Data Management for Data Science

Lecture 16: Intro to ML and Decision Trees

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Today's Lecture

1. Intro to Machine Learning

2. Types of Machine Learning

3. Decision Trees

1. Intro to Machine Learning

What is Machine Learning?

- "Learning is any process by which a system improves performance from experience" – Herbert Simon

- Definition by Tom Mitchell (1998):

Machine Learning is the study of algorithms that

- Improve their performance *P*
- at some task *T*
- with experience *E*

  A well-defined learning task is given by *<P, T, E>*.

What is Machine Learning?

Machine Learning is the study of algorithms that

- Improve their performance P
- at some task T
- with experience E

A well-defined learning task is given by *<P, T, E>.*

Experience: data-driven task, thus statistics, probability

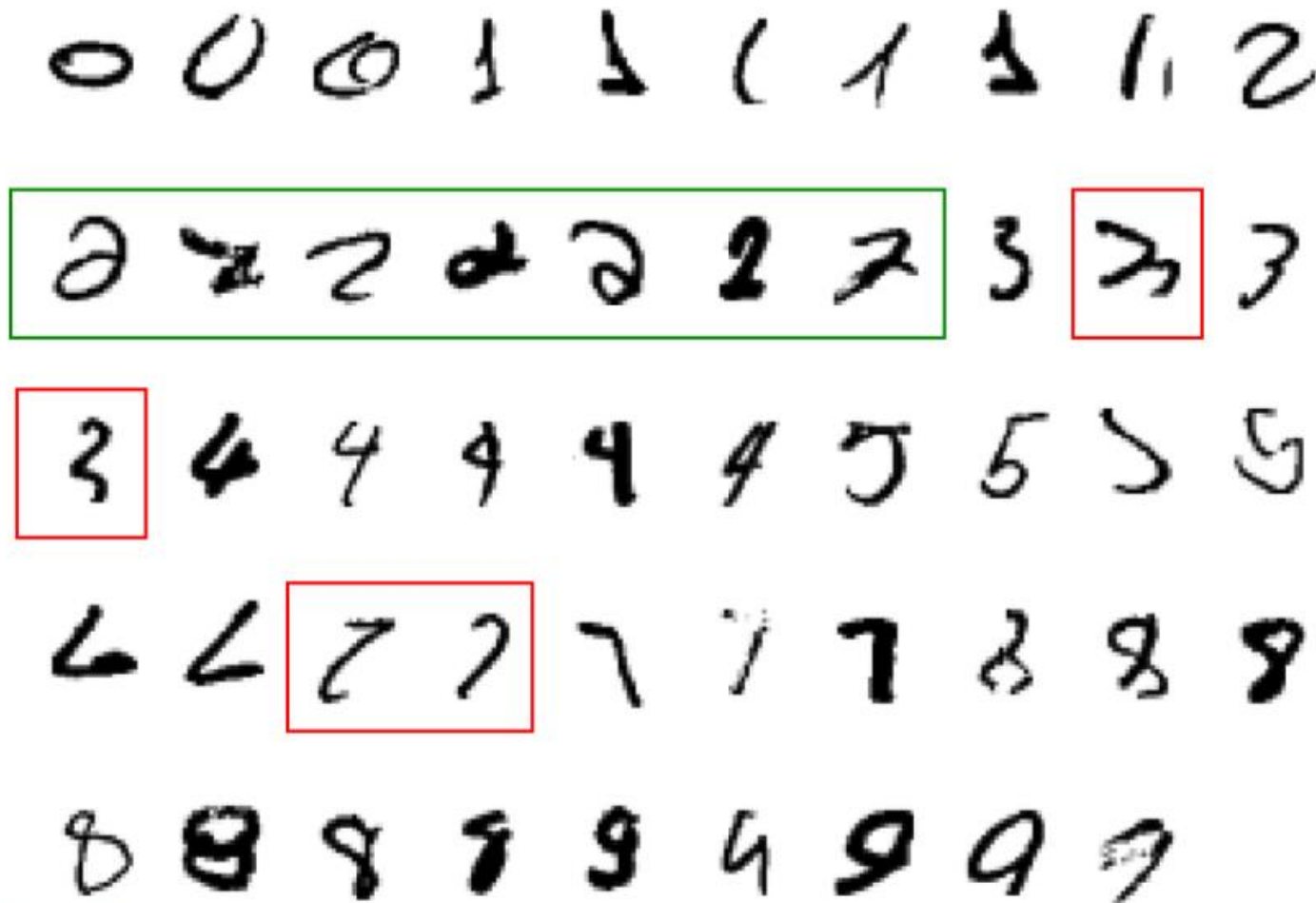**Example:** use height and weight to predict gender

When do we use machine learning?

ML is used when:

- Human expertise does not exist (navigating on Mars)
- Humans can't explain their expertise (speech recognition)
- Models must be customized (personalized medicine)
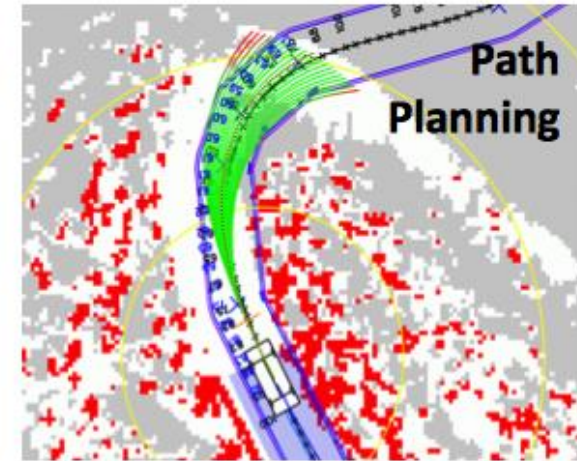- Models are based on huge amounts of data (genomics)
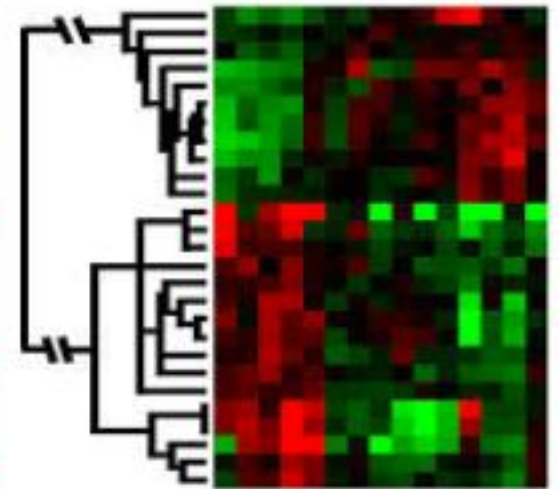
A task that requires machine learning

What makes a hand drawing be 2?

Slide credit: Geoffrey Hinton

Modern machine learning: Autonomous cars

Modern machine learning: Scene Labeling
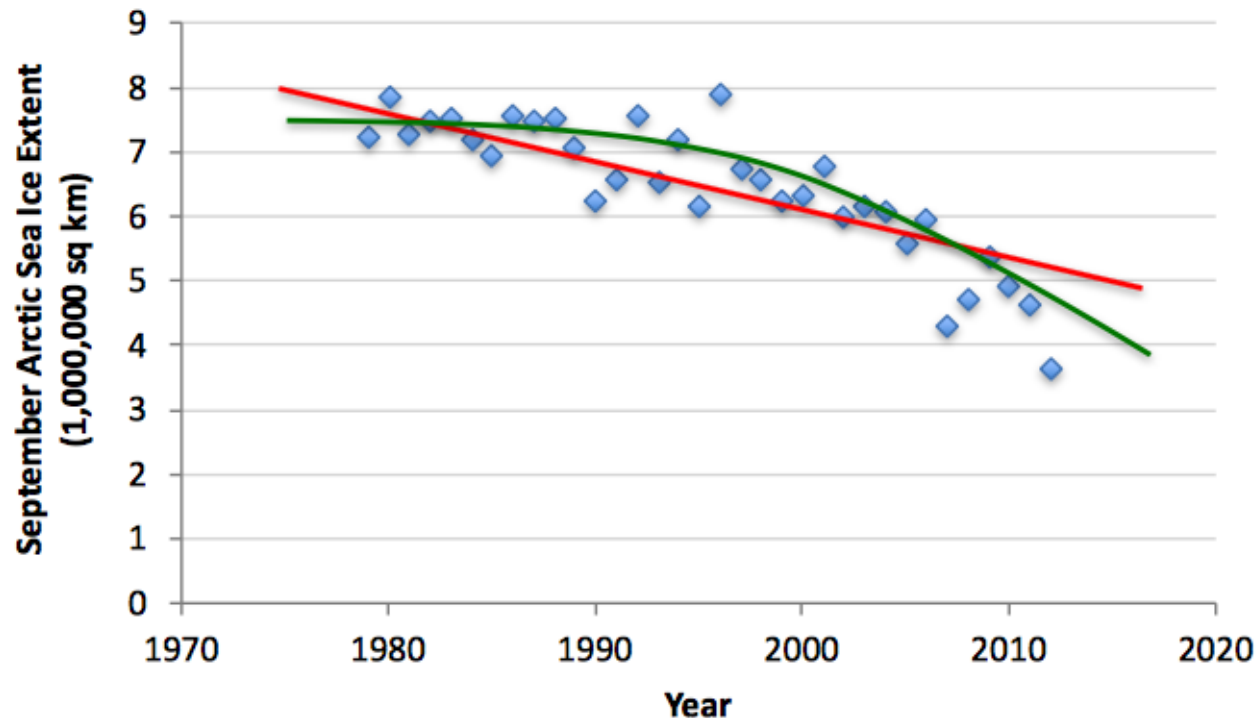
Modern machine learning: Speech Recognition

