Decision trees
Lecture 11

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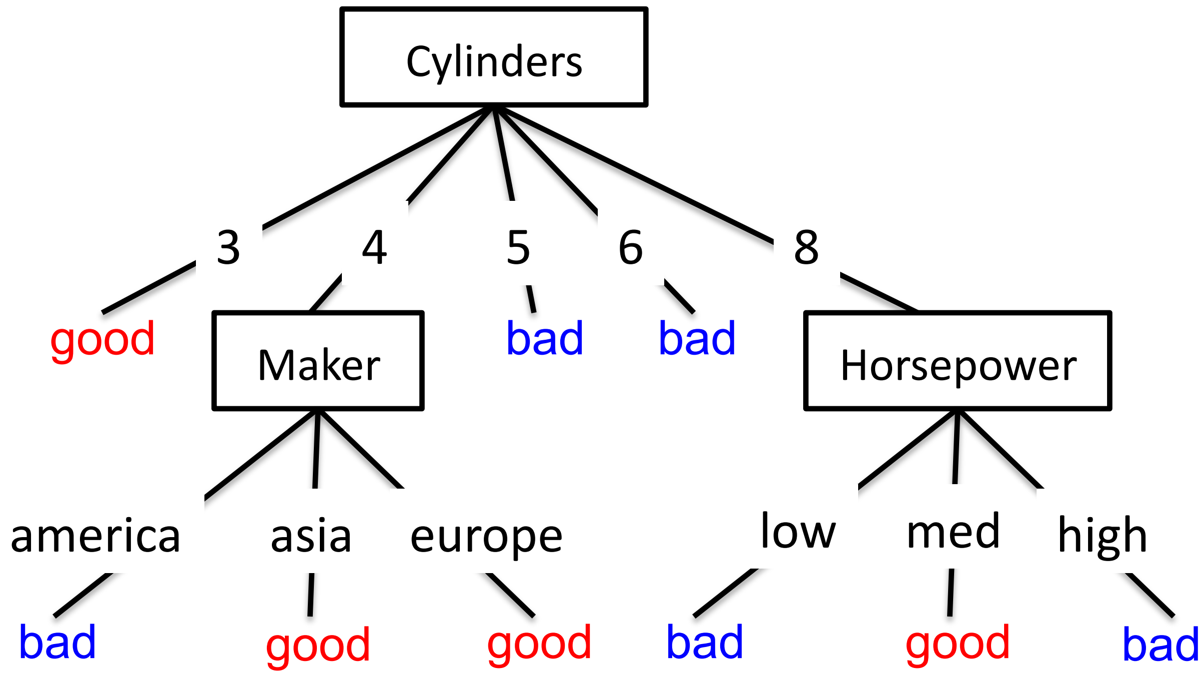
Slides adapted from Luke Zettlemoyer, Carlos Guestrin, and Andrew Moore

Hypotheses: 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

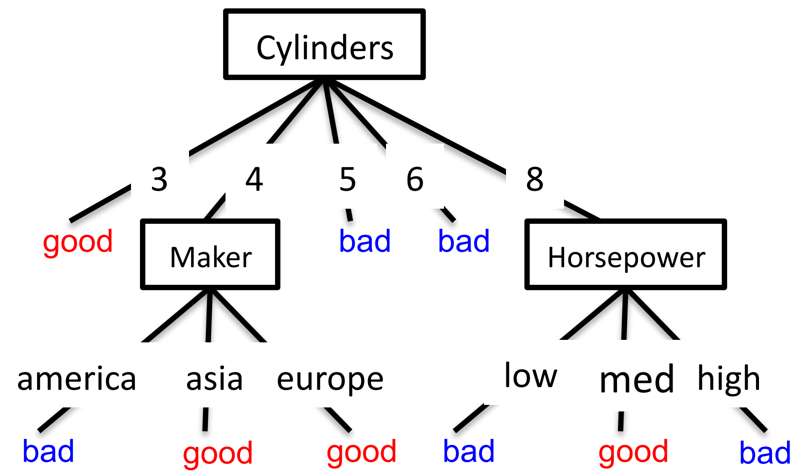


Human interpretable!

Hypothesis space

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

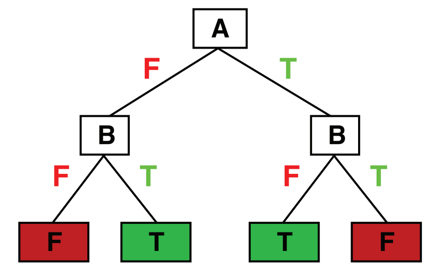
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low	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



What functions can be represented?

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

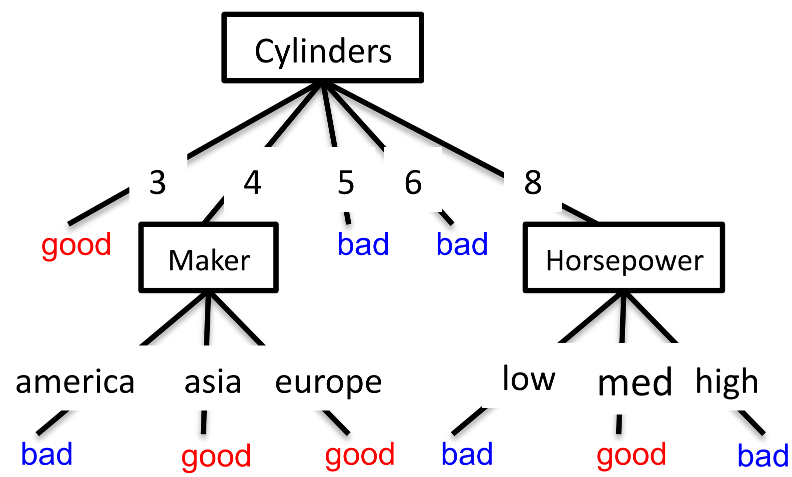
A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



(Figure from Stuart Russell)

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

- Could require exponentially many nodes

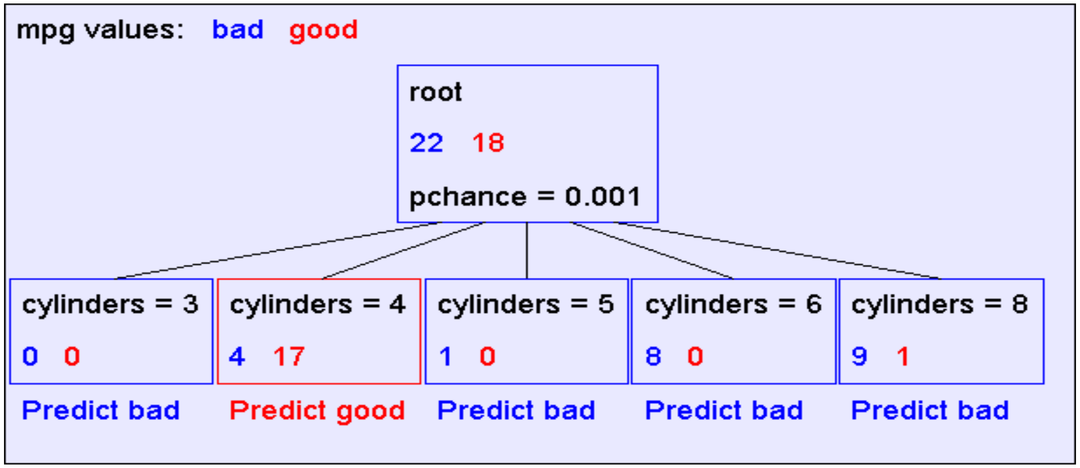


cyl=3 ∨ (cyl=4 ∧ (maker=asia ∨ maker=europe)) ∨ …

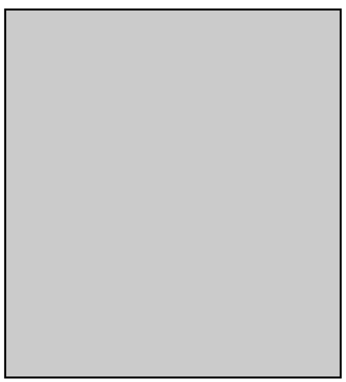
Learning *simplest* decision tree is NP-hard

- 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

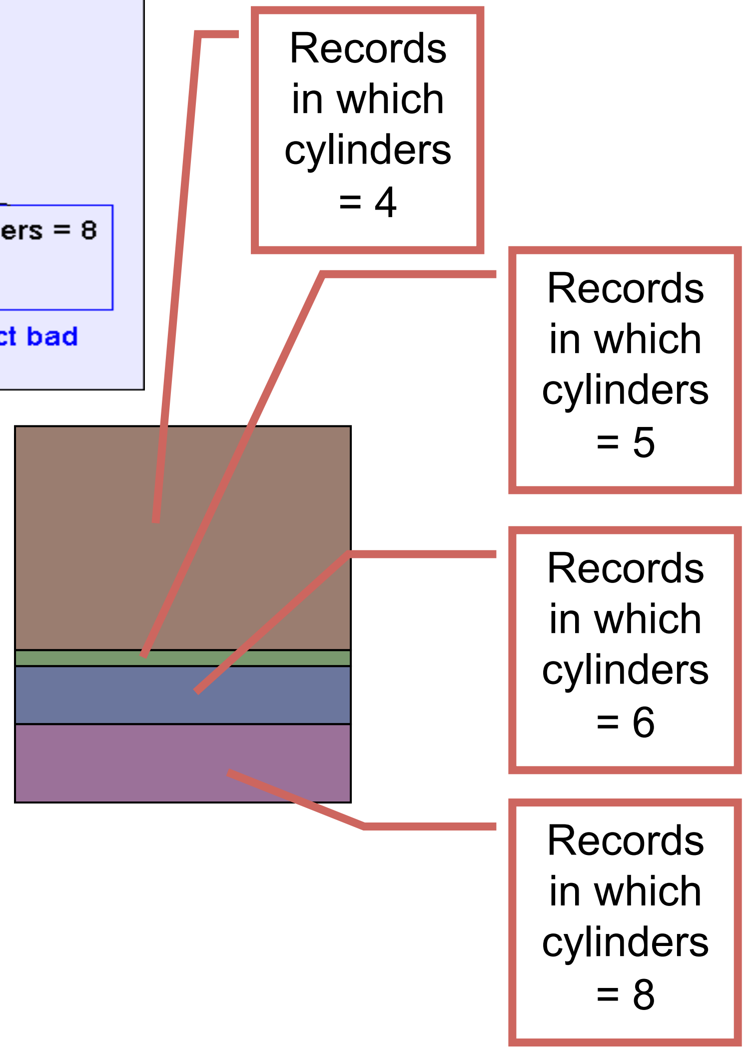
Key idea: Greedily learn trees using **recursion**



