Supervised learning methods
Lecture 5

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

Plan for next few weeks

February 2014

Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
						1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	

Today: nearest neighbor methods, decision trees, random forests

PS4 released tomorrow

Midterm review

March 2014

S	M	T	W	T	F	S
						1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31					

Guest lecture: Yann LeCun on deep learning

Spring break: no class or lab!

Midterm exam: in class

Project proposals due

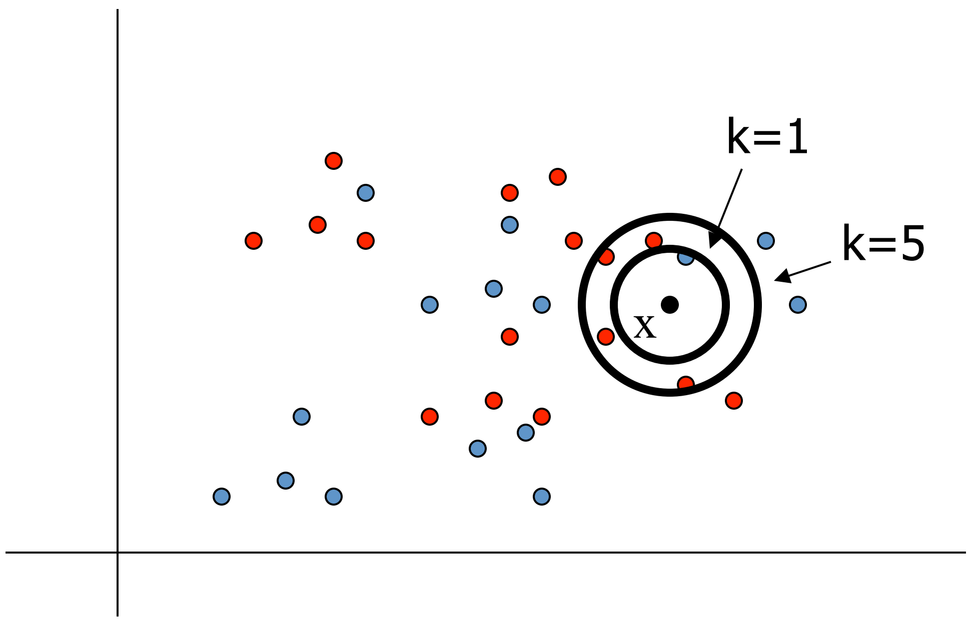
Lab: meet & chat with project advisers (registered students only)

Nearest Neighbor Algorithm

- Learning Algorithm:
  - Store training examples
- Prediction Algorithm:
  - To classify a new example **x** by finding the training example ($\mathbf{x}^i$,y^i) that is *nearest* to **x**
  - Guess the class $y = y^i$

K-Nearest Neighbor Methods

- To classify a new input vector x, examine the k-closest training data points to x and assign the object to the most frequently occurring class

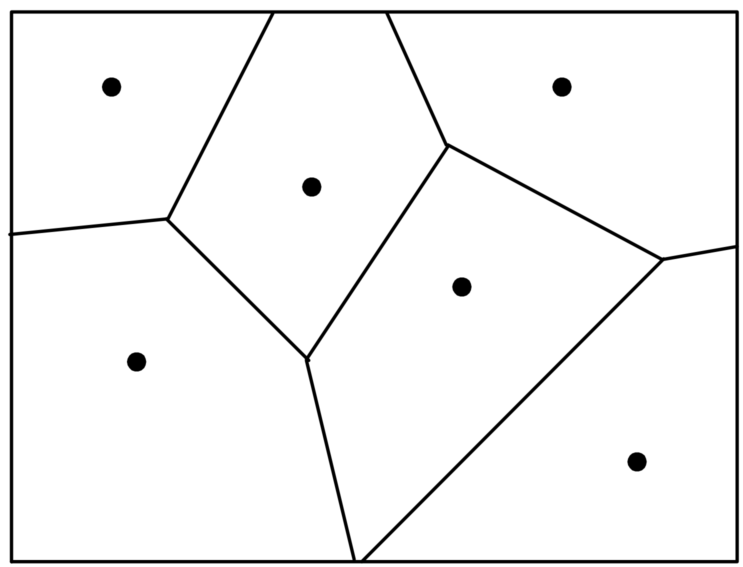


common values for k: 3, 5

Decision Boundaries

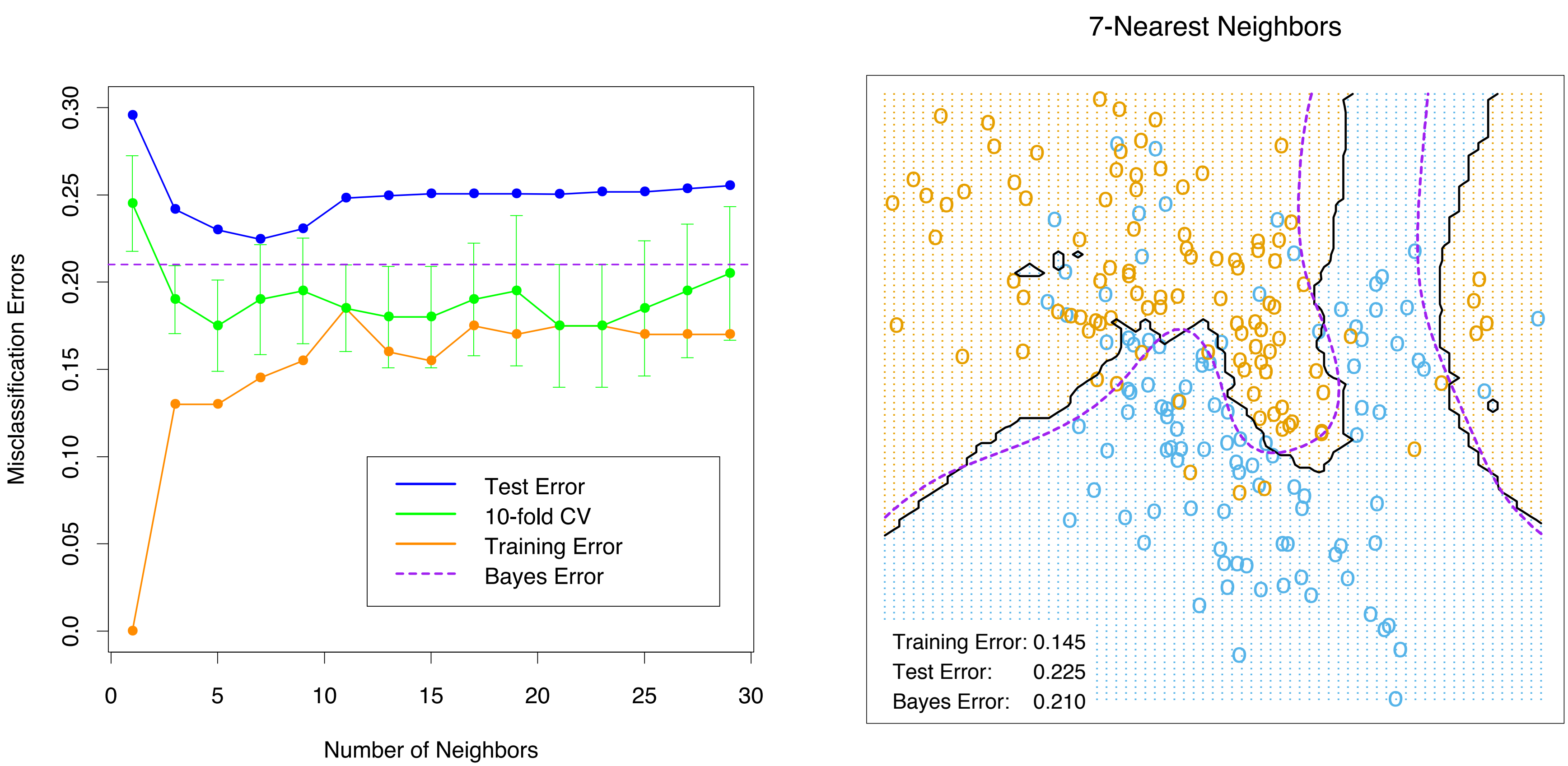
- The nearest neighbor algorithm does not explicitly compute decision boundaries. However, the decision boundaries form a subset of the Voronoi diagram for the training data.

1-NN Decision Surface



- The more examples that are stored, the more complex the decision boundaries can become

Example results for k-NN



[Figures from Hastie and Tibshirani, Chapter 13]

Nearest Neighbor

When to Consider

- Instance maps to points in R^n
- Less than 20 attributes per instance
- Lots of training data

Advantages

- Training is very fast
- Learn complex target functions
- Do not lose information

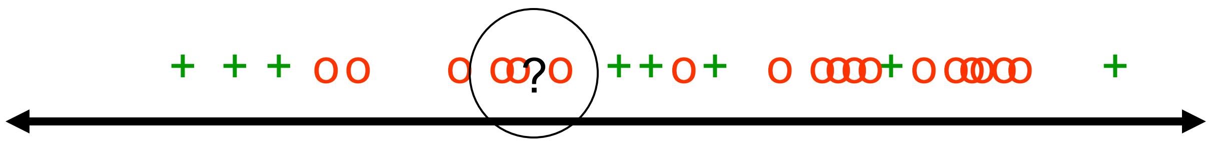
Disadvantages

- Slow at query time
- Easily fooled by irrelevant attributes

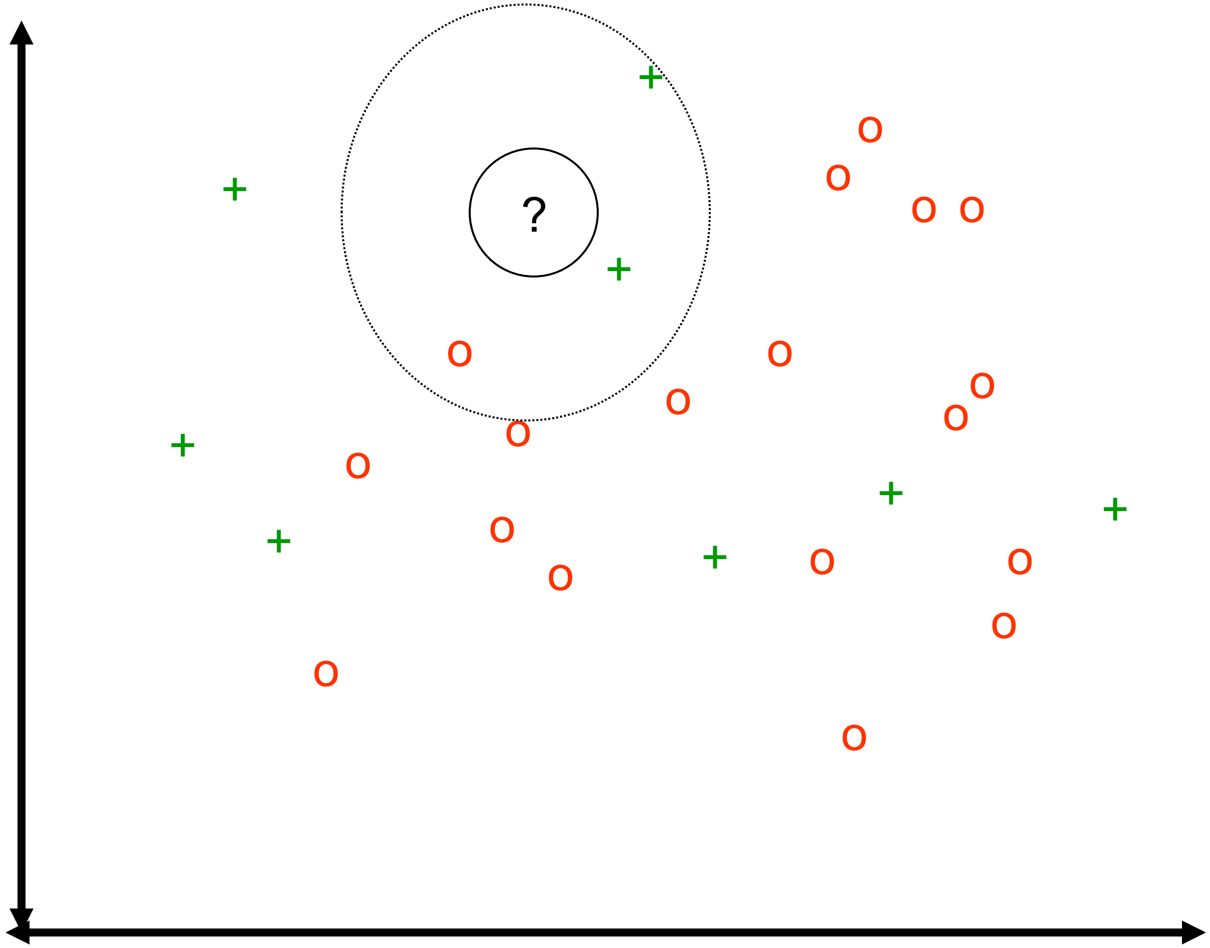
Issues

- Distance measure
  - Most common: Euclidean
- Choosing k
  - Increasing k reduces variance, increases bias
- For high-dimensional space, problem that the nearest neighbor may not be very close at all!
- Memory-based technique. Must make a pass through the data for each classification. This can be prohibitive for large data sets.

k-NN and irrelevant features



k-NN and irrelevant features



Weighted *k*-NN

- Consider the following generalization of the *k*-NN algorithm (specialized to binary classification):

$$\hat{y}(\vec{x}) \leftarrow \operatorname{sign}\left(\sum_{i=1}^{k} y_i s(\vec{x}_i, \vec{x})\right) \text{ with } s(\vec{x}_i, \vec{x}) = \frac{1}{\|\vec{x}_i - \vec{x}\|_2^2} \text{ or... } s(\vec{x}_i, \vec{x}) = \exp\left(-\frac{\|\vec{x}_i - \vec{x}\|_2^2}{2\sigma^2}\right)$$

- Weighs the *i*'th training point's label by how far $\mathbf{x}_i$ is from $\mathbf{x}$

k-NN is similar to SVM with Gaussian kernel!