2. Types of Machine Learning

Types of Learning

- Supervised (inductive) learning
  - Given: training data + desired outputs (labels)

- Unsupervised learning
  - Given: training data (without desired outputs)

- Semi-supervised learning
  - Given: training data + a few desired outputs

- Reinforcement learning
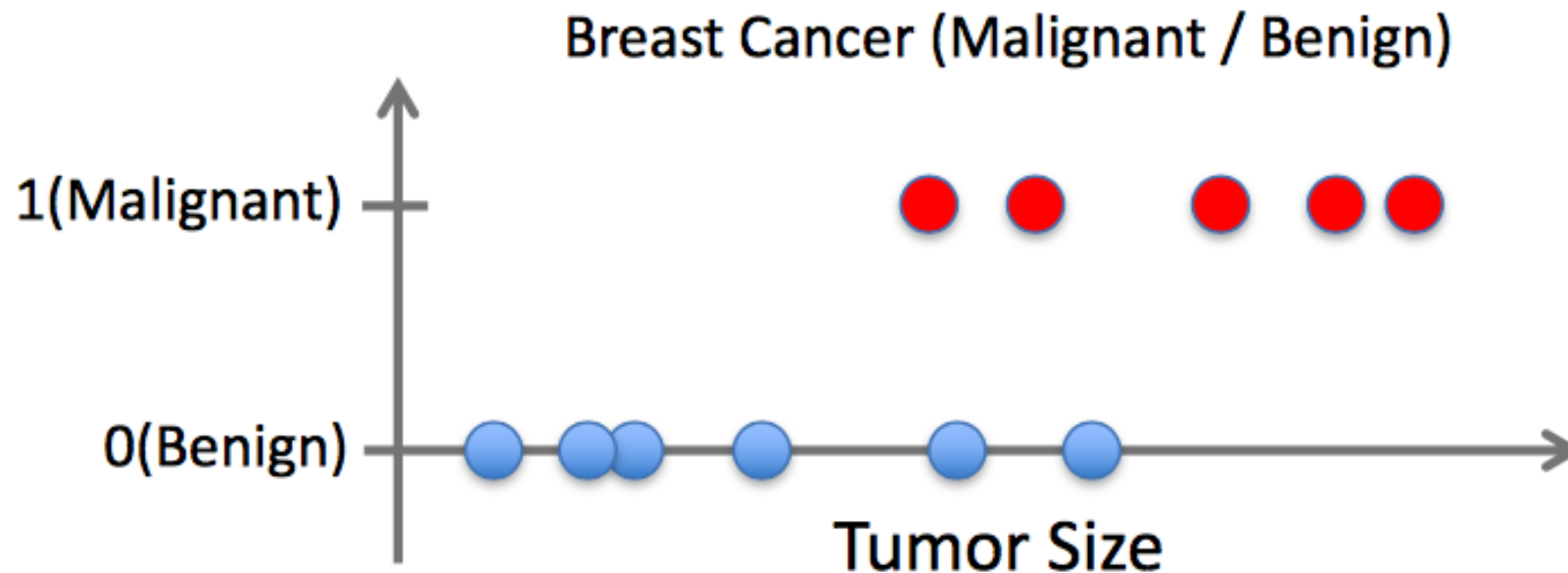 - Rewards from sequence of actions

Supervised Learning: Regression

- Given $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$
- Learn a function *f(x)* to predict *y* given *x*
  - *y* is real-valued == regression

Supervised Learning: Classification

- Given $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$
- Learn a function $f(x)$ to predict y given x
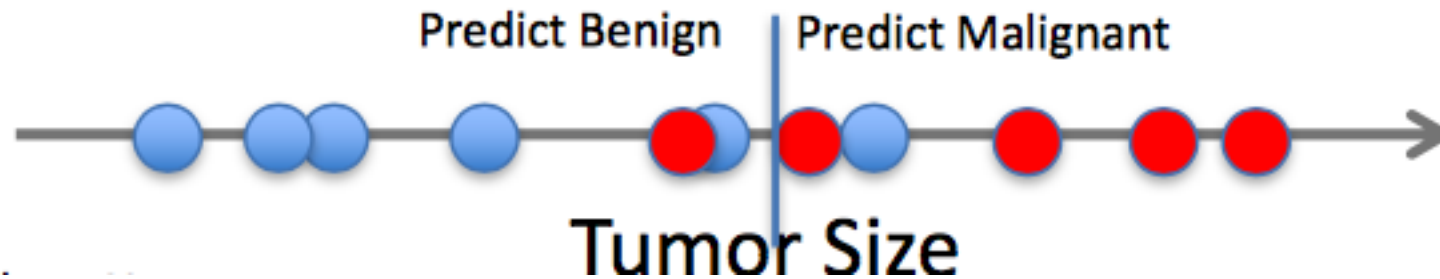 - y is categorical == regression

Breast Cancer (Malignant / Benign)

Supervised Learning: Classification
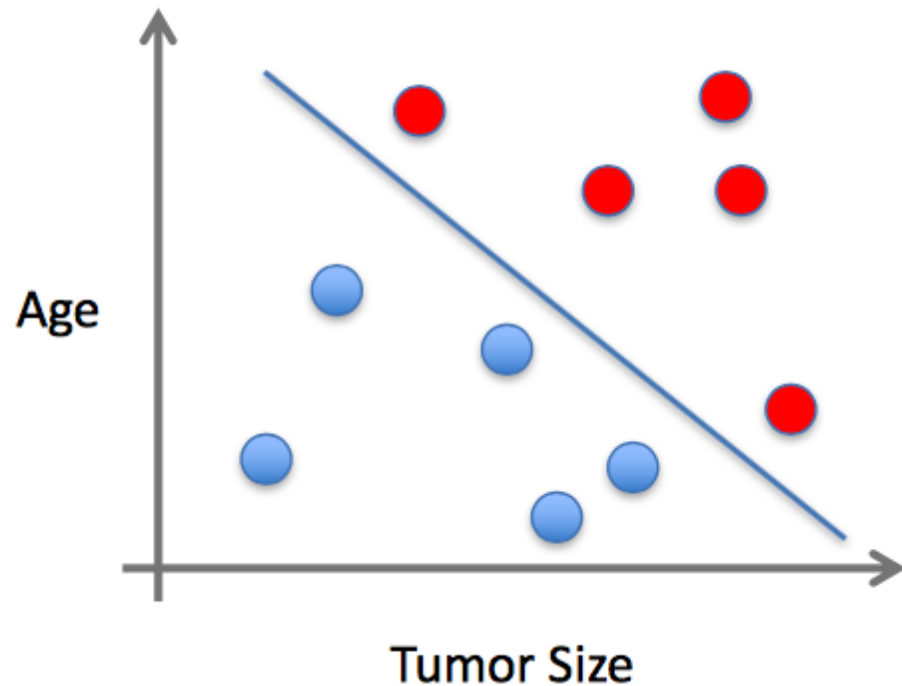
- Given $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$
- Learn a function $f(x)$ to predict y given x
  - y is categorical == regression

Predict Benign   Predict Malignant

Tumor Size

Supervised Learning

- Value *x* can be multi-dimensional.
    - Each dimension corresponds to an attribute

- Clump Thickness
- Uniformity of Cell Size
- Uniformity of Cell Shape

...

