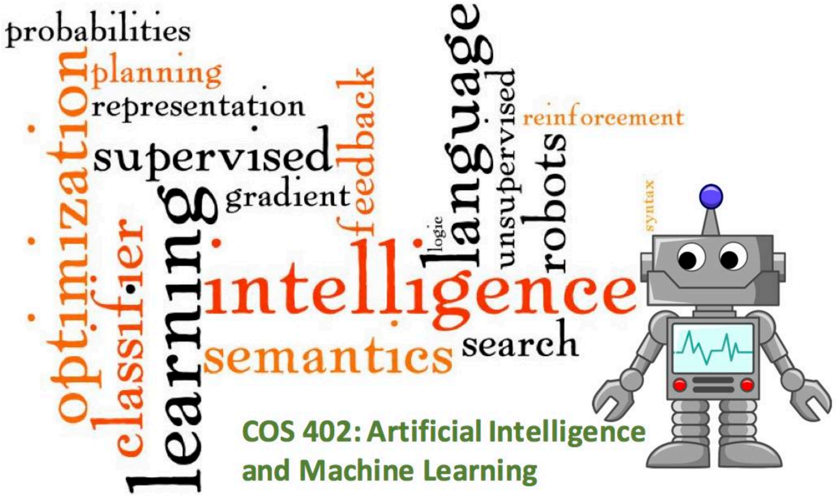


COS 402 – Machine Learning and Artificial Intelligence
Fall 2016

# Lecture 2: Classification and Decision Trees

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This lecture contains material from the
T. Michel text “Machine Learning”, and slides adapted from
David Sontag, Luke Zettlemoyer, Carlos Guestrin, and Andrew Moore

# Admin

- Enrolling to the course – priorities
- Pre-requisites reminder (calculus, linear algebra, discrete math, probability, data structures & graph algorithms)
- Movie tickets
- Slides
- Exercise 1 – theory – due in one week, in class

# Agenda

This course: Basic principles of how to design machines/programs that act “intelligently.”

- Recall crow / fox example.
- Start with simpler task – classification, learning from examples
- Today: still Naive AI.
  Next week: statistical learning theory

# Classification

Goal: Find *best* mapping from domain (features) to output (labels)

- Given a document (email), classify spam or ham.
  Features = words , labels = {spam, ham}

- Given a picture, classify if it contains a chair or not
  features = bits in a bitmap image, labels = {chair, no chair}

GOAL: automatic machine that learns from examples


Terminology for learning from examples:
- Set aside a ”training set” of examples, train a classification machine
- Test on a “test set”, to see how well machine performs on unseen examples

# Classifying fuel efficiency

- 40 data points
- Goal: predict MPG
- Need to find: $f : X \rightarrow Y$
- Discrete data (for now)

| 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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| 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)

# Decision trees for classification

- Why use decision trees?
- What is their expressive power?
- Can they be constructed automatically?
- How accurate can they classify?
- What makes a good decision tree besides accuracy on given examples?

# Decision trees for classification

Some real examples (from Russell & Norvig, Mitchell)

- BP’s GasOIL system for separating gas and oil on offshore platforms - decision trees replaced a hand-designed rules system with 2500 rules. C4.5-based system outperformed human experts and saved BP millions. (1986)
- learning to fly a Cessna on a flight simulator by watching human experts fly the simulator (1992)
- can also learn to play tennis, analyze C-section risk, etc.

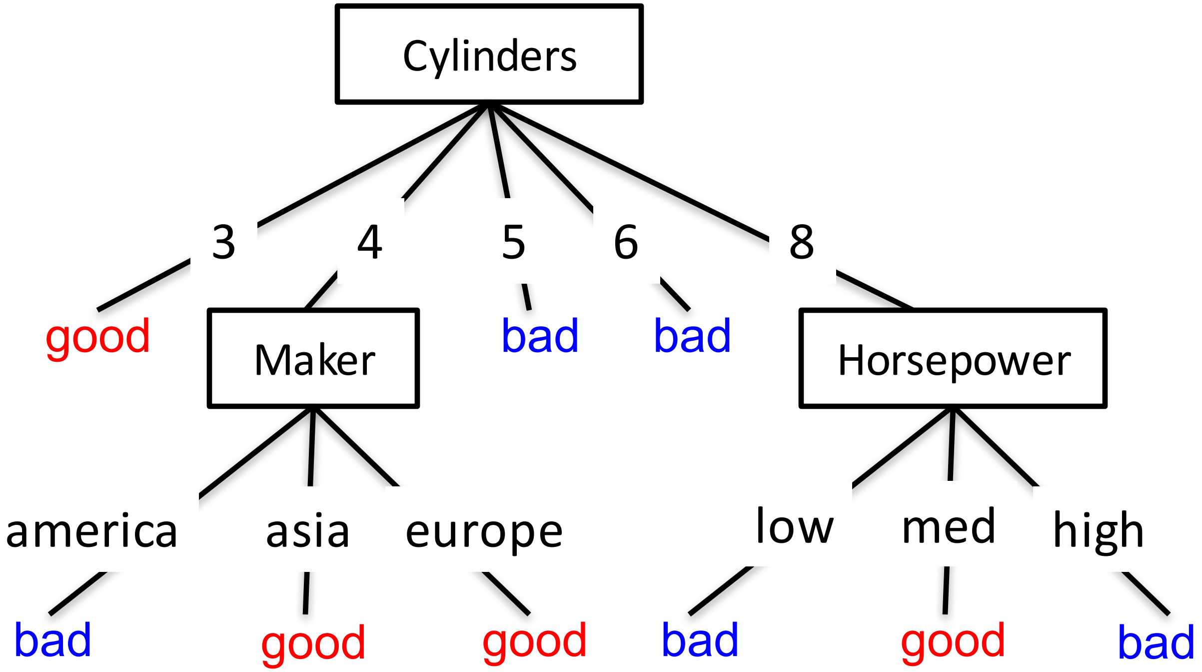
# Decision trees for classification

- interpretable/intuitive, popular in medical applications because they mimic the way a doctor thinks
- model discrete outcomes nicely
- can be very powerful (expressive)
- C4.5 and CART - from “top 10 data mining methods” - very popular

- This Thu: we’ll see why not…

# decision trees $f : X \rightarrow Y$

- Each internal node tests an attribute $x_i$
- One branch for each possible 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 $y$
- Can we construct a tree automatically?

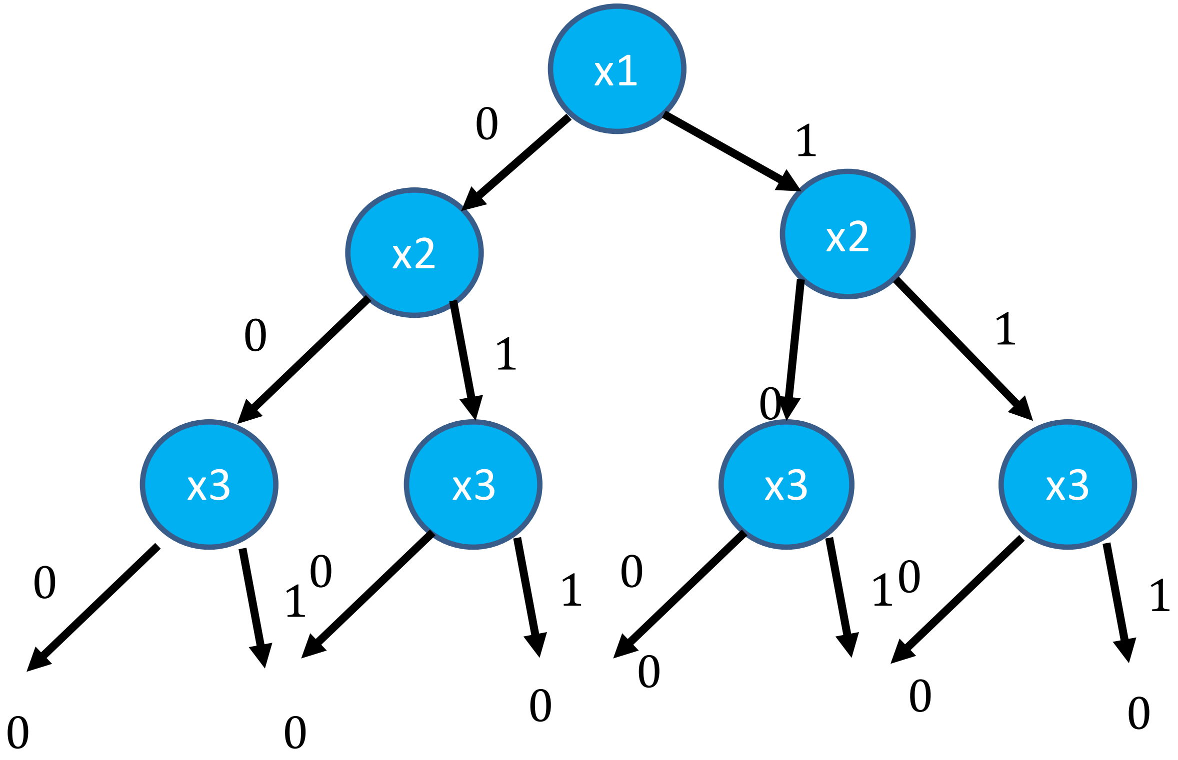



Human interpretable!

# Expressive power of DT

What kind of functions can they potentially represent?

- Boolean functions?
  F = $\{0,1\}^n \mapsto \{0,1\}$

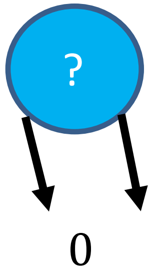



| X1 | X2 | X3 | F(X1,X2,X3) |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 |
| 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | 0 |
| 1 | 0 | 0 | 0 |
| 1 | 0 | 1 | 0 |
| 1 | 1 | 0 | 0 |
| 1 | 1 | 1 | 0 |

# Is simpler better?

What kind of functions can they potentially represent?

- Boolean functions?
  F = $\{0,1\}^n \mapsto \{0,1\}$




| X1 | X2 | X3 | F(X1,X2,X3) |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 |
| 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | 0 |
| 1 | 0 | 0 | 0 |
| 1 | 0 | 1 | 0 |
| 1 | 1 | 0 | 0 |
| 1 | 1 | 1 | 0 |

# What is the Simplest 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 |
| 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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| bad | 8 | high | high | high | low | 70to74 | america |
| good | 4 | low | medium | low | medium | 75to78 | europe |
| bad | 5 | medium | medium | medium | medium | 75to78 | europe |

predict
mpg=bad

## Is this a good tree?

[22+, 18-]

