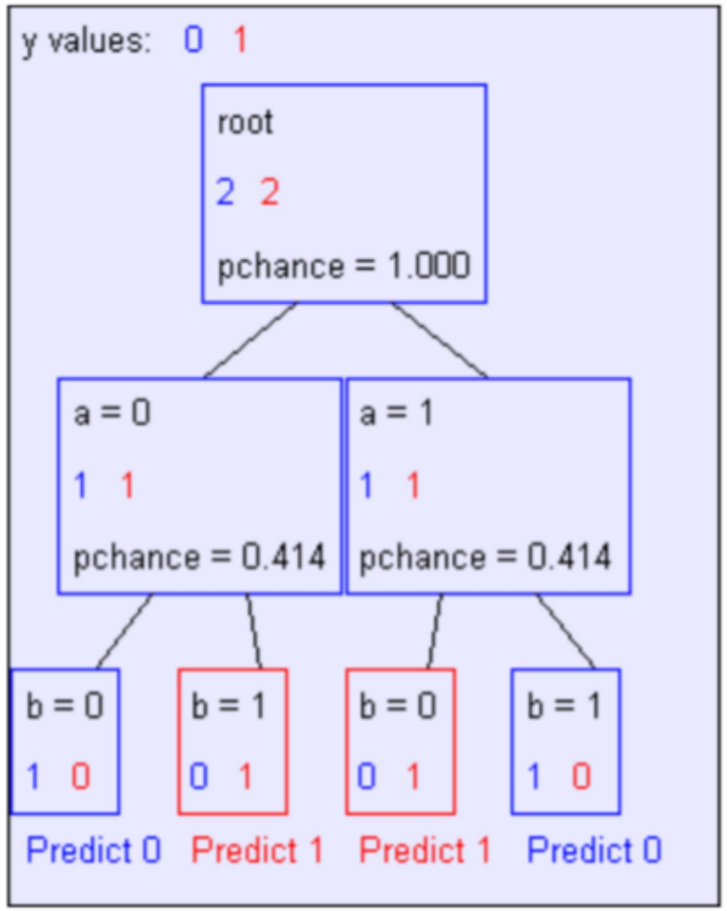
But *Without* Base Case 3:

y = a XOR b

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

So: Base Case 3?
Include or Omit?

The resulting decision tree:

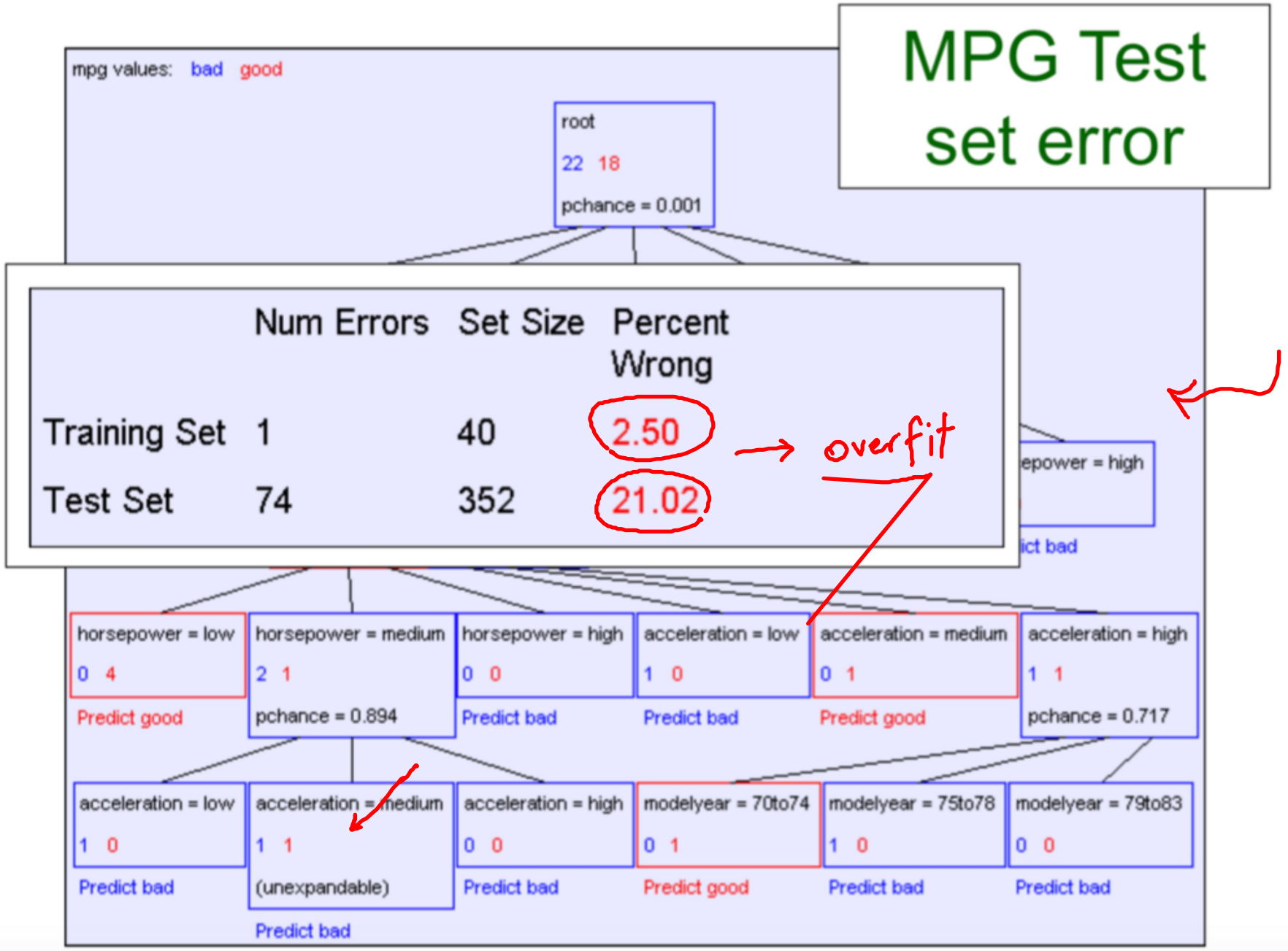


X_2 X_1 Y

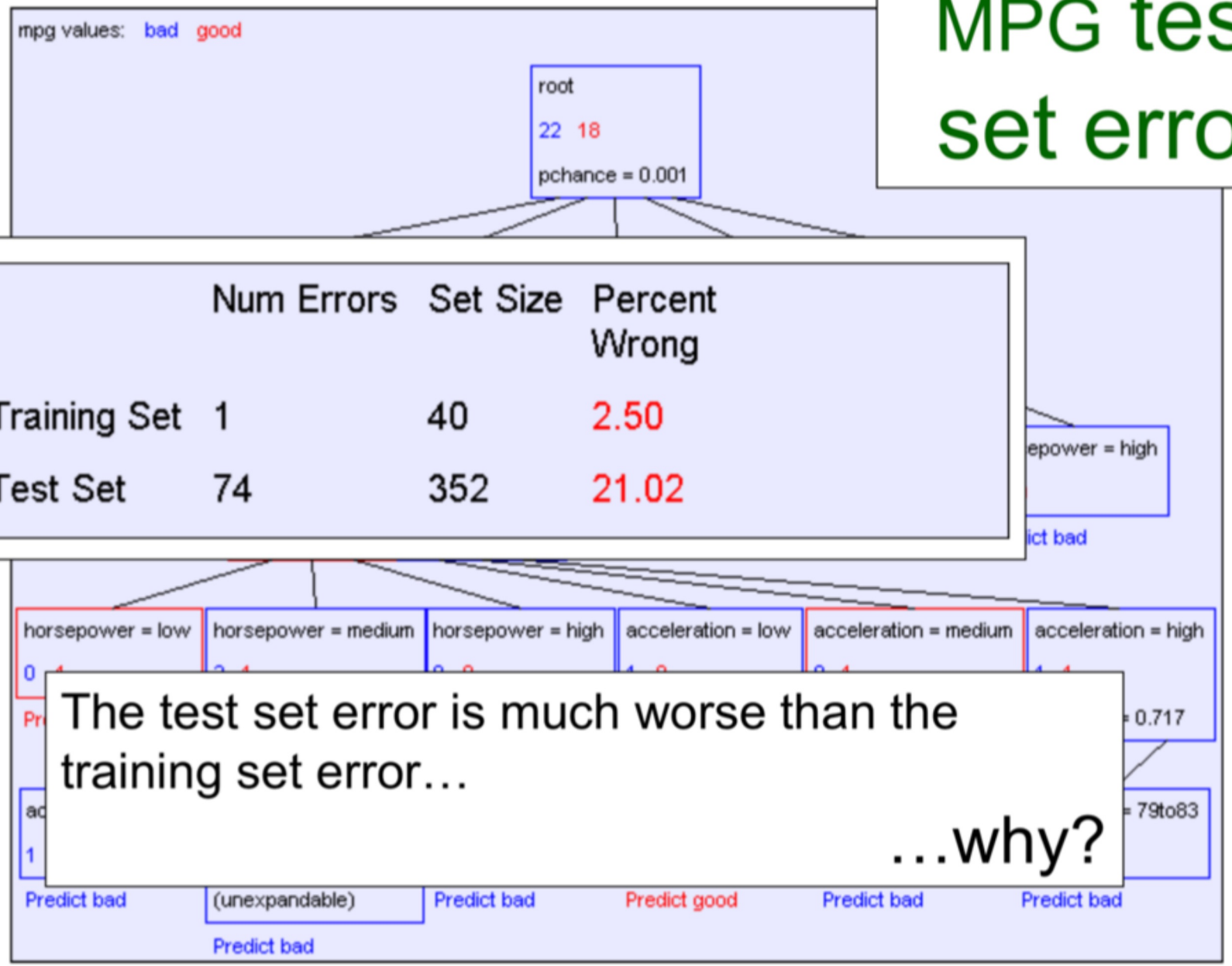
IG → empirical

0% error

MPG Test set error



MPG test set error



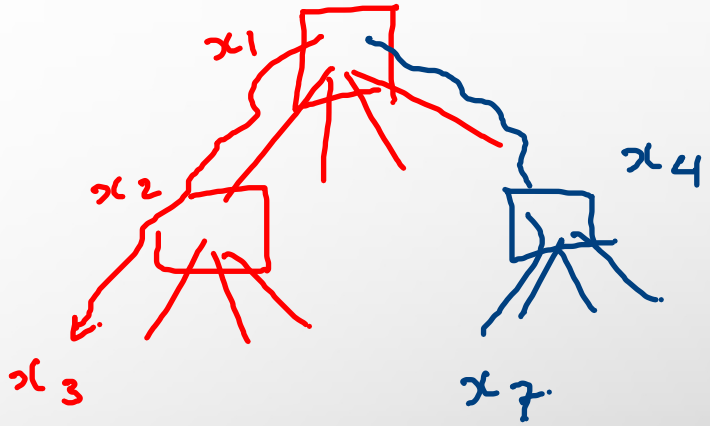
	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

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

…why?