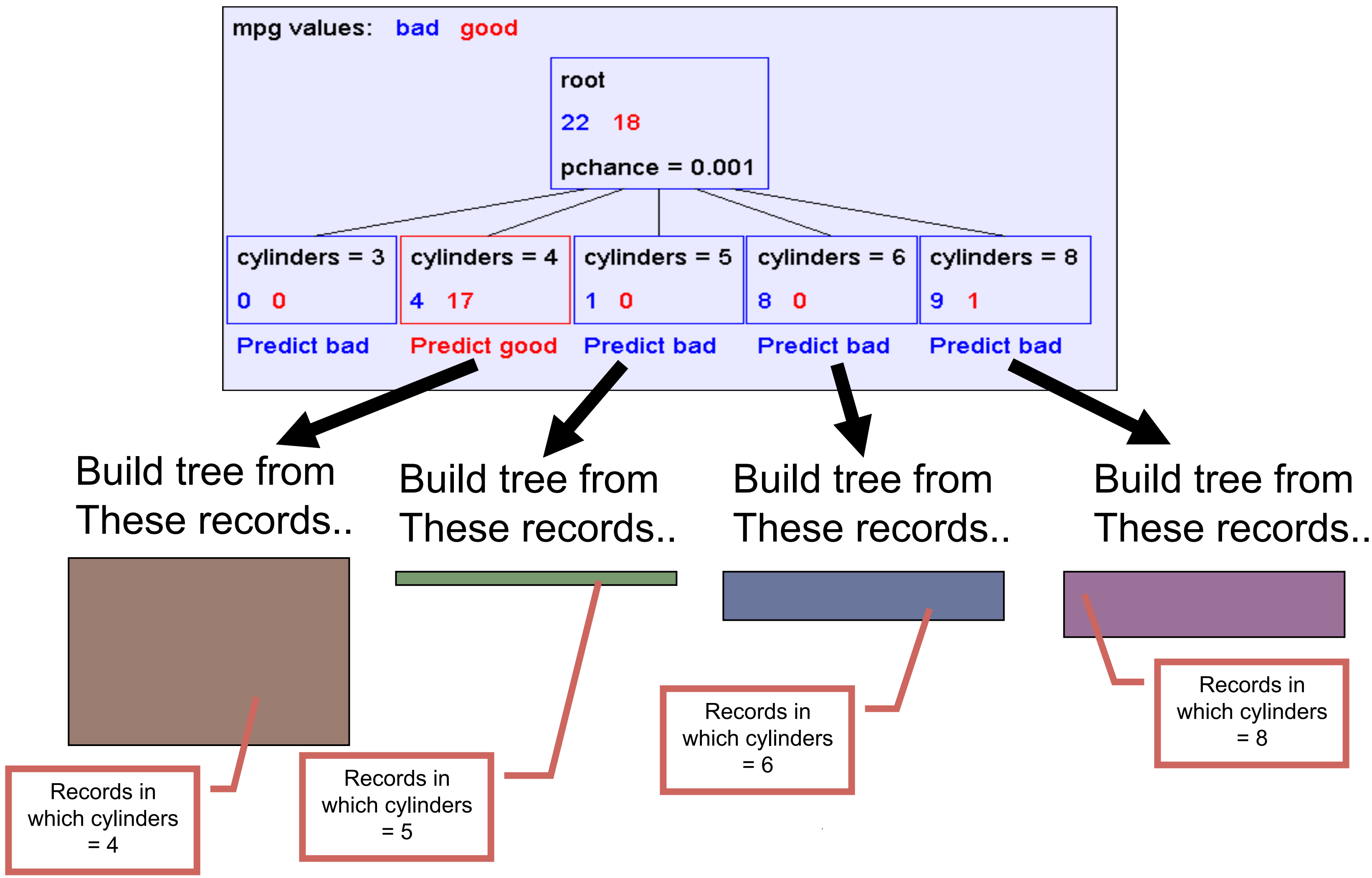
Take the Original Dataset..



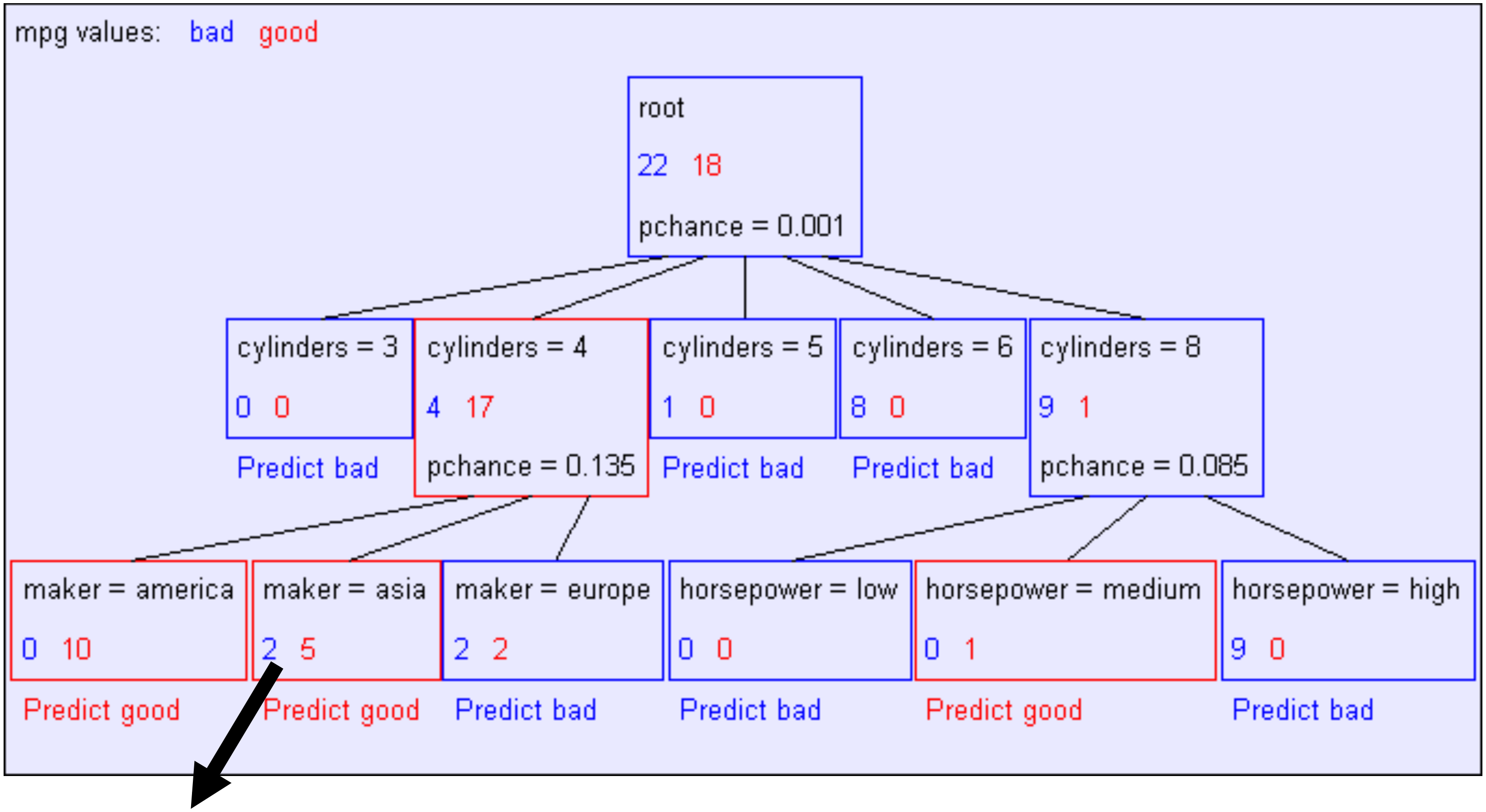
And partition it according to the value of the attribute we split on