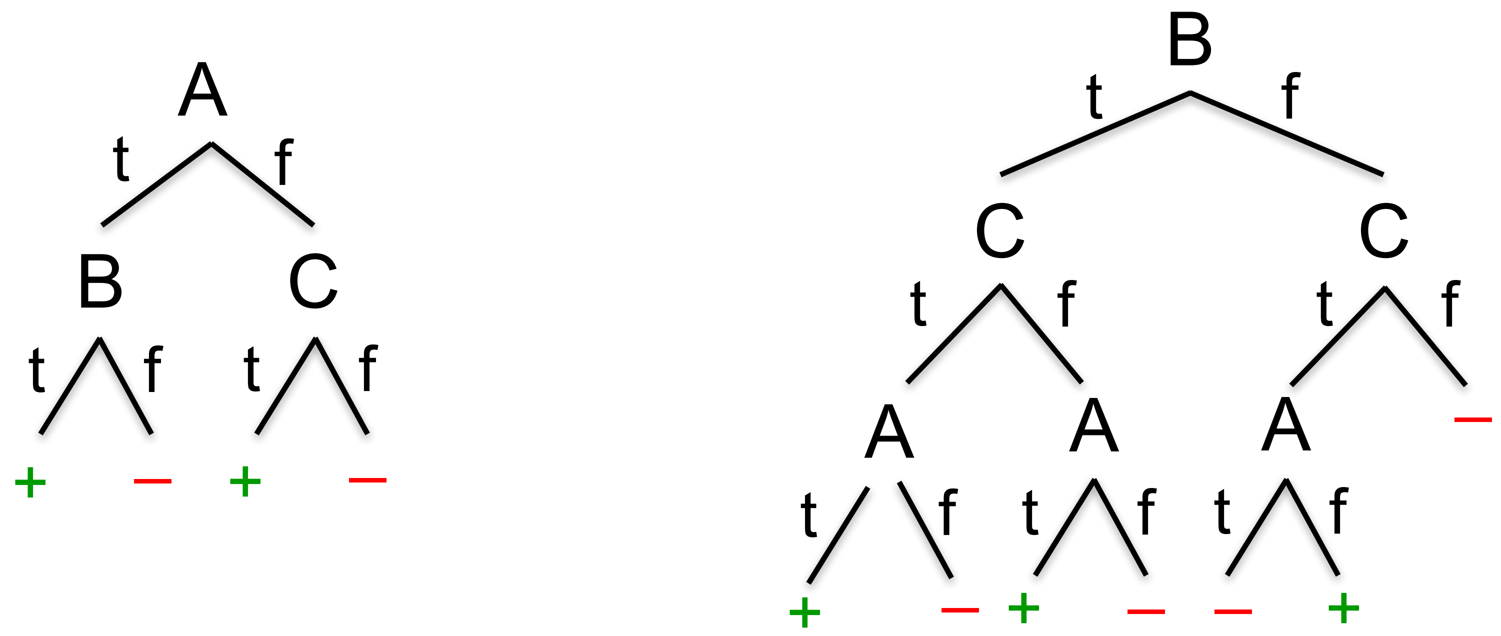
Means:

correct on 22 examples

incorrect on 18 examples

# Are all decision trees equal?

- Many trees can represent the same concept
- But, not all trees will have the same size!
  – e.g., ((A and B) or (not A and C))




- Which tree do we prefer?

# Learning *simplest* decision tree is NP-hard

- Formal justification - statistical learning theory (next lecture)
- 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)**
  - Recurs

# Learning Algorithm for Decision Trees

$$S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$$

$$\mathbf{x} = (x_1, \ldots, x_d)$$

$$x_j, y \in \{0,1\}$$

$\textsc{GrowTree}(S)$

**if** $(y = 0 \text{ for all } \langle \mathbf{x}, y \rangle \in S)$ **return** new leaf(0)

**else if** $(y = 1 \text{ for all } \langle \mathbf{x}, y \rangle \in S)$ **return** new leaf(1)

**else**

choose best attribute $x_j$

$S_0 = \text{all } \langle \mathbf{x}, y \rangle \in S \text{ with } x_j = 0;$

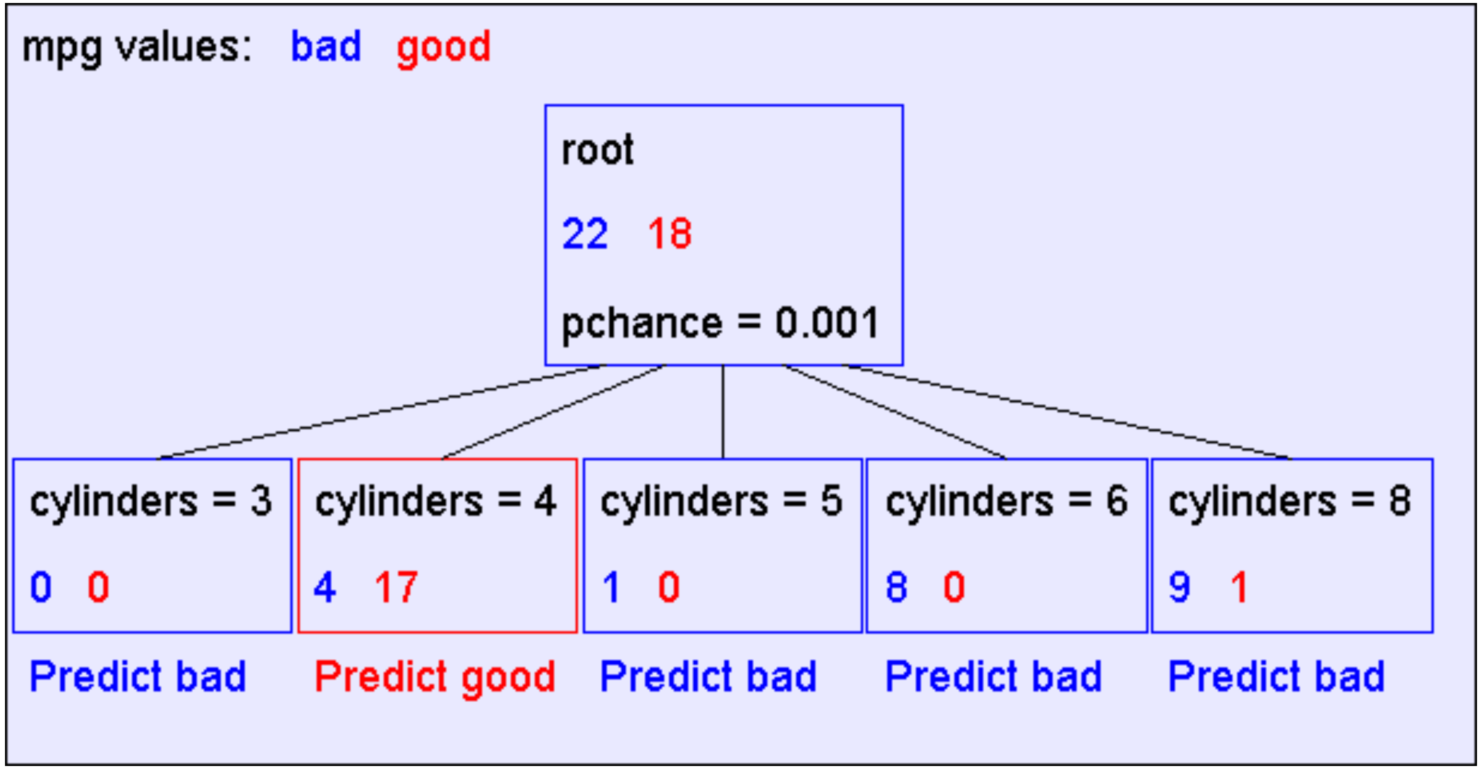
$S_1 = \text{all } \langle \mathbf{x}, y \rangle \in S \text{ with } x_j = 1;$

**return** new node$(x_j, \textsc{GrowTree}(S_0), \textsc{GrowTree}(S_1))$

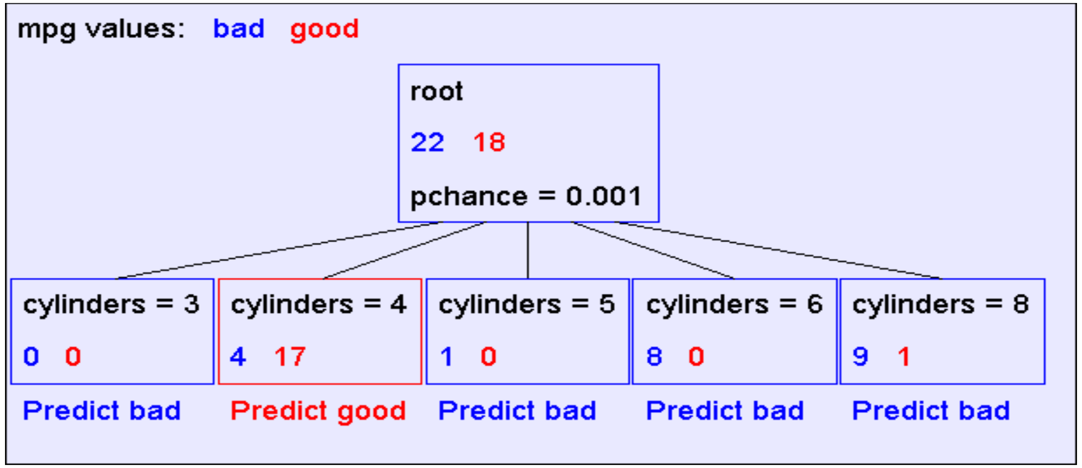
DT algs differ on this choice!

- ID3
- CAT4.5
- CART

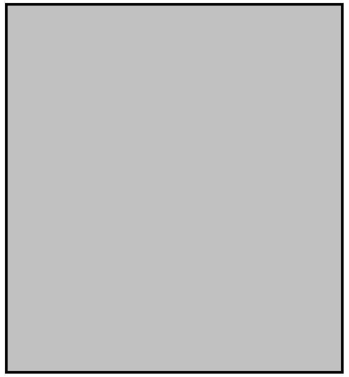
# A Decision Stump



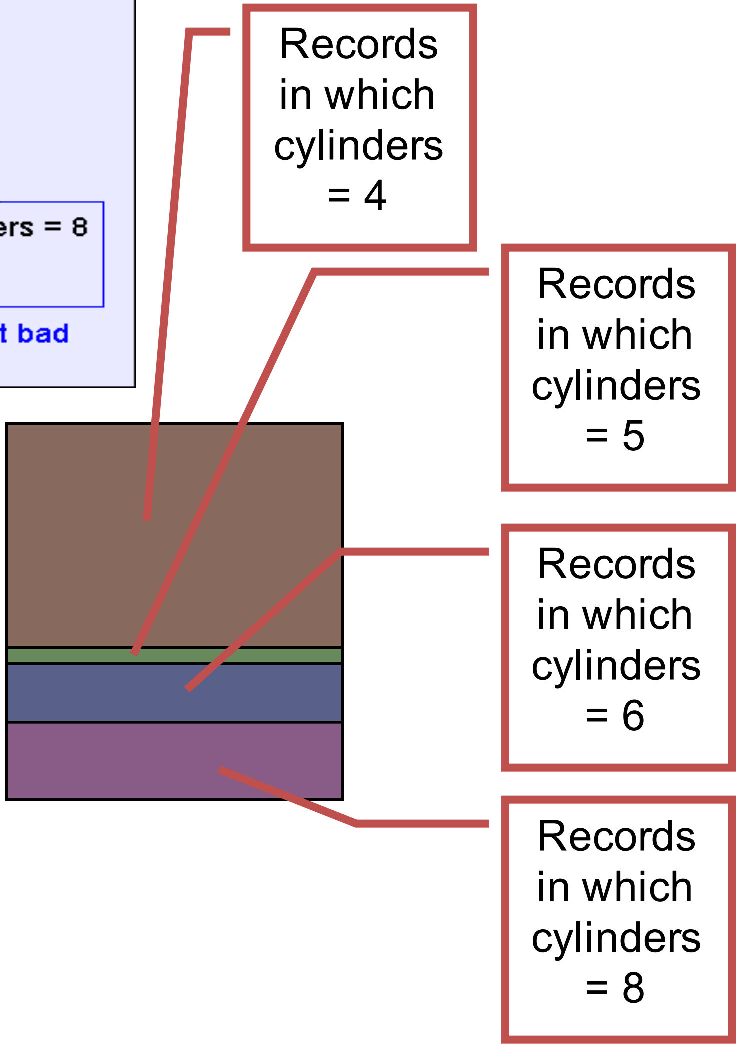
# Key idea: Greedily learn trees using **recursion**