Types of Learning

- Supervised (inductive) learning
  - Given: training data + desired outputs (labels)

- Unsupervised learning
  - Given: training data (without desired outputs)

- Semi-supervised learning
  - Given: training data + a few desired outputs

- Reinforcement learning
  - Rewards from sequence of actions

We will cover later in the class

3. Decision Trees

A learning problem: predict 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
good	8	high	medium	high	high	79to83	america
bad	8	high	high	high	low	75to78	america
good	4	low	low	low	low	79to83	america
bad	6	medium	medium	medium	high	75to78	america
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 X

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
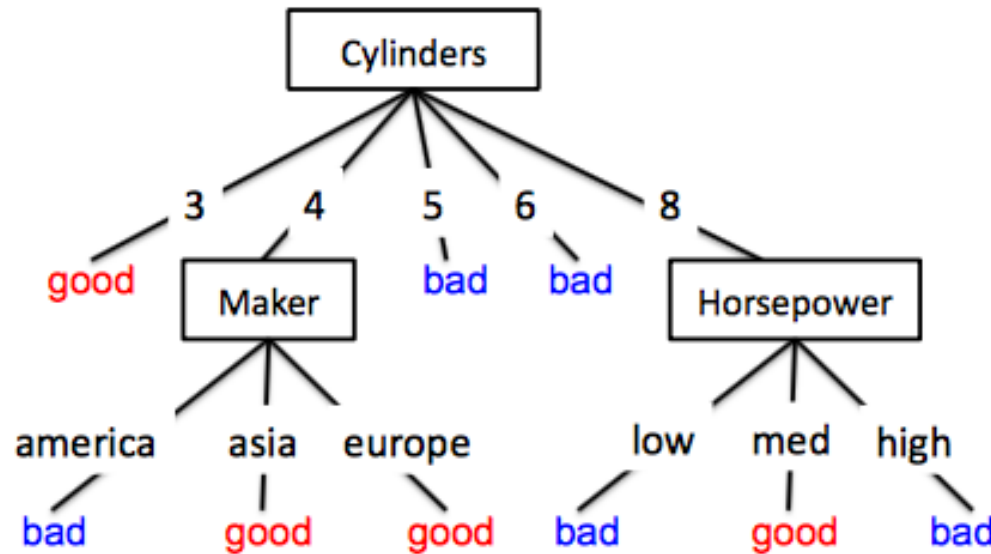

Human interpretable!

Informal
A hypothesis is a certain function that we believe (or hope) is similar to the true function, the *target function* that we want to model.

What functions can Decision Trees represent?

- Decision trees can represent any function of the input attributes!

- For Boolean functions, path to leaf gives truth table row

- But, could require exponentially many nodes...

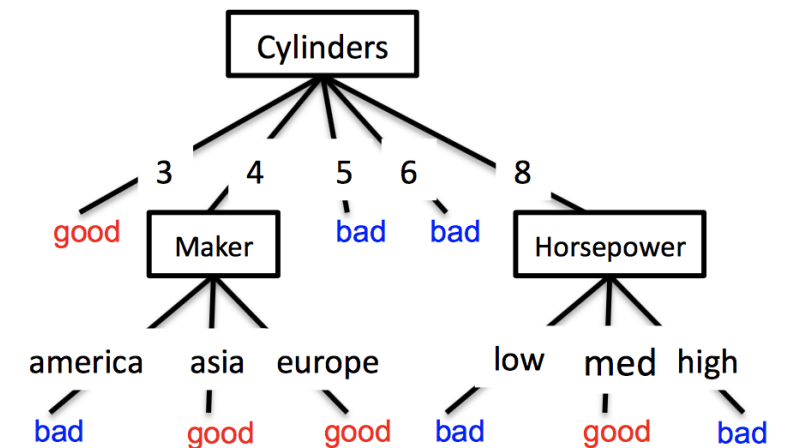| A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F
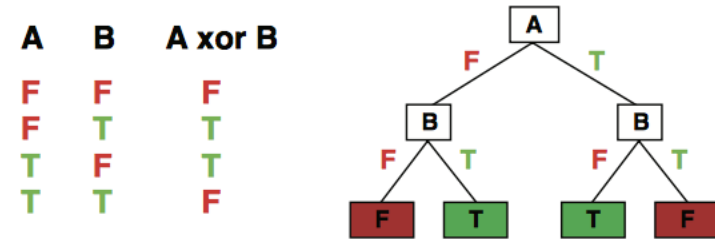
(Figure from Stuart Russell)
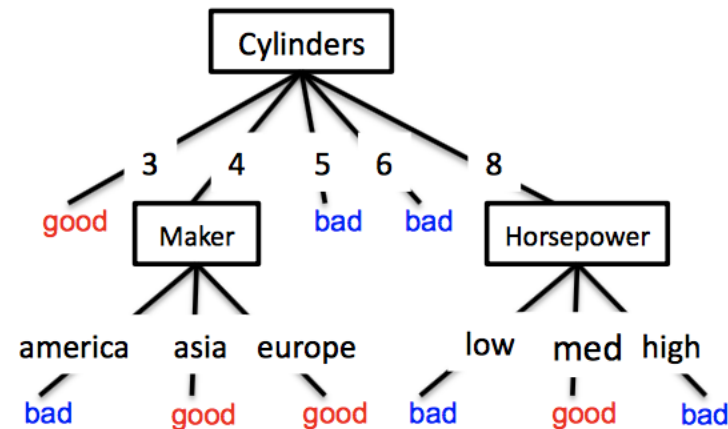
cyl=3 ∨ (cyl=4 ∧ (maker=asia ∨ maker=europe)) ∨ …

Space of possible decision trees

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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- How will we choose the best one?
- Lets first look at how to split nodes, then consider how to find the best tree
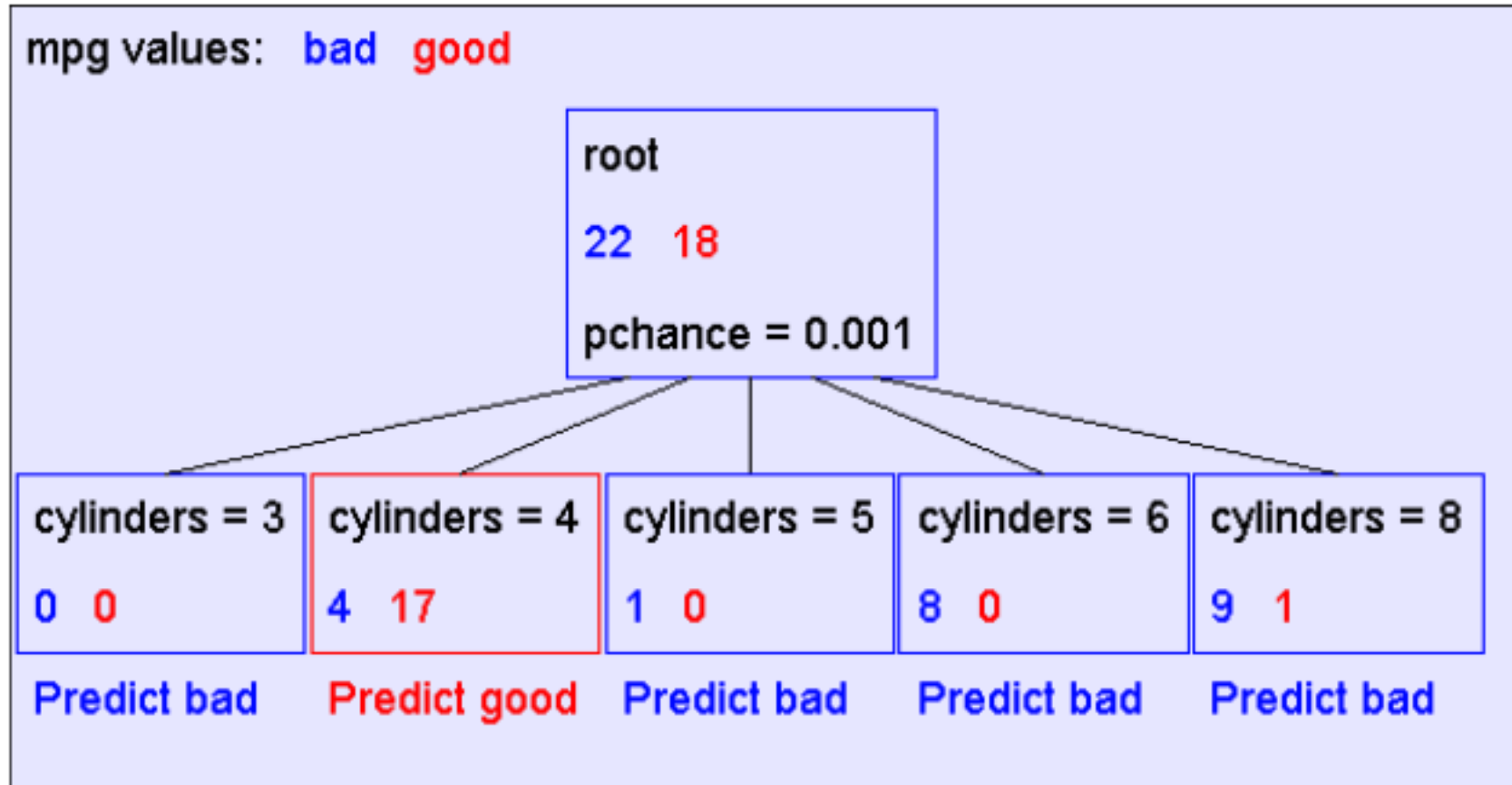
What is the simplest tree?

