Machine Learning: Decision Trees

CS540

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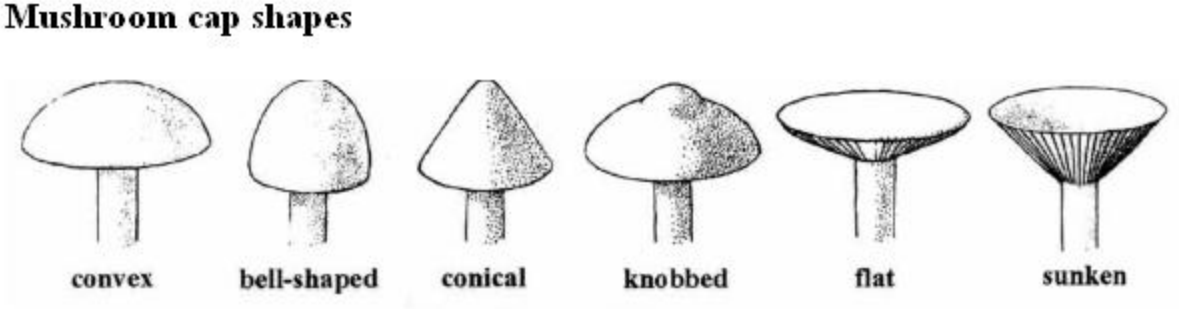
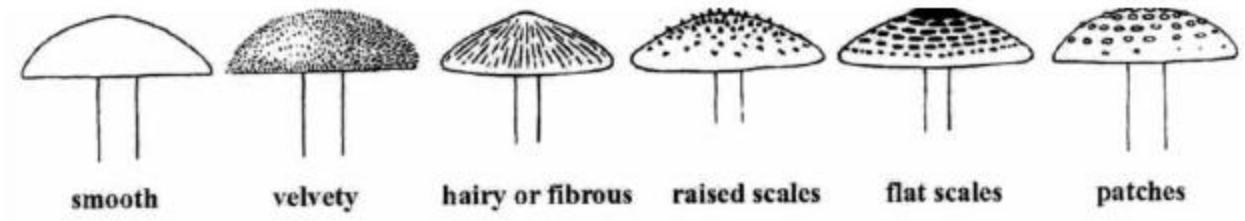
[Some slides from Andrew Moore http://www.cs.cmu.edu/~awm/tutorials and Chuck Dyer, with permission.]

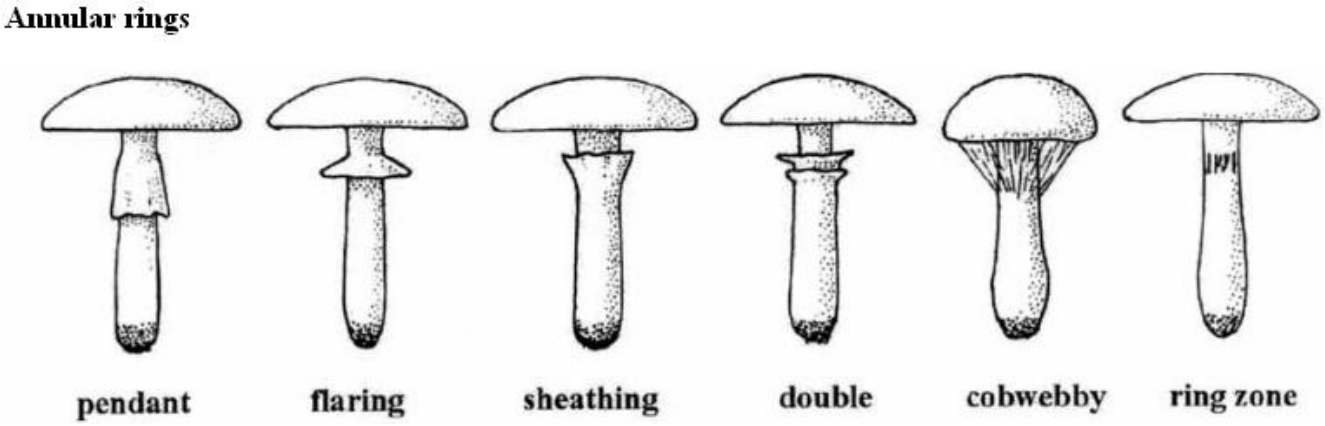
x

- The input
- These names are the same: example, point, instance, item, input
- Usually represented by a feature vector
  - These names are the same: attribute, feature
  - For decision trees, we will especially focus on *discrete* features (though continuous features are possible, see end of slides)