Recursive Step



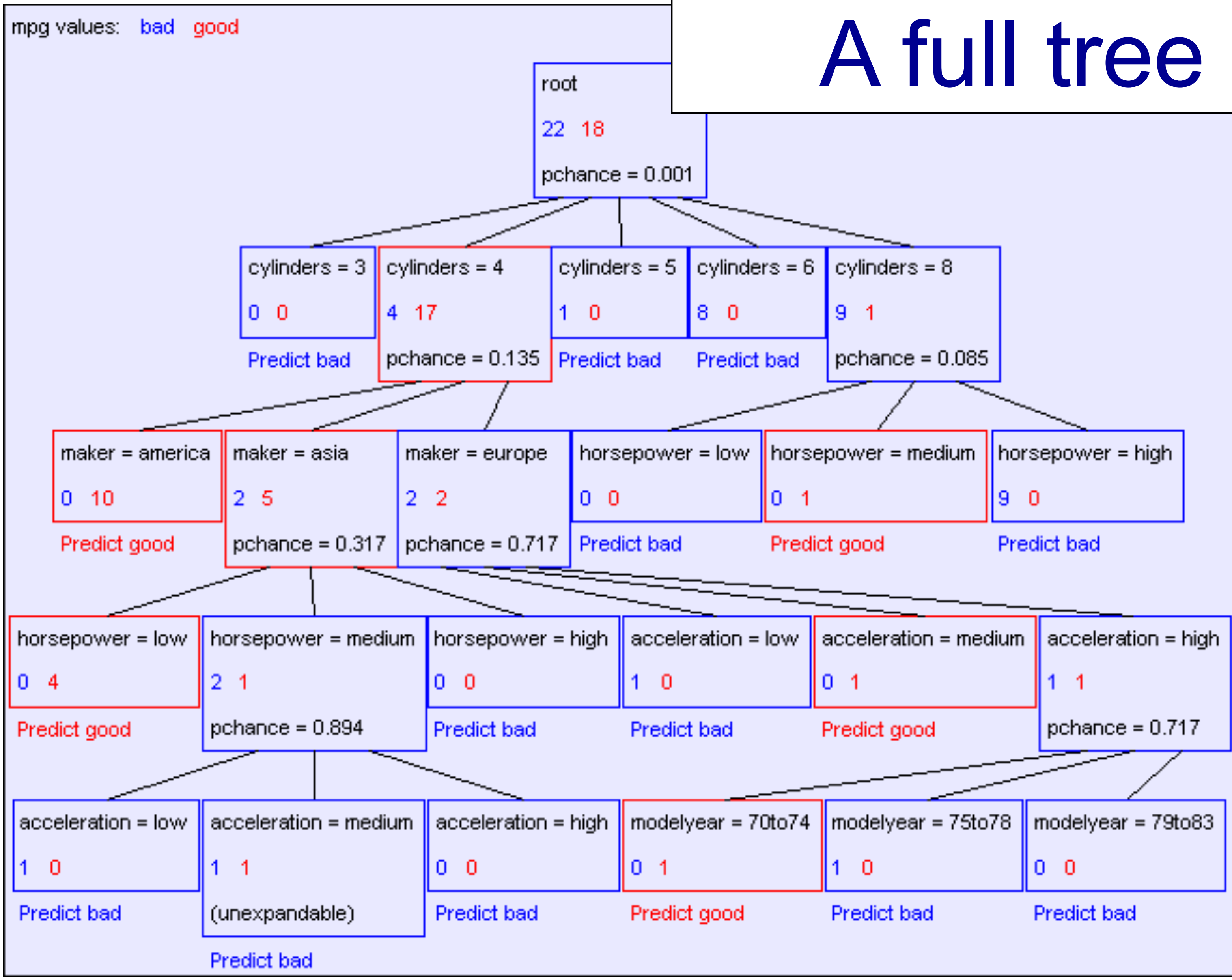
Second level of tree



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

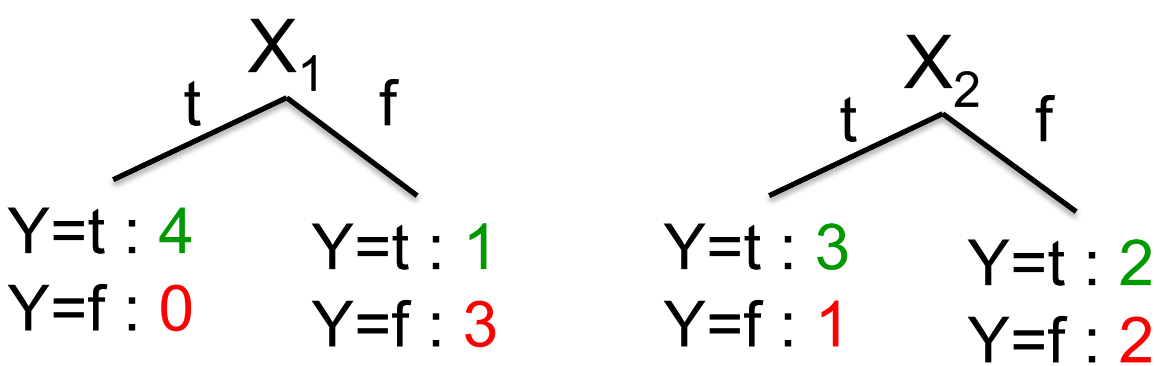
(Similar recursion in the other cases)

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

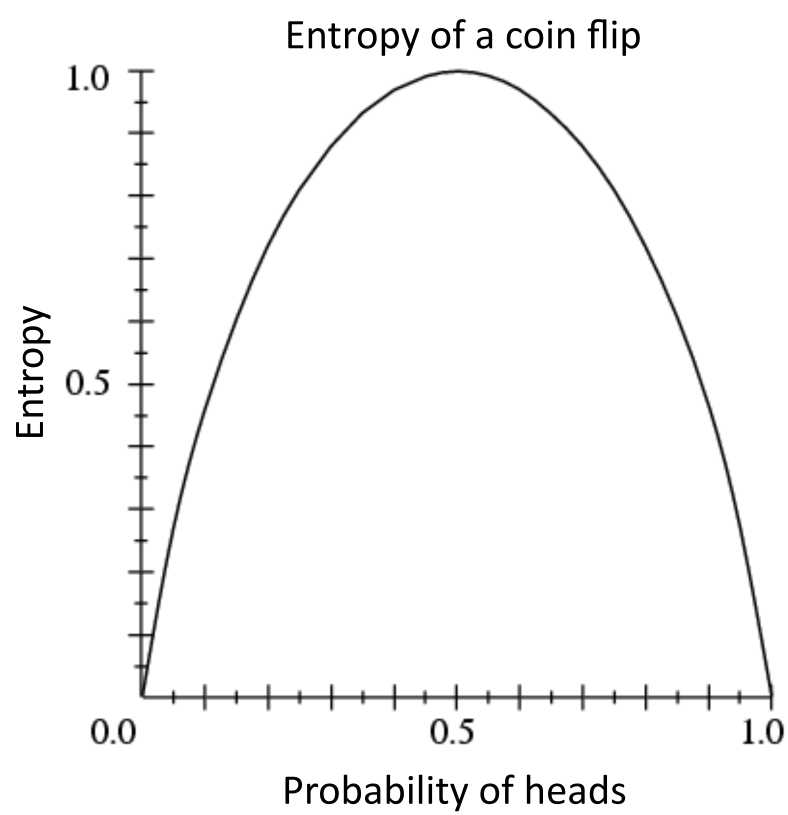
Entropy

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)

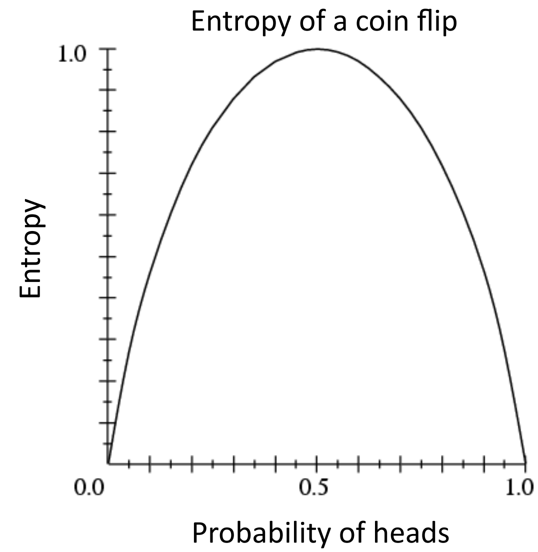


High, Low Entropy

- “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

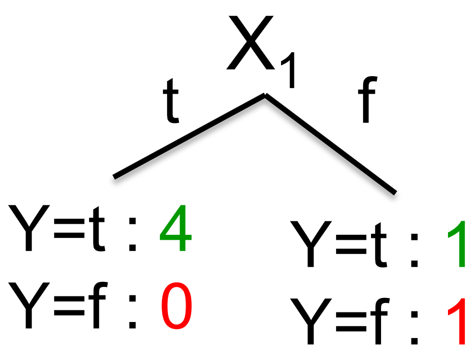
Conditional Entropy $H(Y|X)$ of a random variable Y conditioned on a random variable X