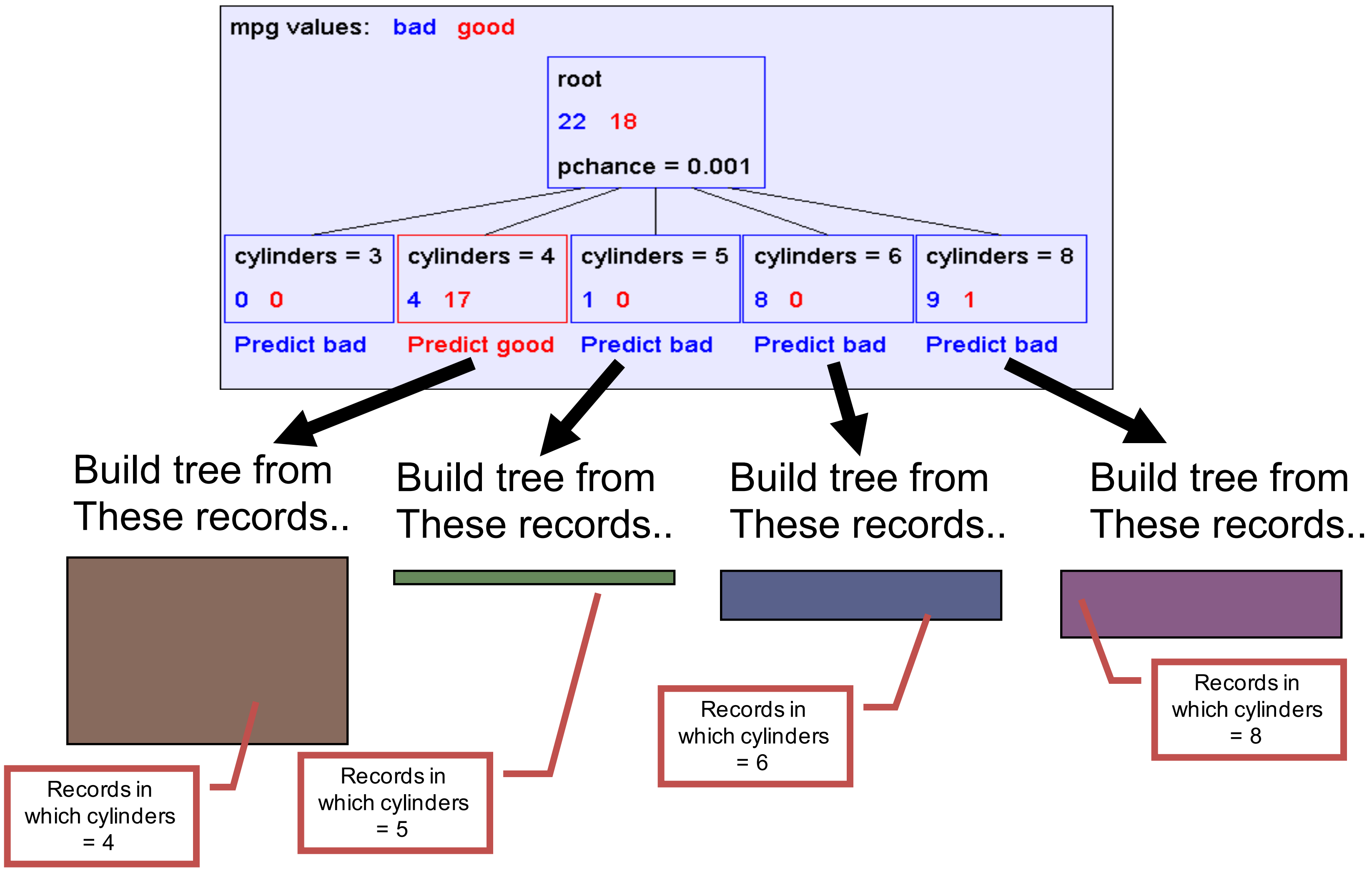

Take the Original Dataset..



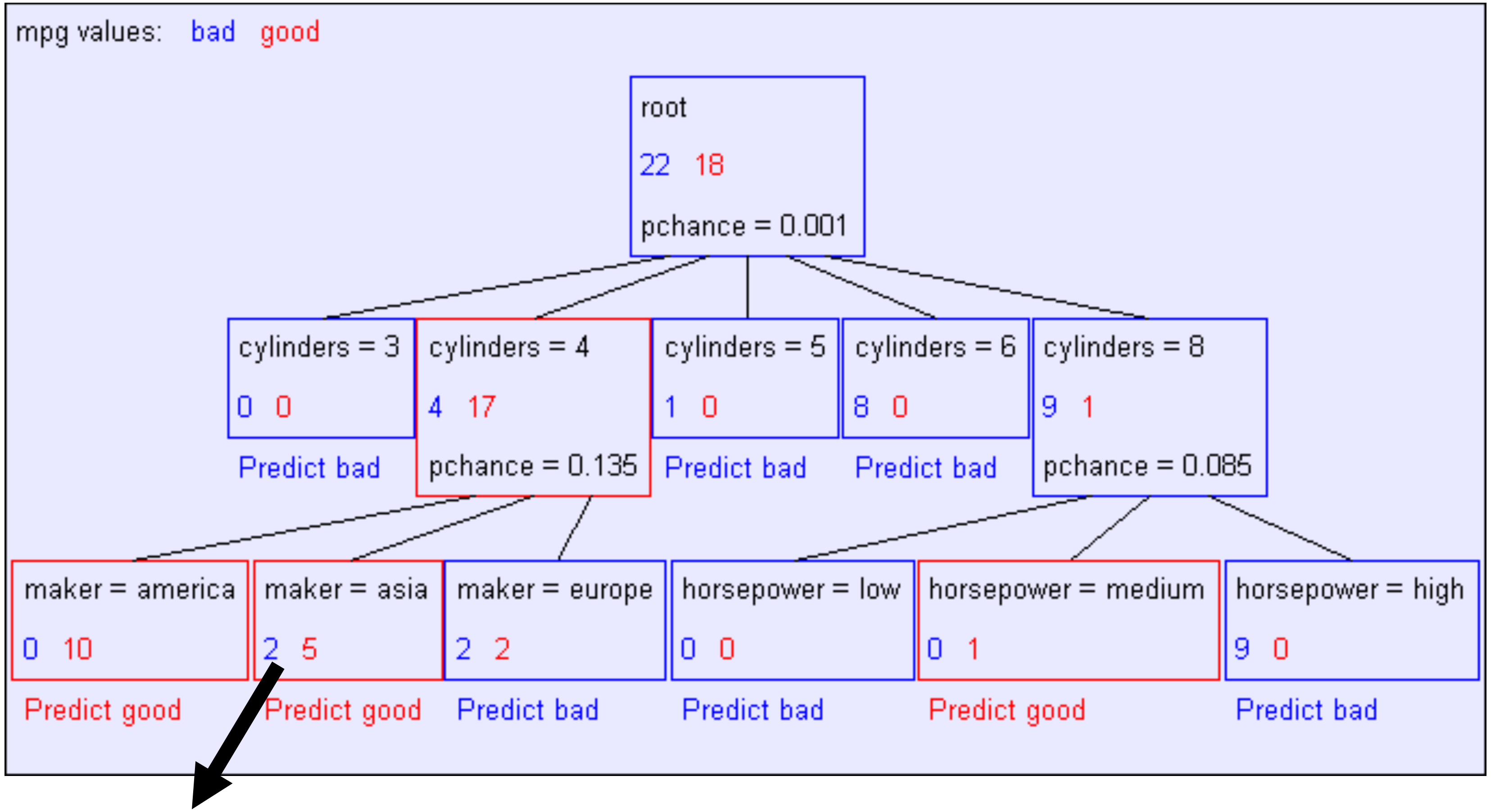
And partition it according to the value of the attribute we split on



# Recursive Step



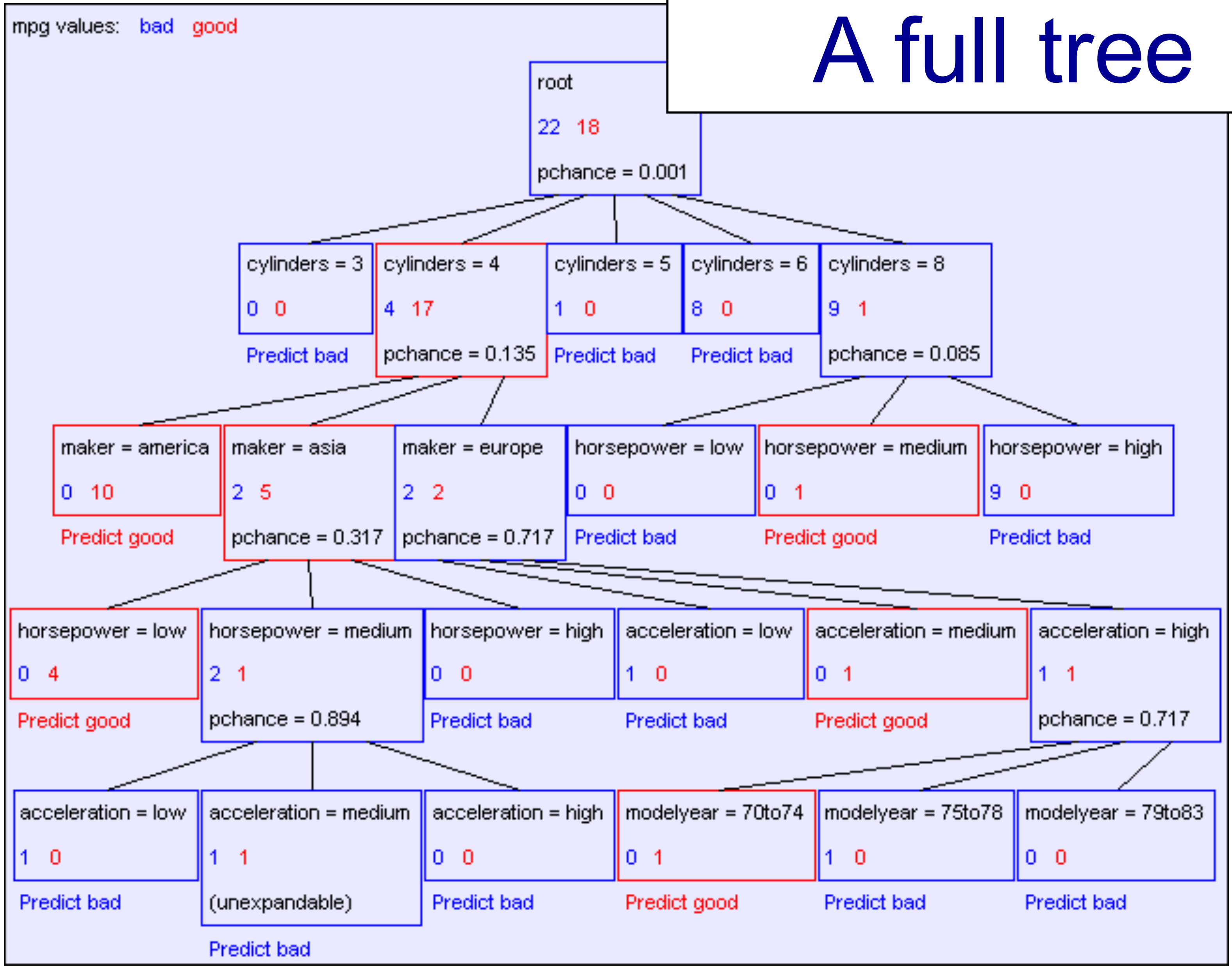
# Second level of tree




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)