- Consider the following generalization of the k-NN algorithm (specialized to binary classification):

$$\hat{y}(\vec{x}) \leftarrow \text{sign}\left(\sum_{i=1}^{\text{N}} y_i s(\vec{x}_i, \vec{x})\right) \text{ with } s(\vec{x}_i, \vec{x}) = \frac{1}{\|\vec{x}_i - \vec{x}\|_2^2} \text{ or... } s(\vec{x}_i, \vec{x}) = \exp\left(-\frac{\|\vec{x}_i - \vec{x}\|_2^2}{2\sigma^2}\right)$$

- Looks at *all* training points (i.e., k=N), but weighs the *i*'th training point's label by how far $\mathbf{x}_i$ is from $\mathbf{x}$

- Now compare this to classification with SVM and a Gaussian kernel:

$$\hat{y}(\vec{x}) \leftarrow \text{sign}\left(\sum_{i=1}^{N} \alpha_i y_i K(\vec{x}_i, \vec{x})\right) \qquad K(\vec{u}, \vec{v}) = \exp\left(-\frac{||\vec{u} - \vec{v}||_2^2}{2\sigma^2}\right) \qquad 0 \leq \alpha_i \leq C$$

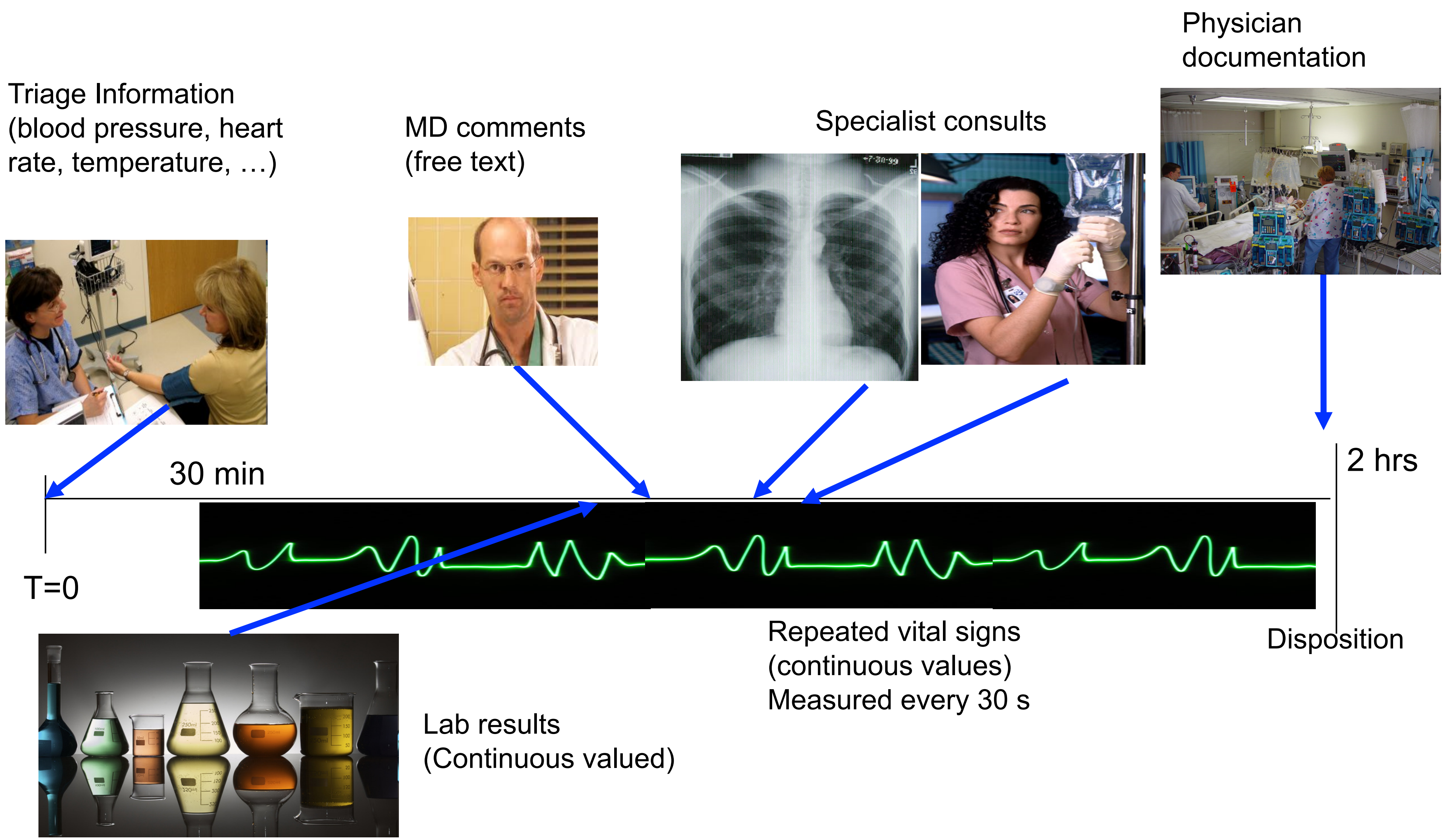
- The discriminant functions are nearly identical! The SVM has parameters α_i that can be learned

KNN Advantages

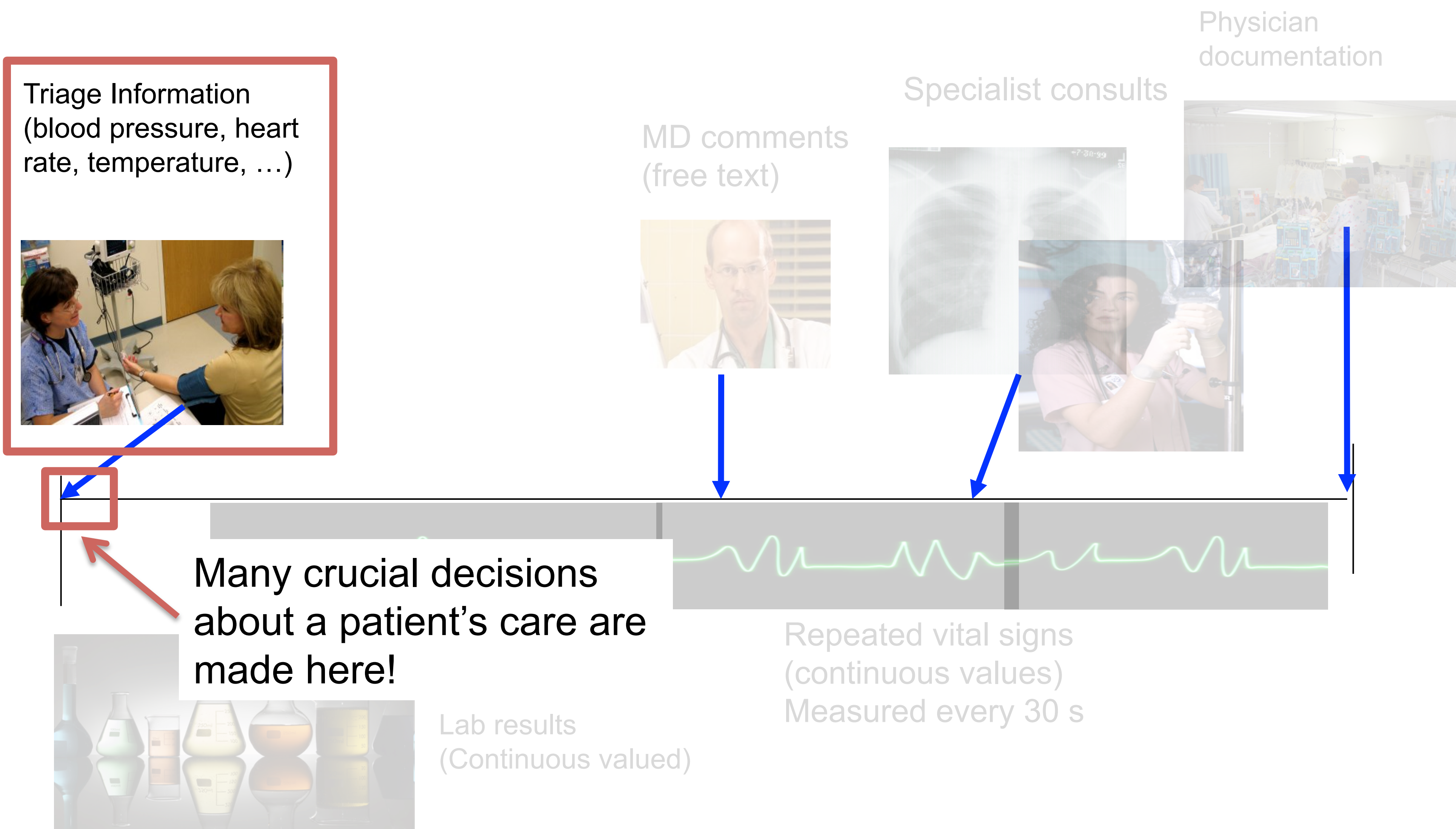
- Easy to program
- No optimization or training required
- Classification accuracy can be very good; can outperform more complex models

Decision Trees

Machine Learning in the ER

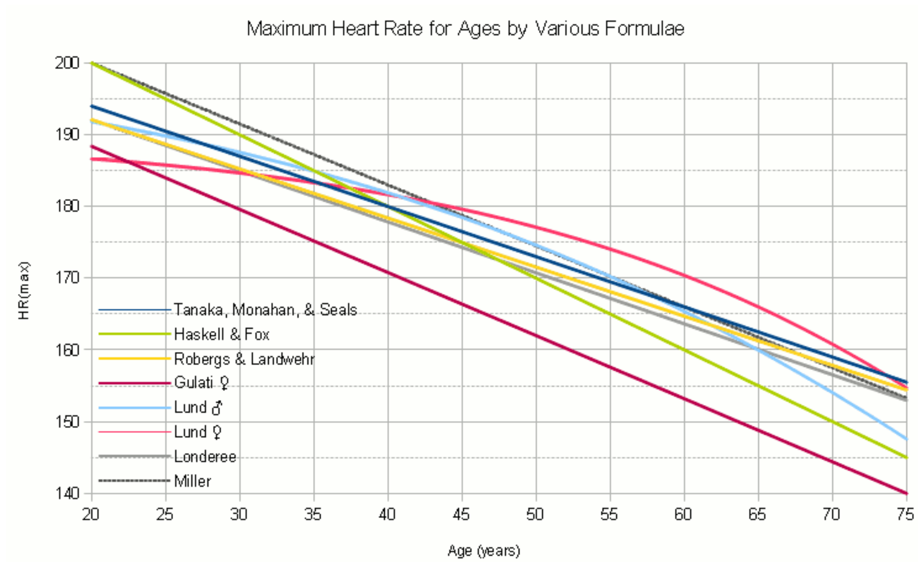


Can we predict infection?



Can we predict infection?

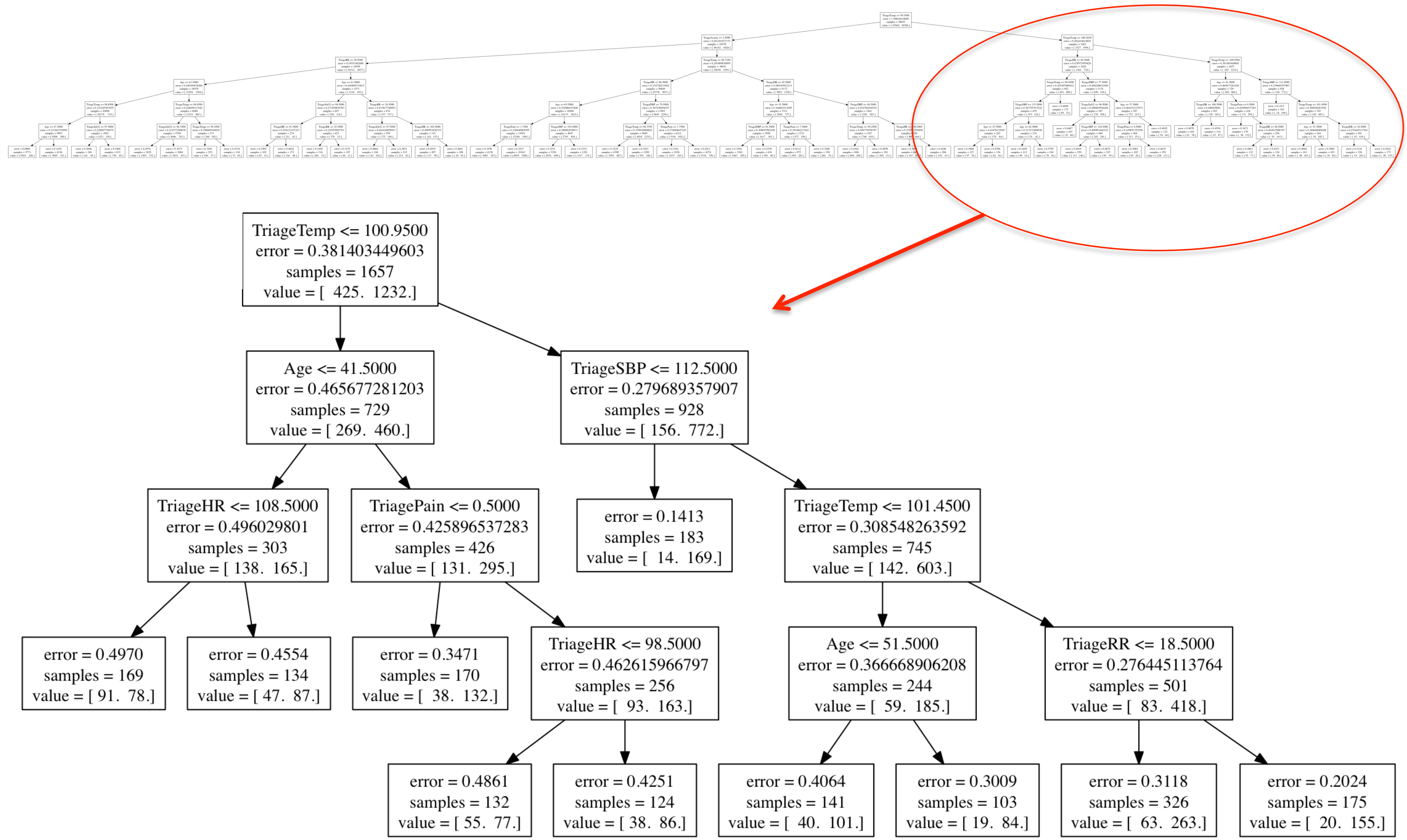
- Previous automatic approaches based on simple criteria:
  - Temperature < 96.8 °F or > 100.4 °F
  - Heart rate > 90 beats/min
  - Respiratory rate > 20 breaths/min
- Too simplified… e.g., heart rate depends on age!