Example: mushrooms







http://www.usask.ca/biology/fungi/

Mushroom features

1. cap-shape: bell=b,conical=c,convex=x,flat=f, knobbed=k,sunken=s
2. cap-surface: fibrous=f,grooves=g,scaly=y,smooth=s
3. cap-color: brown=n,buff=b,cinnamon=c,gray=g,green=r, pink=p,purple=u,red=e,white=w,yellow=y
4. bruises?: bruises=t,no=f
5. odor: almond=a,anise=l,creosote=c,fishy=y,foul=f, musty=m,none=n,pungent=p,spicy=s
6. gill-attachment: attached=a,descending=d,free=f,notched=n
7. …

y

- The output
- These names are the same: label, target, goal
- It can be
  - Continuous, as in our population prediction➔Regression
  - Discrete, e.g., is this mushroom x edible or poisonous? ➔ Classification

Two mushrooms

x_1=x,s,n,t,p,f,c,n,k,e,e,s,s,w,w,p,w,o,p,k,s,u

y_1=p

x_2=x,s,y,t,a,f,c,b,k,e,c,s,s,w,w,p,w,o,p,n,n,g

y_2=e

1. cap-shape: bell=b,conical=c,convex=x,flat=f, knobbed=k,sunken=s
2. cap-surface: fibrous=f,grooves=g,scaly=y,smooth=s
3. cap-color: brown=n,buff=b,cinnamon=c,gray=g,green=r, pink=p,purple=u,red=e,white=w,yellow=y
4. …

Supervised Learning

- Training set: n pairs of example, label: $(x_1,y_1)…(x_n,y_n)$
- A function (=hypothesis) $f: x \rightarrow y$
- Hypothesis space: e.g., the set of *d*-th order polynomials.
- Find the best function in the hypothesis space that generalizes well.
- Performance measure: MSE for regression, accuracy or error rate for classification

Evaluating classifiers

- During training
  - Train a classifier from a training set (x_1,y_1), (x_2,y_2), …, (x_n,y_n).
- During testing
  - For new test data $x_{n+1}…x_{n+m}$, your classifier generates predicted labels $y'_{n+1}… y'_{n+m}$
- Test set accuracy:
  - You need to know the true test labels $y_{n+1}… y_{n+m}$
  - Test set accuracy: $acc = \frac{1}{m}\sum_{i=n+1}^{n+m} 1_{y_i = y'_i}$
  - Test set error rate = 1 – acc

Decision Trees

- One kind of classifier (supervised learning)
- Outline:
  - The tree
  - Algorithm
  - Mutual information of questions
  - Overfitting and Pruning
  - Extensions: real-valued features, tree→rules, pro/con