Decision trees will overfit

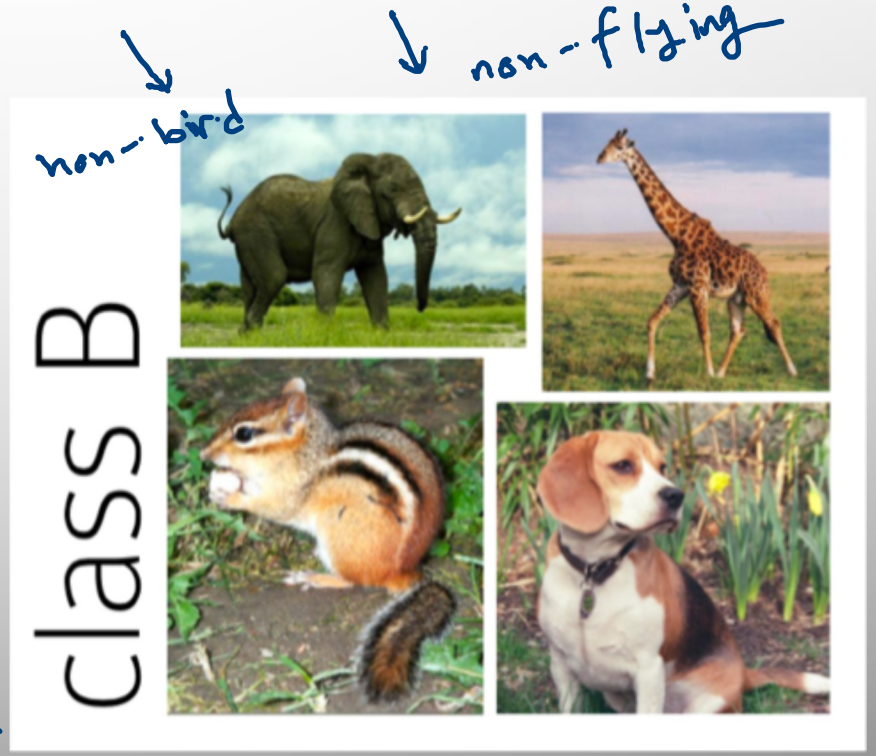
- Our decision trees have no learning bias
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Will definitely overfit!!!
  - Must introduce some bias towards *simpler* trees → restrict the depth
- Why might one pick simpler trees?



Small # of features are suff. for the classification of each data point!

Inductive bias

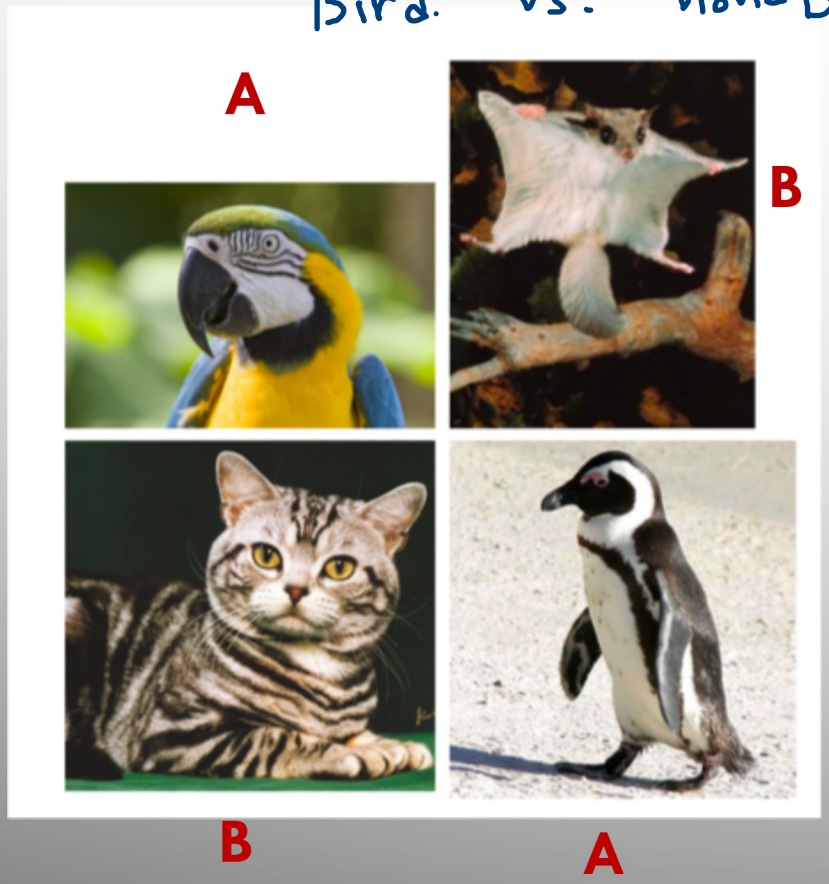
- Suppose that you are given 8 training samples for two classes A and B.