- Always predict mpg = bad
  - We just take the majority class

- Is this a good tree?
  - We need to evaluate its performance

- Performance: We are correct on 22 examples and incorrect on 18 examples
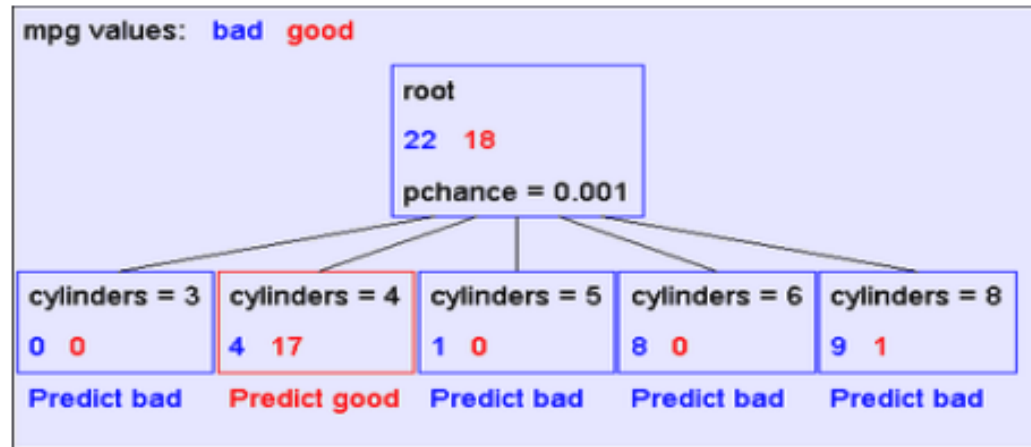
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
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bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
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:	:	:	:	:	:	:	:
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A decision stump

Recursive step
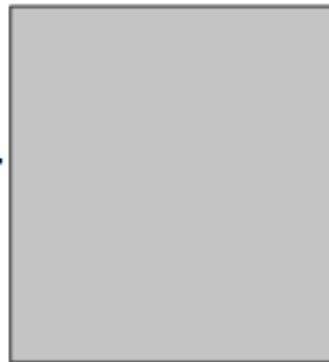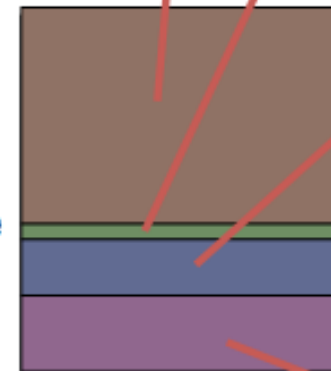
Recursive step

Second level of tree

mpg values: bad good

root
22 18
pchance = 0.001

cylinders = 3	cylinders = 4	cylinders = 5	cylinders = 6	cylinders = 8
0 0	4 17	1 0	8 0	9 1
Predict bad	pchance = 0.135	Predict bad	Predict bad	pchance = 0.085