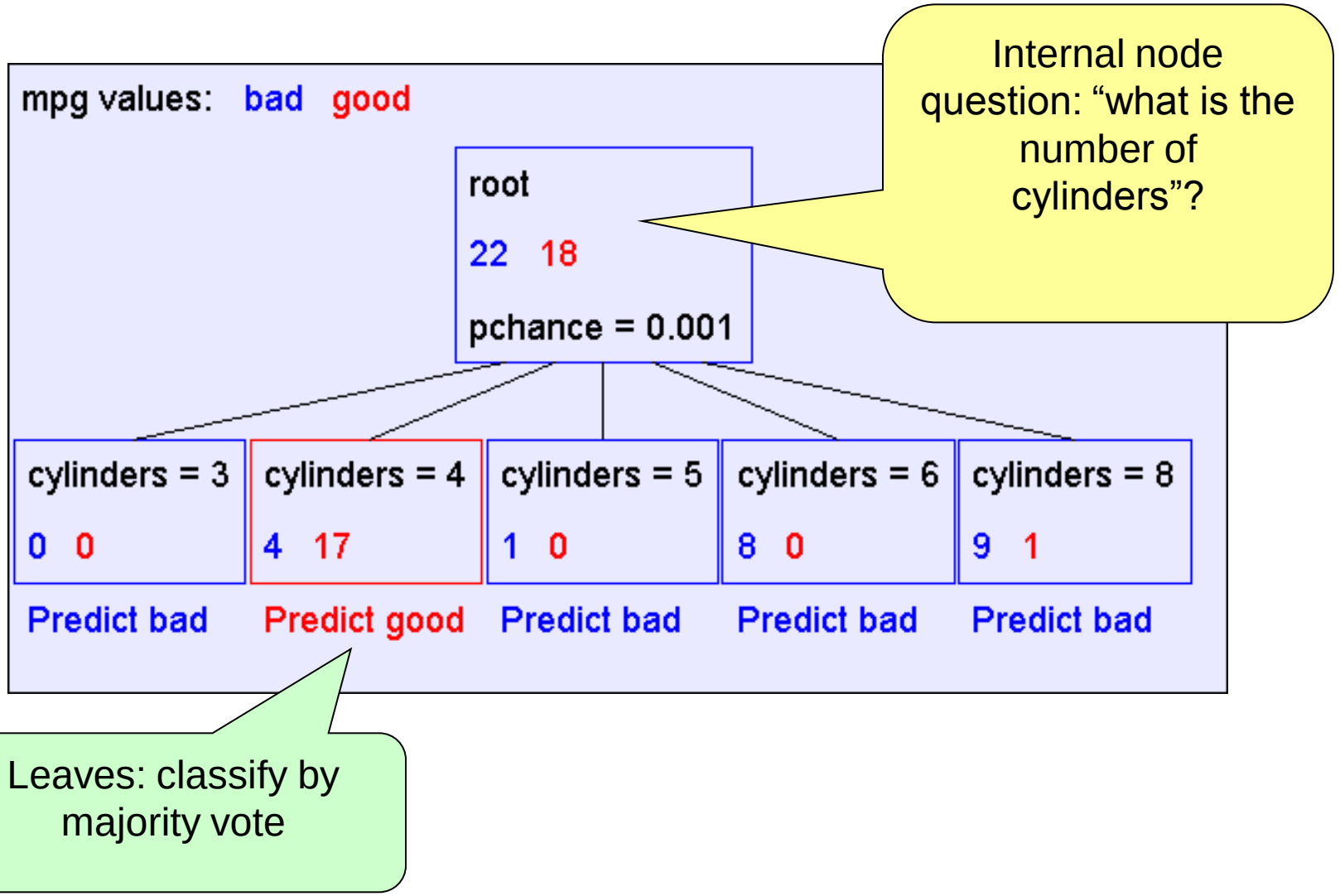
A Decision Tree

- A decision tree has 2 kinds of nodes
  1. Each leaf node has a class label, determined by majority vote of training examples reaching that leaf.
  2. Each internal node is a question on features. It branches out according to the answers.