Can we predict infection?

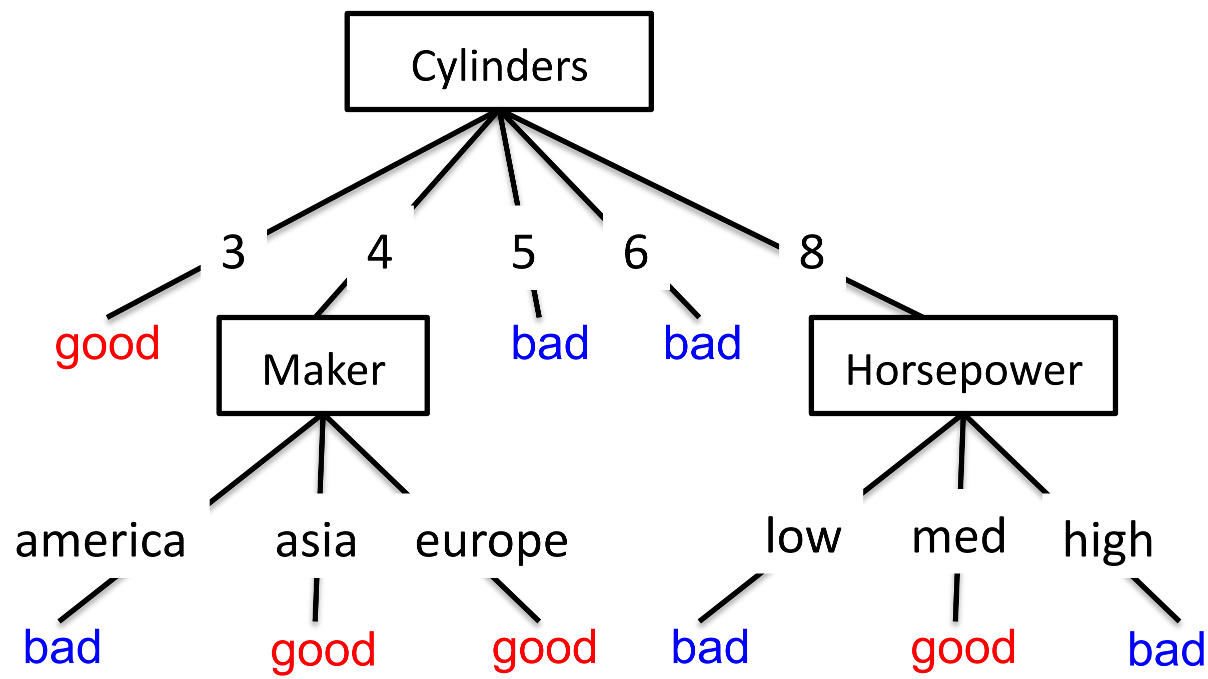
- These are the attributes we have for each patient:
  - Temperature
  - Heart rate (HR)
  - Respiratory rate (RR)
  - Age
  - Acuity and pain level
  - Diastolic and systolic blood pressure (DBP, SBP)
  - Oxygen Saturation (SaO2)
- We have these attributes + label (infection) for 200,000 patients!
- Let’s **learn** to classify infection

Predicting infection using decision trees



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

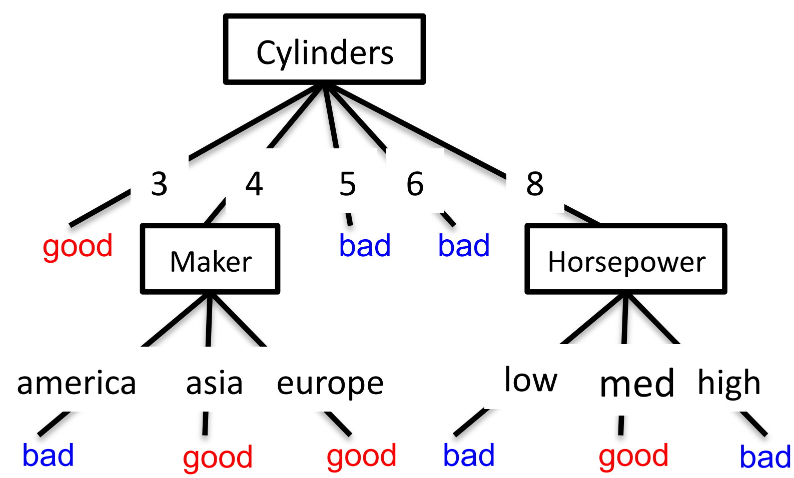


Human interpretable!

Hypothesis space

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

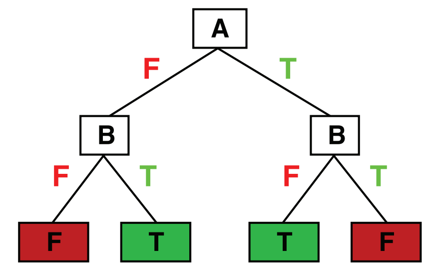
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low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



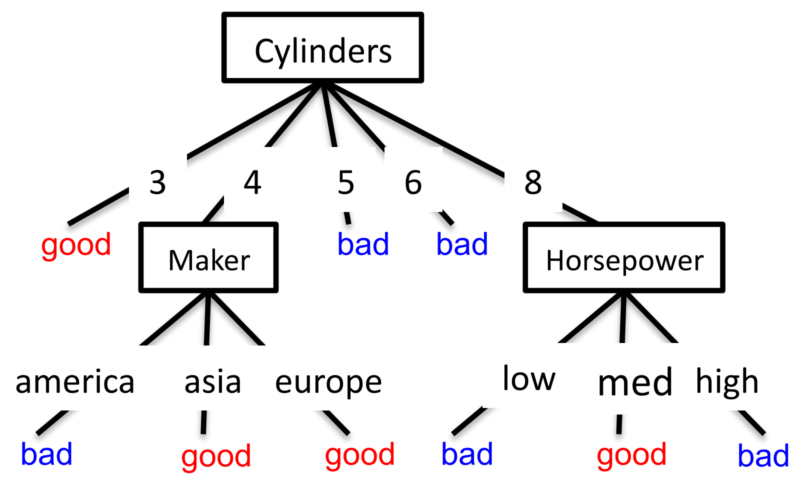
What functions can be represented?

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



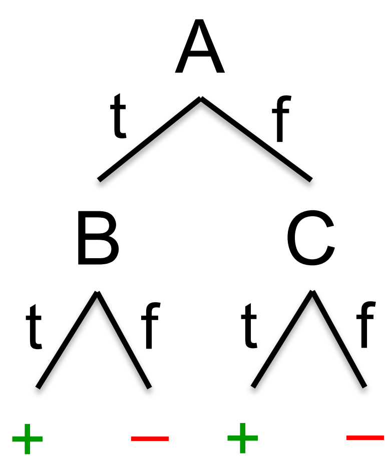
(Figure from Stuart Russell)

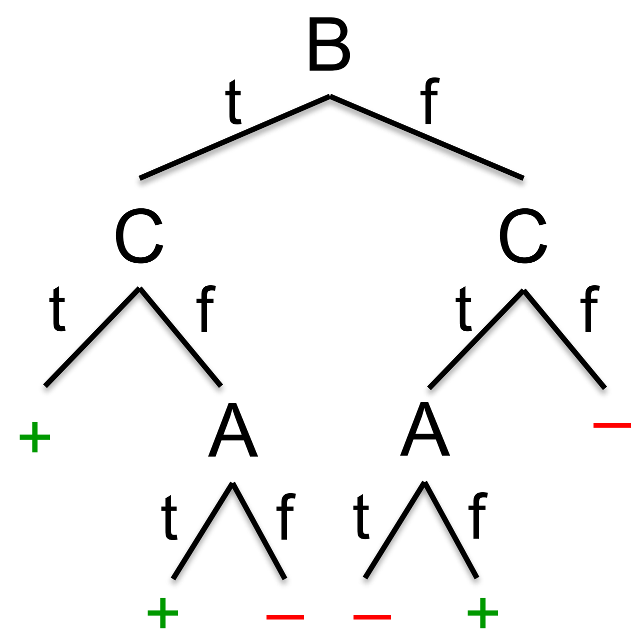


$$cyl{=}3 \lor (cyl{=}4 \land (maker{=}asia \lor maker{=}europe)) \lor \ldots$$

Are all decision trees equal?

- Many trees can represent the same concept
- But, not all trees will have the same size!
  - e.g., $\phi = (A \wedge B) \vee (\neg A \wedge C)$ -- ((A and B) or (not A and C))



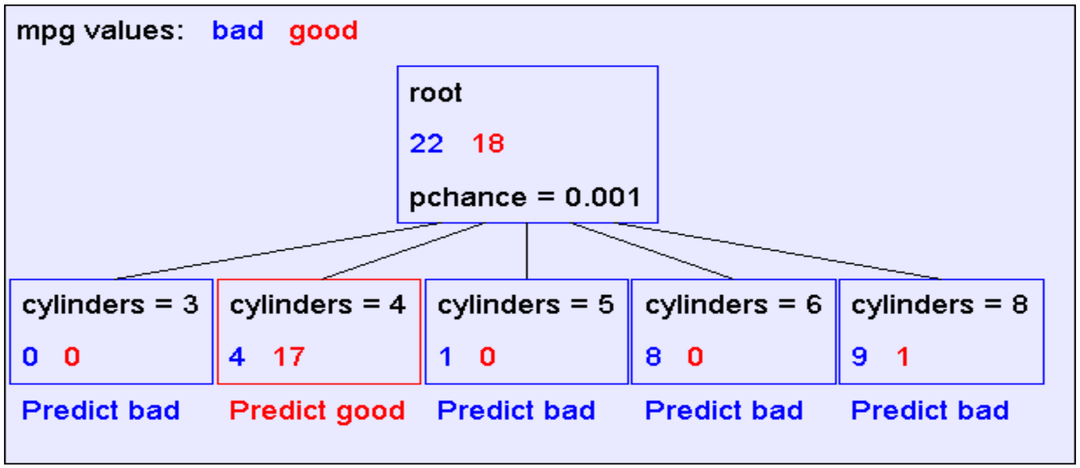


- Which tree do we prefer?

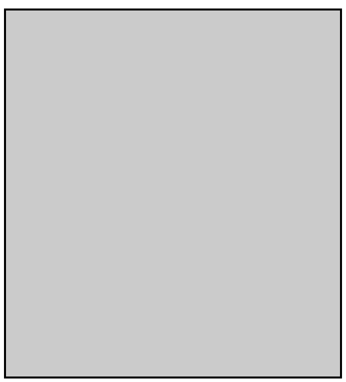
Learning decision trees is hard!!!

- 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

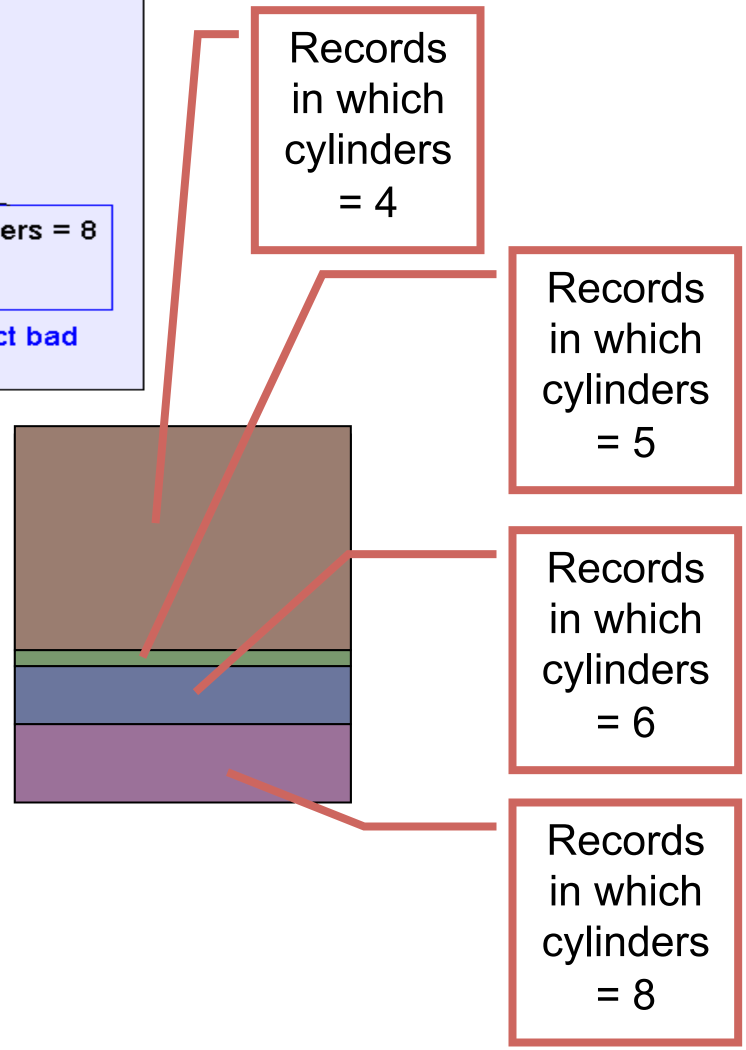
Key idea: Greedily learn trees using **recursion**