Inductive bias (cont.)

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

Bird vs. non-Bird



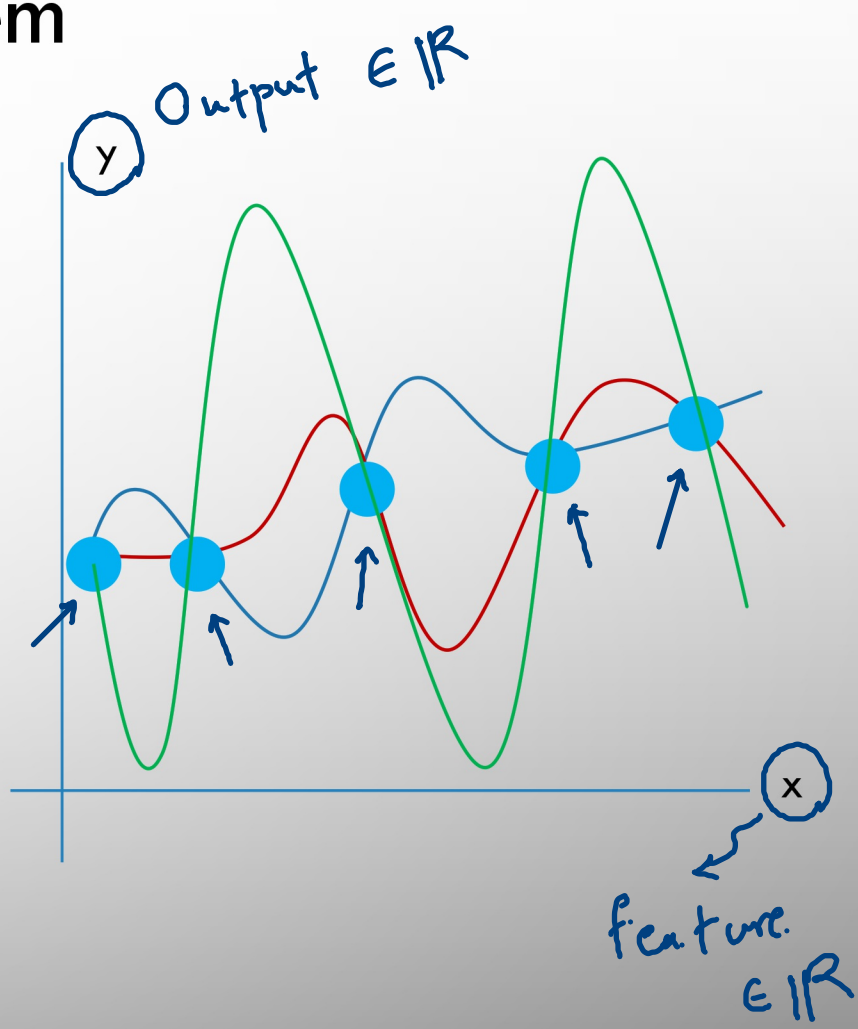
Flying vs. non-Flying

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 narrow 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 in 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!