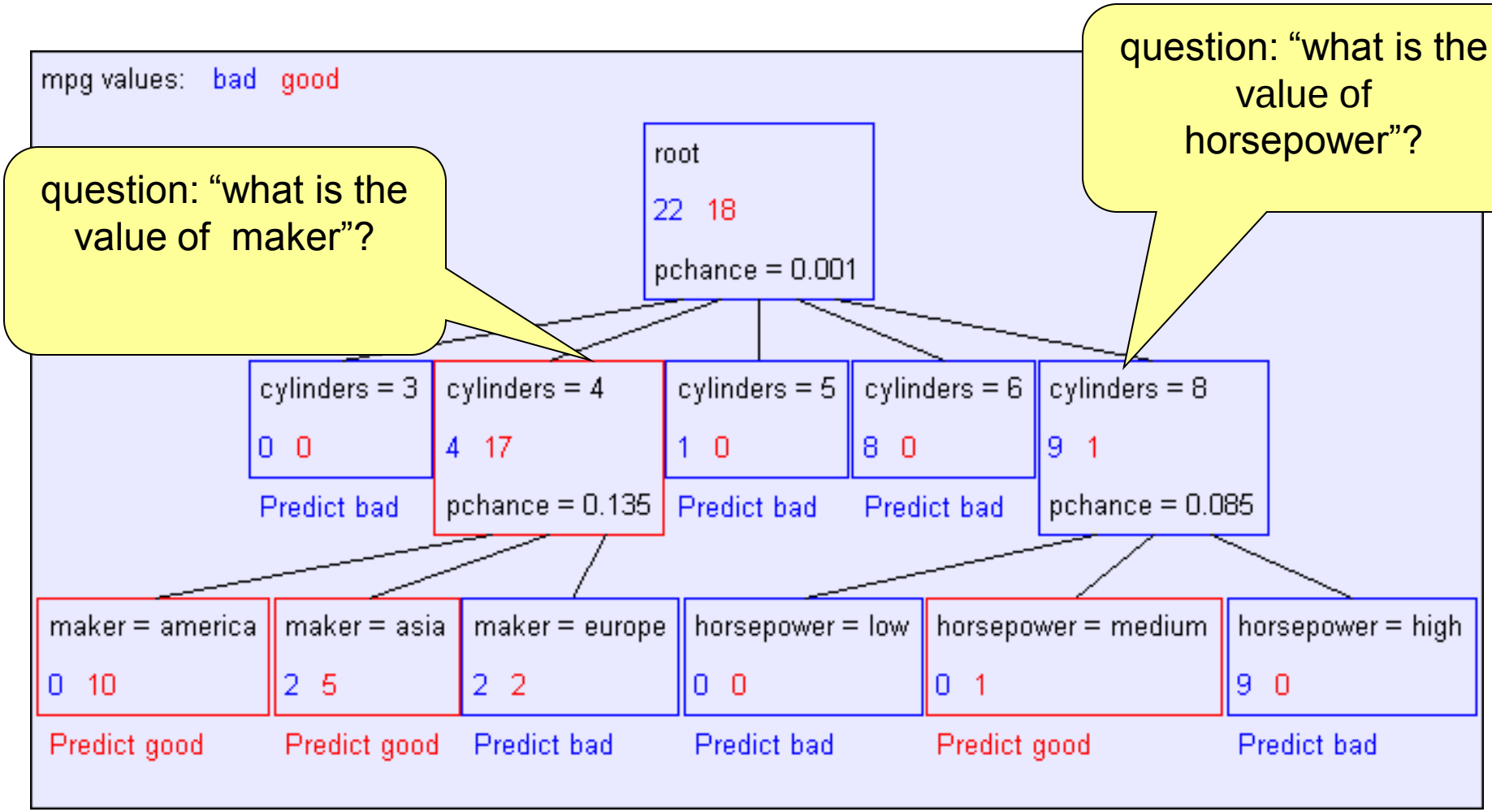
Automobile Miles-per-gallon prediction

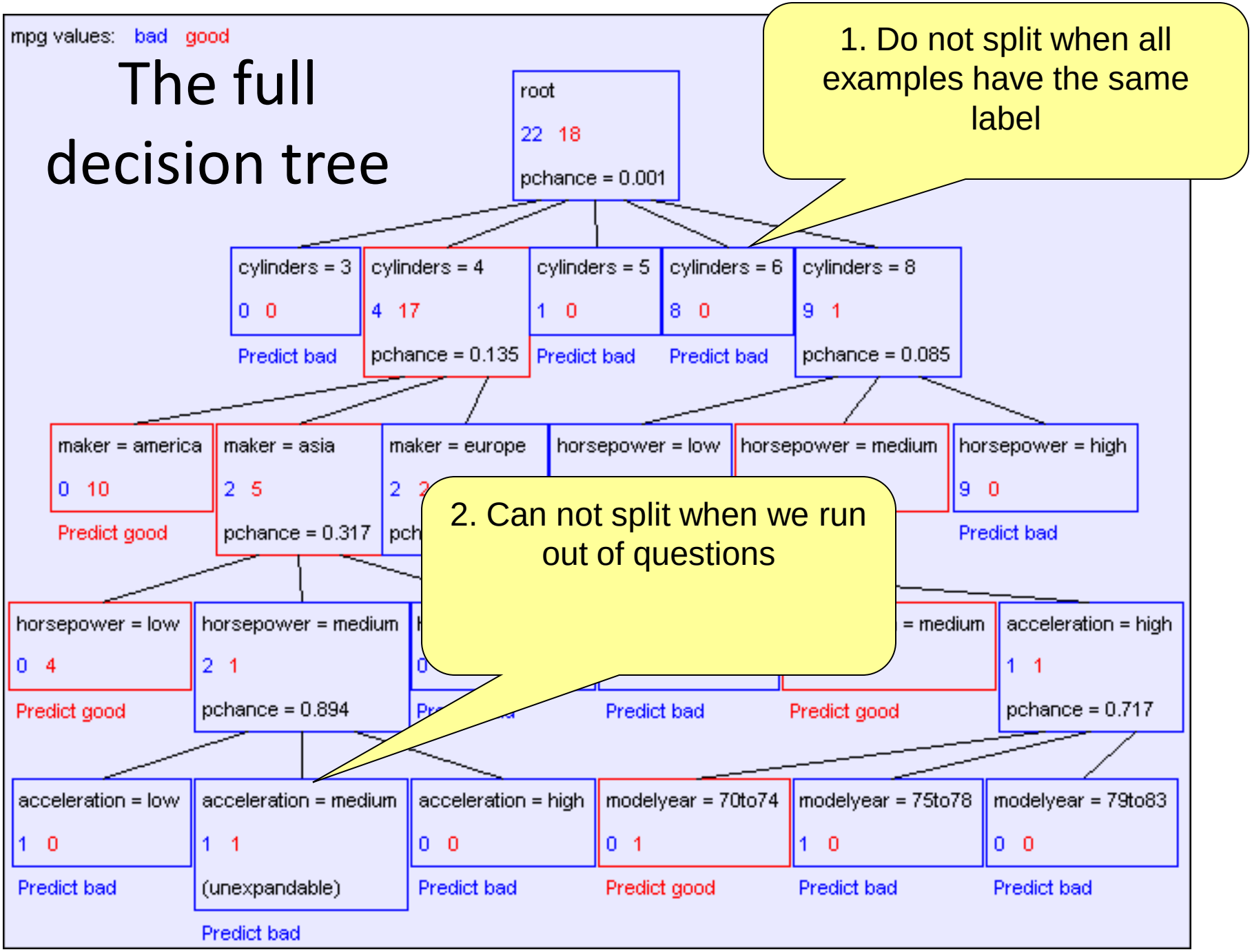
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low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