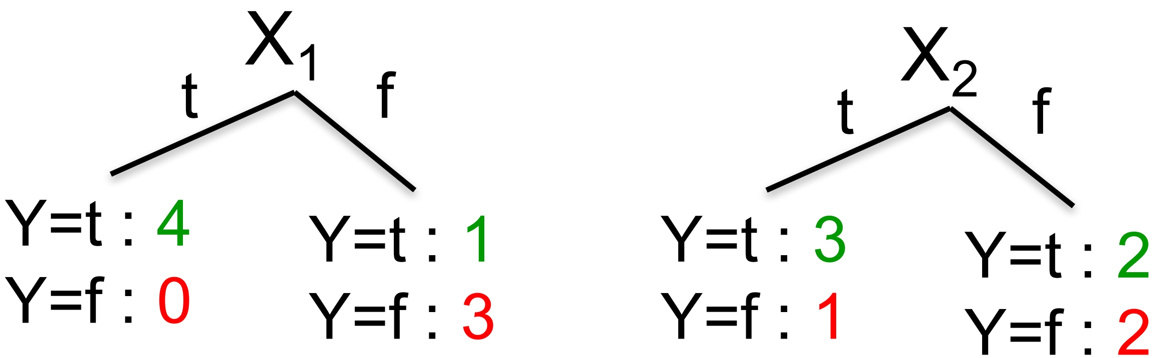
# A full tree



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

# 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 |

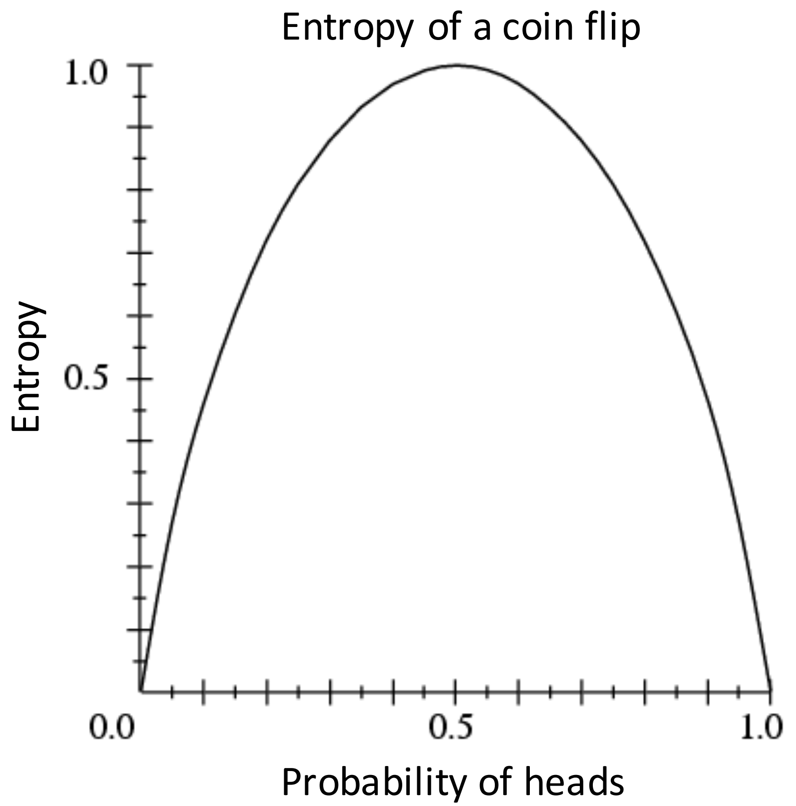
# Entropy

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)

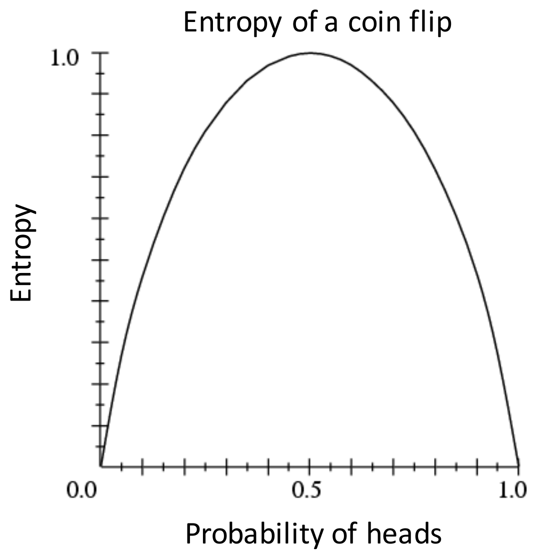


# High, Low Entropy

- "High Entropy"
  - Y is from a uniform like distribution
  - Flat histogram
  - Values sampled from it are less predictable
- "Low Entropy"
  - Y is from a varied (peaks and valleys) distribution
  - Histogram has many lows and highs
  - Values sampled from it are more predictable

(Slide from Vibhav Gogate)

# 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

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

$= 0.65$

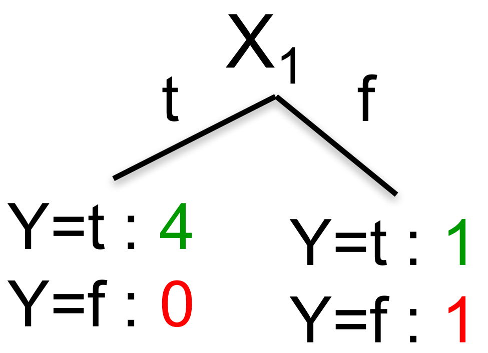
| $X_1$ | $X_2$ | Y |
|---|---|---|
| T | T | T |
| T | F | T |
| T | T | T |
| T | F | T |
| F | T | T |
| F | F | F |

# 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:




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

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

| $X_1$ | $X_2$ | $Y$ |
|---|---|---|
| T | T | T |
| T | F | T |
| T | T | T |
| T | F | T |
| F | T | T |
| F | F | F |

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

# Information gain

- Decrease in entropy (uncertainty) after splitting

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

In our running example:

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

$IG(X_1) > 0$ → 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

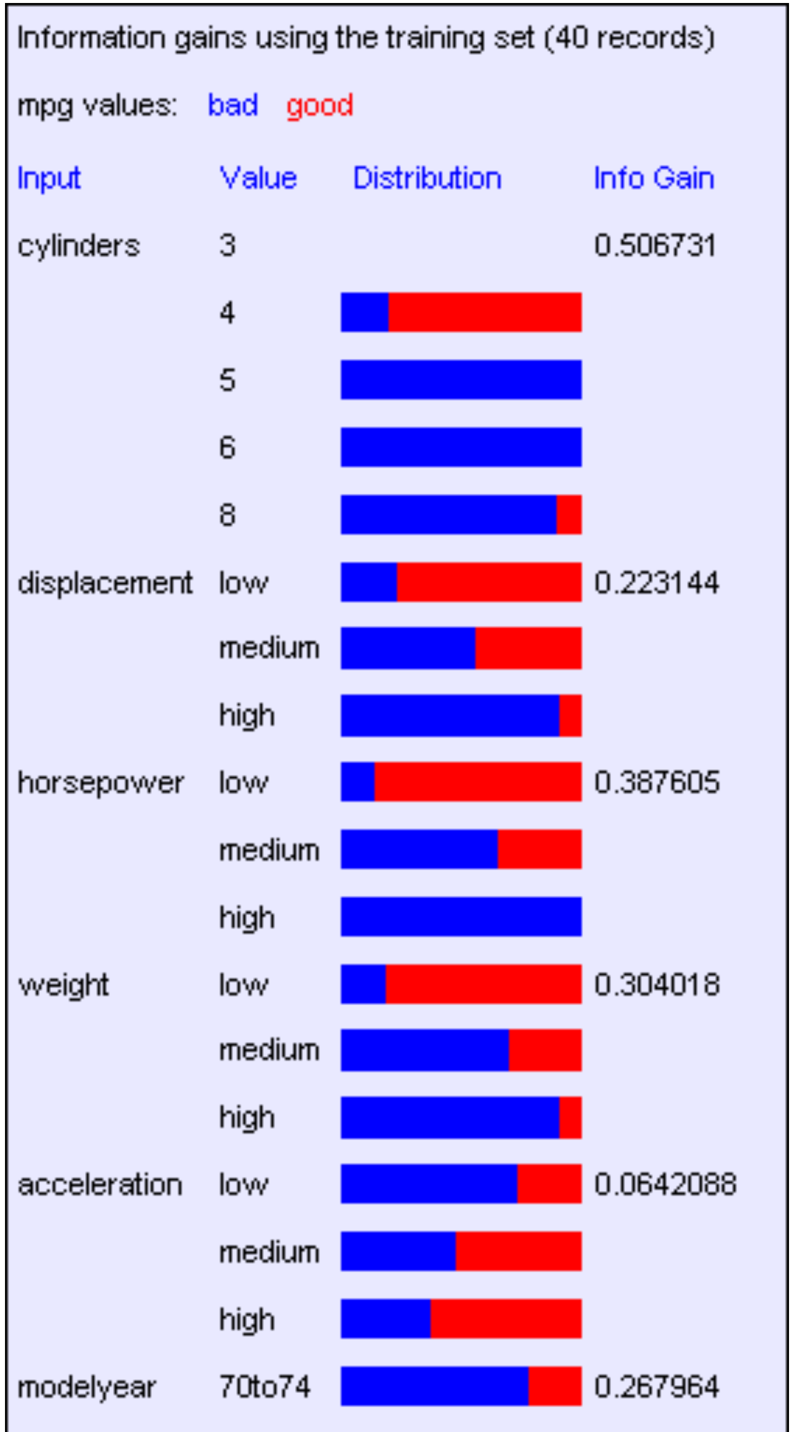
- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