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

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

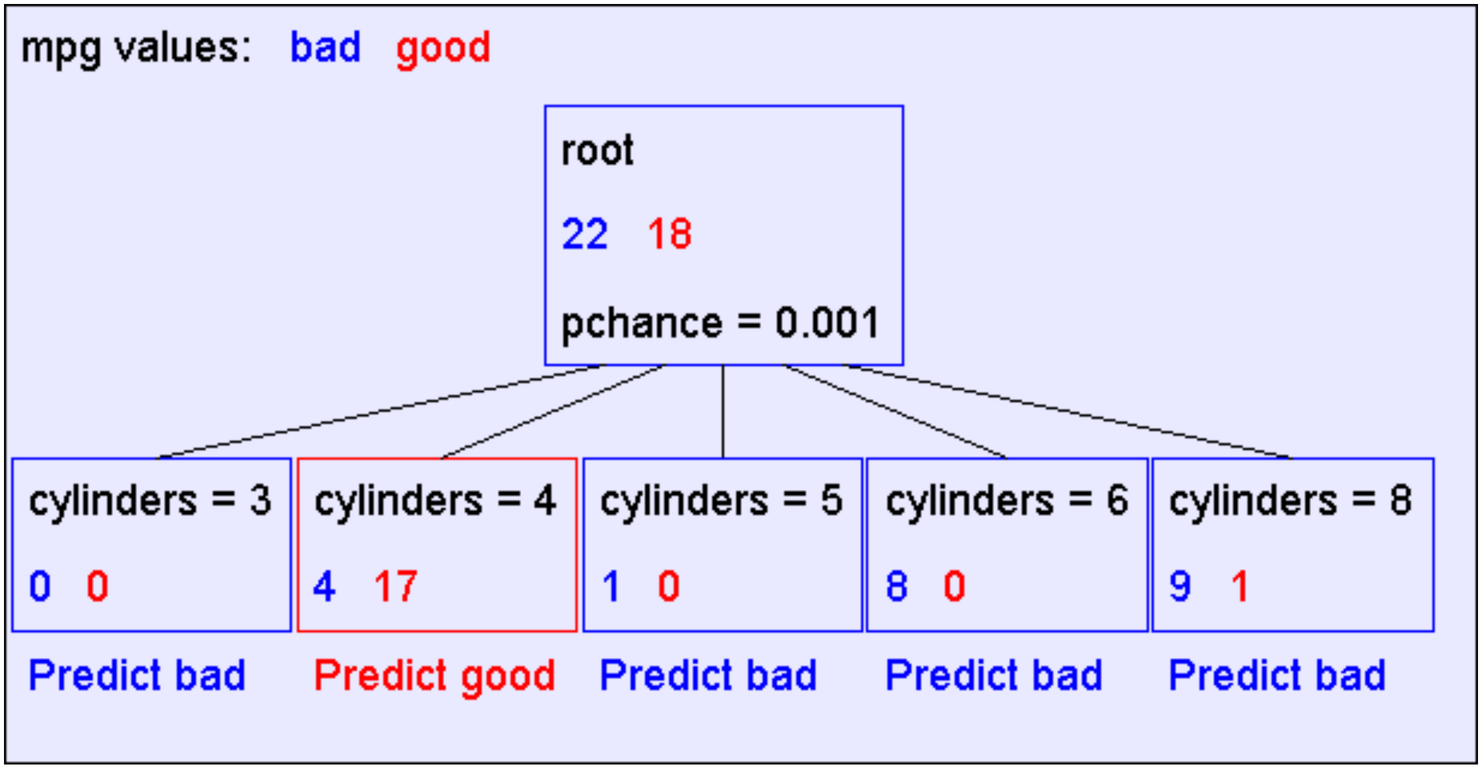
Learning decision trees

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

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

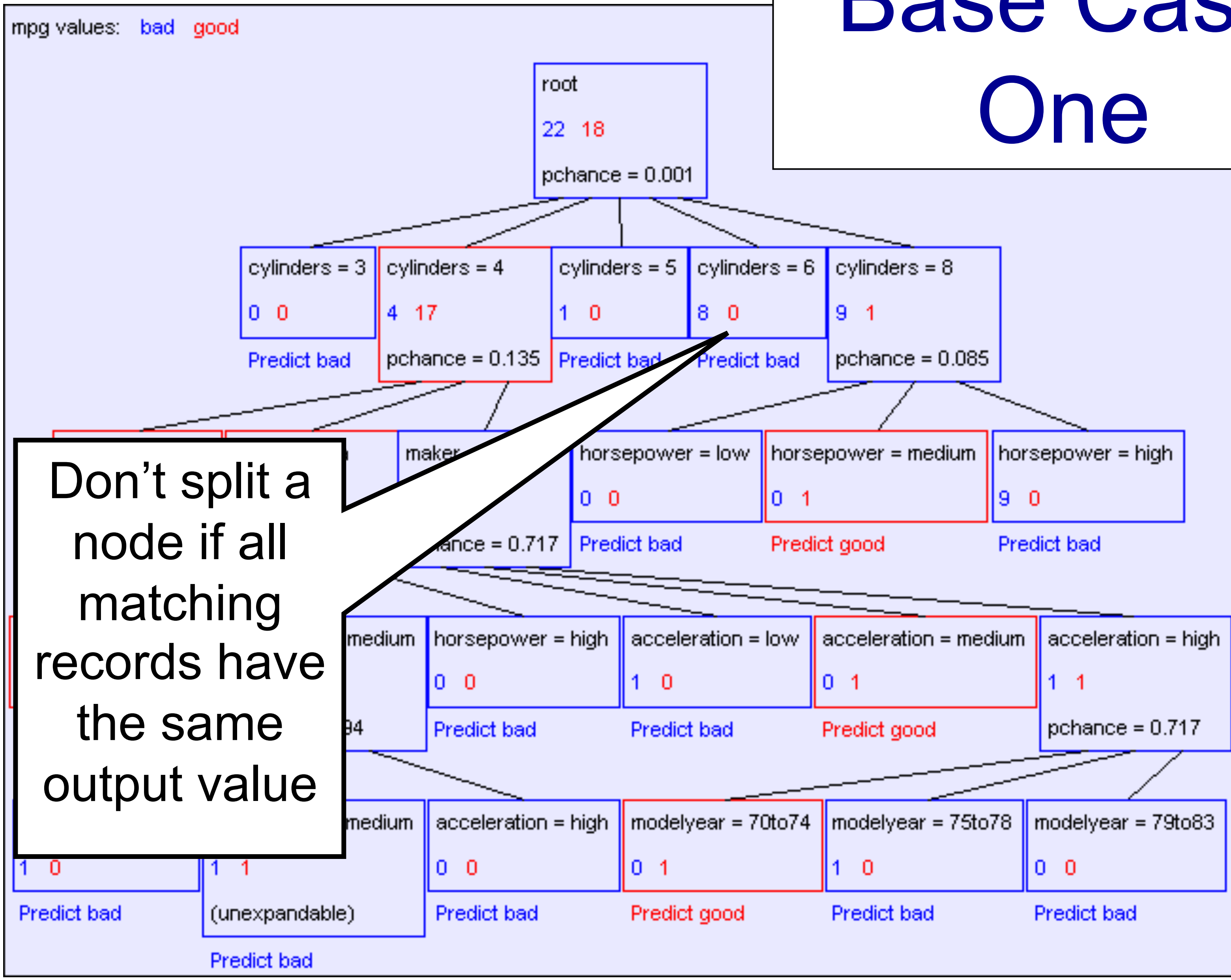
- Recurse

When to stop?



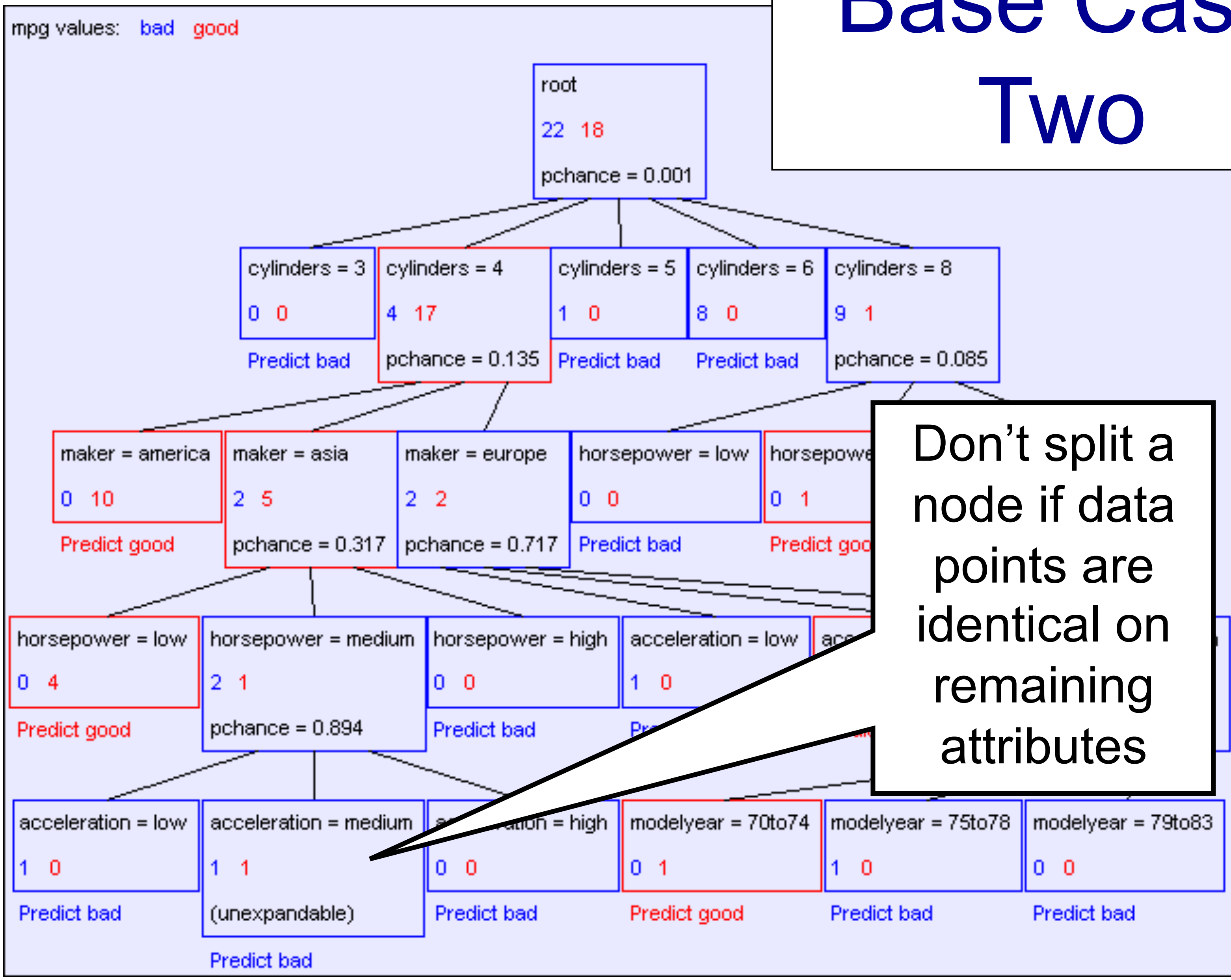
First split looks good! But, when do we stop?