A very small decision tree



A bigger decision tree




mpg values: bad good
The full decision tree
root
22 18
pchance = 0.001
1. Do not split when all examples have the same label
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
horsepower = low
horsepower = medium
horsepower = high
9 0
Predict bad
2. Can not split when we run out of questions
horsepower = low
0 4
Predict good
horsepower = medium
2 1
pchance = 0.894
= medium
Predict good
acceleration = high
1 1
pchance = 0.717
Predict bad
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

Decision tree algorithm

buildtree(*examples*, *questions*, *default*)

/* examples: a list of training examples

questions: a set of candidate questions, e.g., "what's the value of feature x_i?"

default: default label prediction, e.g., over-all majority vote */

IF empty(*examples*) THEN return(*default*)

IF (*examples* have same label y) THEN return(y)

IF empty(*questions*) THEN return(majority vote in *examples*)

q = best_question(*examples, questions*)

Let there be n answers to q

- Create and return an internal node with n children
- The i^{th} child is built by calling

buildtree({*example*|q=i^{th} answer}, *questions*\{q}, *default*)

The best question

- What do we want: pure leaf nodes, i.e. all examples having (almost) the same y.
- A good question → a split that results in pure child nodes
- How do we measure the degree of purity induced by a question? Here's one possibility (Max-Gain in book):

mutual information
= information gain
A quantity from information theory

Entropy

- At the current node, there are $n=n_1+\ldots+n_k$ examples
  - n_1 examples have label y_1
  - n_2 examples have label y_2
  - …
  - n_k examples have label y_k
- What's the impurity of the node?
- Turn it into a game: if I put these examples in a bag, and grab one at random, what is the probability the example has label y_i?

Entropy

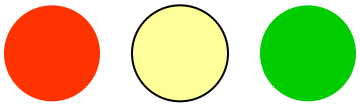
- Probability estimated from samples:
  - with probability $p_1=n_1/n$ the example has label y_1
  - with probability $p_2=n_2/n$ the example has label y_2
  - …
  - with probability $p_k=n_k/n$ the example has label y_k
- $p_1+p_2+…+p_k=1$
- The "outcome" of the draw is a random variable y with probability $(p_1, p_2, …, p_k)$
- What's the impurity of the node ➔ what's the uncertainty of y in a random drawing?

Entropy

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

$$= \sum_{i=1}^{k} -p_i \log_2 p_i$$

- Interpretation: The number of yes/no questions (bits) needed on average to pin down the value of y in a random drawing



H(y)=

H(y)=

H(y)=

Entropy

p(head)=0.5
p(tail)=0.5
H=1

biased coin

p(head)=0.51
p(tail)=0.49
H=0.9997

Jerry's coin

p(head)=?
p(tail)=?
H=?

Conditional entropy

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

$$H(Y \mid X) = \sum_{v: \text{values of } X} \Pr(X = v) H(Y \mid X = v)$$

- Y: label. X: a question (e.g., a feature). v: an answer to the question
- Pr(Y|X=v): conditional probability