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

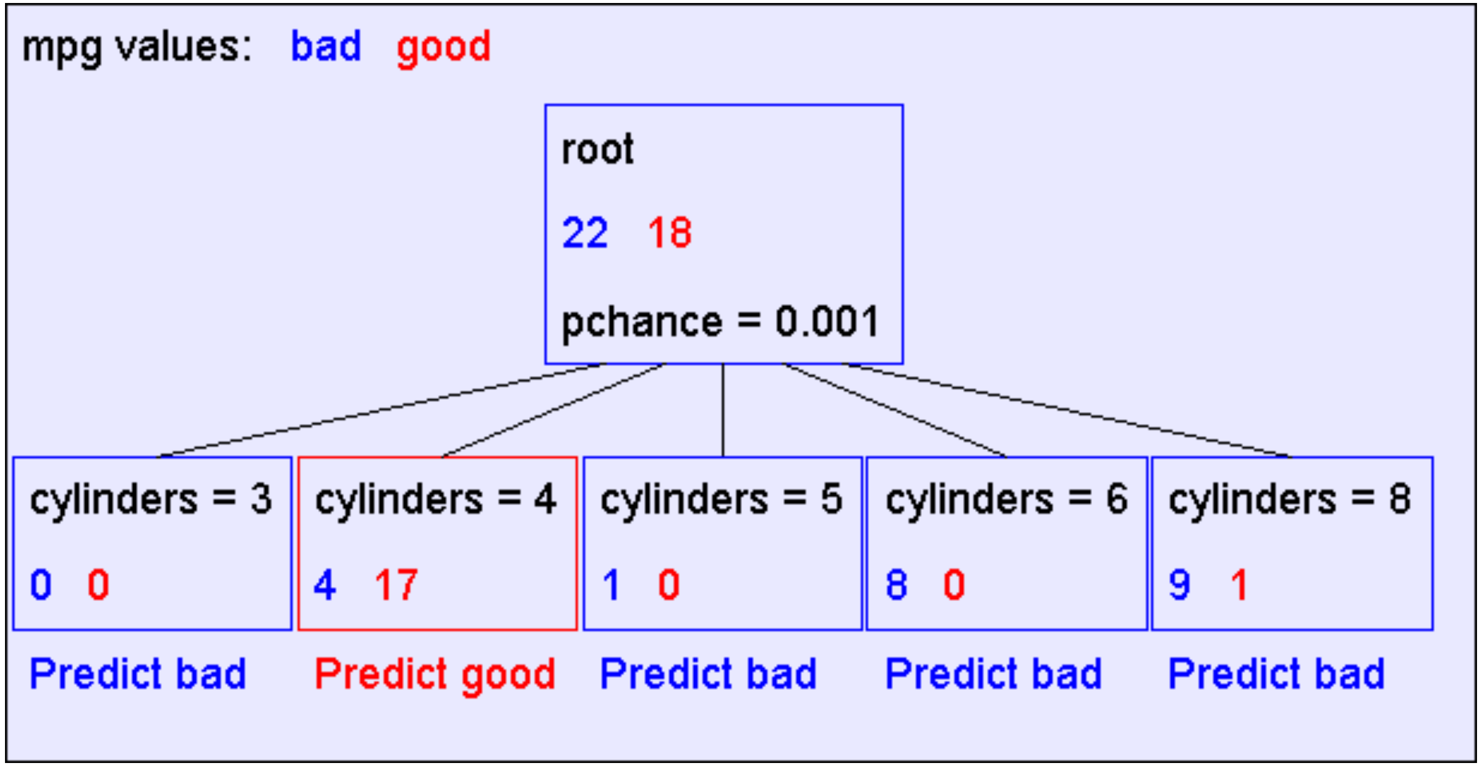
- Recurs

Suppose we want
to predict MPG

Look at all the
information
gains…

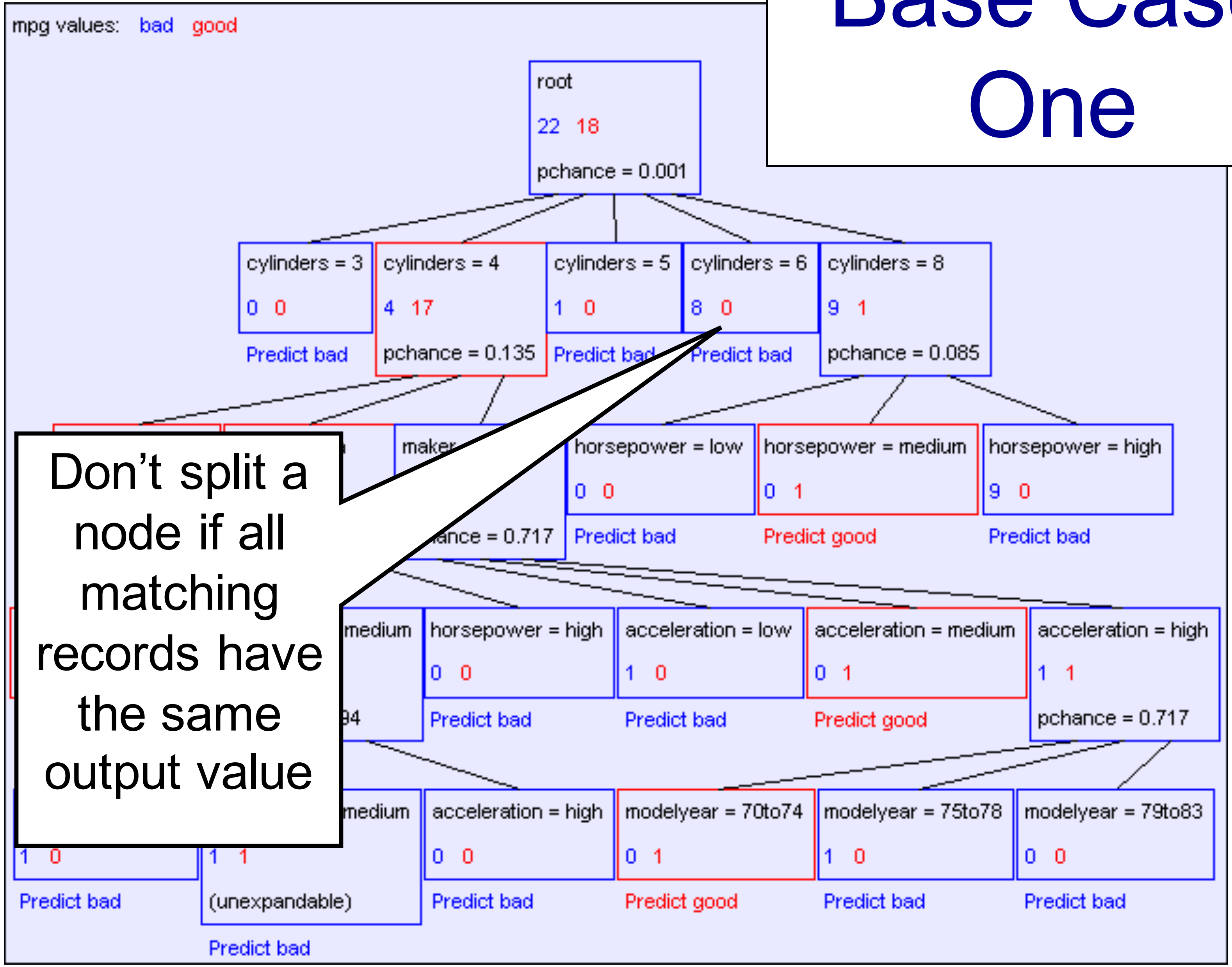


# When to stop?



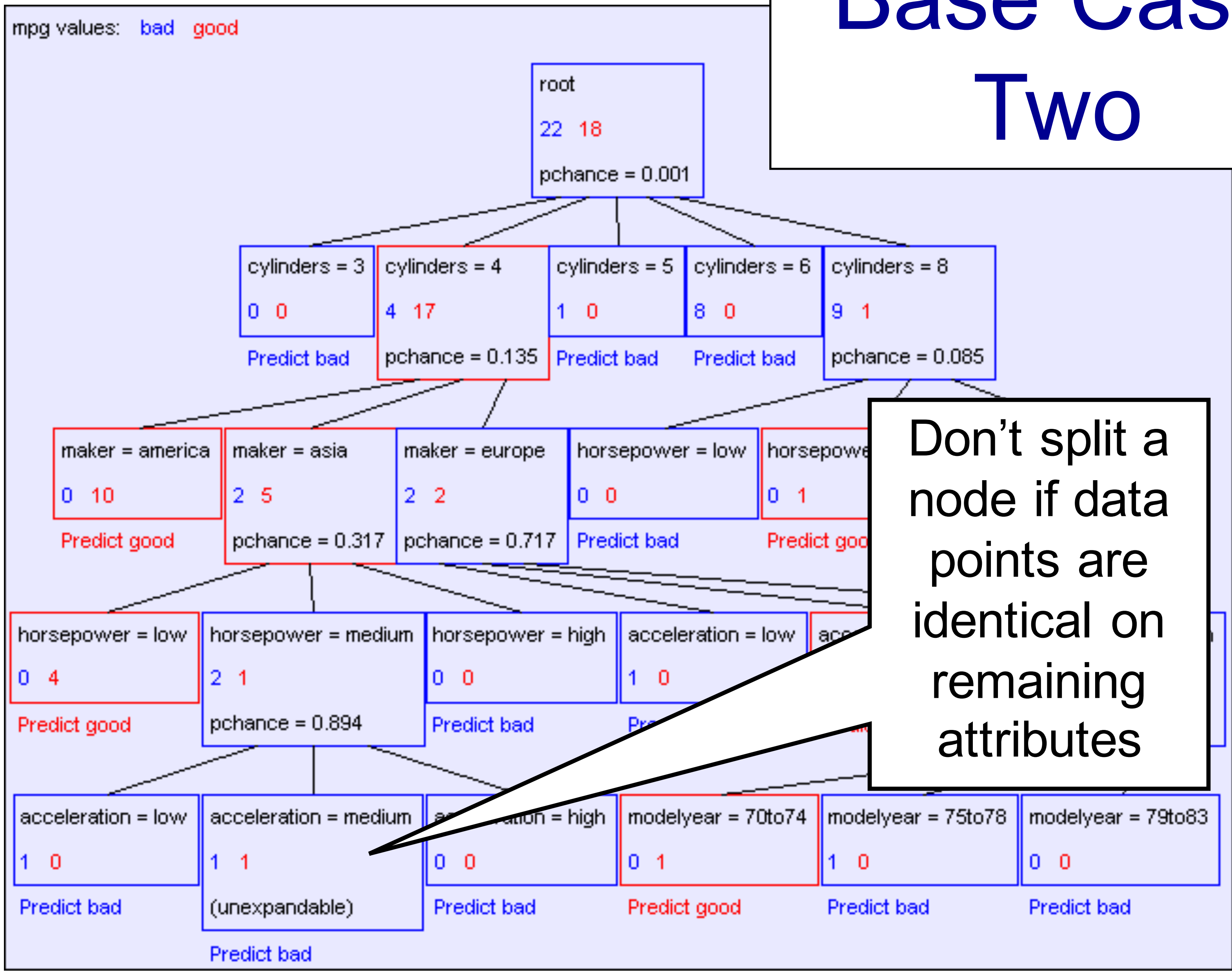

First split looks good! But, when do we stop?

# Base Case One




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

# Base Case Two



# Base Cases: An idea

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

Proposed Base Case 3:
If all attributes have small
information gain then don’t recurs

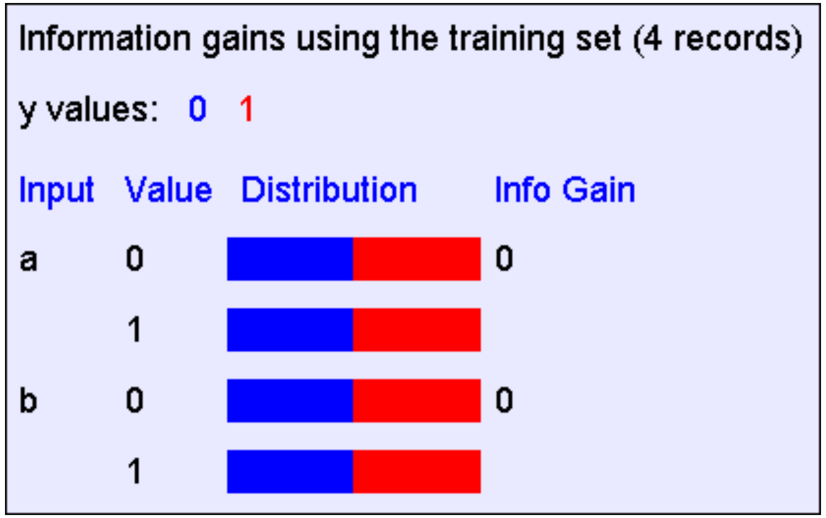
- *This is not a good idea*

# The problem with proposed 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:



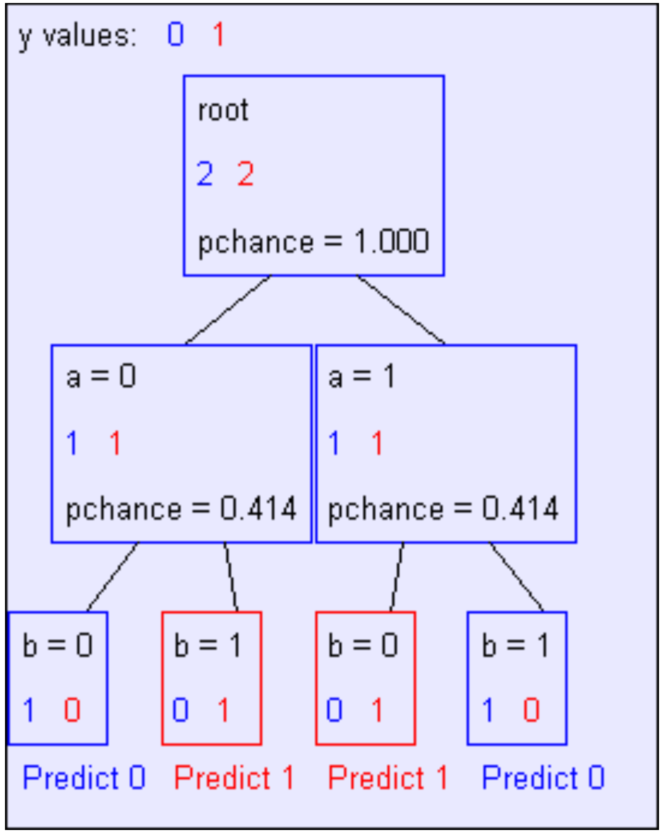
# If we omit proposed case 3:

y = a XOR b

| a | b | y |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

Instead, perform **pruning** after building a tree

The resulting decision tree:



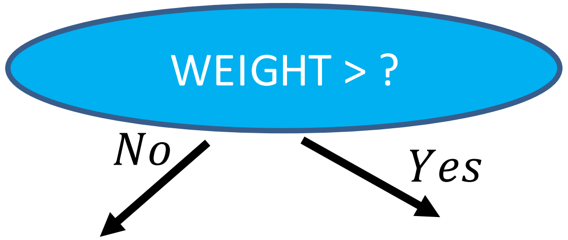
# Non-Boolean Features

- Real-valued features?