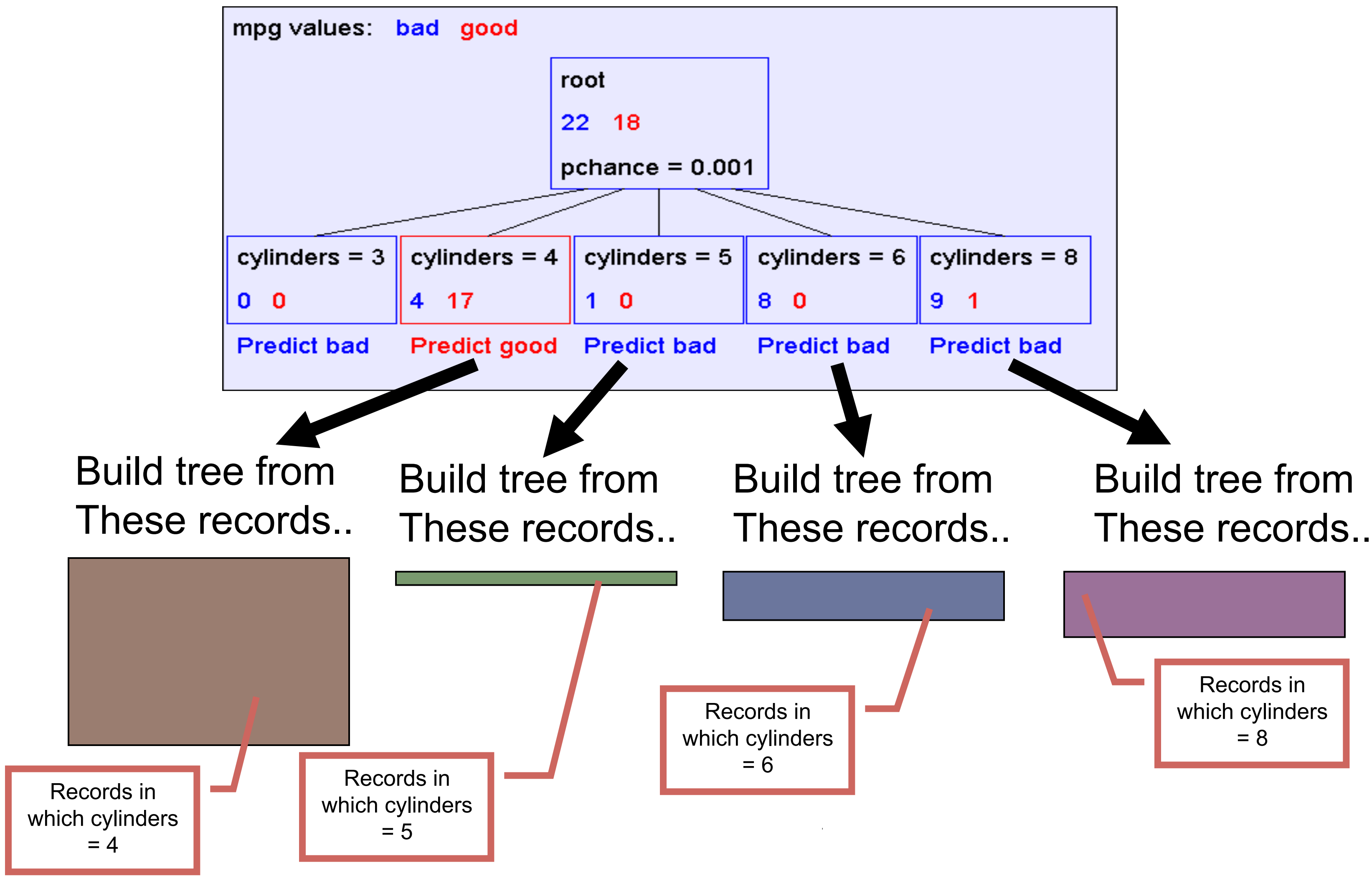
Take the Original Dataset..



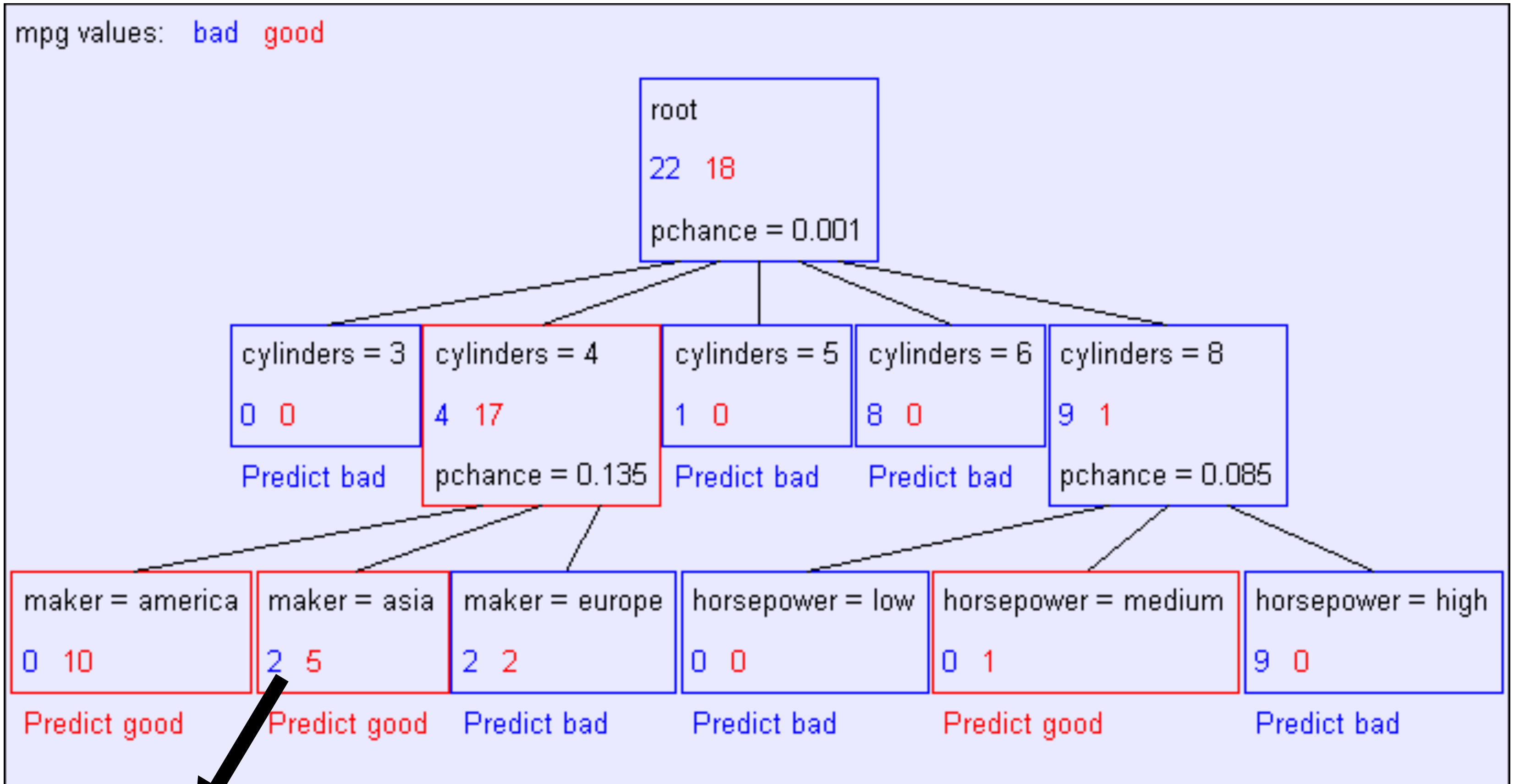
And partition it according to the value of the attribute we split on



Recursive Step



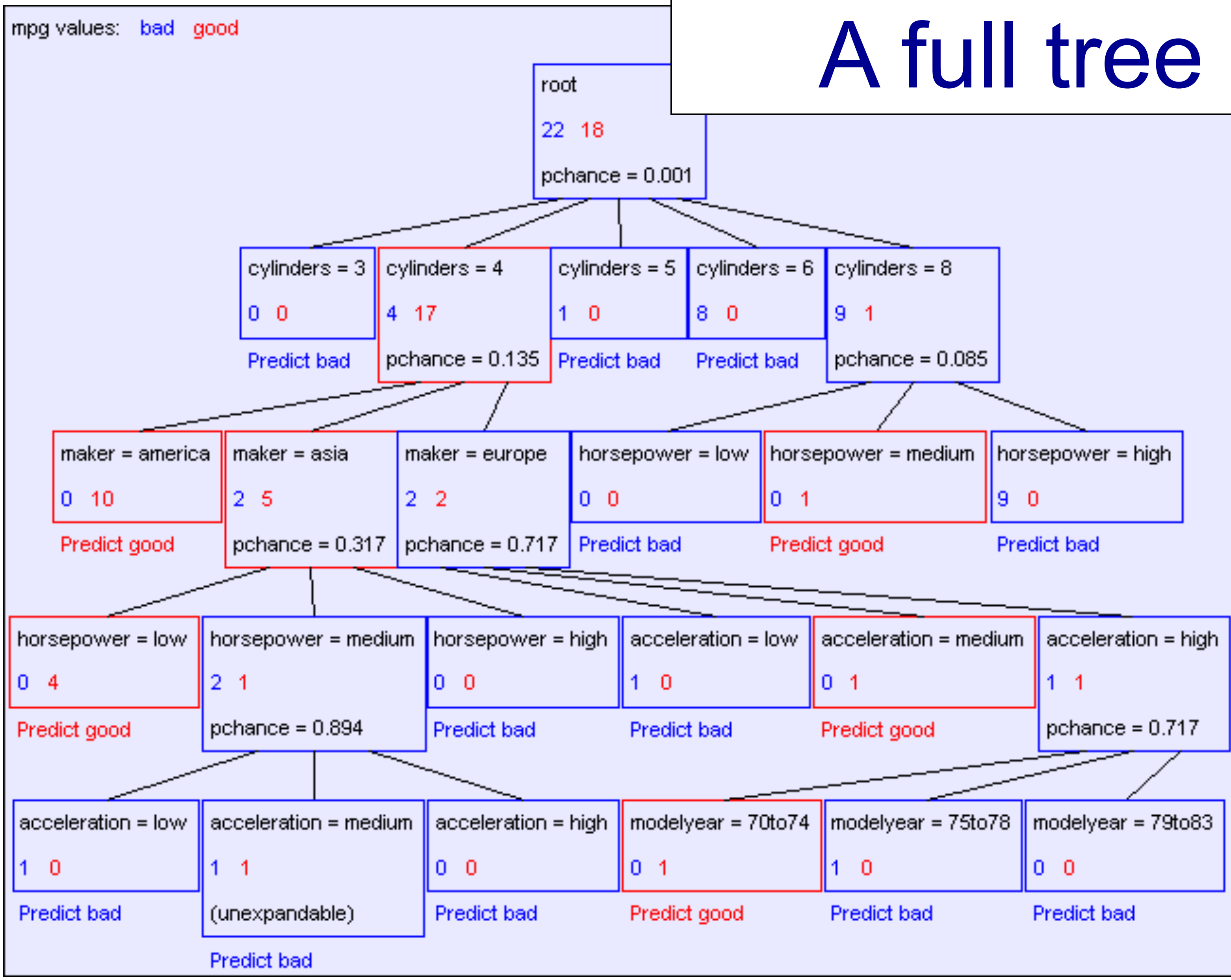
Second level of tree



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)

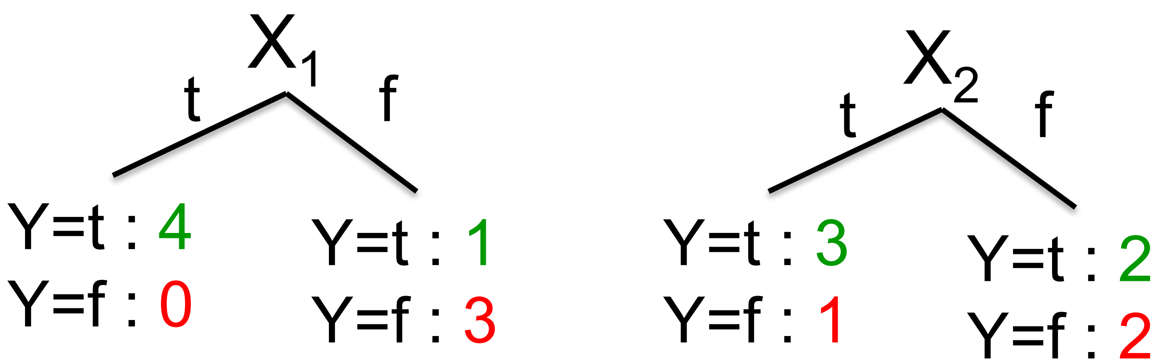
A full tree



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

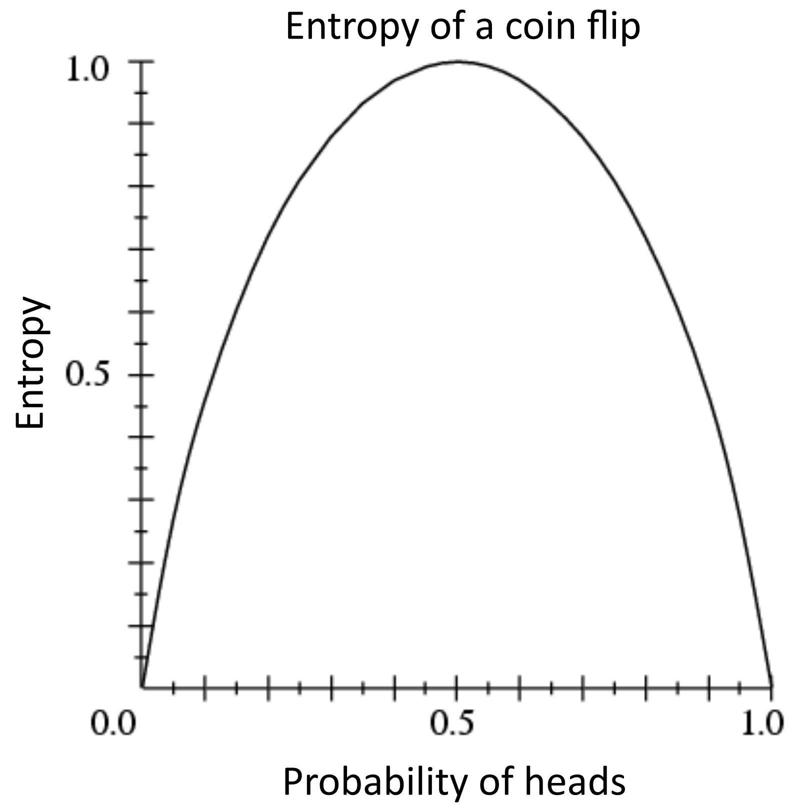
Entropy

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)