Information gain

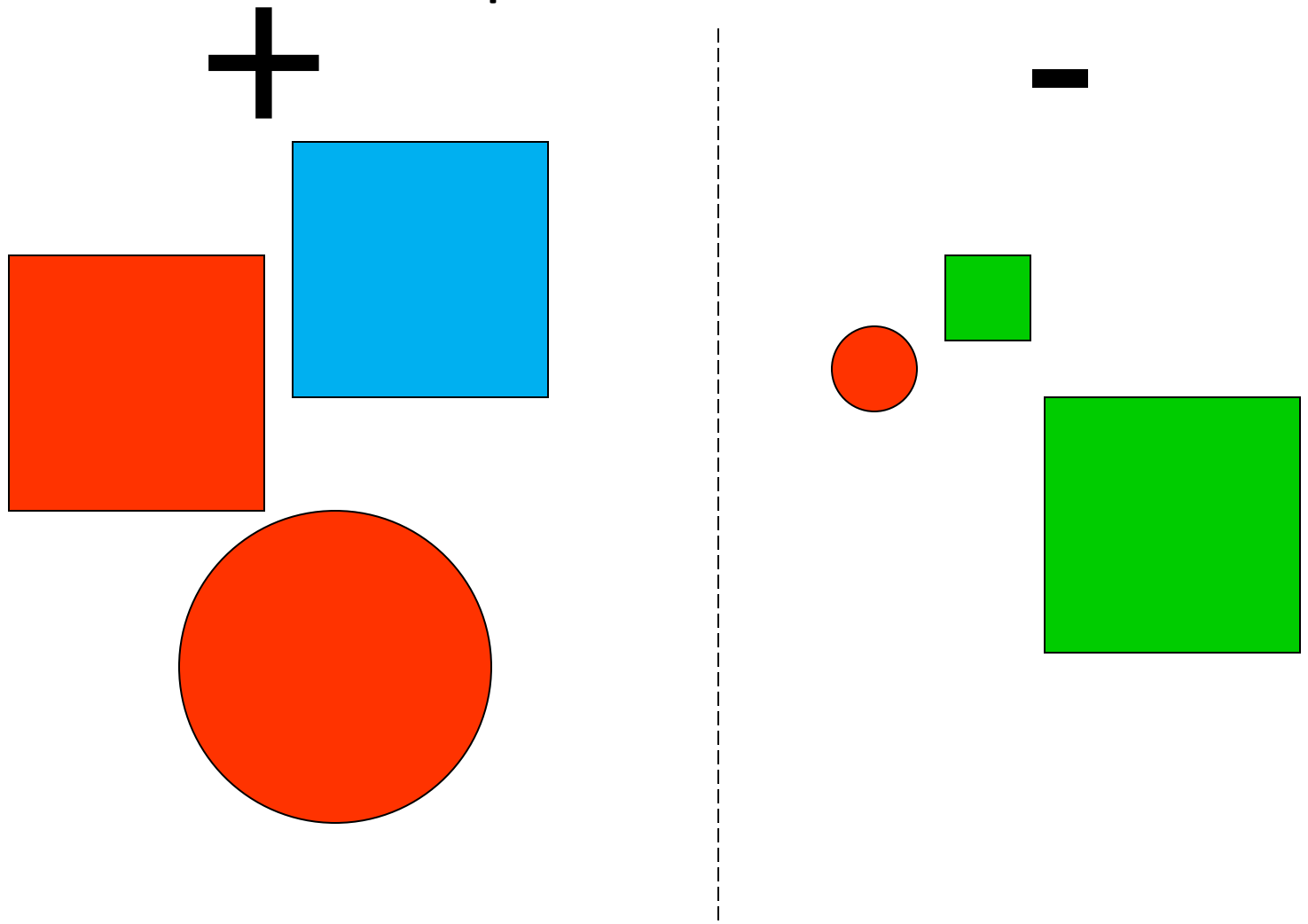
- Information gain, or mutual information

$$I(Y;X) = H(Y) - H(Y \mid X)$$

- Choose question (feature) X which maximizes I(Y;X).

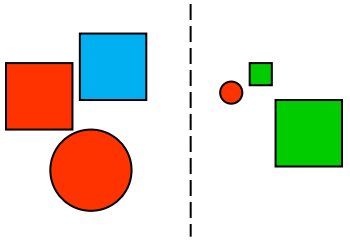
Example

- Features: color, shape, size
- What's the best question at root?



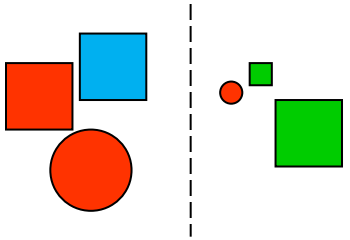
The training set

Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



H(class)=
H(class | color)=

Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



H(class)= H(3/6,3/6) = 1

H(class | color)= 3/6 * H(2/3,1/3) + 1/6 * H(1,0) + 2/6 * H(0,1)

3 out of 6 are red

2 of the red are +

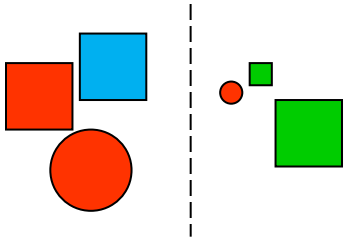
1 out of 6 is blue

blue is +

2 out of 6 are green

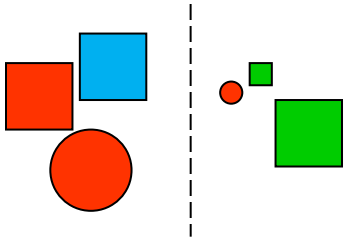
green is -

Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



H(class)= H(3/6,3/6) = 1
H(class | color)= 3/6 * H(2/3,1/3) + 1/6 * H(1,0) + 2/6 * H(0,1)
I(class; color) = H(class) – H(class | color) = 0.54 bits