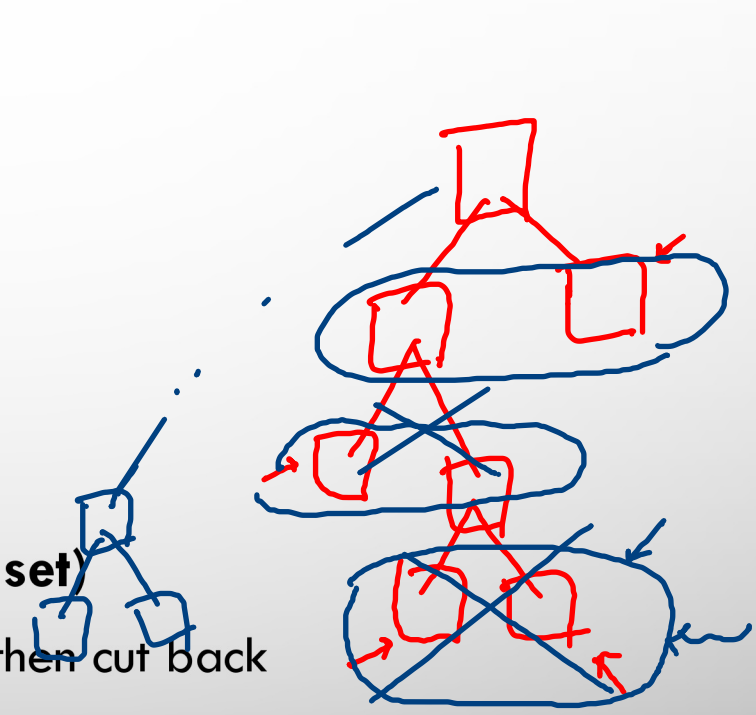


Occam's Razor

- 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!



IG ↑

H_0 / H_1 { t-test, Fisher ←, χ^2 ←, …

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***

χ^2 - test

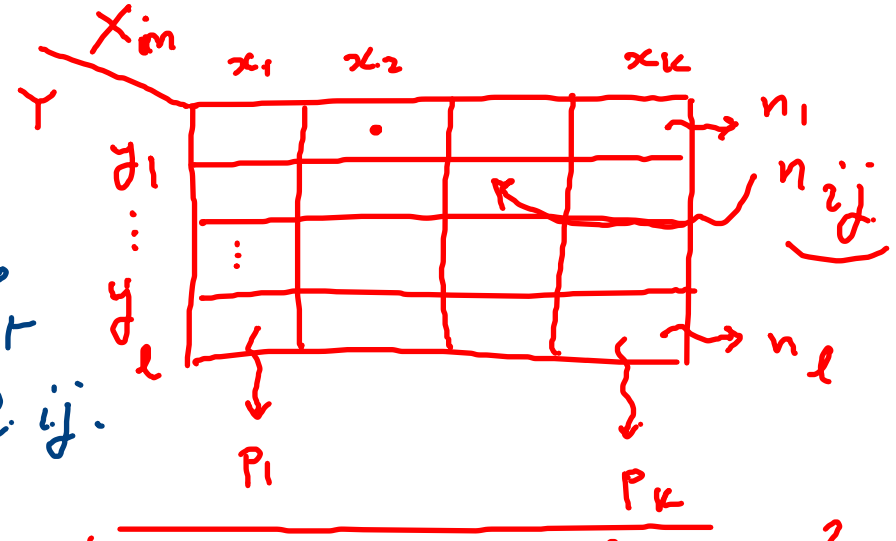
$$\begin{cases} H_0 : & X_i \perp\!\!\!\perp Y \\ H_1 : & X_i \not\perp\!\!\!\perp Y \end{cases} \rightsquigarrow \begin{array}{ll} \text{p-val} \uparrow & H_0 \\ \text{p-val} \downarrow & H_1 \end{array}$$

builds a Statistic $\rightsquigarrow f(D)$

if H_0 holds, $f(D) \sim \chi^2_K$

$$\chi^2 = \sum_{i,j} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$$

n_{ij} ← if $X_m \perp\!\!\!\perp Y$ how many samples do you expect to get @ ij.