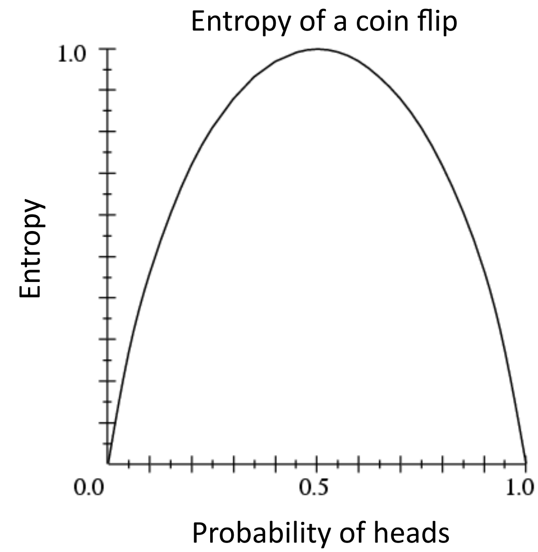


High, Low Entropy

- “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

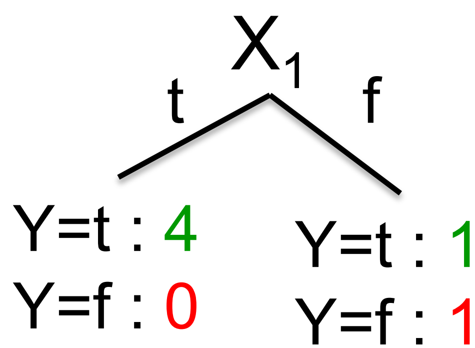
Conditional Entropy $H(Y|X)$ of a random variable Y conditioned on a random variable X

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

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:

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

$IG(X_1) > 0 \rightarrow$ 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

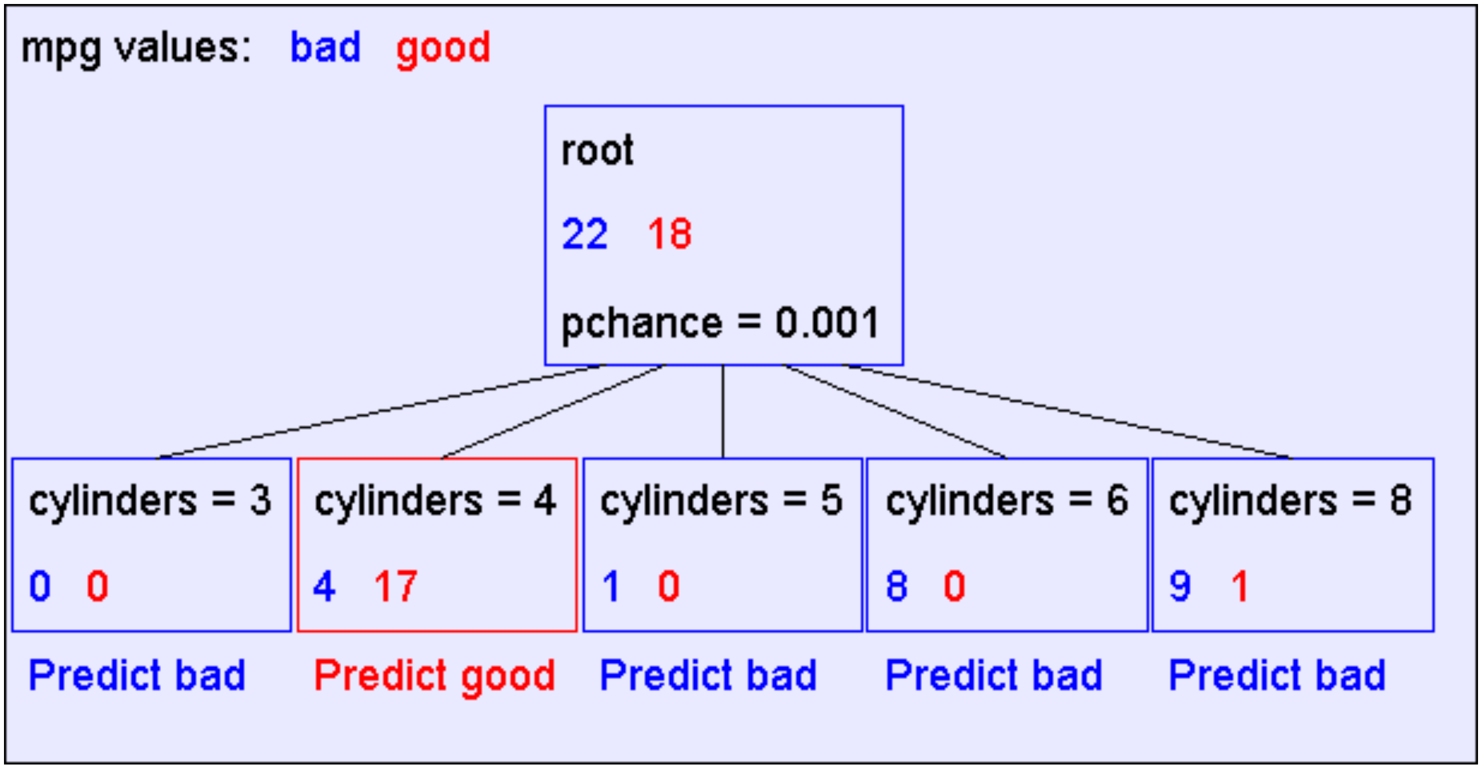
Learning decision trees

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

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

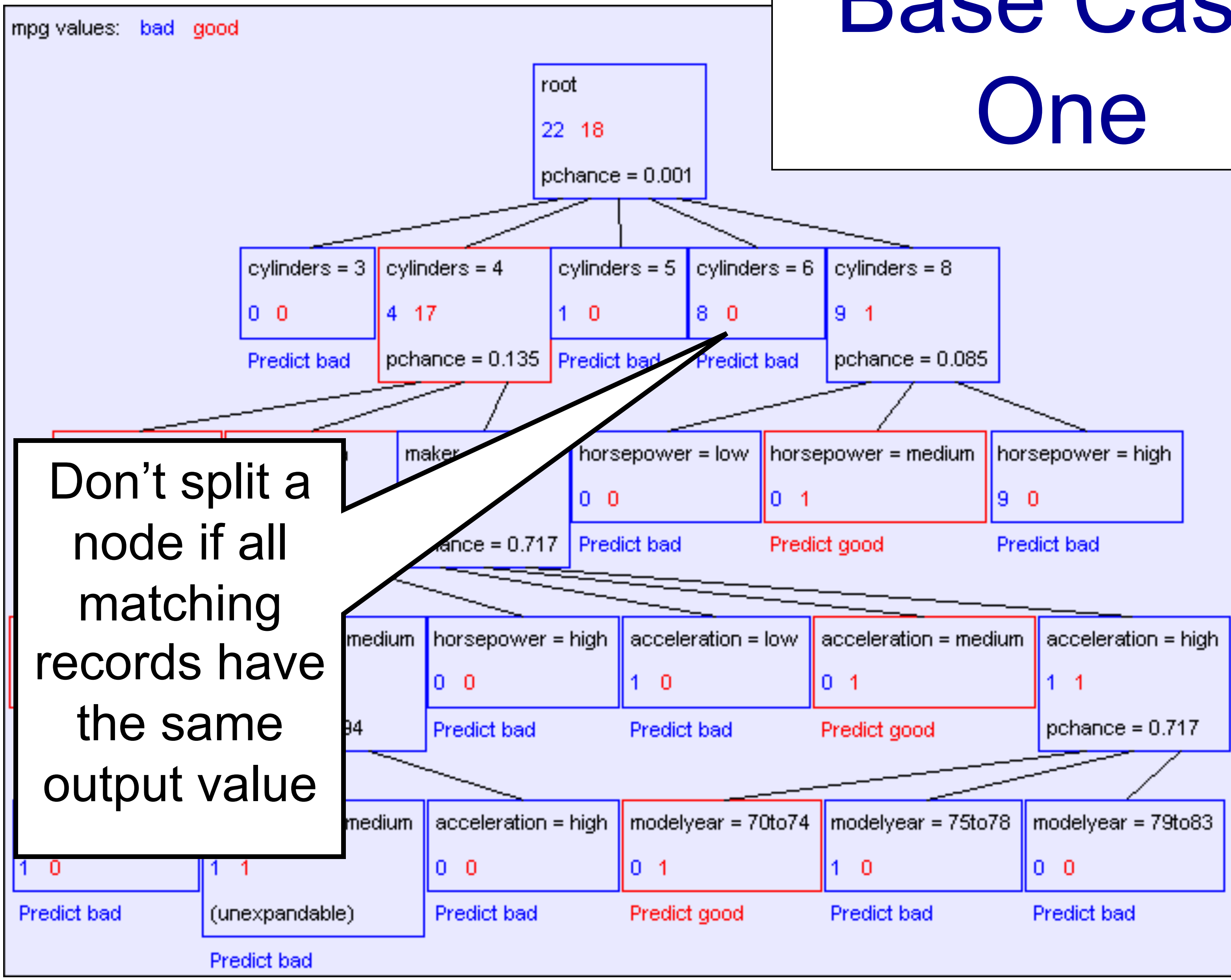
- Recurse

When to stop?



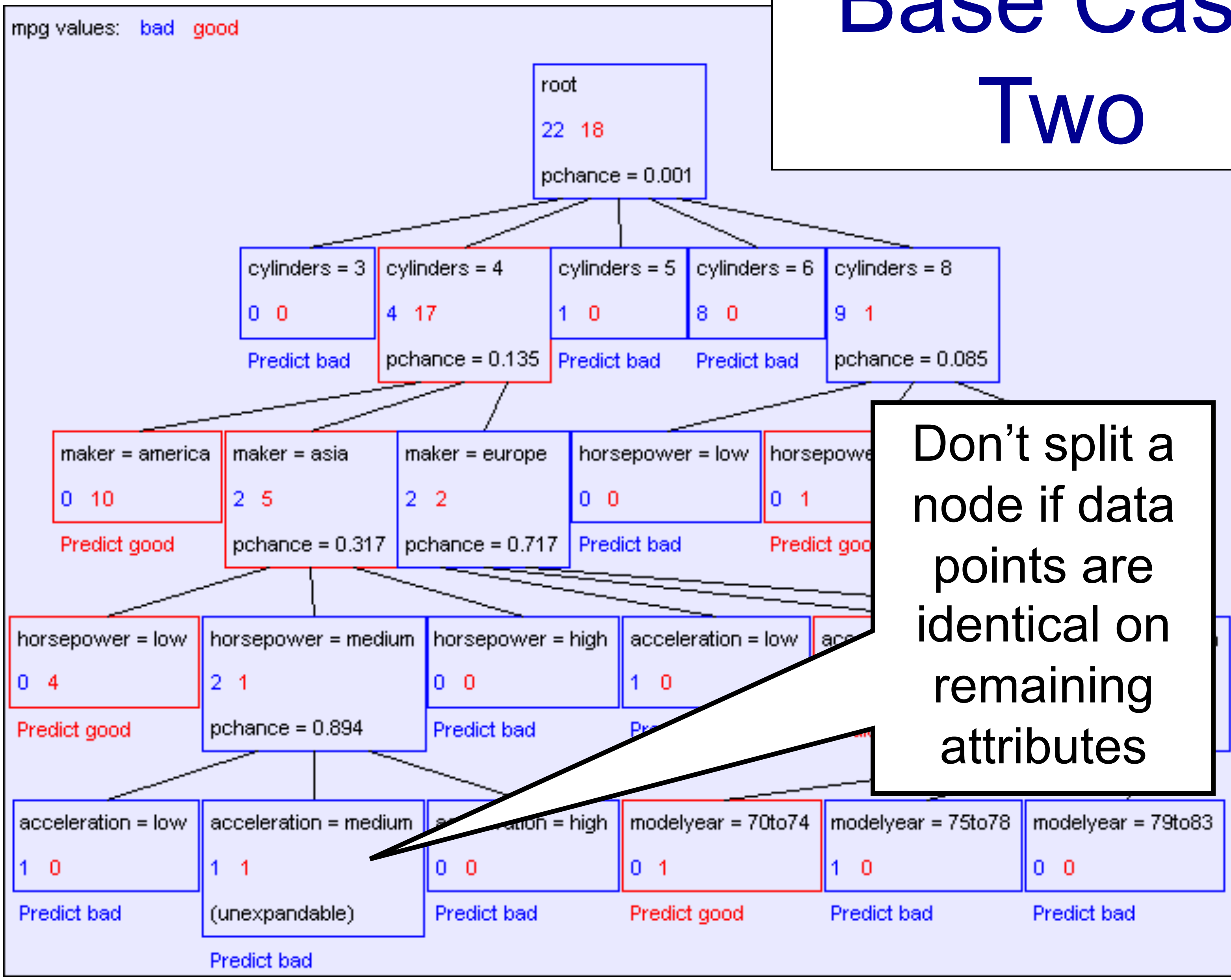
First split looks good! But, when do we stop?