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 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 small information gain then don't recurse

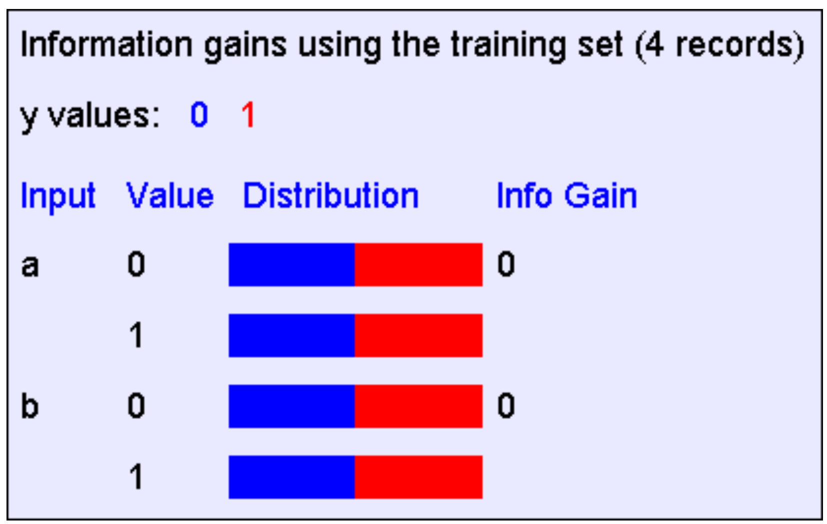
- *This is not a good idea*

The problem with proposed case 3

y = a XOR b

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

The information gains:



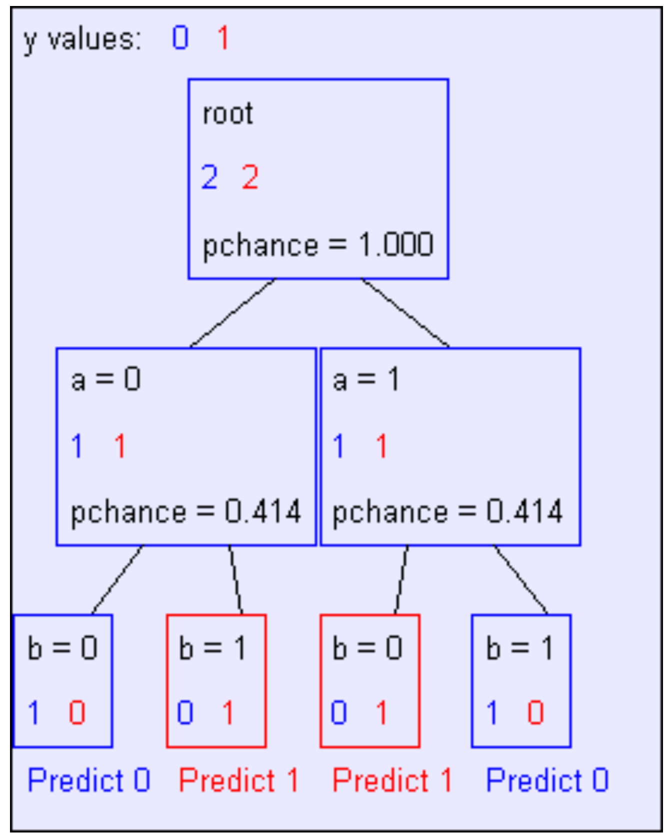
If we omit proposed case 3:

y = a XOR b

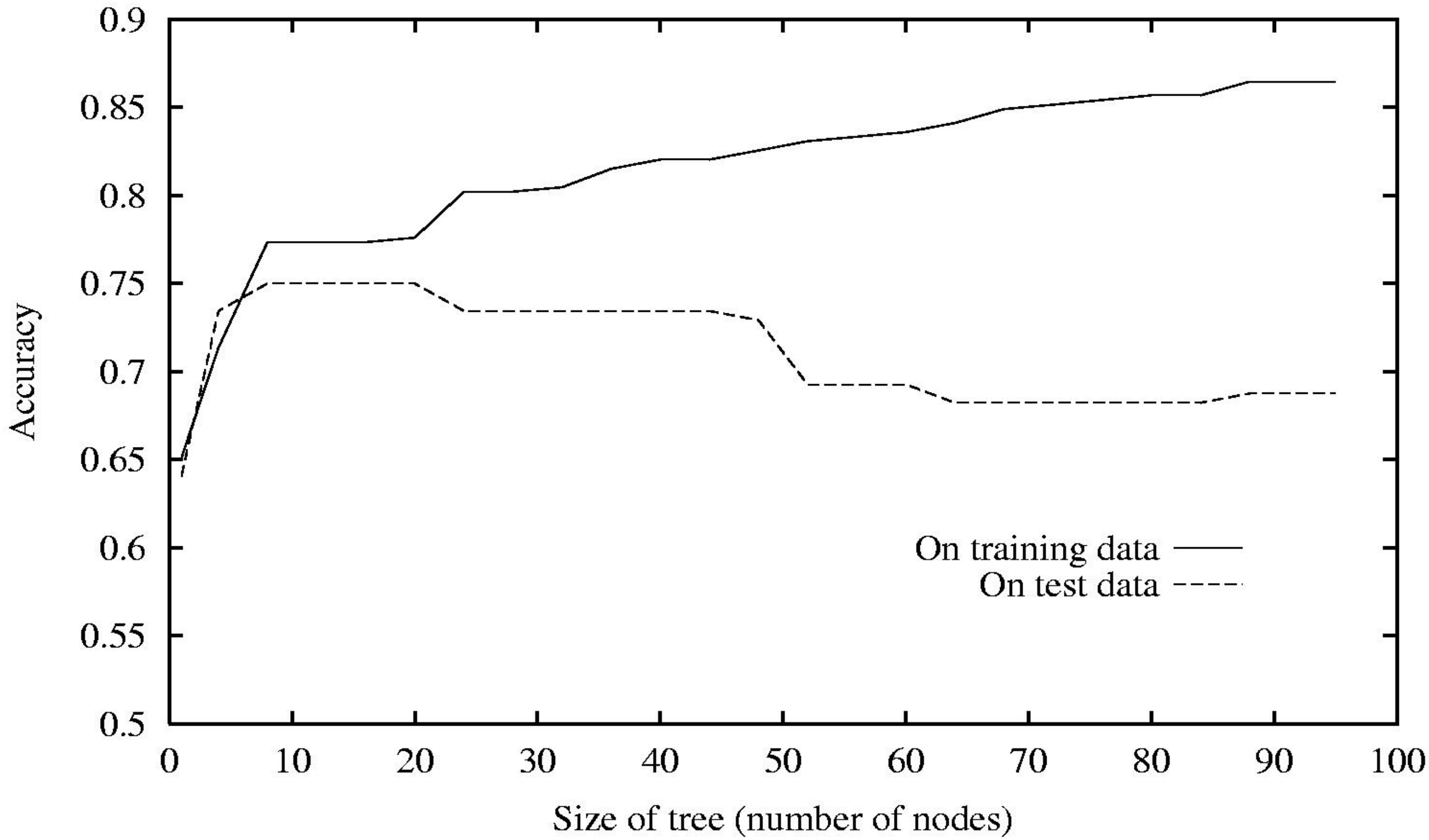
a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

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

The resulting decision tree:



Decision trees will overfit



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
  - Minimum number of samples per leaf
- Random forests

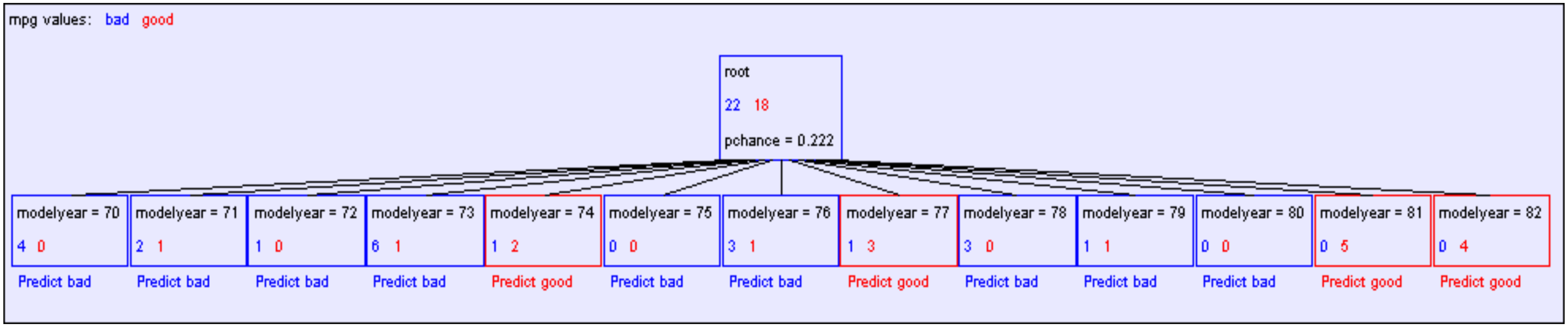
Real-Valued inputs

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

Infinite number of possible split values!!!