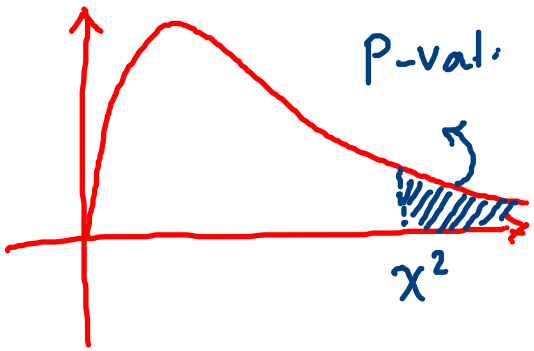


$$E_{ij} = \bigcirc \times n = \frac{n_i p_j}{n} \qquad n = \sum_{i,j=1}^{\cdot\cdot} n_{ij}$$

$\bigcirc$: $\mathbb{P}(Y=i, X_m=j)$

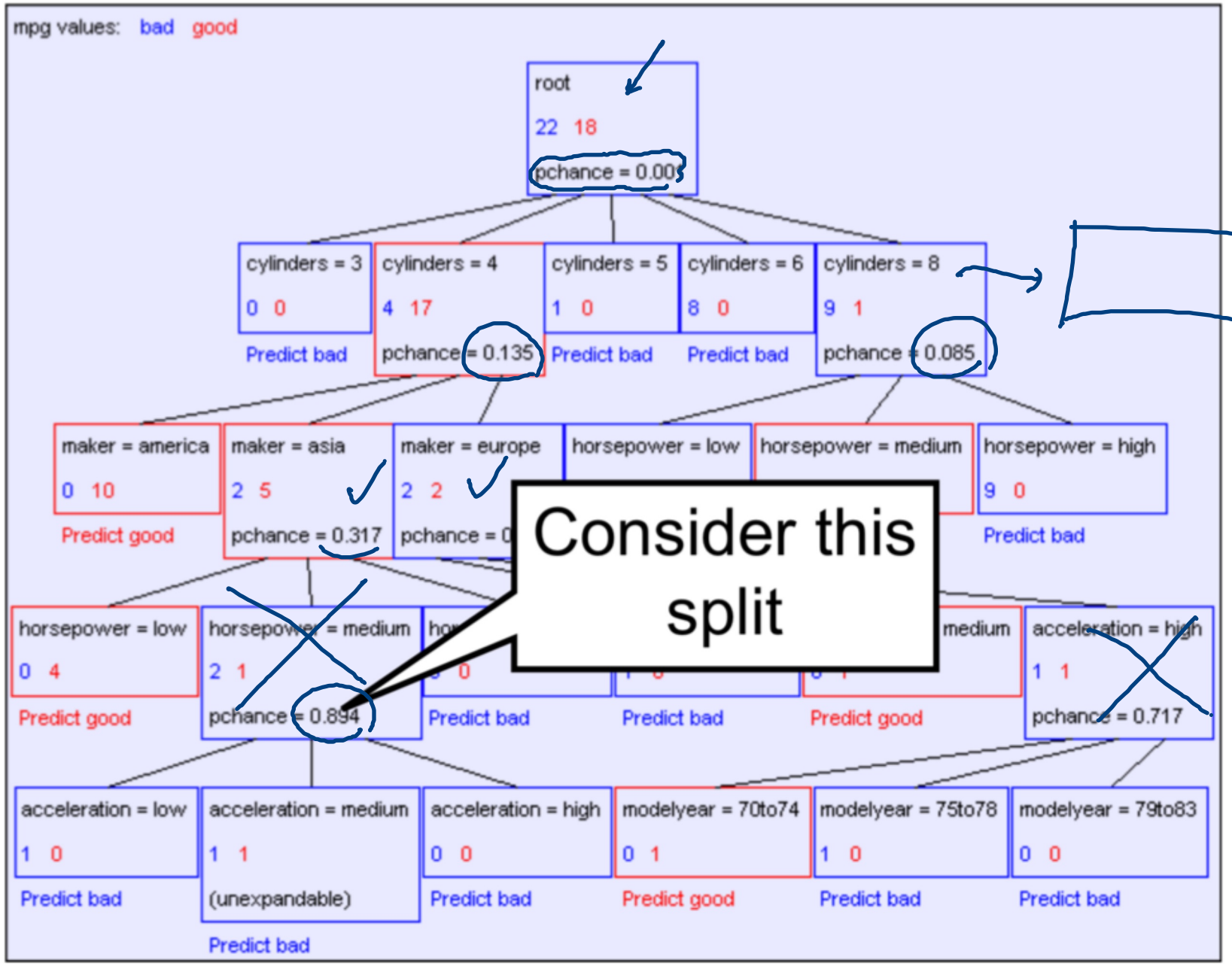
$= \mathbb{P}(Y=i) \cdot \mathbb{P}(X_m=j) = \left(\frac{n_i}{n}\right) \cdot \left(\frac{p_j}{n}\right)$