Base Case One



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

Base Case Two



Don't split a node if data points are identical on remaining attributes

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

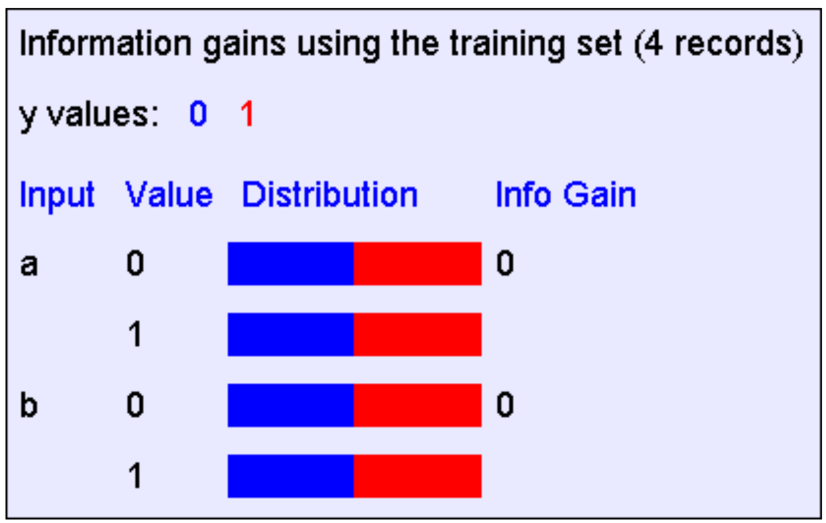
- *This is not a good idea*

The problem with proposed case 3

$y = a \text{ XOR } b$

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

The information gains:



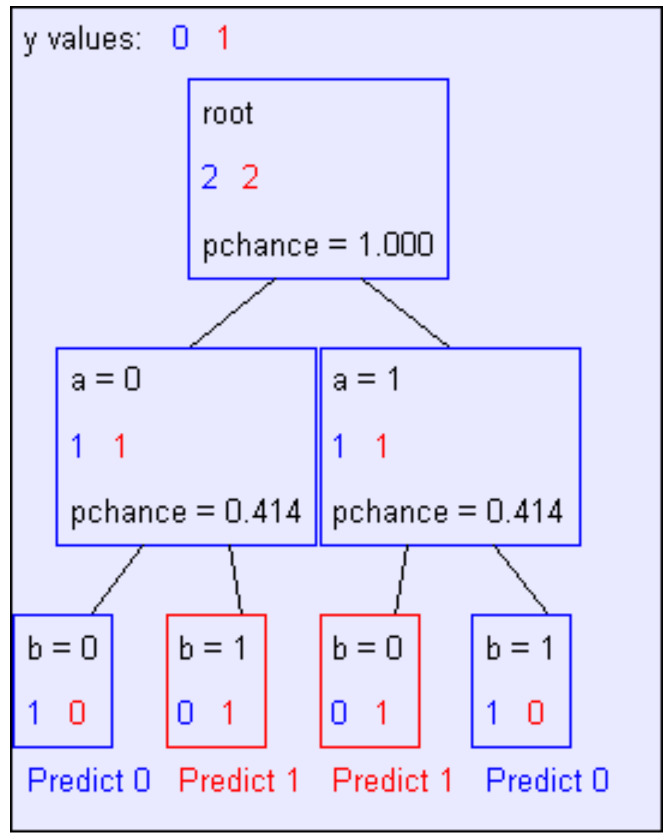
If we omit proposed case 3:

y = a XOR b

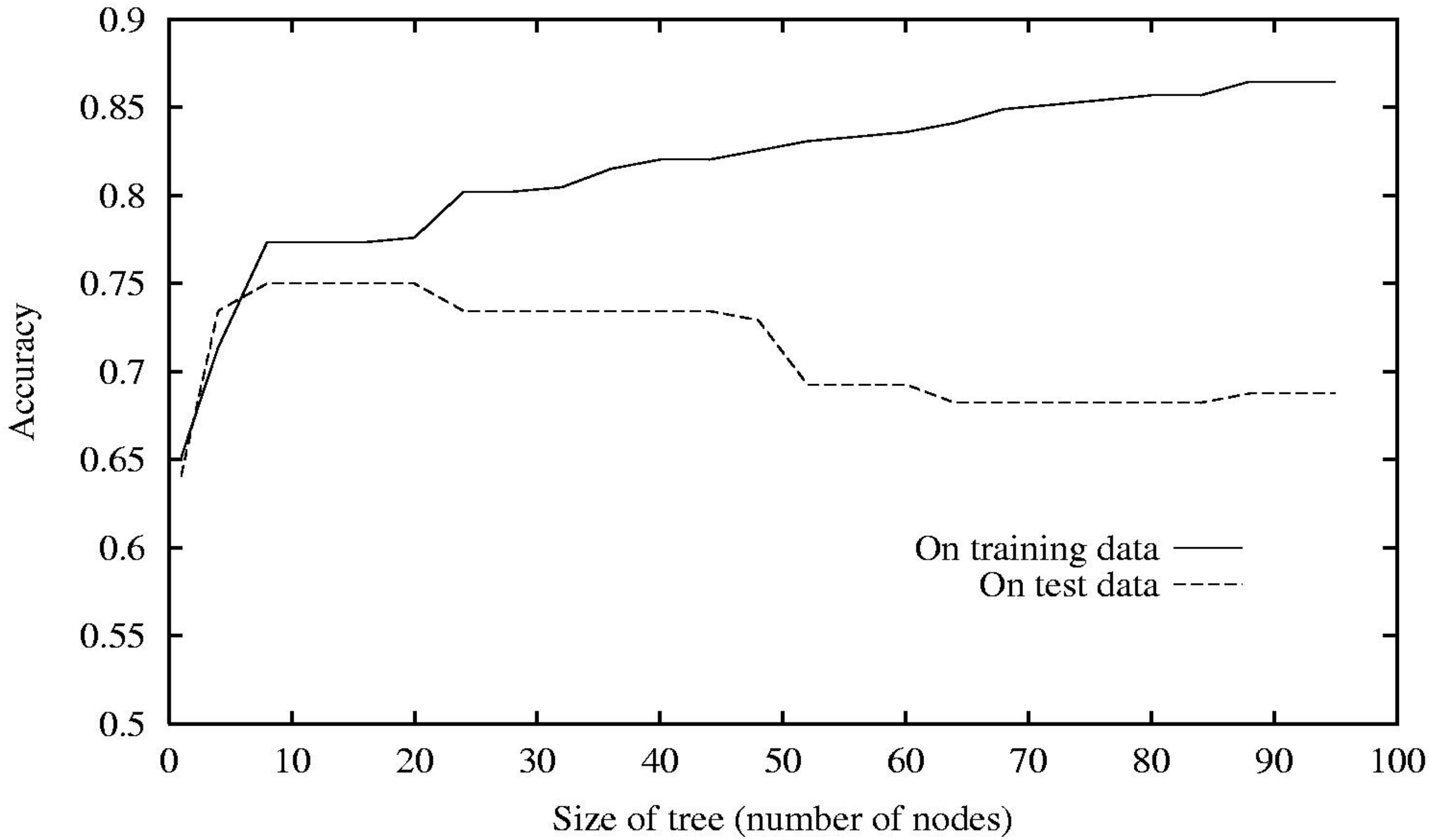
a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

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

The resulting decision tree:



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
  - Fixed number of leaves
- Random forests

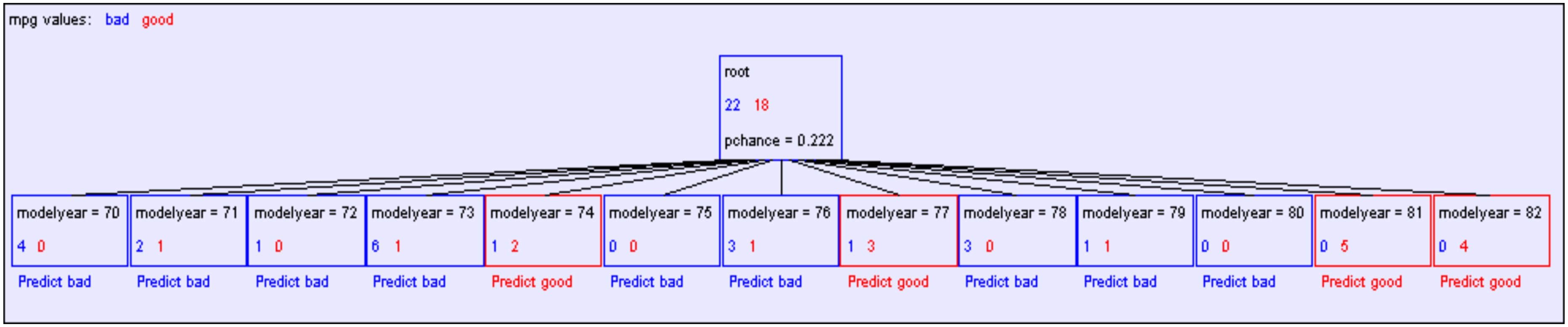
Real-Valued inputs

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:

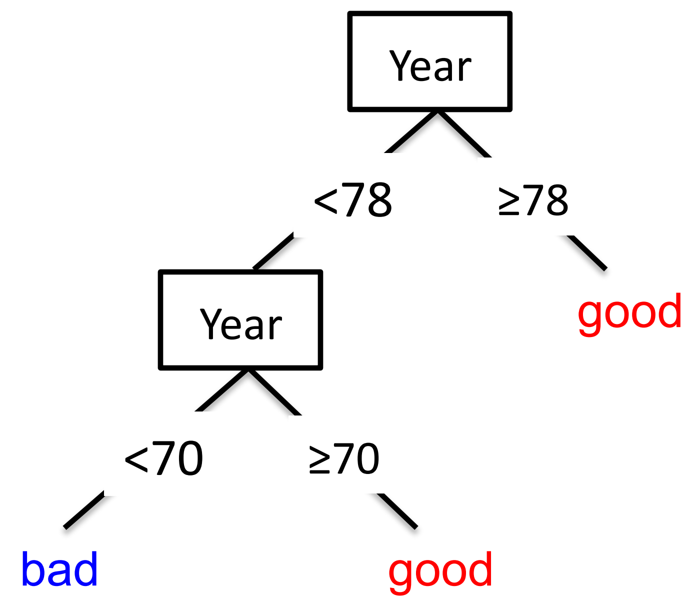


Hopeless: hypothesis with such a high branching factor will shatter *any* dataset and overfit

Threshold splits

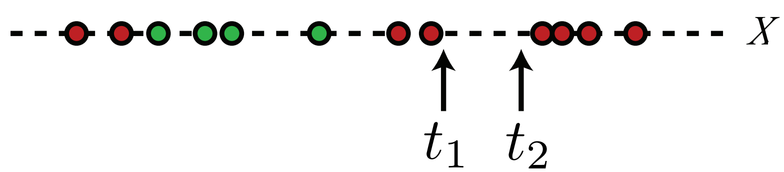
- Binary tree: split on attribute X at value t
  - One branch: X < t
  - Other branch: X ≥ t

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

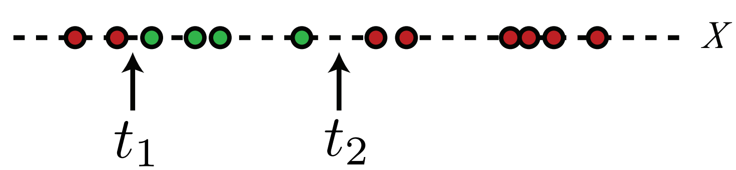


The set of possible thresholds

- 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!

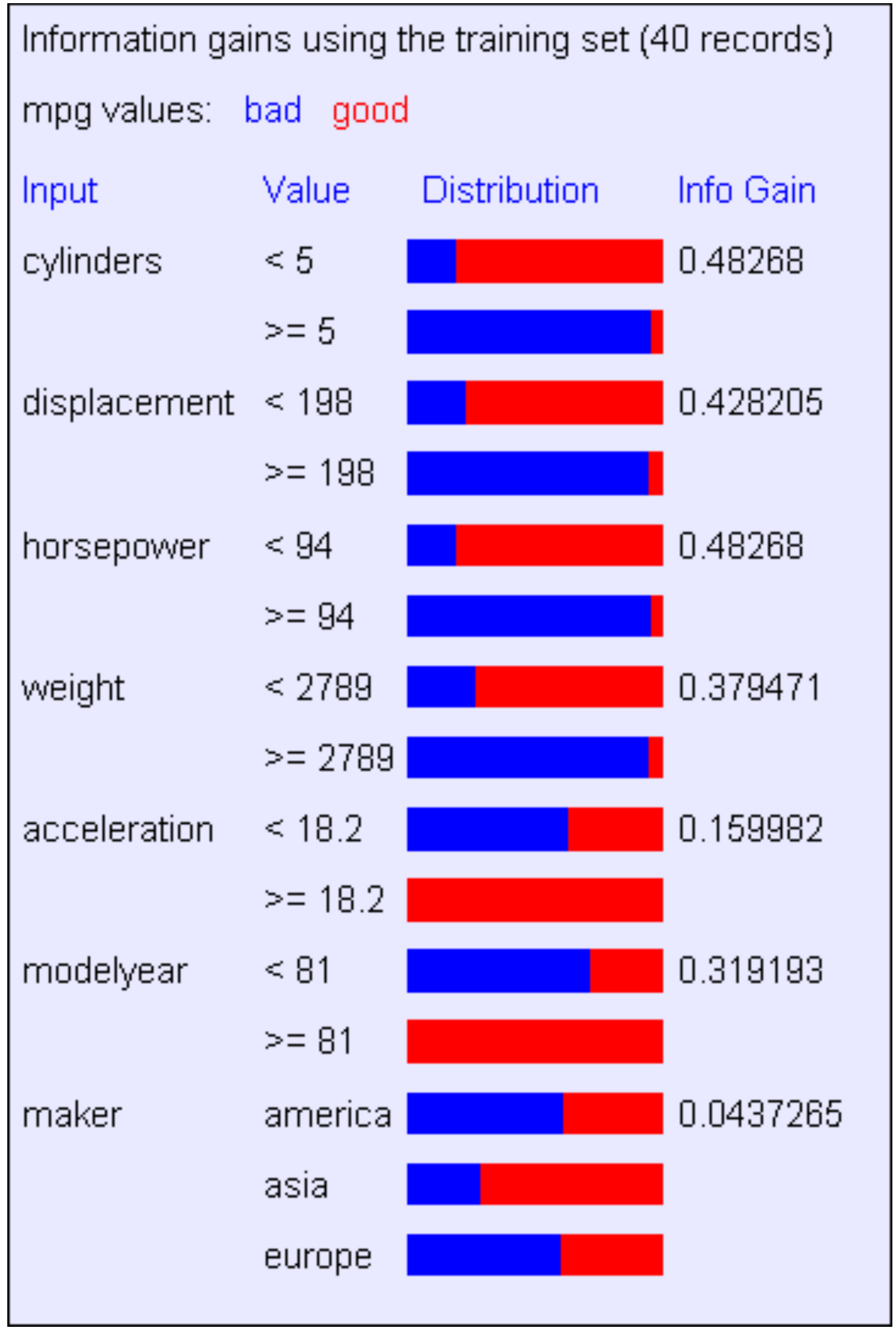


(Figures from Stuart Russell)