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:

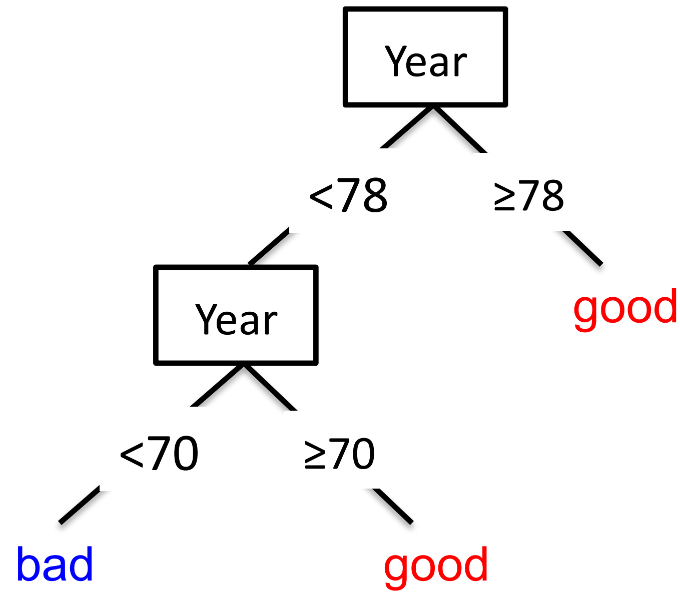


Hopeless: hypothesis with such a high branching factor will shatter *any* dataset and overfit

Threshold splits

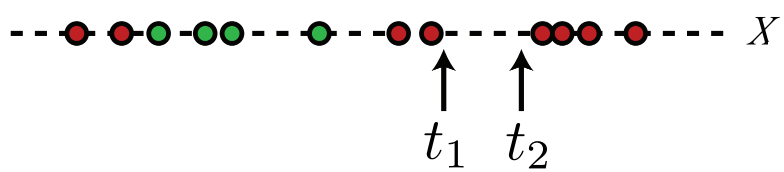
- **Binary tree:** split on attribute X at value t
  - One branch: $X < t$
  - Other branch: $X \geq t$

- Requires small change
  - Allow repeated splits on same variable **along a path**

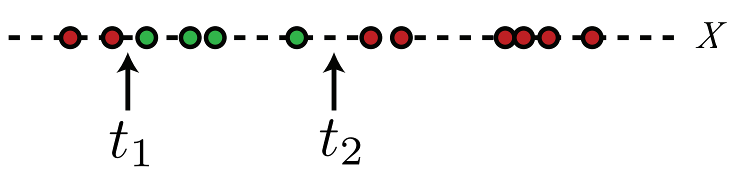


The set of possible thresholds

- Binary tree, split on attribute X
  - One branch: X < t
  - Other branch: X ≥ t
- Search through possible values of *t*
  - Seems hard!!!
- But only a finite number of *t*'s are important:



  - Sort data according to X into $\{x_1,\ldots,x_m\}$
  - Consider split points of the form $x_i + (x_{i+1} - x_i)/2$
  - Morever, only splits between examples of different classes matter!



(Figures from Stuart Russell)

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:
  - $H(Y|X:t) = p(X < t) H(Y|X < t) + p(X >= t) H(Y|X >= t)$
  - $IG(Y|X:t) = H(Y) - H(Y|X:t)$
  - $IG^*(Y|X) = \max_t IG(Y|X:t)$
- Use: $IG^*(Y|X)$ for continuous variables

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
  - Or, use ensembles of different trees (random forests)

Ensemble learning

Slides adapted from Navneet Goyal, Tan, Steinbach, Kumar, Vibhav Gogate

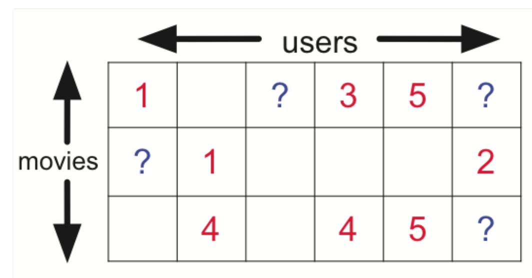
Ensemble methods

Machine learning competition with a $1 million prize

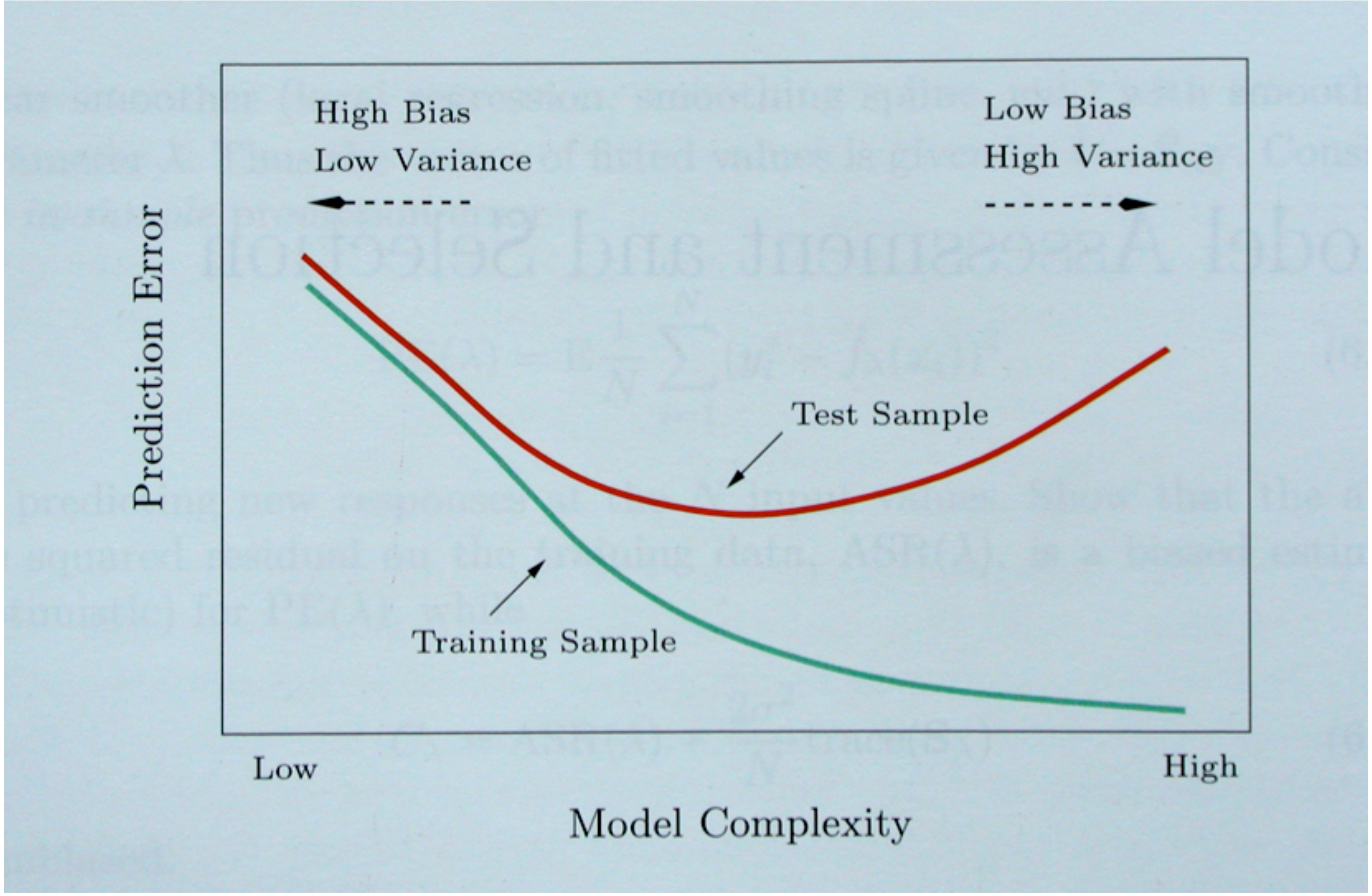
Leaderboard

Display top 20 leaders.

Rank	Team Name	Best Score	% Improvement	Last Submit Time
1	The Ensemble	0.8553	10.10	2009-07-26 18:38:22
2	BellKor's Pragmatic Chaos	0.8554	10.09	2009-07-26 18:18:28
Grand Prize - RMSE <= 0.8563				
3	Grand Prize Team	0.8571	9.91	2009-07-24 13:07:49
4	Opera Solutions and Vandelay United	0.8573	9.89	2009-07-25 20:05:52
5	Vandelay Industries !	0.8579	9.83	2009-07-26 02:49:53
6	PragmaticTheory	0.8582	9.80	2009-07-12 15:09:53
7	BellKor in BigChaos	0.8590	9.71	2009-07-26 12:57:25
8	Dace_	0.8603	9.58	2009-07-24 17:18:43
9	Opera Solutions	0.8611	9.49	2009-07-26 18:02:08
10	BellKor	0.8612	9.48	2009-07-26 17:19:11
11	BigChaos	0.8613	9.47	2009-06-23 23:06:52
12	Feeds2	0.8613	9.47	2009-07-24 20:06:46
Progress Prize 2008 - RMSE = 0.8616 - Winning Team: BellKor in BigChaos				
13	xiangliang	0.8633	9.26	2009-07-21 02:04:40
14	Gravity	0.8634	9.25	2009-07-26 15:58:34
15	Ces	0.8642	9.17	2009-07-25 17:42:38
16	Invisible Ideas	0.8644	9.14	2009-07-20 03:26:12
17	Just a guy in a garage	0.8650	9.08	2009-07-22 14:10:42
18	Craig Carmichael	0.8656	9.02	2009-07-25 16:00:54
19	J Dennis Su	0.8658	9.00	2009-03-11 09:41:54
20	acmehill	0.8659	8.99	2009-04-16 06:29:35
Progress Prize 2007 - RMSE = 0.8712 - Winning Team: KorBell				
Cinematch score on quiz subset - RMSE = 0.9514				



Bias/Variance Tradeoff



Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

Reduce Variance Without Increasing Bias

- Averaging reduces variance:

$$Var(\overline{X}) = \frac{Var(X)}{N}$$

(when predictions are **independent**)