# Real-> threshold

- Number of thresholds <= # of different values in dataset

- Can choose threshold based on information gain



# Summary: Building Decision Trees

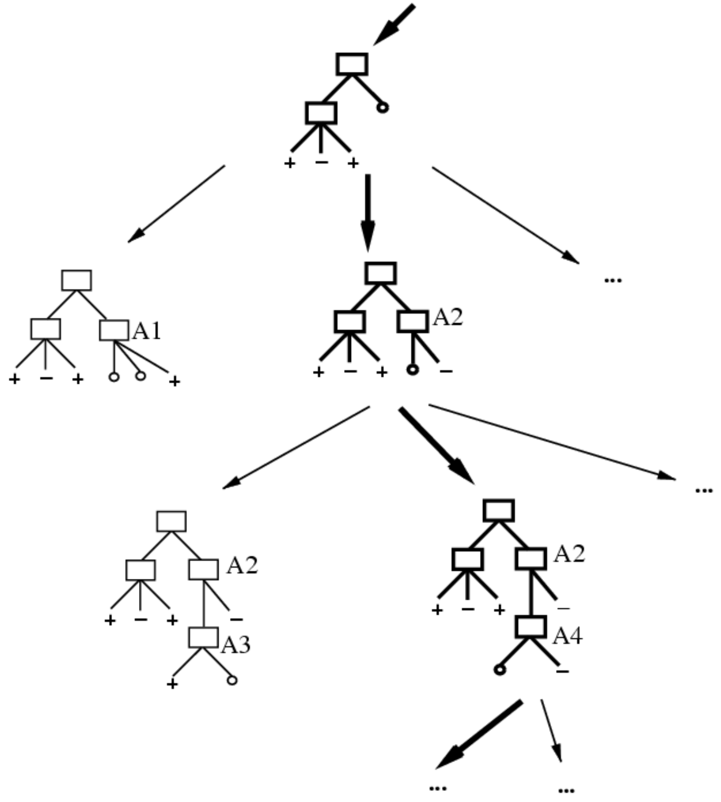
BuildTree(*DataSet*,*Output*)

- 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*)

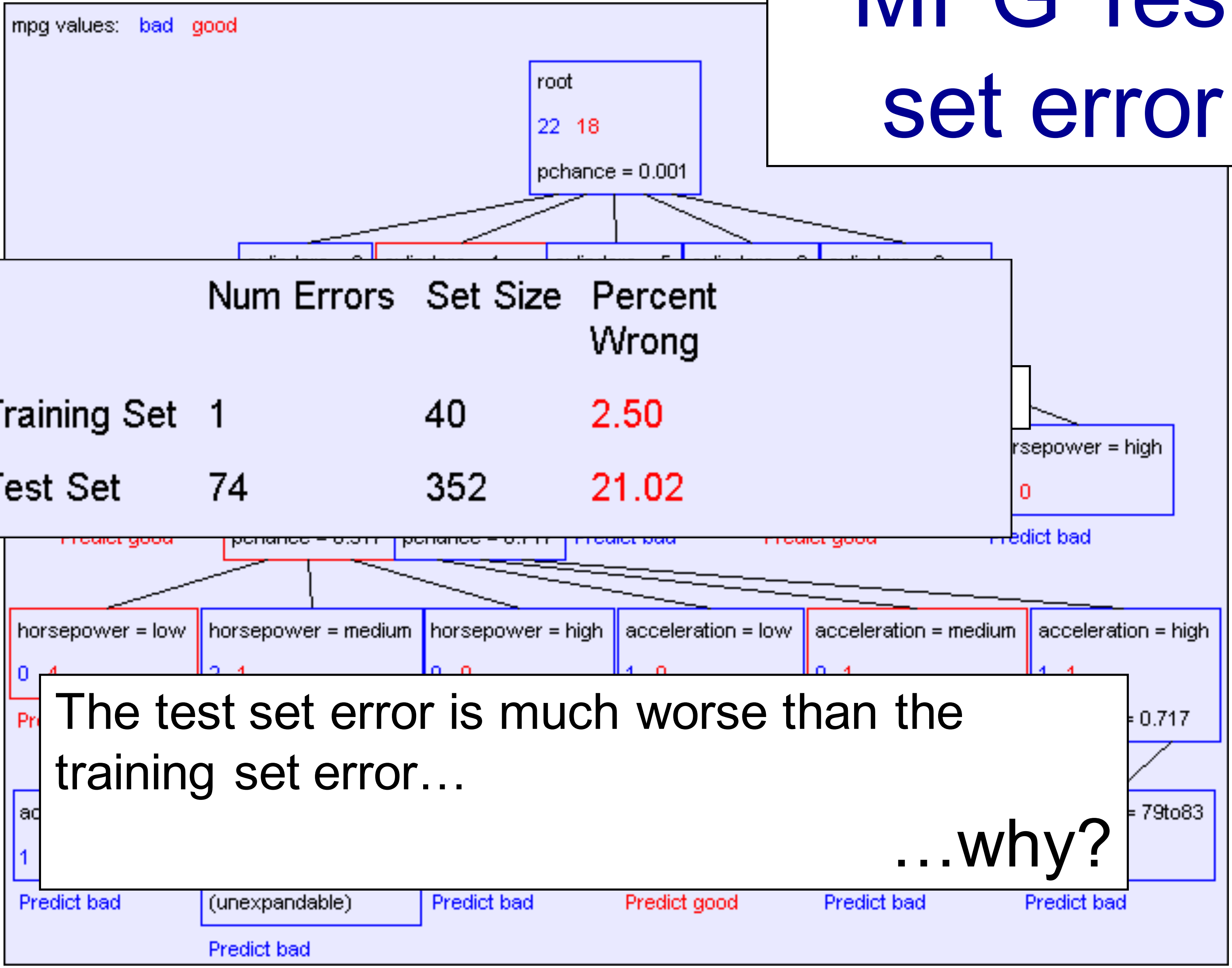
    Where $DS_i$ contains the records in DataSet where X = *i*th value of X.

# Machine Space Search




- ID3 / C4.5 / CART search for a succinct tree that perfectly fits the data.
- They are not going to find it in general (NP-hard)
- Entropy-guided splitting – well-performing heuristic. Exists others.
- Why should we search for a small tree at all?

# MPG Test set error

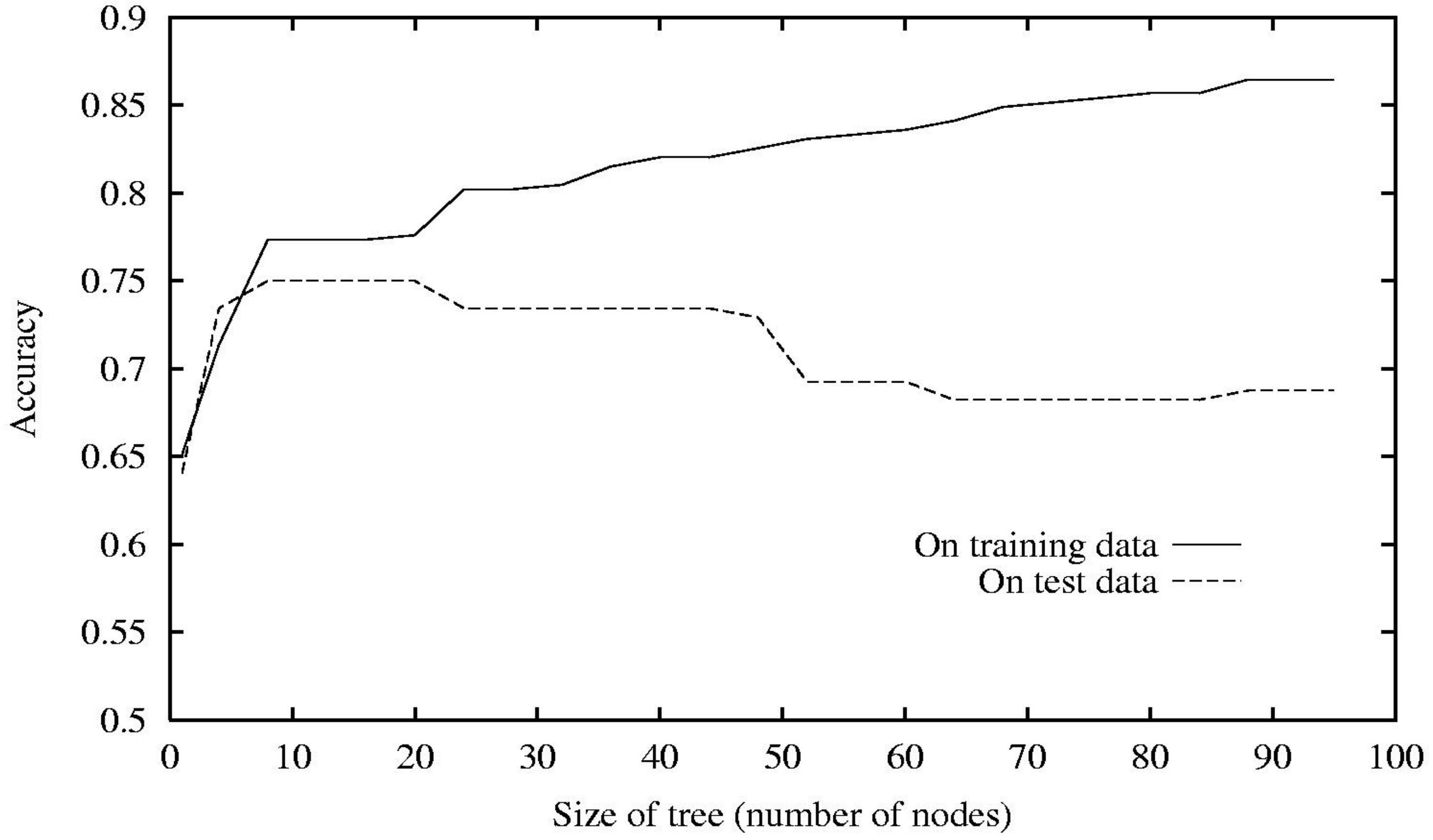



| | Num Errors | Set Size | Percent Wrong |
|---|---|---|---|
| Training Set | 1 | 40 | 2.50 |
| Test Set | 74 | 352 | 21.02 |

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

…why?