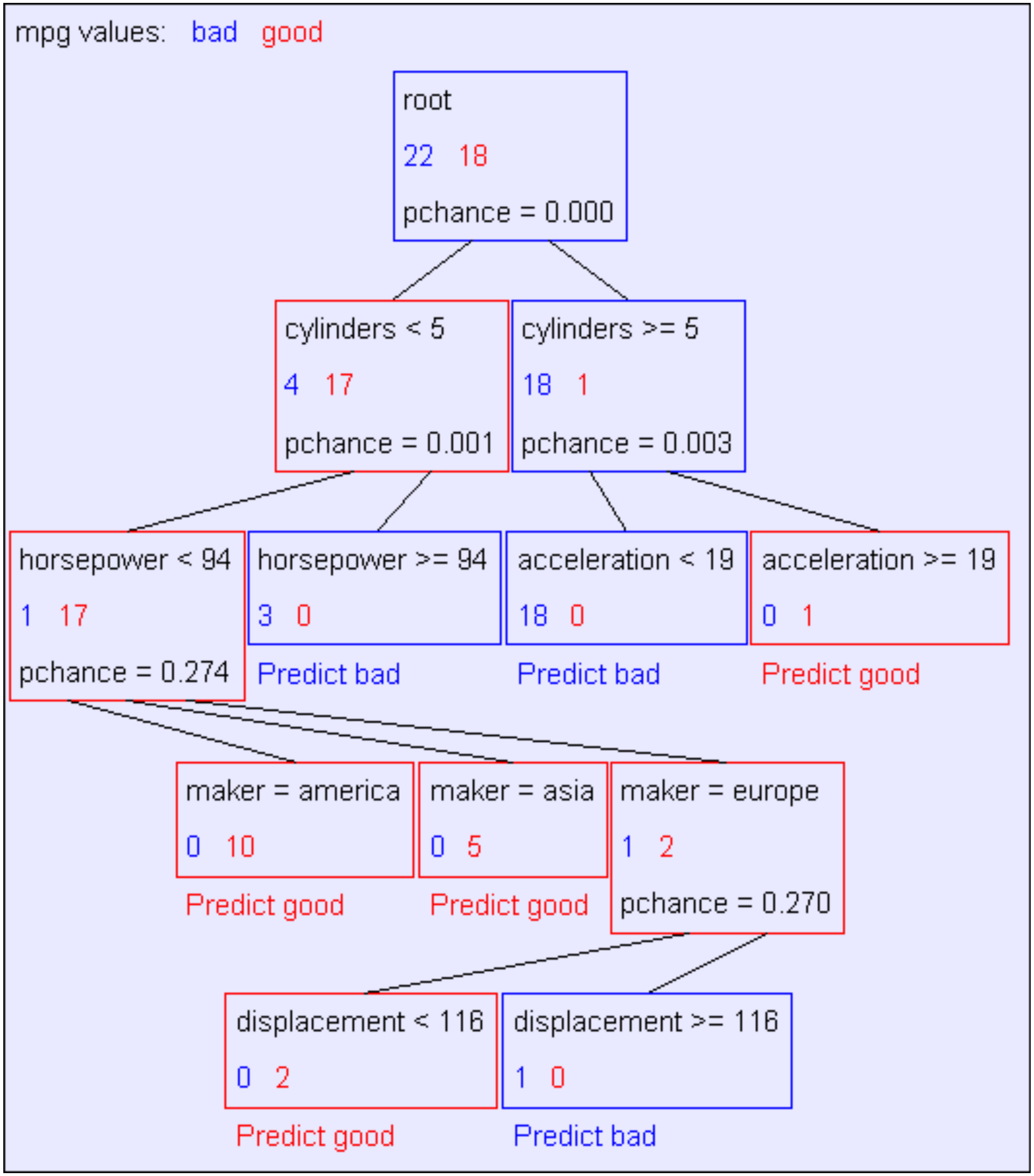
Picking the best threshold

- 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

Example with MPG



Example tree for our continuous dataset



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

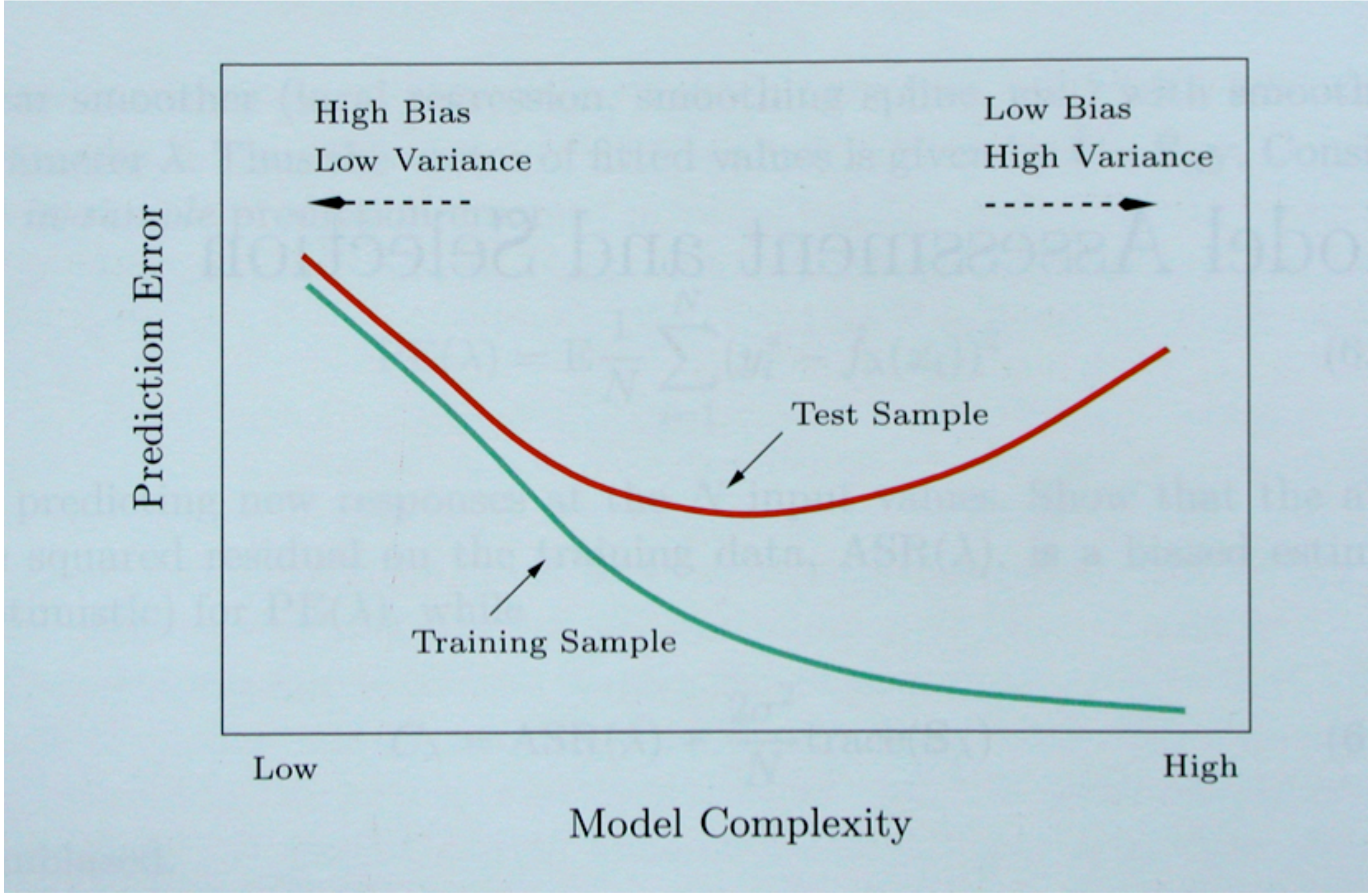
Leaderboard

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				

	users →					
movies ↓	1		?	3	5	?
	?	1				2
		4		4	5	?

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

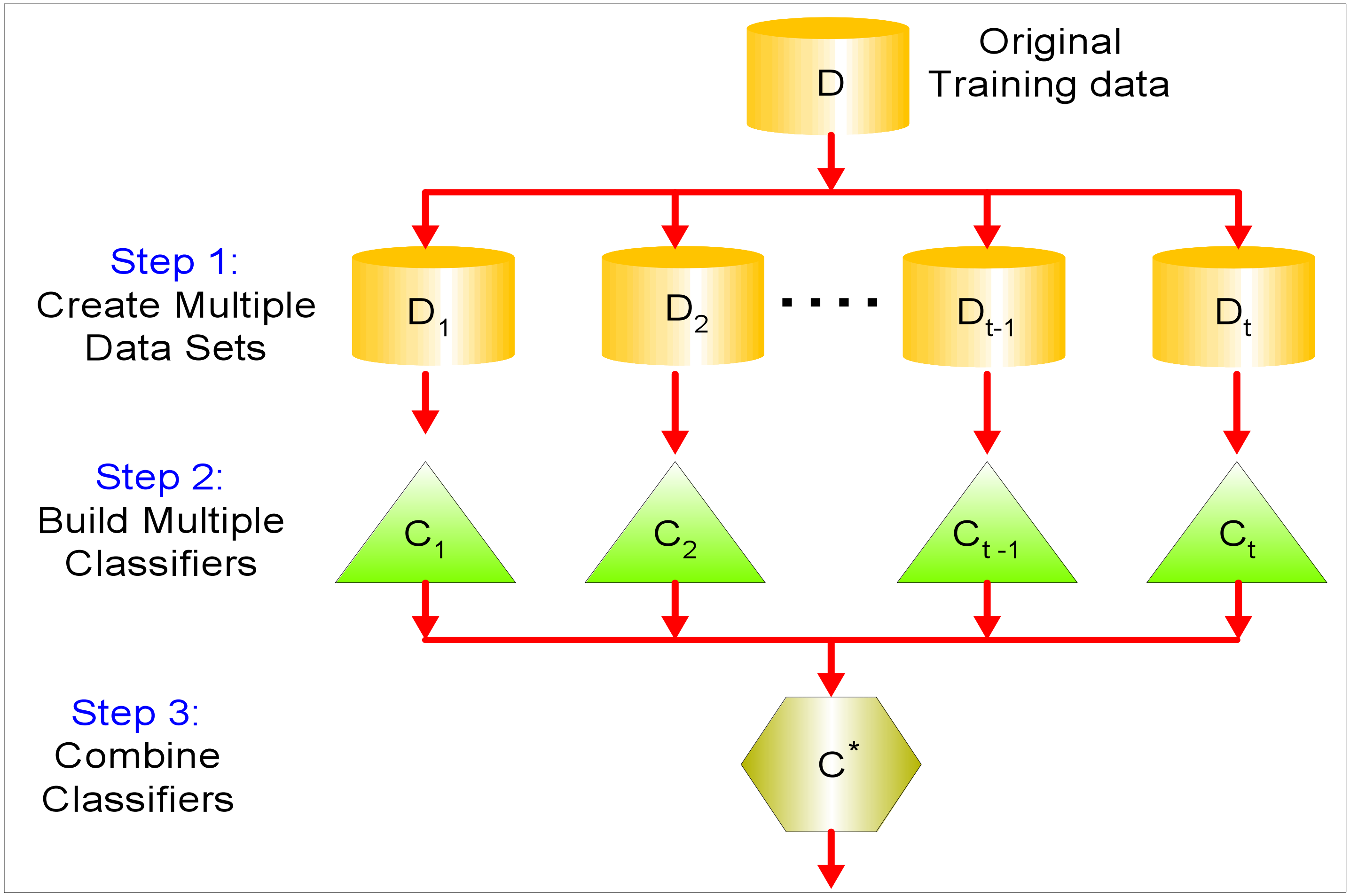
where do multiple models come from?

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 … D_k.
  - Train distinct classifier on each D_i.
  - Classify new instance by majority vote / average.