Average models to reduce model variance

One problem:

only one training set

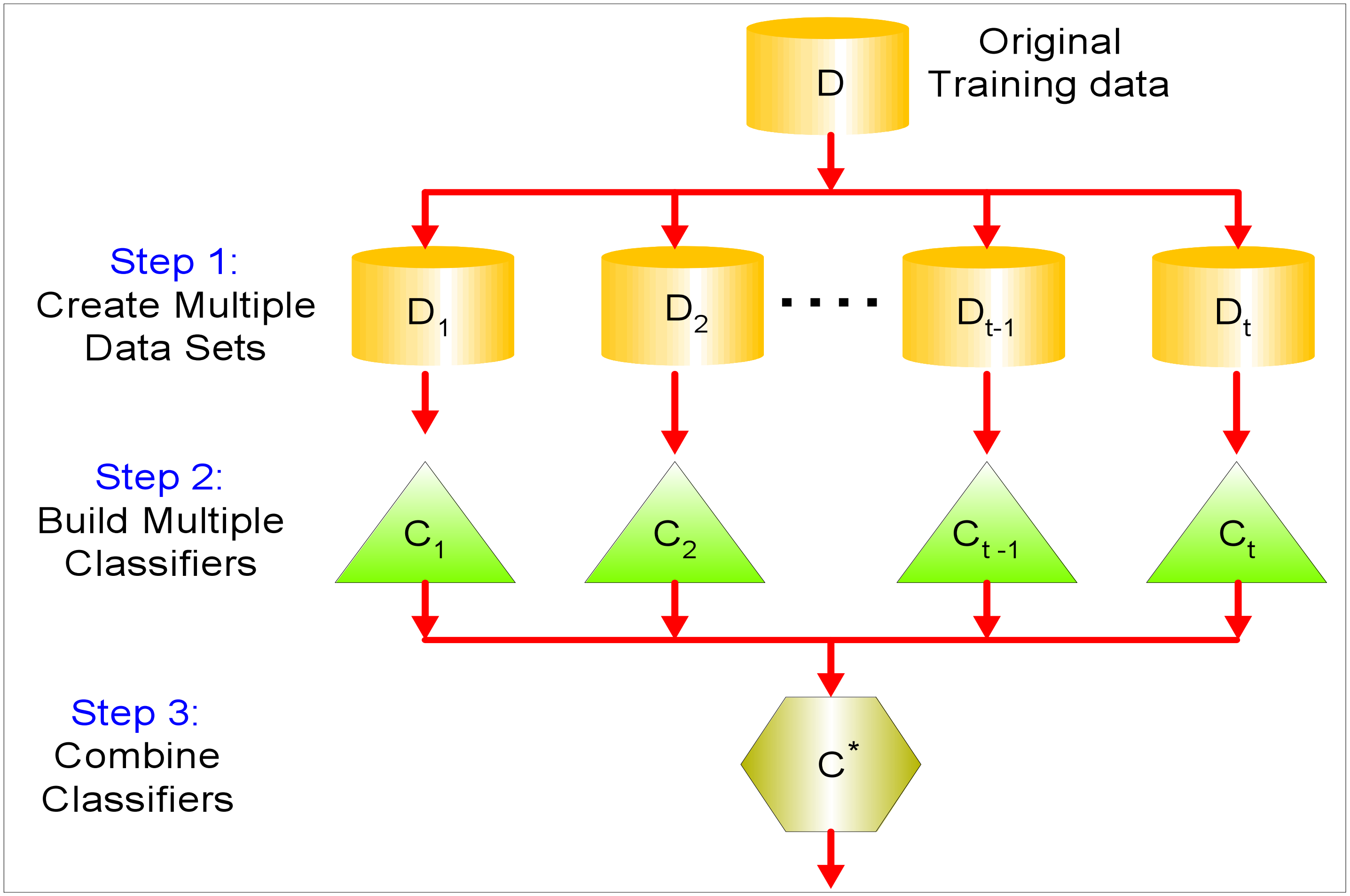
where do multiple models come from?

Bagging: Bootstrap Aggregation

- Leo Breiman (1994)
- Take repeated bootstrap samples from training set *D*
- *Bootstrap sampling*: Given set *D* containing *N* training examples, create *D*' by drawing *N* examples at random with replacement from *D*.

- Bagging:
  - Create *k* bootstrap samples $D_1 \ldots D_k$.
  - Train distinct classifier on each D_i.
  - Classify new instance by majority vote / average.