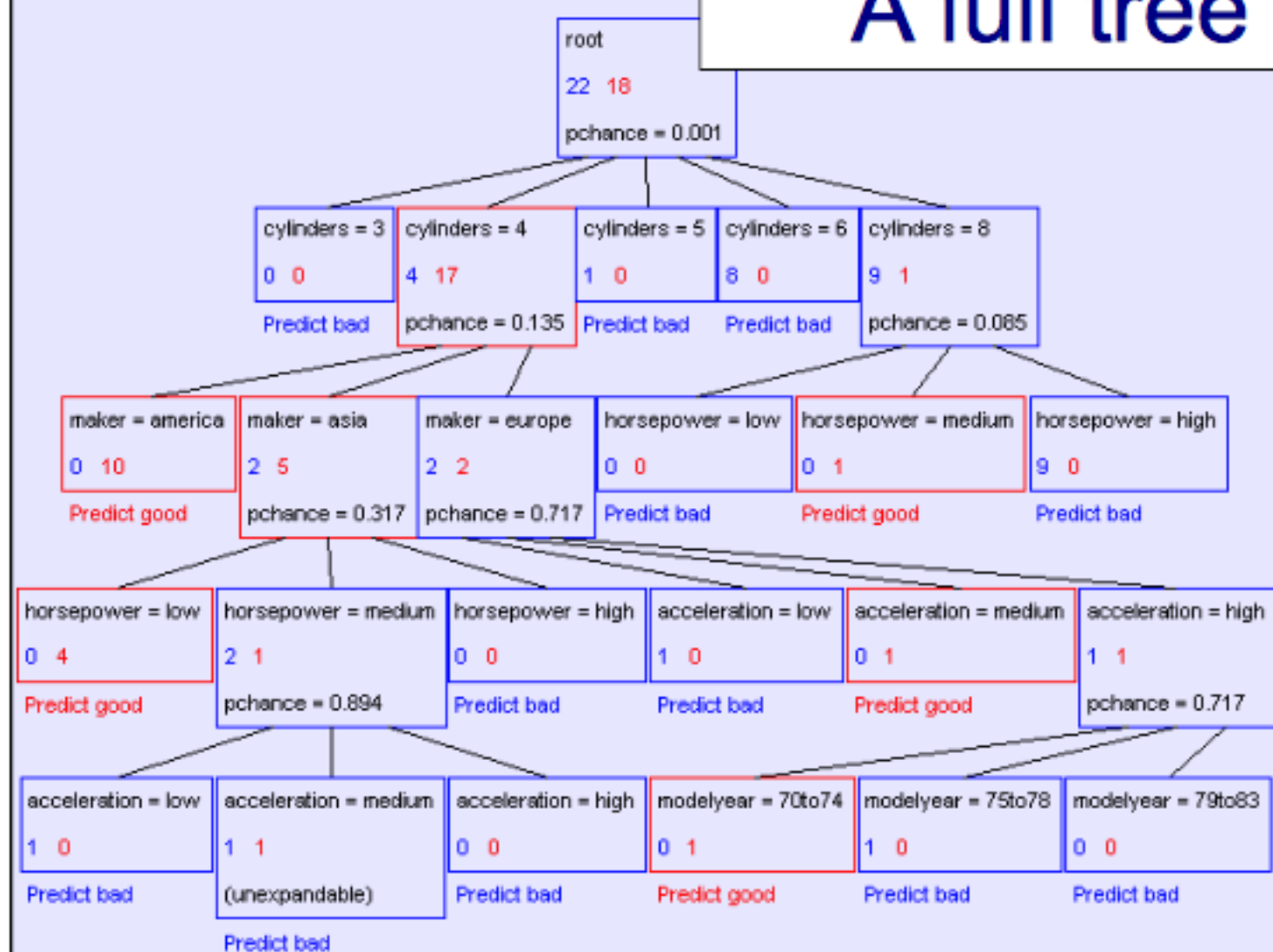| maker = america	maker = asia	maker = europe	horsepower = low	horsepower = medium	horsepower = high
0 10	2 5	2 2	0 0	0 1	9 0
Predict good	Predict good	Predict bad	Predict bad	Predict good	Predict bad
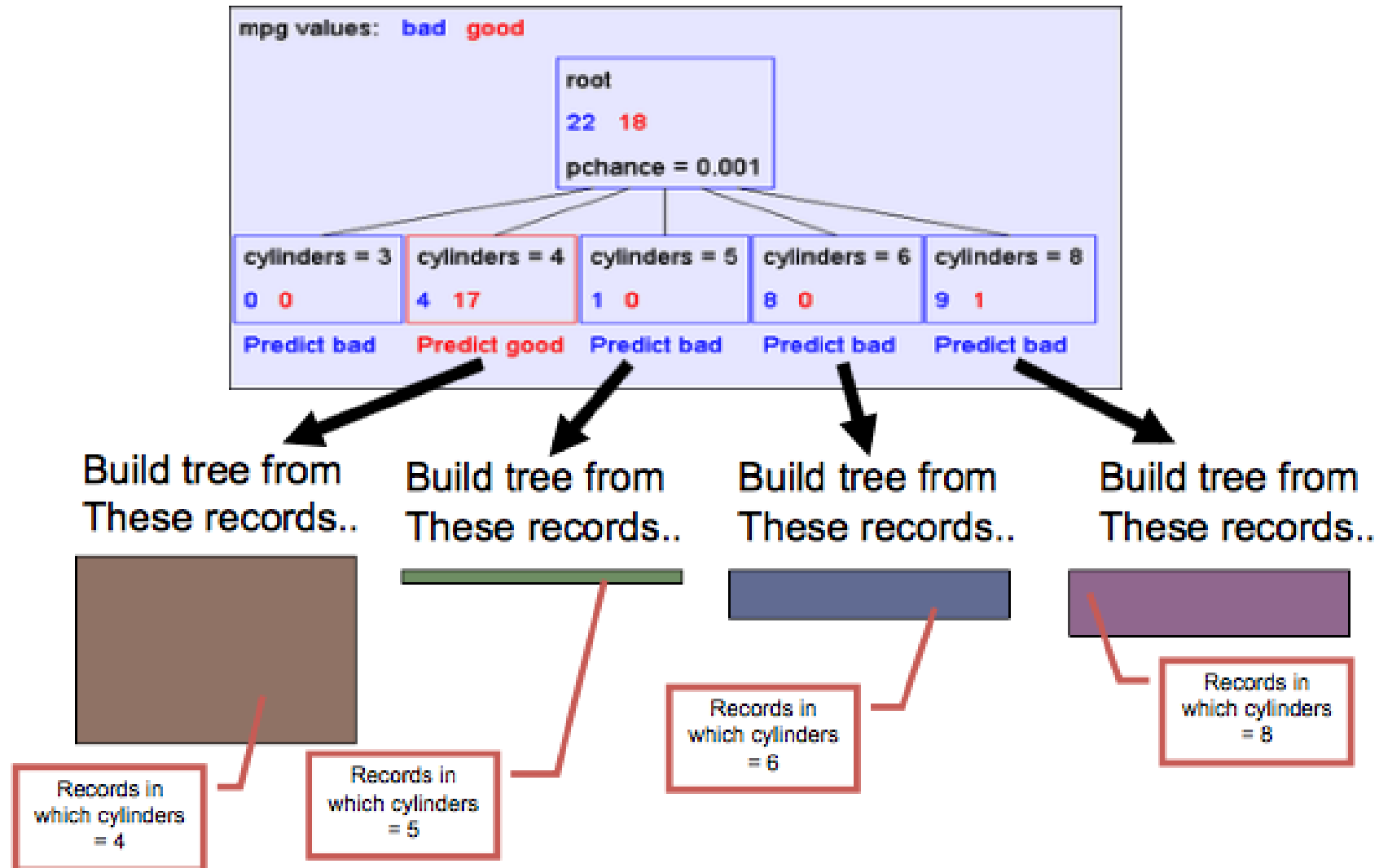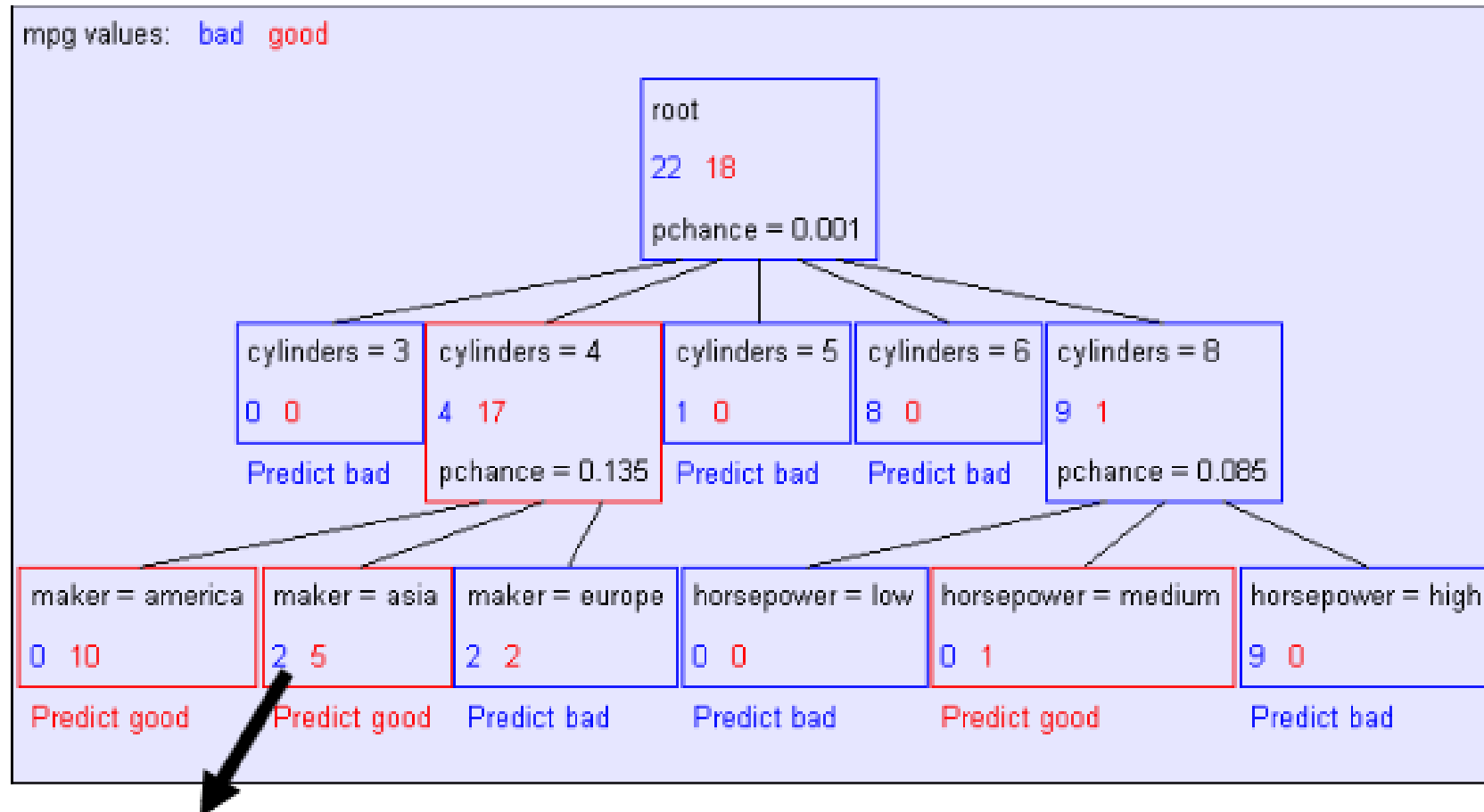
Recursively build a tree from the seven records in which there are four cylinders and the maker was based in Asia
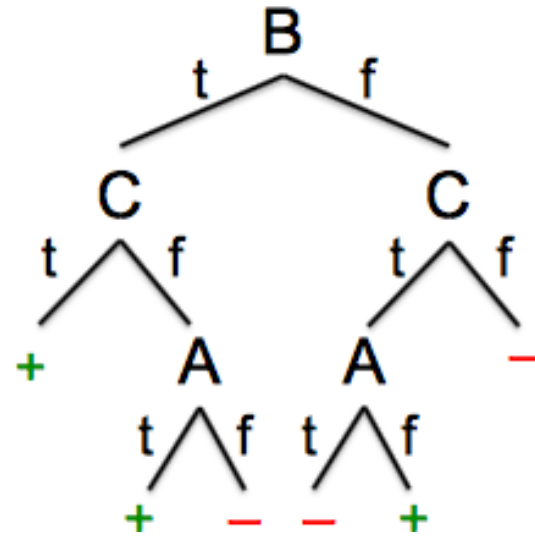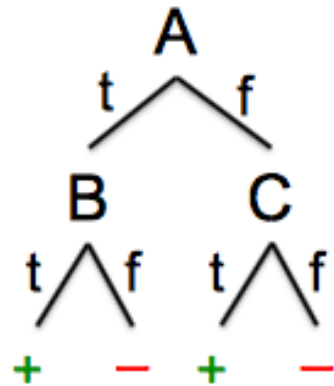
(Similar recursion in the other cases)

Are all decision trees equal?