General Idea



Example of Bagging

- Sampling with replacement

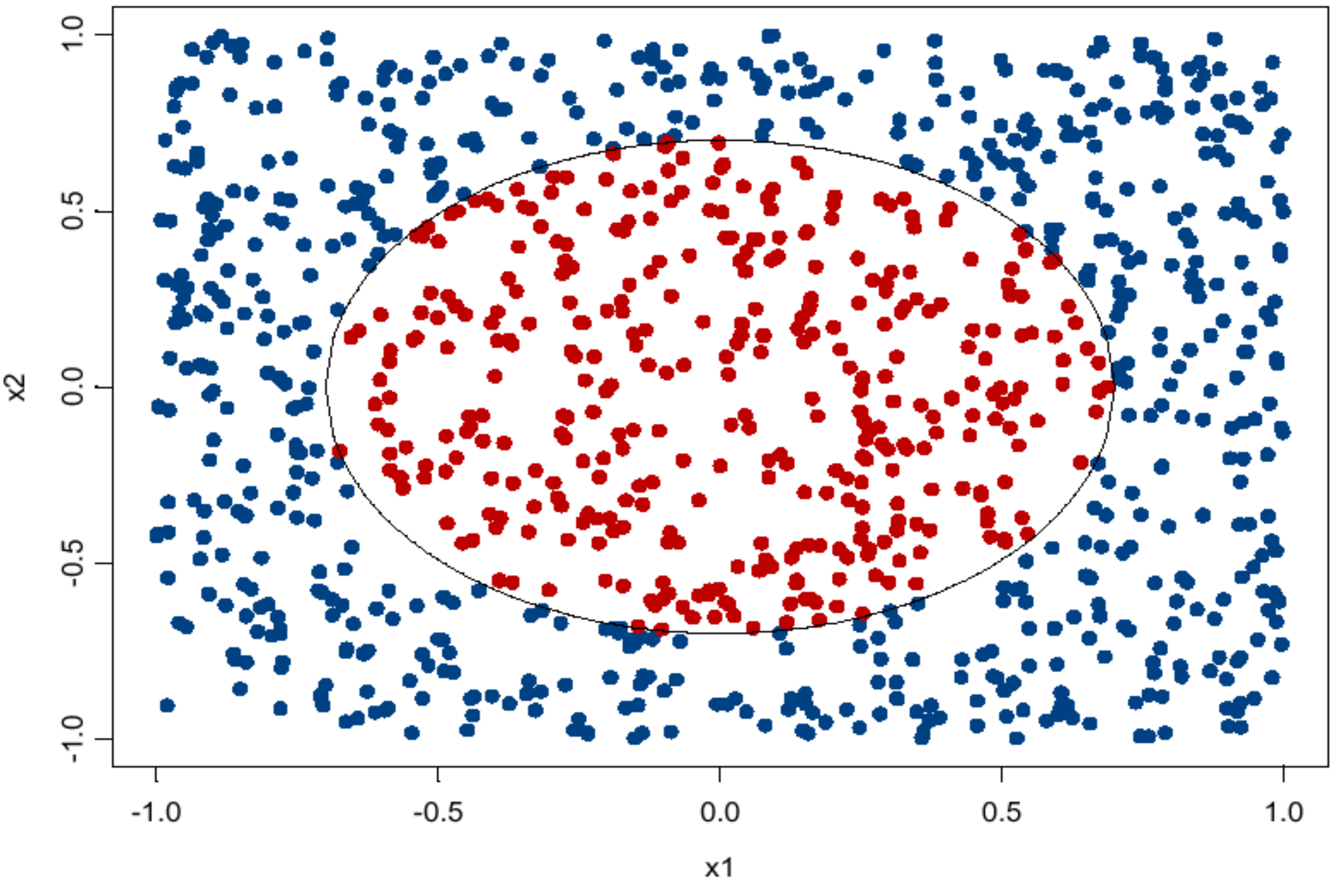
Training Data

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

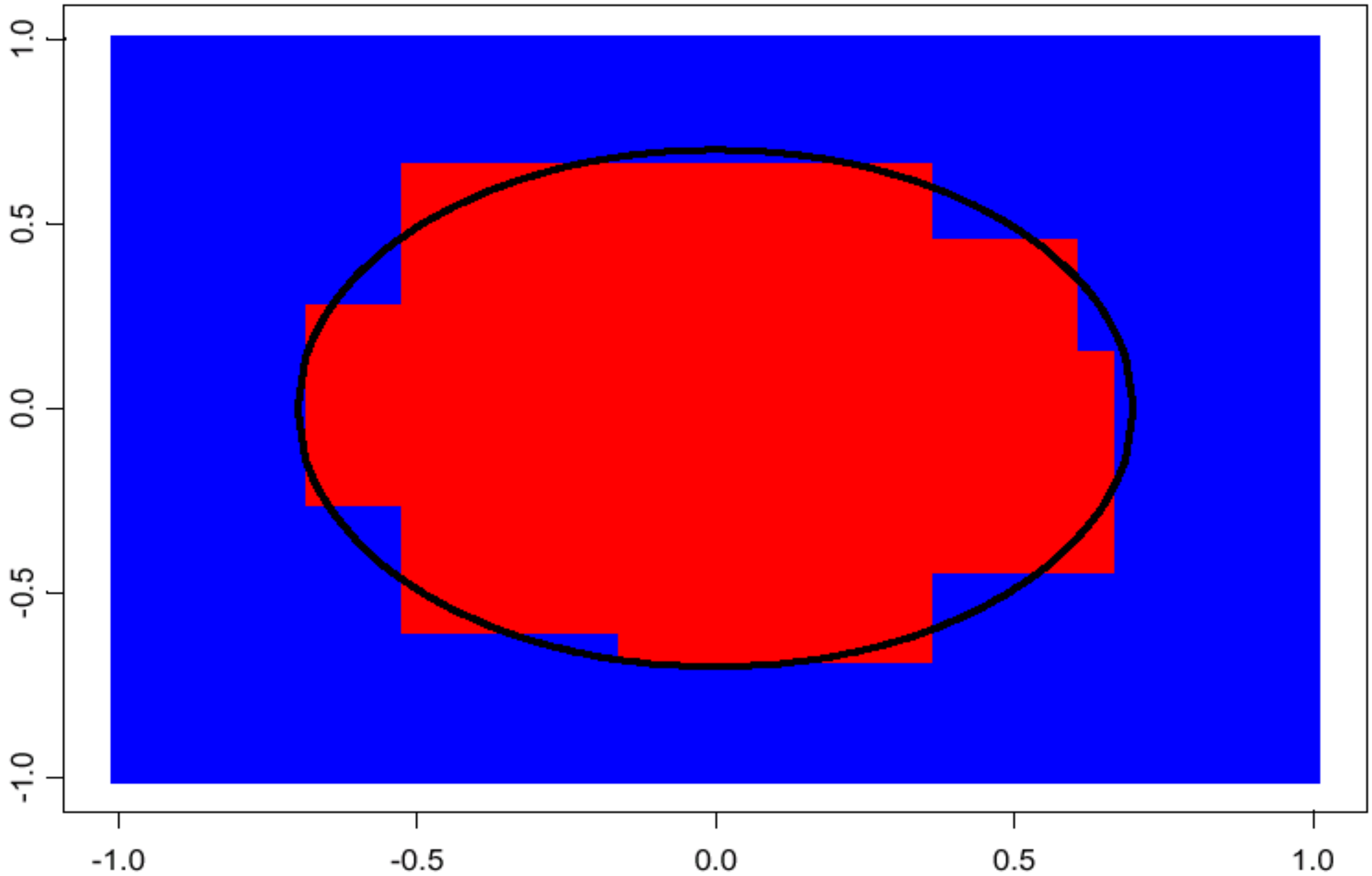
- Build classifier on each bootstrap sample
- Each data point has probability $(1 – 1/n)^n$ of being selected as test data
- Training data = $1- (1 – 1/n)^n$ of the original data

Bagging Example

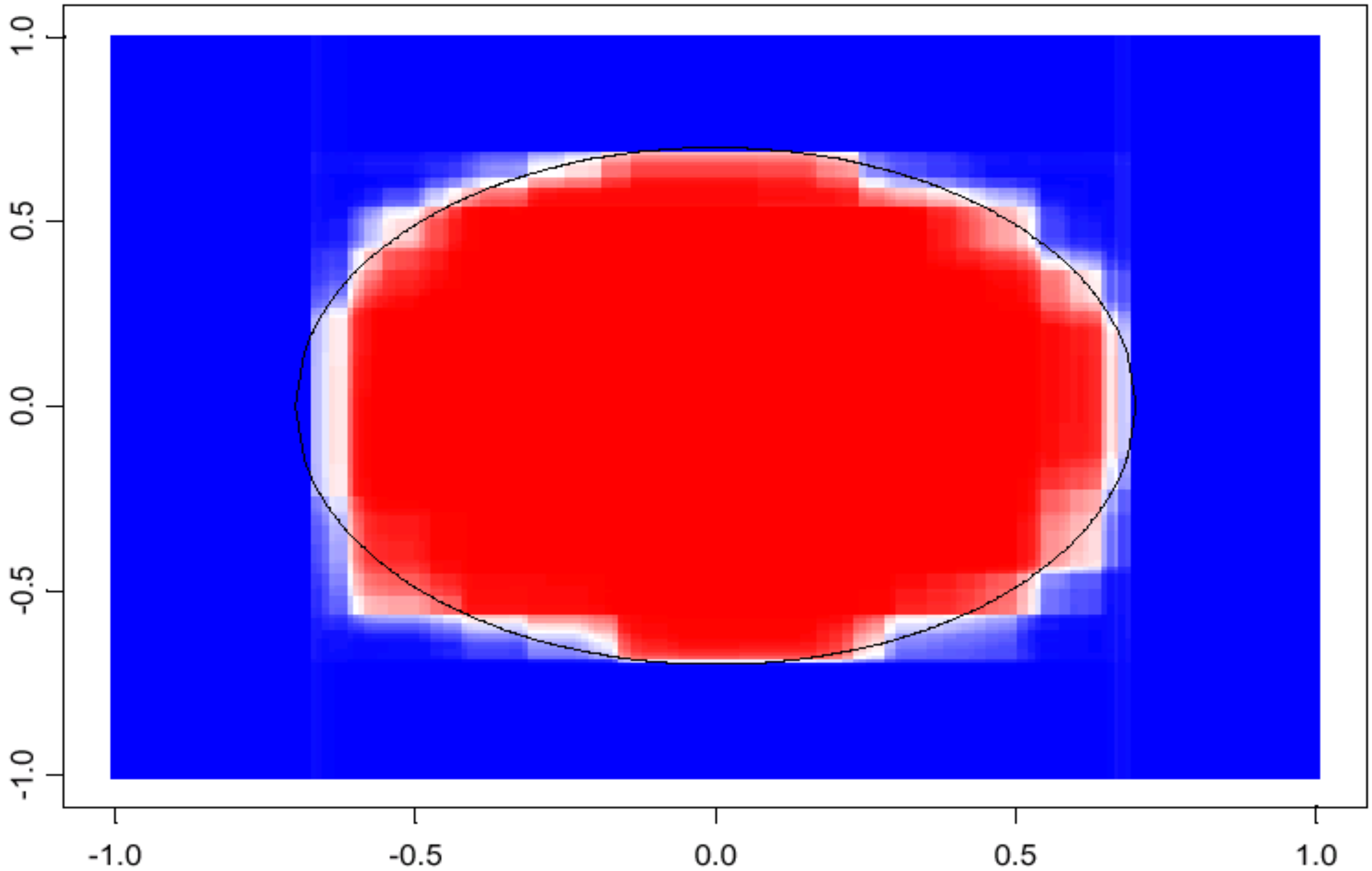


decision tree learning algorithm; very similar to ID3

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

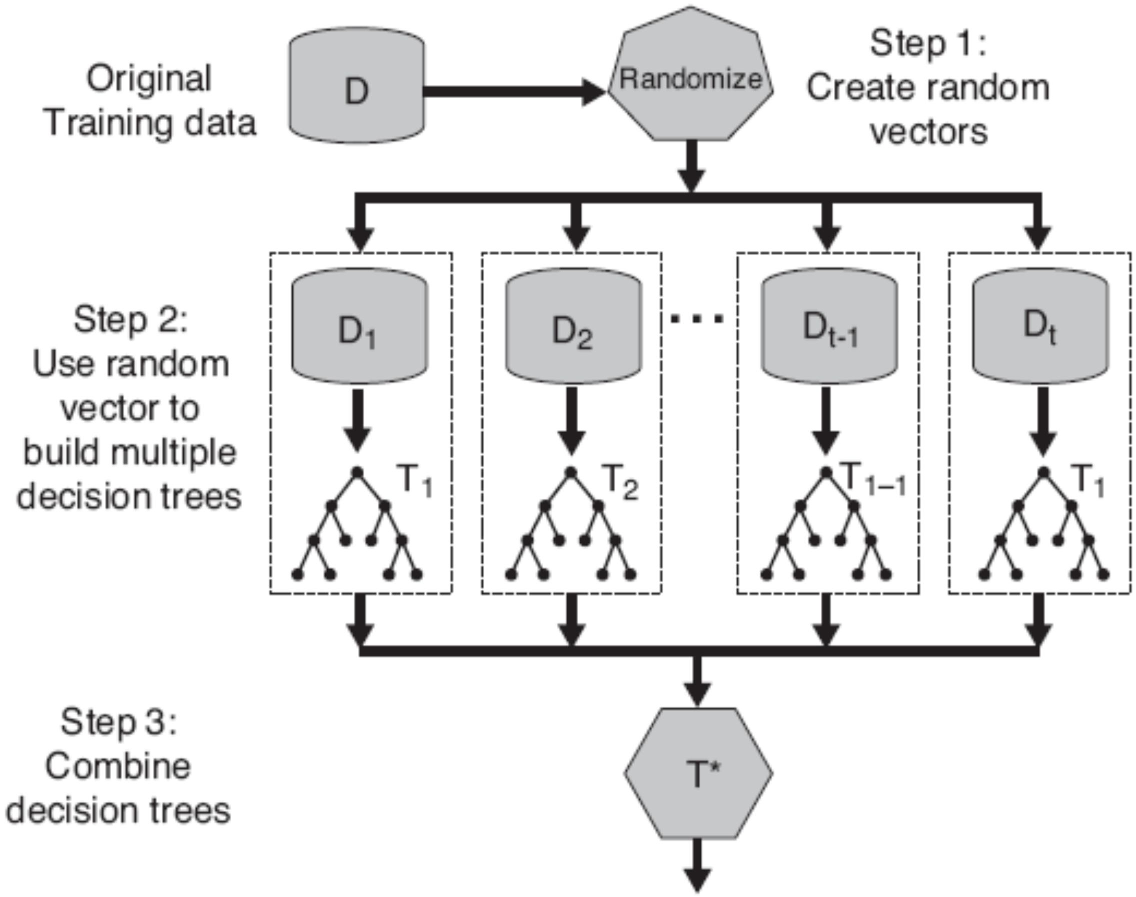


Figure 5.40. Random forests.

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

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