General Idea



Example of Bagging

- Sampling with replacement

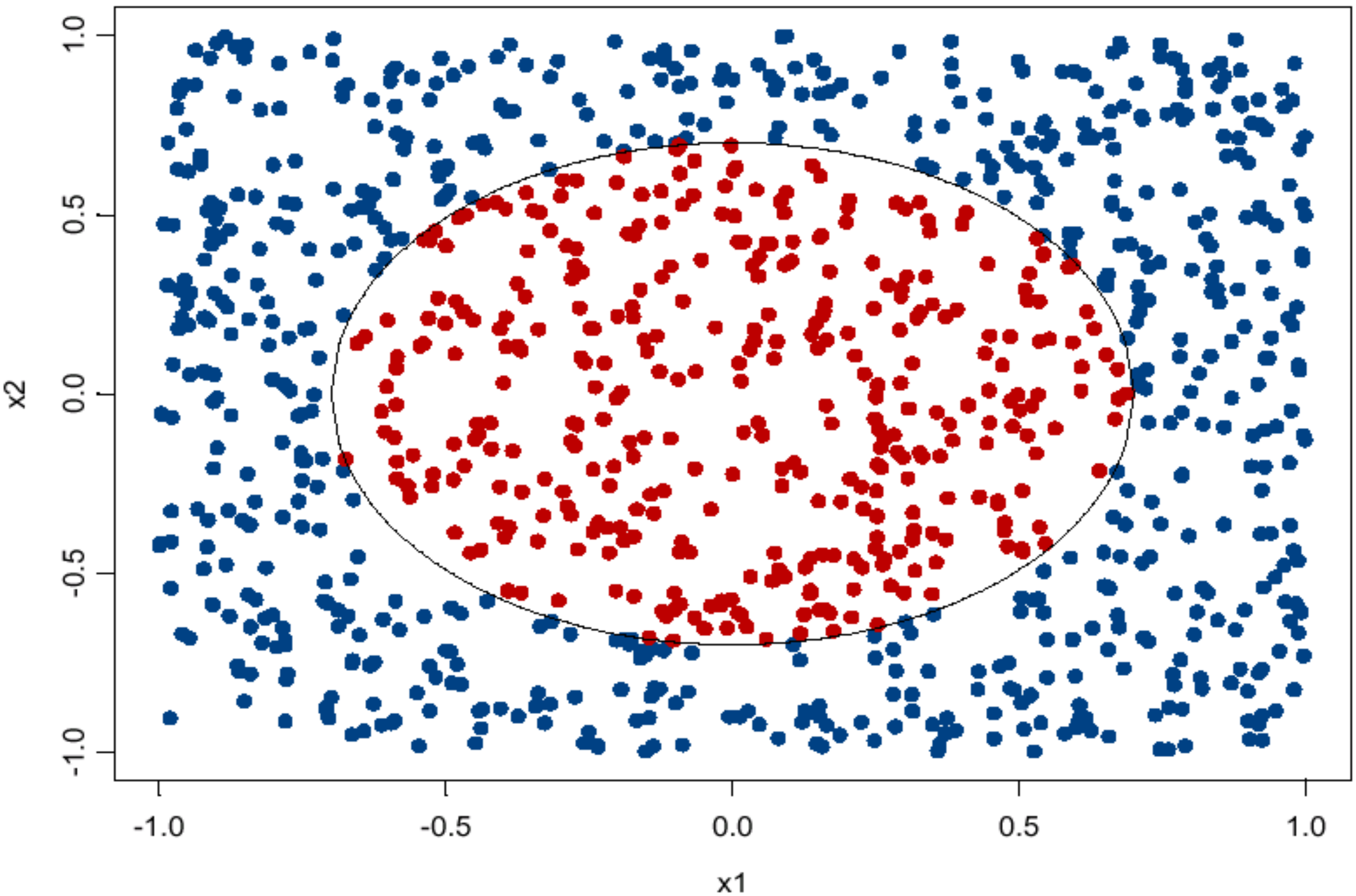
Training Data

Data ID

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

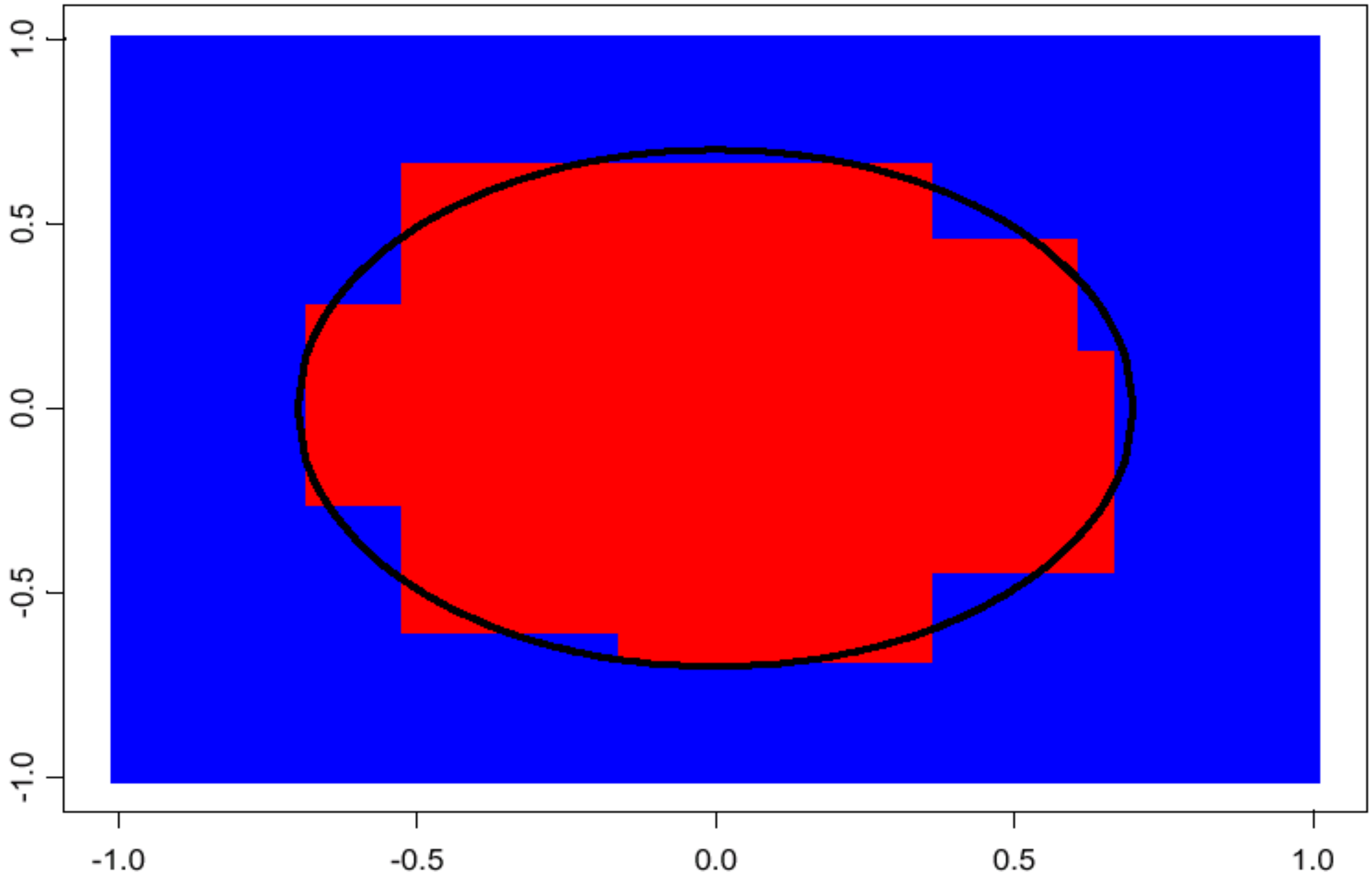
- Build classifier on each bootstrap sample
- Each data point has probability $(1 – 1/n)^n$ of being selected as test data
- Training data = 1- $(1 – 1/n)^n$ of the original data

Bagging Example

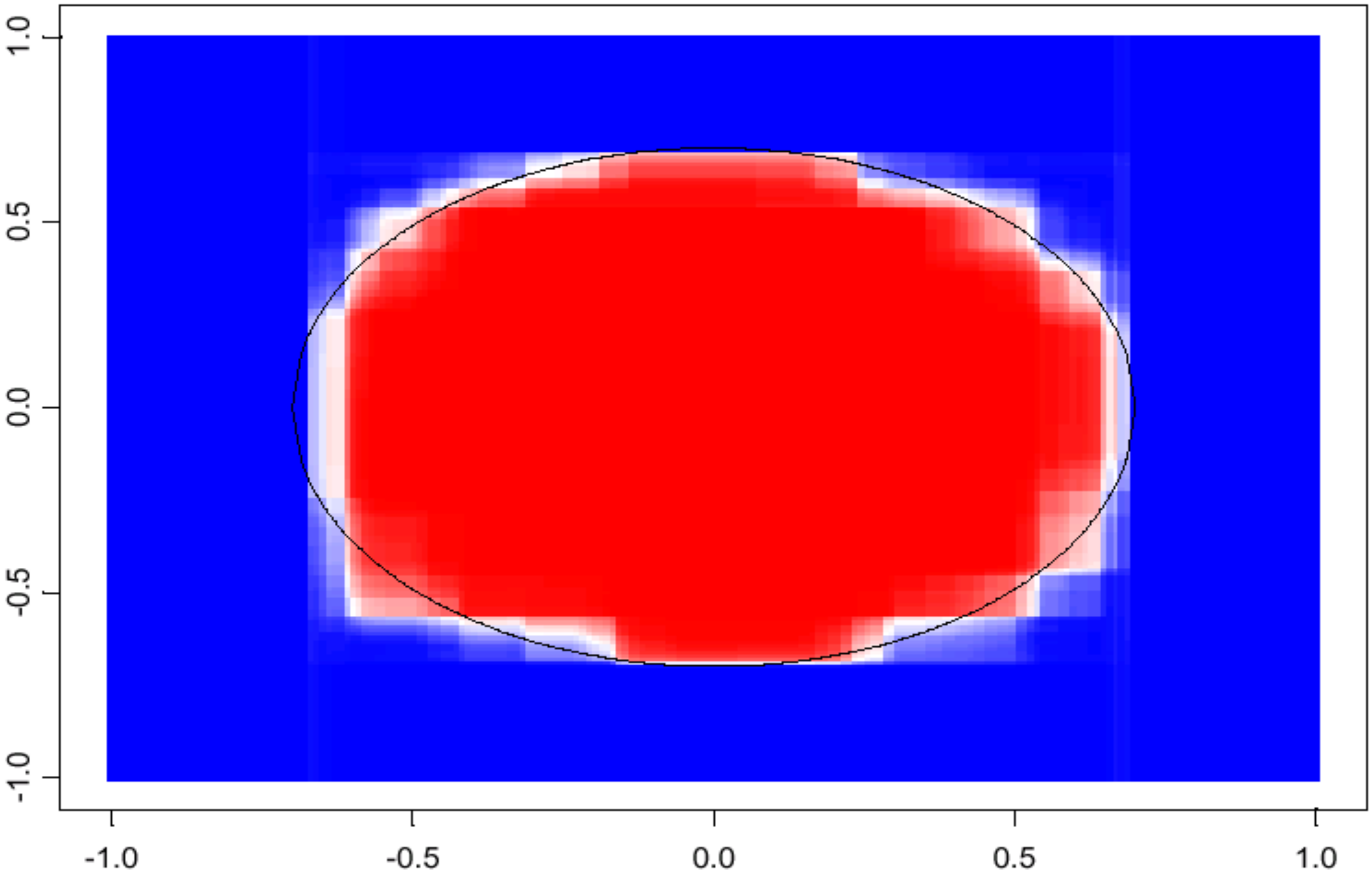


decision tree learning algorithm; very similar to ID3

CART decision boundary



100 bagged trees



shades of blue/red indicate strength of vote for particular classification

Random Forests

- Ensemble method specifically designed for decision tree classifiers

- Introduce two sources of randomness: "Bagging" and "Random input vectors"
  - Bagging method: each tree is grown using a bootstrap sample of training data
  - Random vector method: At each node, best split is chosen from a random sample of *m* attributes instead of all attributes

Random Forests

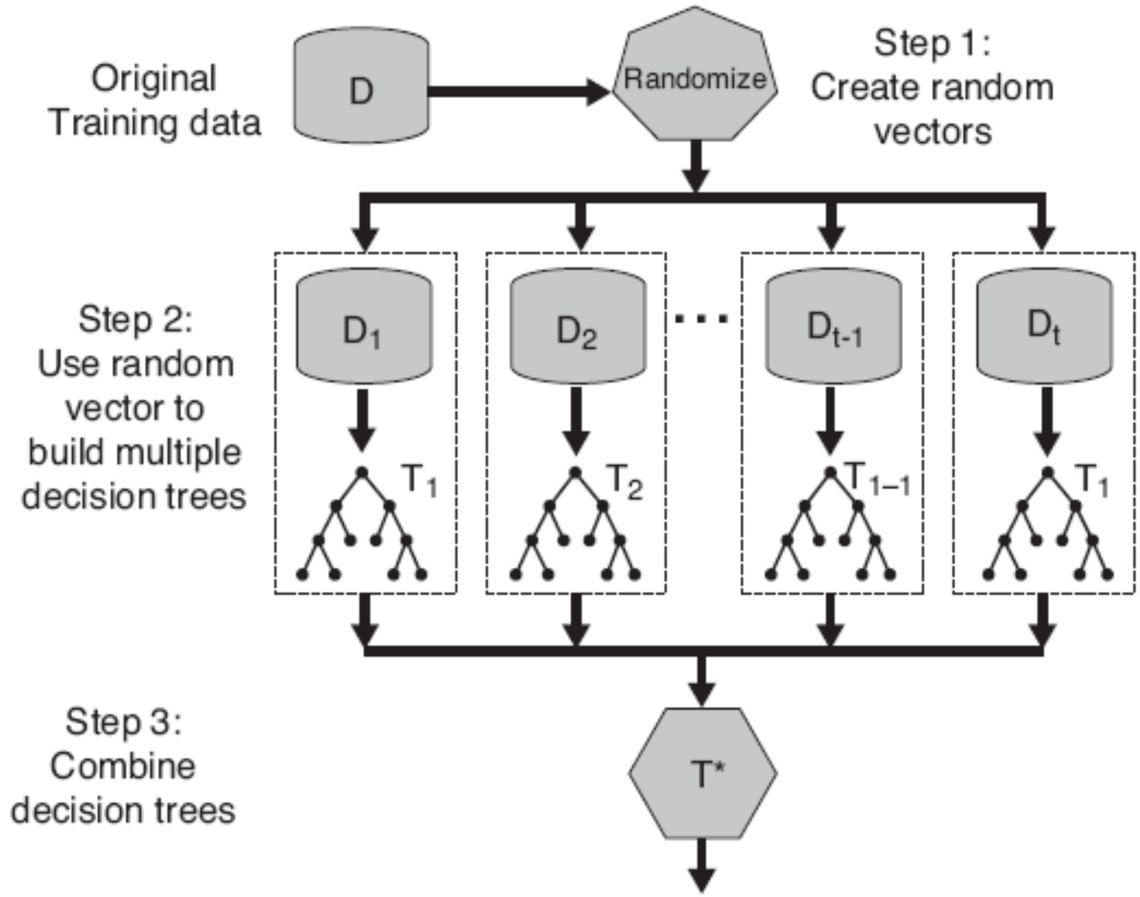


Figure 5.40. Random forests.

Random Forests Algorithm

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.