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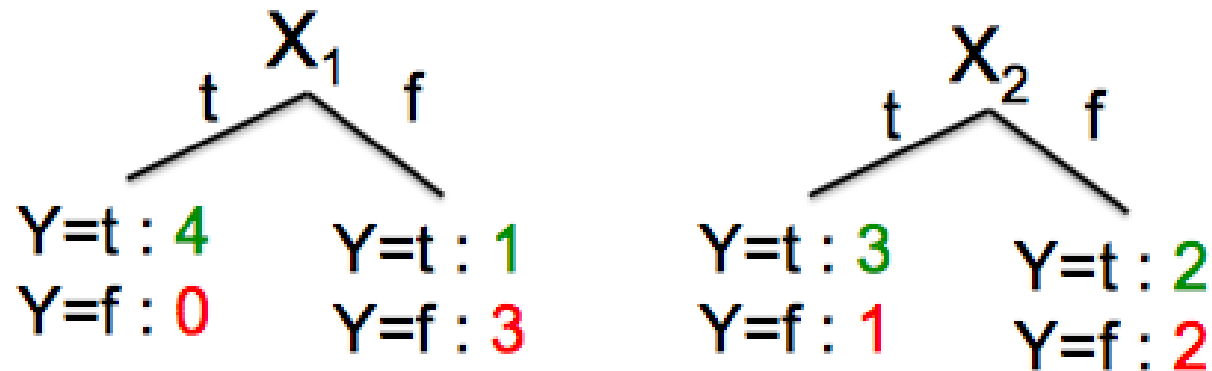 - e.g., φ = (A ∧ B)∨(¬A ∧ C) -- ((A and B) or (not A and C))

- Which tree do we prefer?

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

X_1
t   f

Y=t : 4   Y=t : 1
Y=f : 0   Y=f : 3

X_2
t   f

Y=t : 3   Y=t : 2
Y=f : 1   Y=f : 2

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

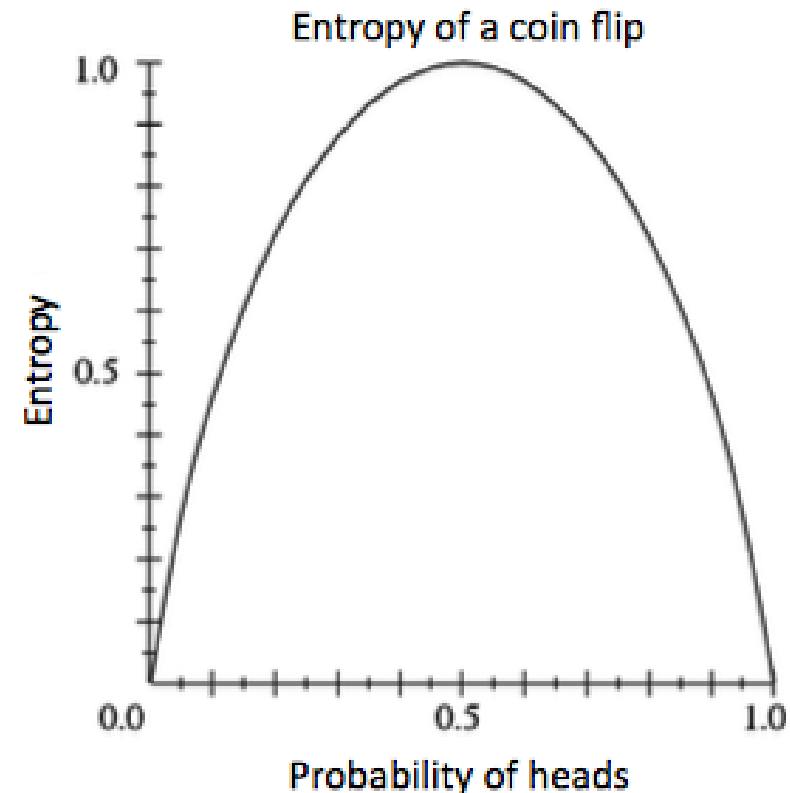| P(Y=A) = 1/4	P(Y=B) = 1/4	P(Y=C) = 1/4	P(Y=D) = 1/4

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 of a coin flip

Entropy (y-axis), Probability of heads (x-axis)

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
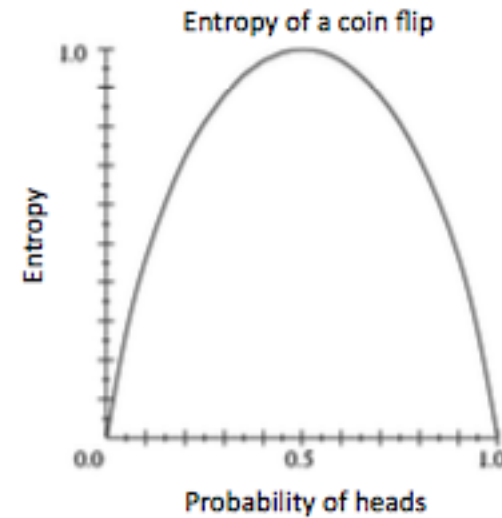 - Values sampled from it are more predictable

Entropy Example

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

Entropy of a coin flip

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

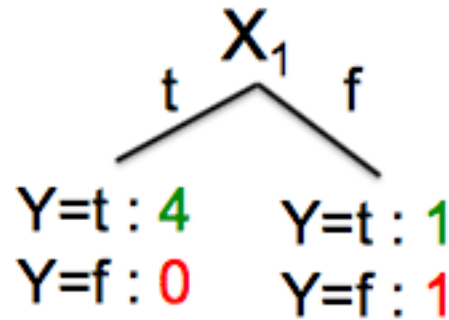Conditional Entropy $H(Y|X)$ of a random variable Y conditioned on a random variable X

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

Example:

$P(X_1=t) = 4/6$
$P(X_1=f) = 2/6$

X_1
t   f

Y=t : 4   Y=t : 1
Y=f : 0   Y=f : 1

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

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

Information gain

- Decrease in entropy (uncertainty) after splitting

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

In our running example:

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

$IG(X_1) > 0$ → we prefer the split!

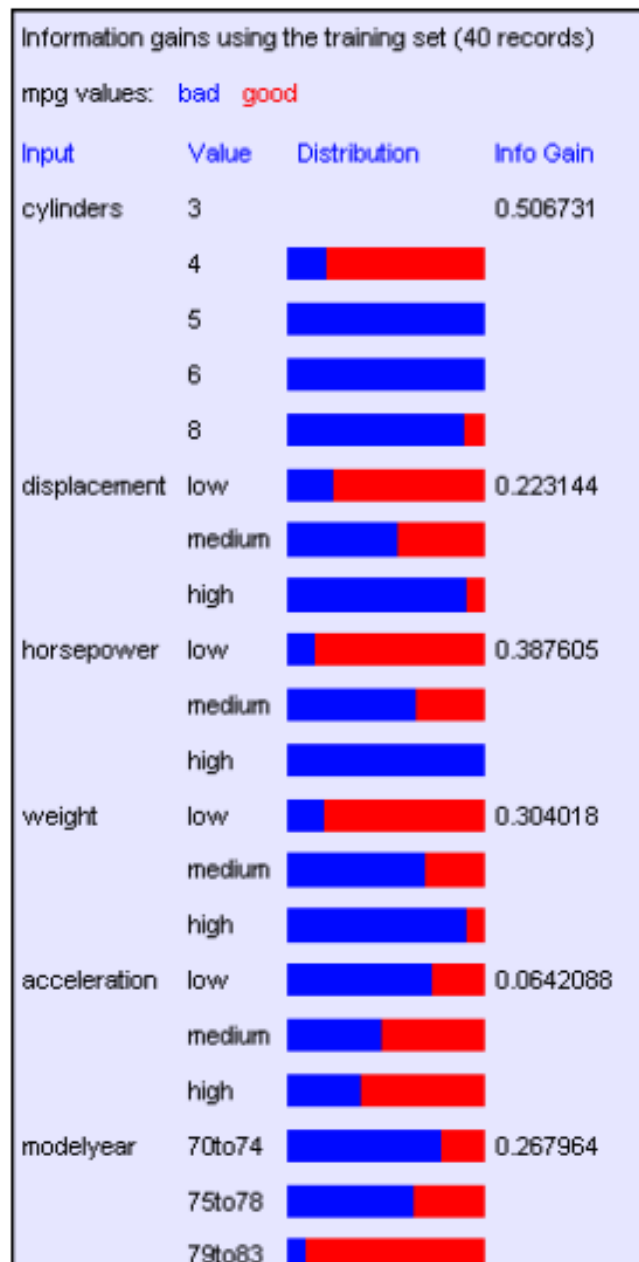| X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