# Decision trees will overfit



# Fitting a polynomial

$$t = \sin(2\pi x) + \epsilon$$

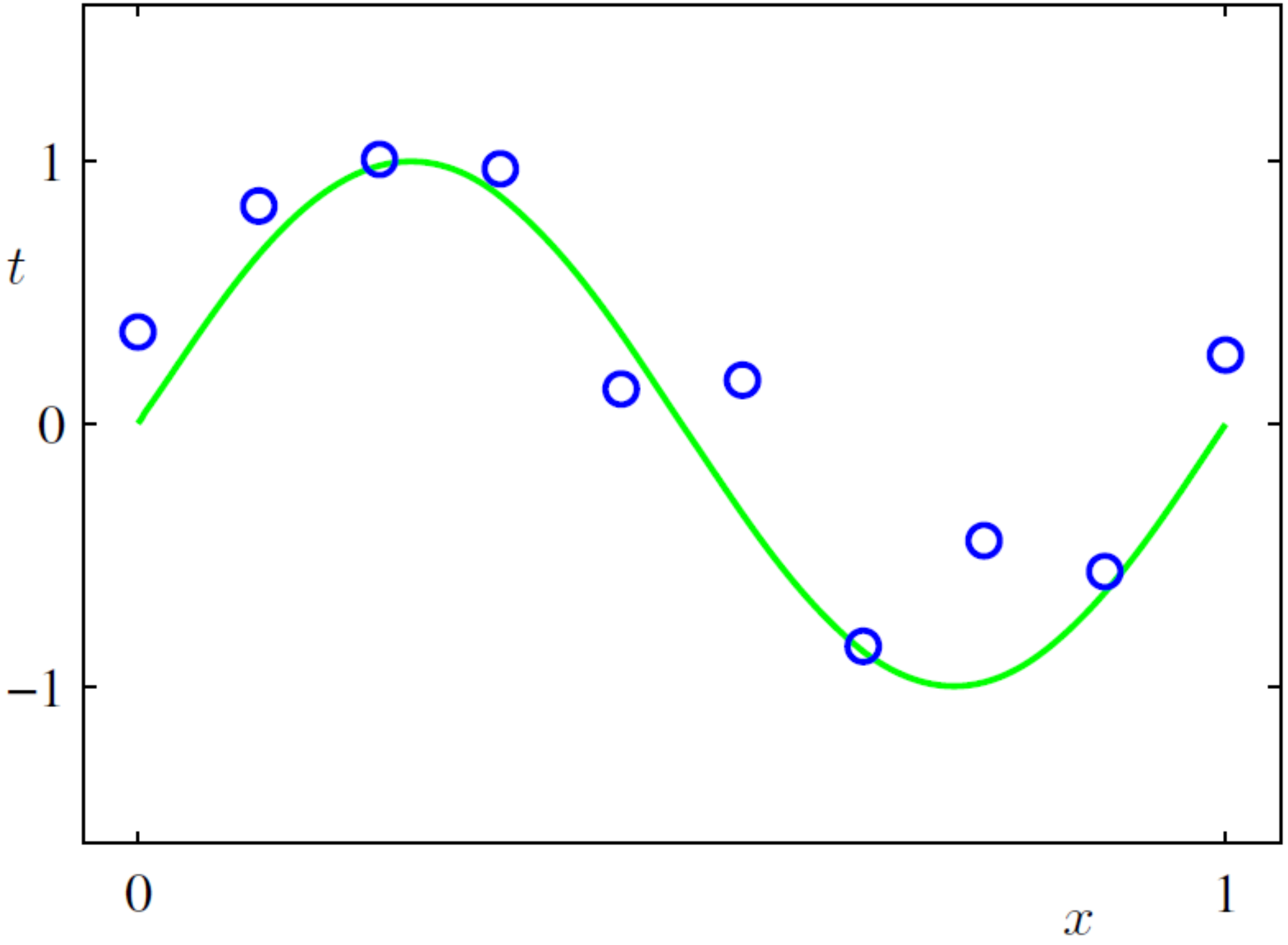
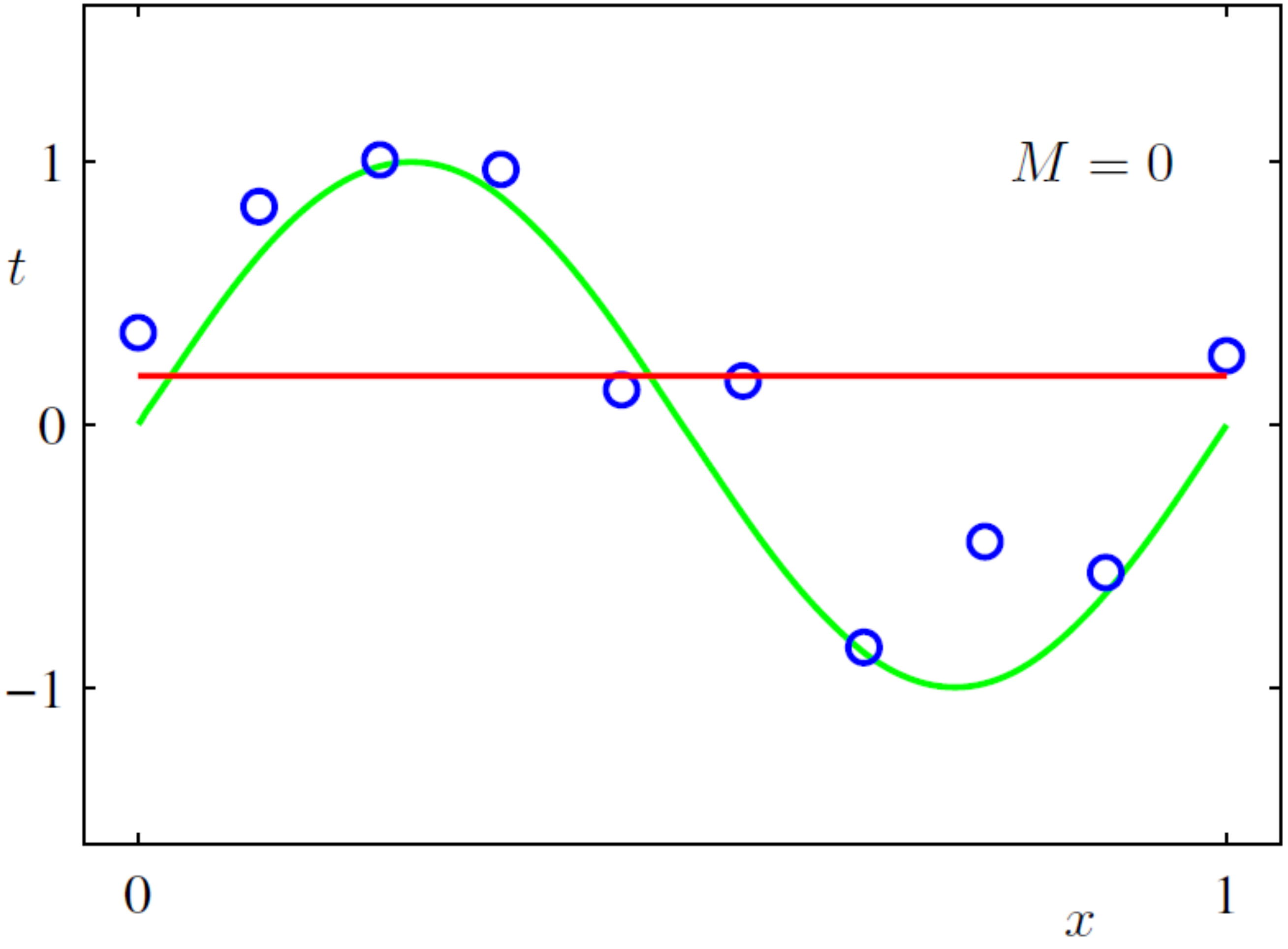