under H_0 $\chi^2 \sim \chi^2_{(K-1)(l-1)}$

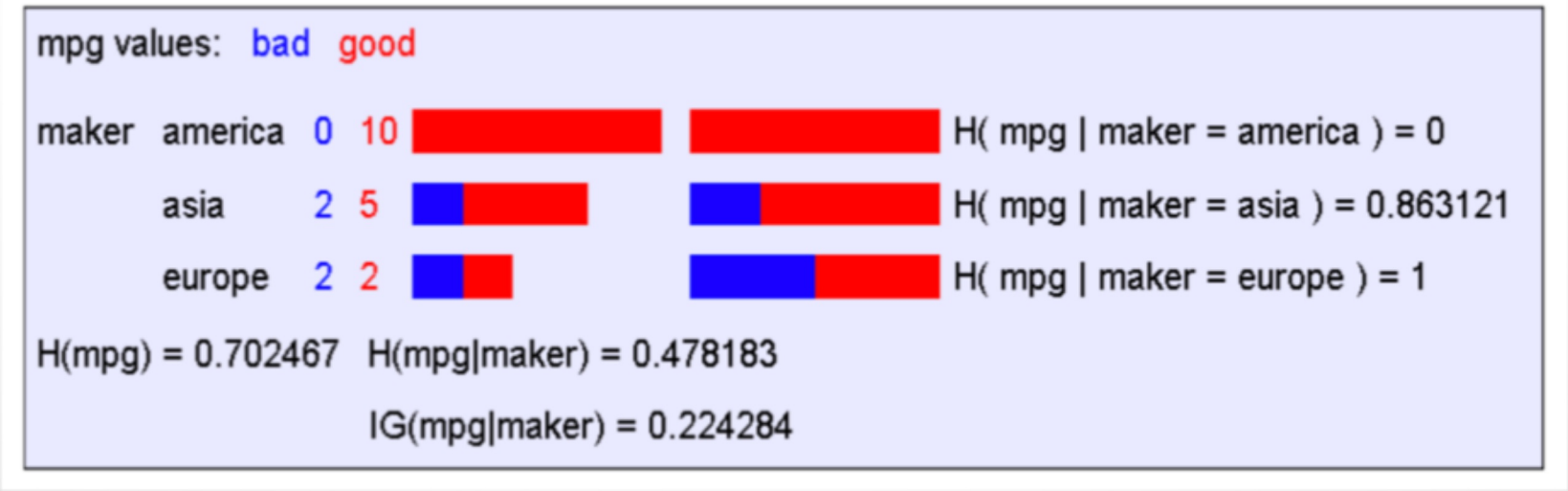


Alternatively

- Chi-squared pruning
  - Grow tree fully
  - Consider leaves in turn
    - Is parent split worth it?


mpg values: bad good
root
22 18
pchance = 0.005
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
horsepower = low
horsepower = medium
horsepower = high
9 0
Predict bad
Consider this split
horsepower = low
0 4
Predict good
horsepower = medium
2 1
pchance = 0.894
Predict bad
Predict bad
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
χ²
P-val.

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

Validation

Regularization