Learning decision trees

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

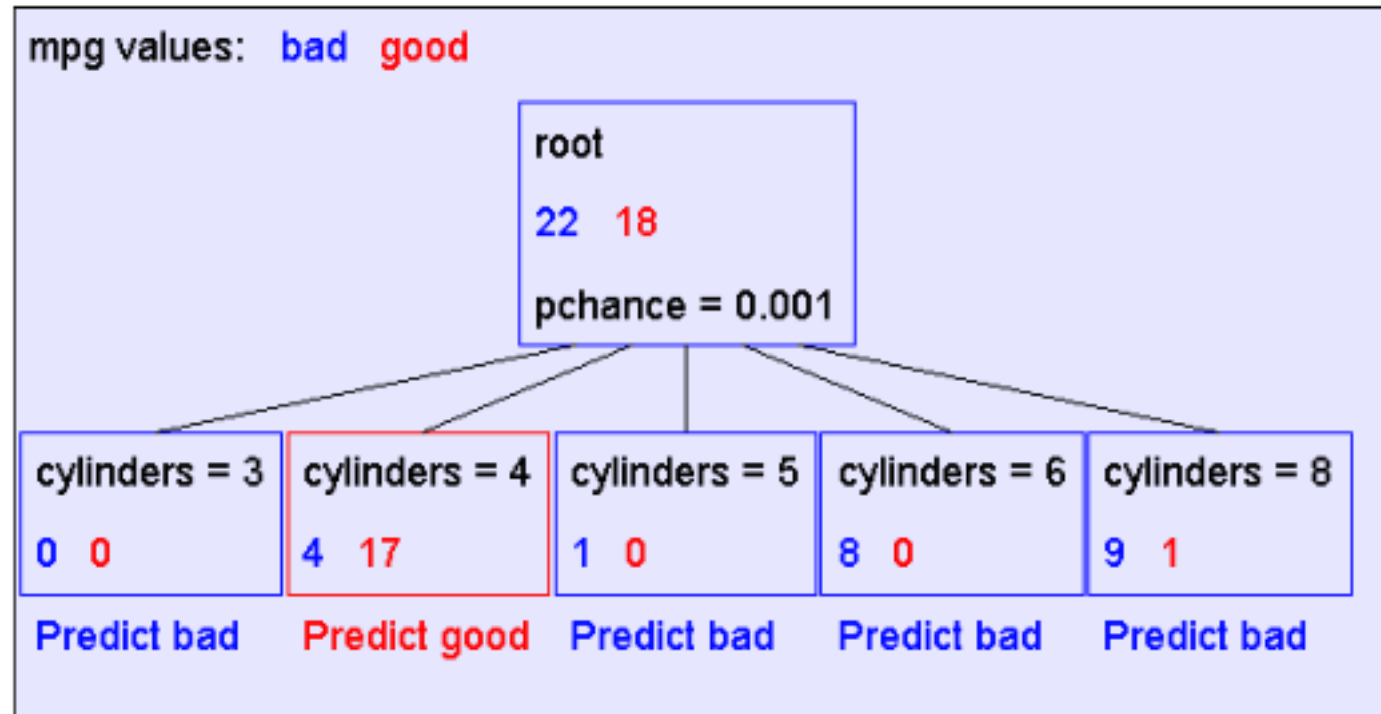$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

- Recurse

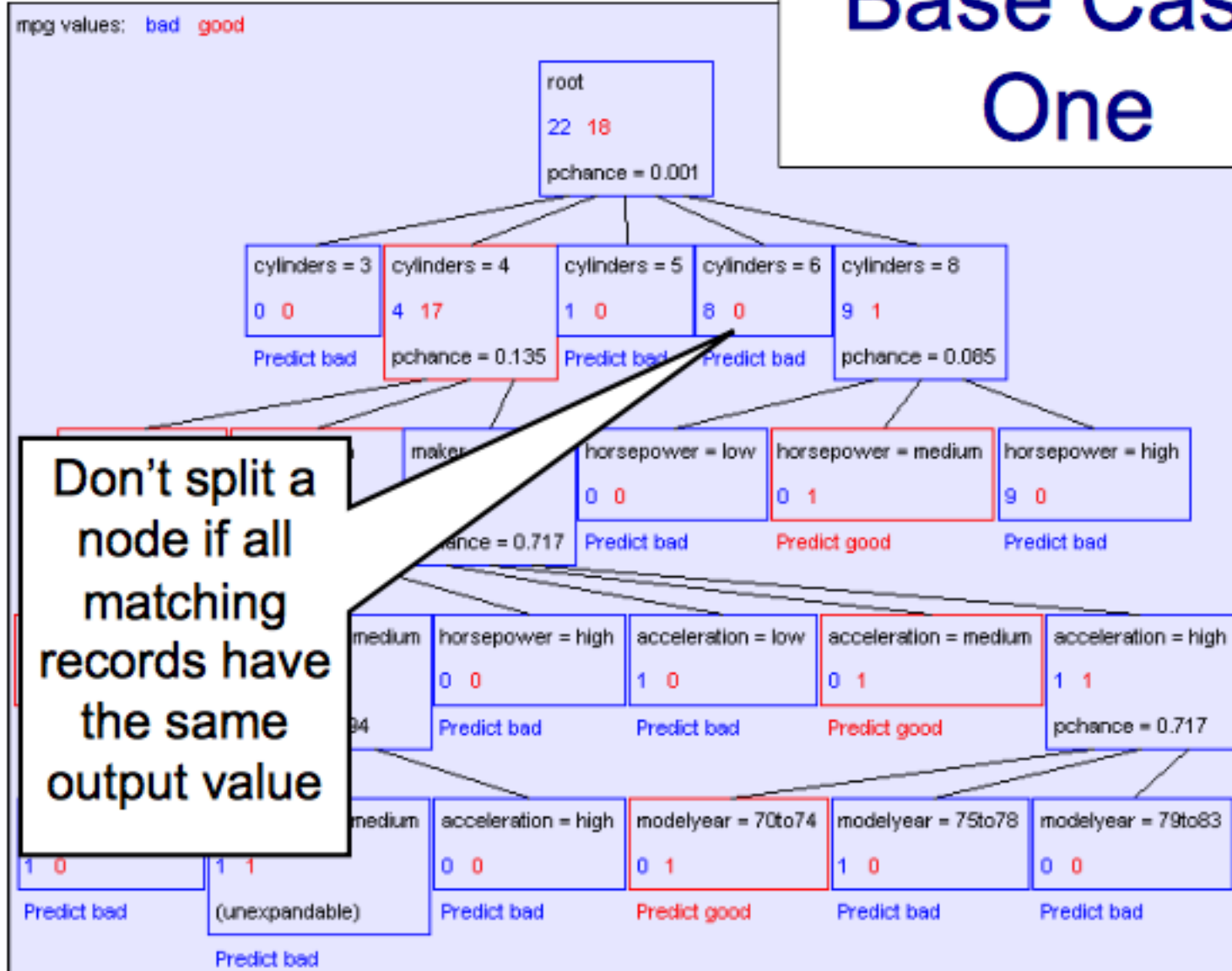Suppose we want to predict MPG

Look at all the information gains…

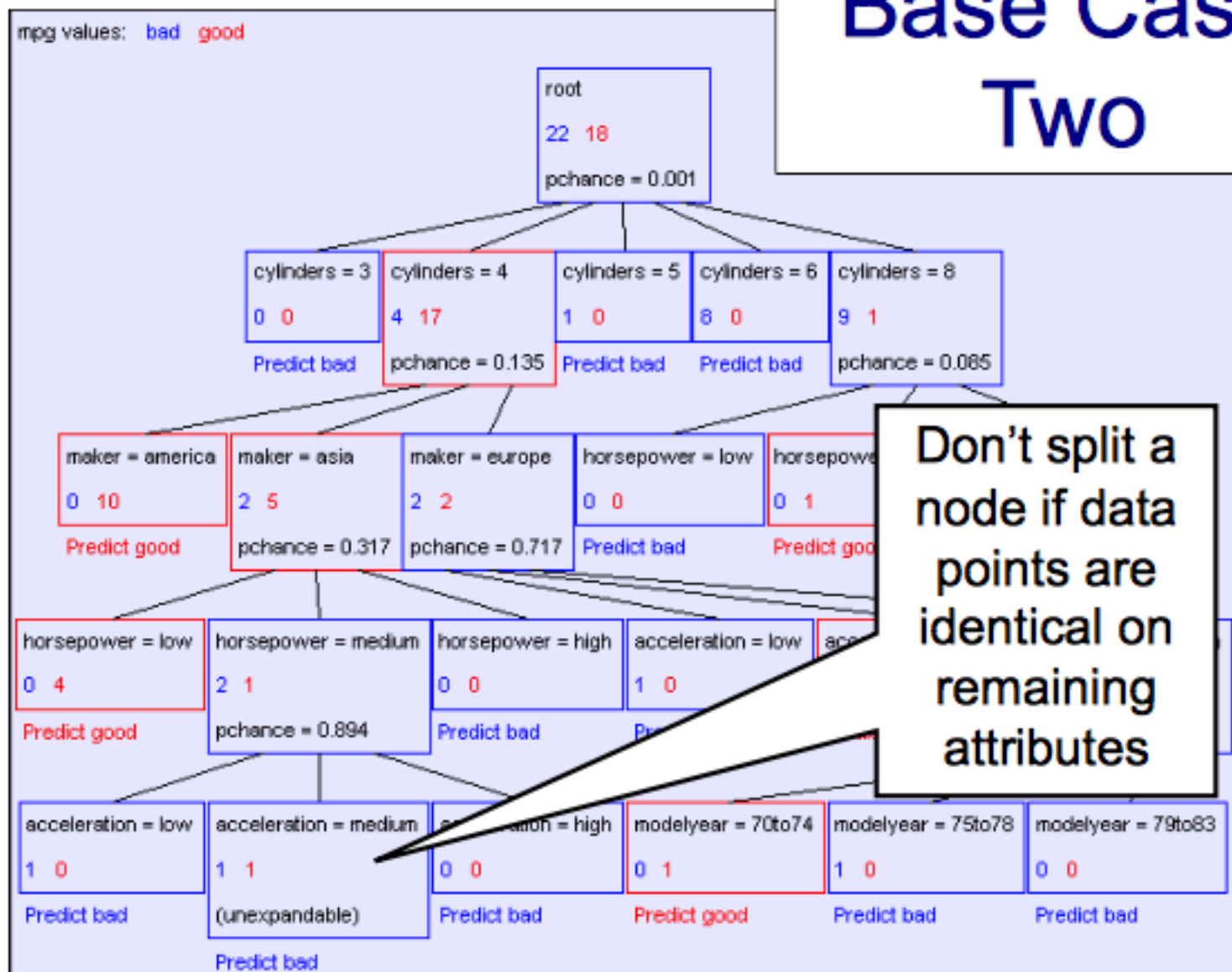Information gains using the training set (40 records)