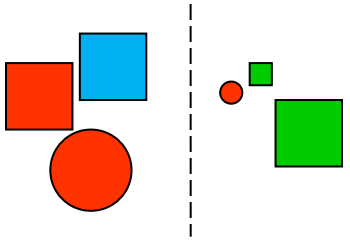
Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



H(class)= H(3/6,3/6) = 1
H(class | shape)= 4/6 * H(1/2, 1/2) + 2/6 * H(1/2,1/2)
I(class; shape) = H(class) – H(class | shape) = 0 bits

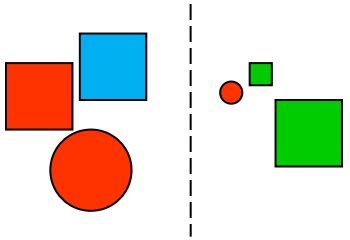
Shape tells us nothing about the class!

Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



H(class)= H(3/6,3/6) = 1
H(class | size)= 4/6 * H(3/4, 1/4) + 2/6 * H(0,1)
I(class; size) = H(class) – H(class | size) = 0.46 bits

Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



I(class; color) = H(class) – H(class | color) = 0.54 bits
I(class; shape) = H(class) – H(class | shape) = 0 bits
I(class; size) = H(class) – H(class | size) = 0.46 bits

➔ We select color as the question at root

Overfitting Example: Predicting US Population

x=Year	*y*=Million
1900	75.995
1910	91.972
1920	105.71
1930	123.2
1940	131.67
1950	150.7
1960	179.32
1970	203.21
1980	226.51
1990	249.63
2000	281.42

- We have some training data (*n*=11)
- What will the population be in 2020?

Regression: Polynomial fit

- The degree *d* (complexity of the model) is important

$$f(x) = c_d x^d + c_{d-1} x^{d-1} + \cdots + c_1 x + c_0$$

- Fit (=learn) coefficients c_d, … c_0 to minimize Mean Squared Error (MSE) on training data

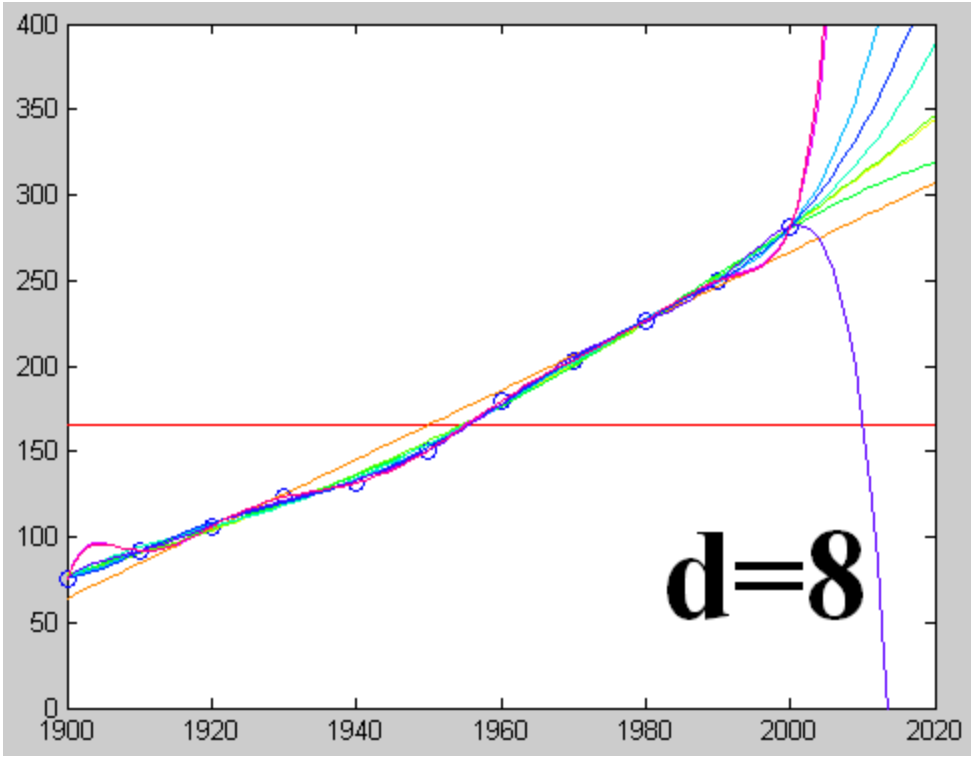
$$MSE = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f(x_i) \right)^2$$