Figure from *Machine Learning and Pattern Recognition*, Bishop

# Fitting a polynomial

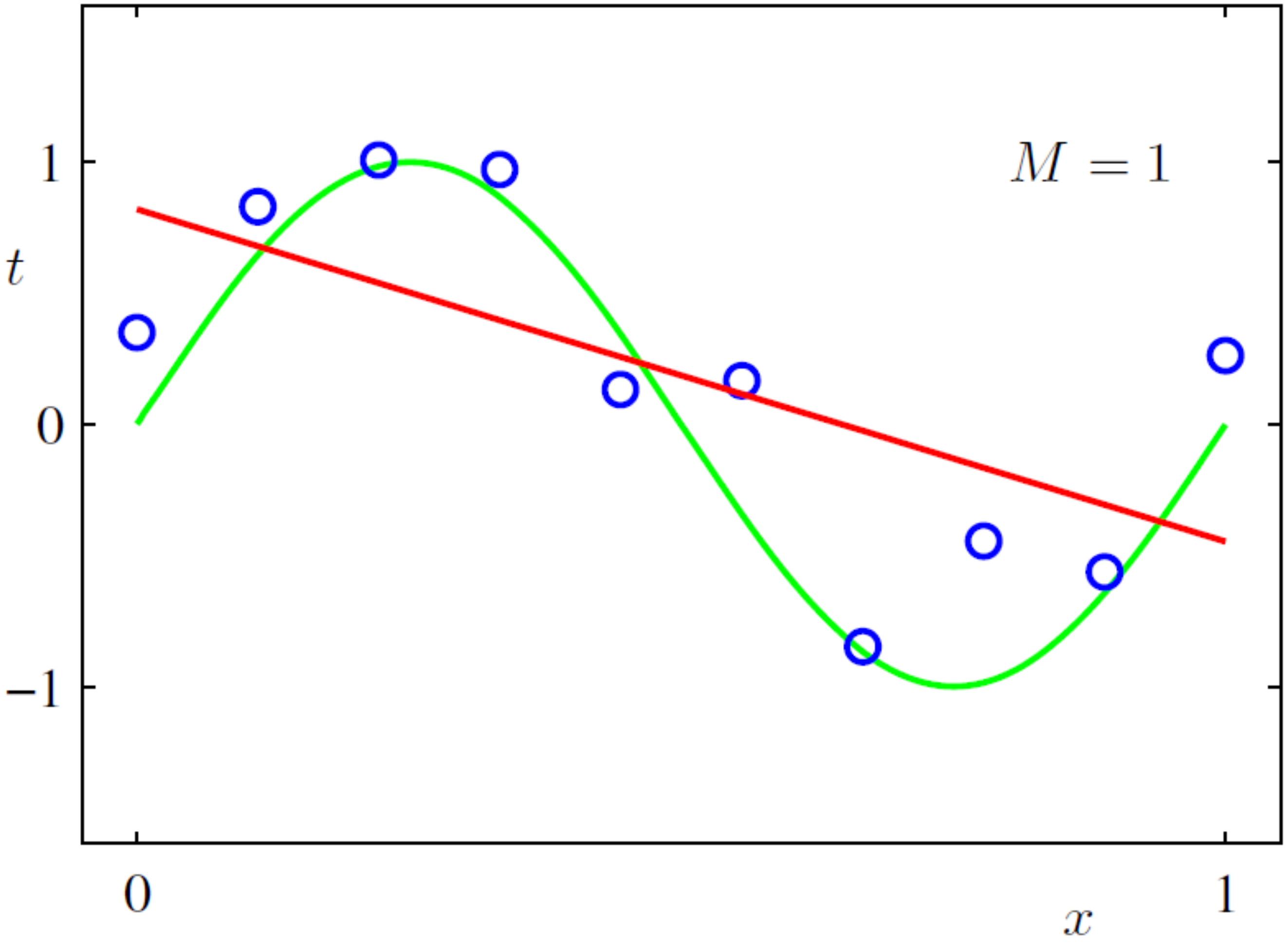
$$t = \sin(2\pi x) + \epsilon$$




Regression using polynomial of degree *M*

Figure from *Machine Learning and Pattern Recognition*, Bishop

$$t = \sin(2\pi x) + \epsilon$$

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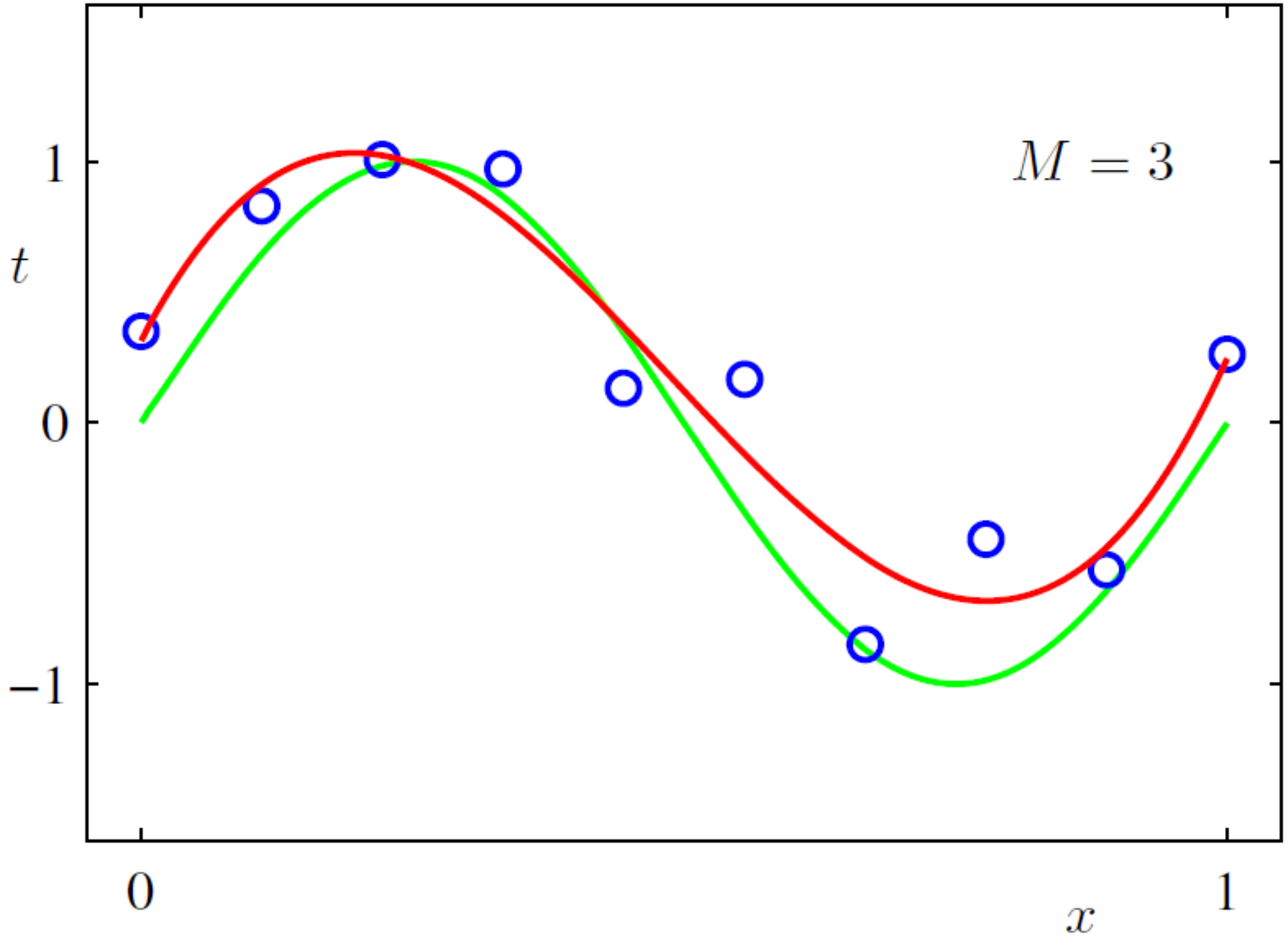


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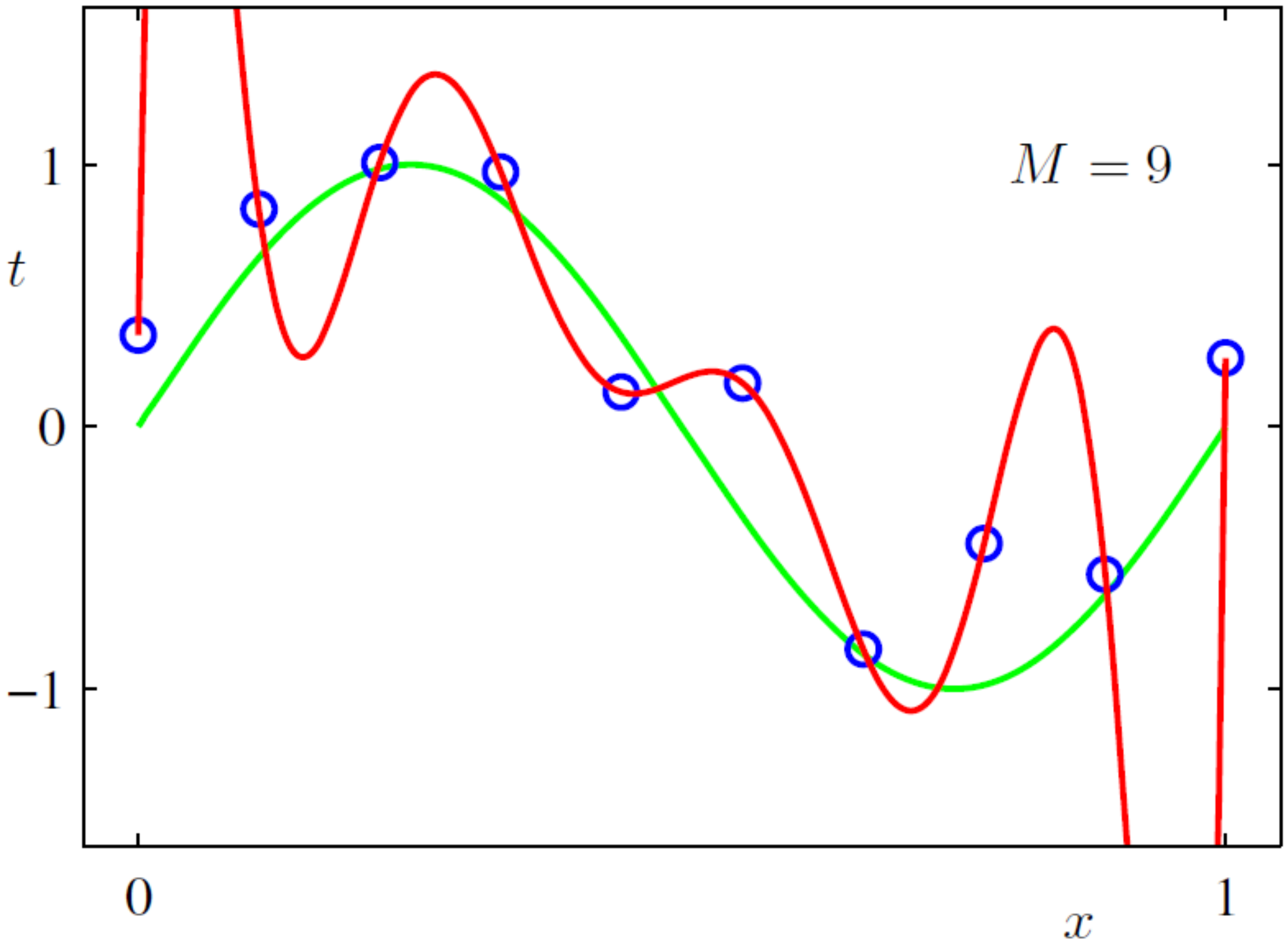


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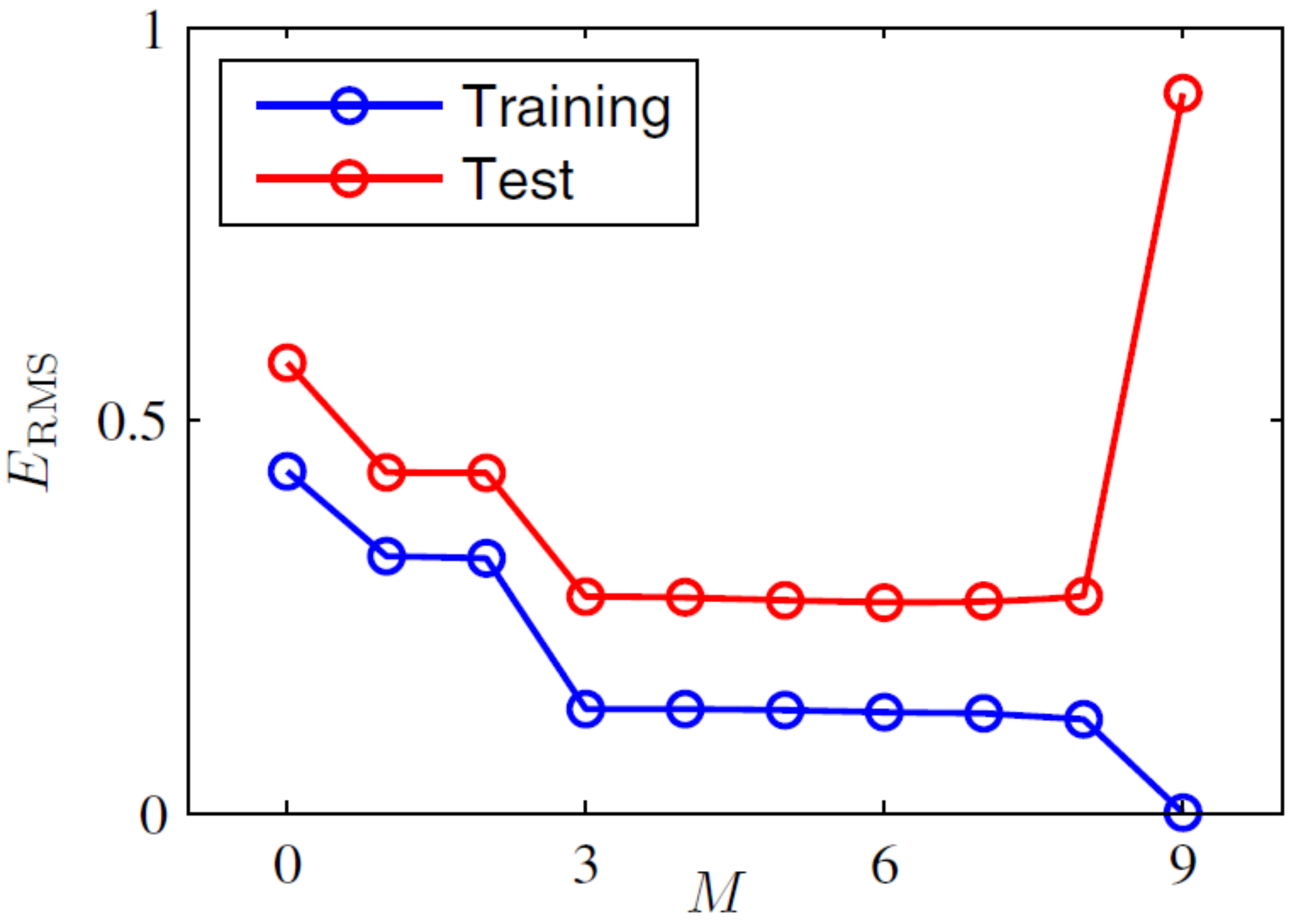


Figure from *Machine Learning and Pattern Recognition*, Bishop

# Overfitting

- Precise characterization – statistical learning theory
- Special technics to prevent overfitting in DT learning
  - Pruning the tree, e.g. “reduced error” pruning:
    Do until further pruning is harmful:
    1. Evaluate the impact on validation (test) set of the data of pruning each possible node (and it’s subtree)
    2. Greedily remove one that most improves validation (test) error

# Concepts we have encountered (and will appear again in the course!)

- Greedy algorithm.
- Trying to find succinct machines.
- Computational efficiency of an algorithm (running time).
- Overfitting.

# Questions

- Why are smaller trees (theory) preferable to large trees (theory)?
- When can a tree generalize to unseen examples, and how well?
- How many examples are needed to build a tree that generalizes well?
- How to identify and prevent overfitting?
- Are there other natural classification machines and how do they compare?

Need to reason more generally about “what learning means”, TBC on Thu…