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
	75to78		
	79to83		

A decision stump

mpg values: bad good

root
22 18
pchance = 0.001

cylinders = 3	cylinders = 4	cylinders = 5	cylinders = 6	cylinders = 8
0 0	4 17	1 0	8 0	9 1
Predict bad	Predict good	Predict bad	Predict bad	Predict bad

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

Base Cases: An Idea

- **Base Case One:** If all records in current data subset have the same output then do not recurse

- **Base Case Two:** If all records have exactly the same set of input attributes then do not recurse

Proposed Base Case 3:
If all attributes have zero information gain then don't recurse
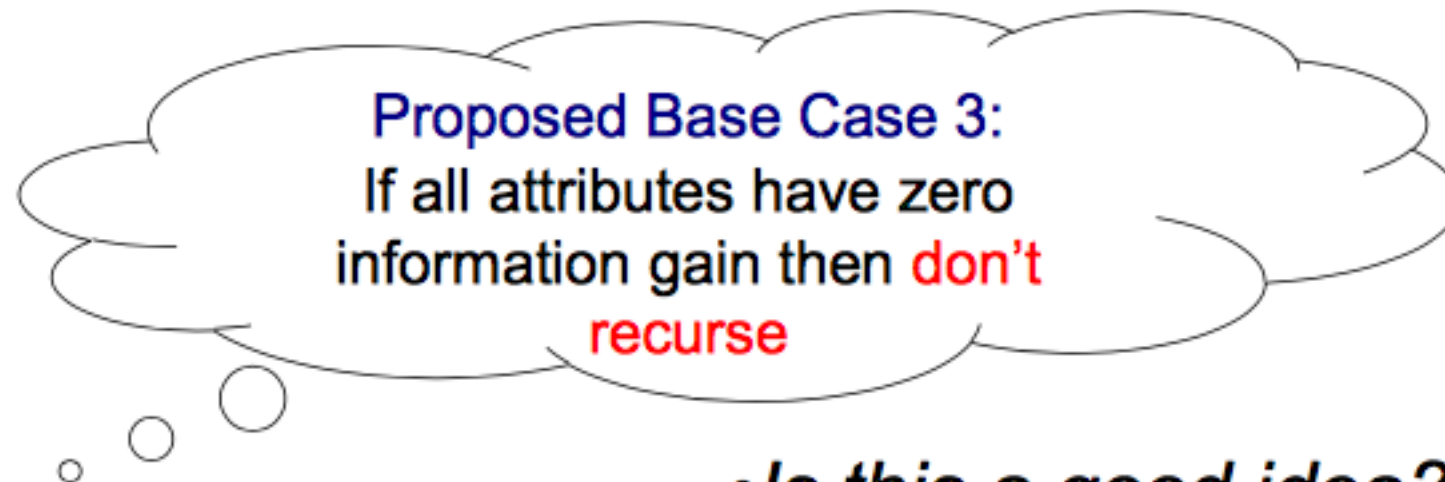
- *Is this a good idea?*

The problem with Base Case 3

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

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

The information gains:

The resulting decision tree:

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		

y values: 0 1

root

2 2
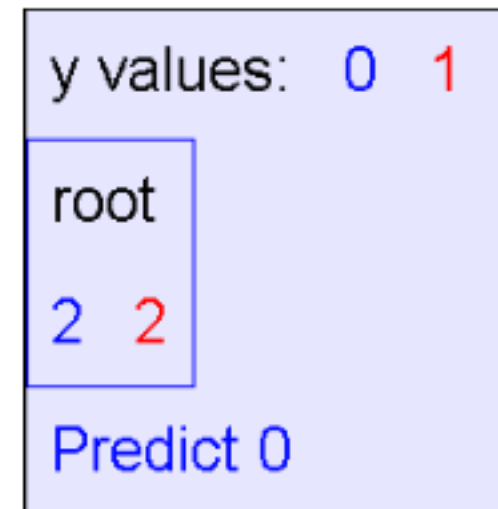
Predict 0

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

Is it OK to omit Base Case 3?

The resulting decision tree:
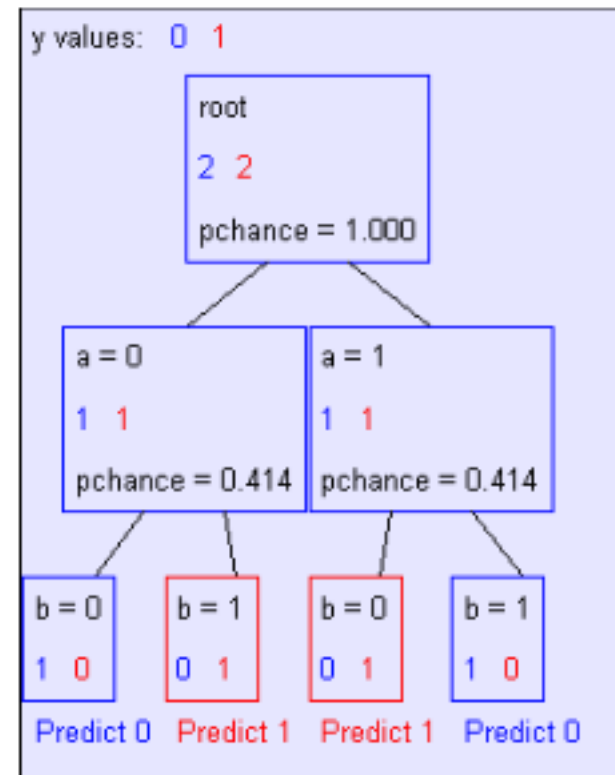
Summary: Building Decision Trees

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 = ith value of X.

From categorical to real-valued attributes

- **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?
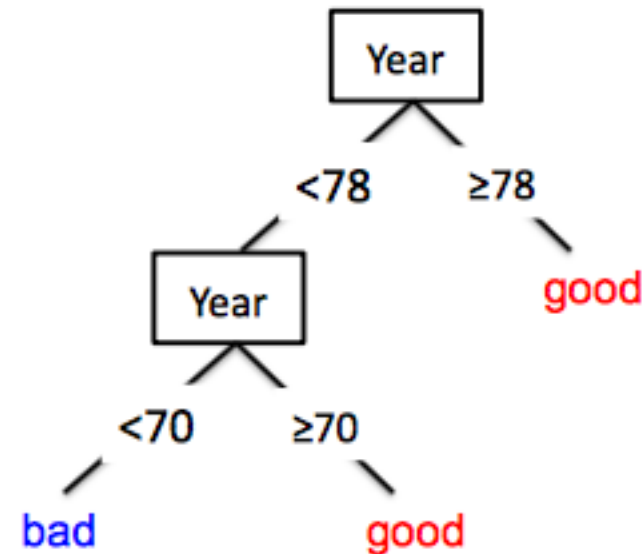
What you need to know about decision trees

- 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
- Presented for classification but can be used for regression and density estimation too
- Decision trees will overfit!!!
  - We will see the definition of overfitting and related concepts later in class.