- Matlab demo: USpopulation.m

Overfitting

- As *d* increases, MSE on training data improves, but prediction outside training data worsens

degree=0 MSE=4181.451643
degree=1 MSE=79.600506
degree=2 MSE=9.346899
degree=3 MSE=9.289570
degree=4 MSE=7.420147
degree=5 MSE=5.310130
degree=6 MSE=2.493168
degree=7 MSE=2.278311
degree=8 MSE=1.257978
degree=9 MSE=0.001433
degree=10 MSE=0.000000



Overfit a decision tree

Five inputs, all bits, are generated in all 32 possible combinations

Output y = copy of e, Except a random 25% of the records have y set to the opposite of e

32 records

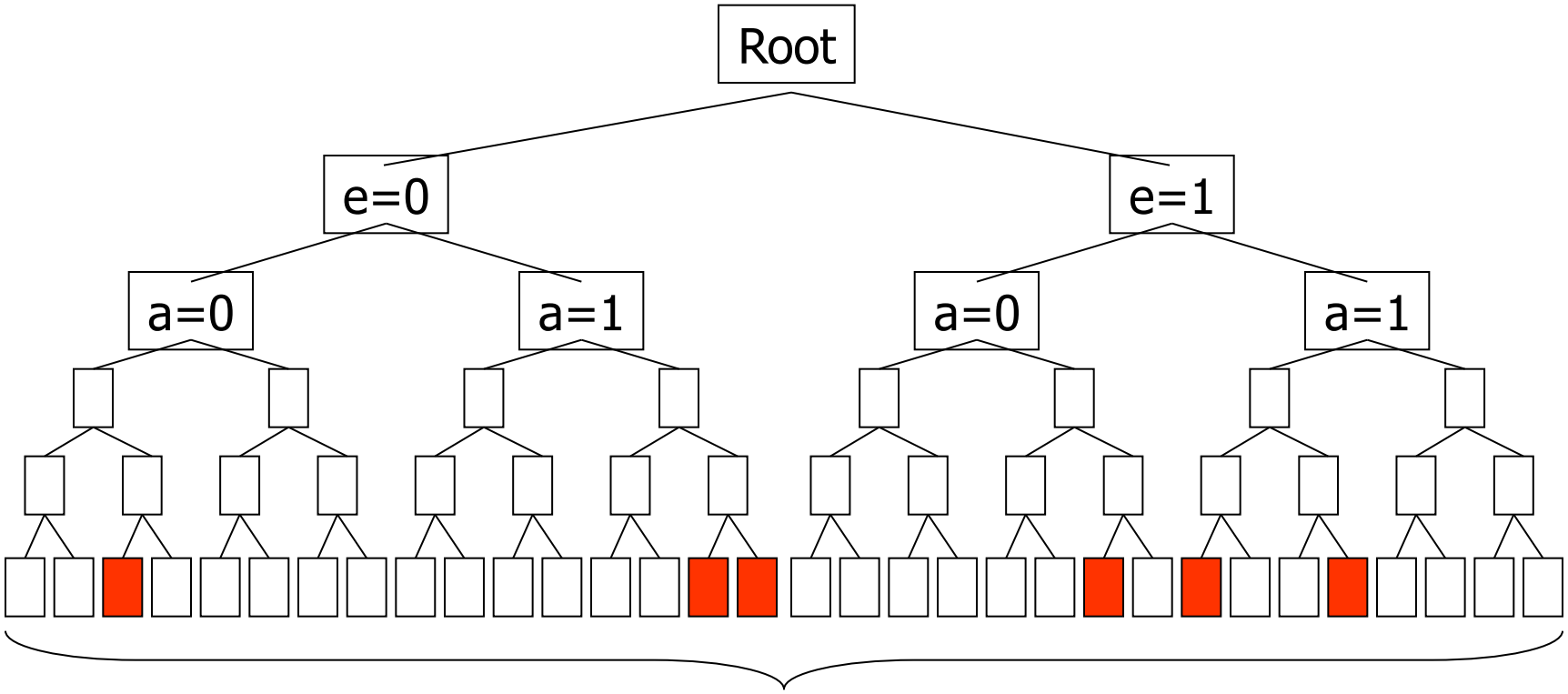
a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

Overfit a decision tree

- The test set is constructed similarly
  - y=e, but 25% the time we corrupt it by y=¬e
  - The corruptions in training and test sets are independent
- The training and test sets are the same, except
  - Some y's are corrupted in training, but not in test
  - Some y's are corrupted in test, but not in training

Overfit a decision tree

- We build a full tree on the training set

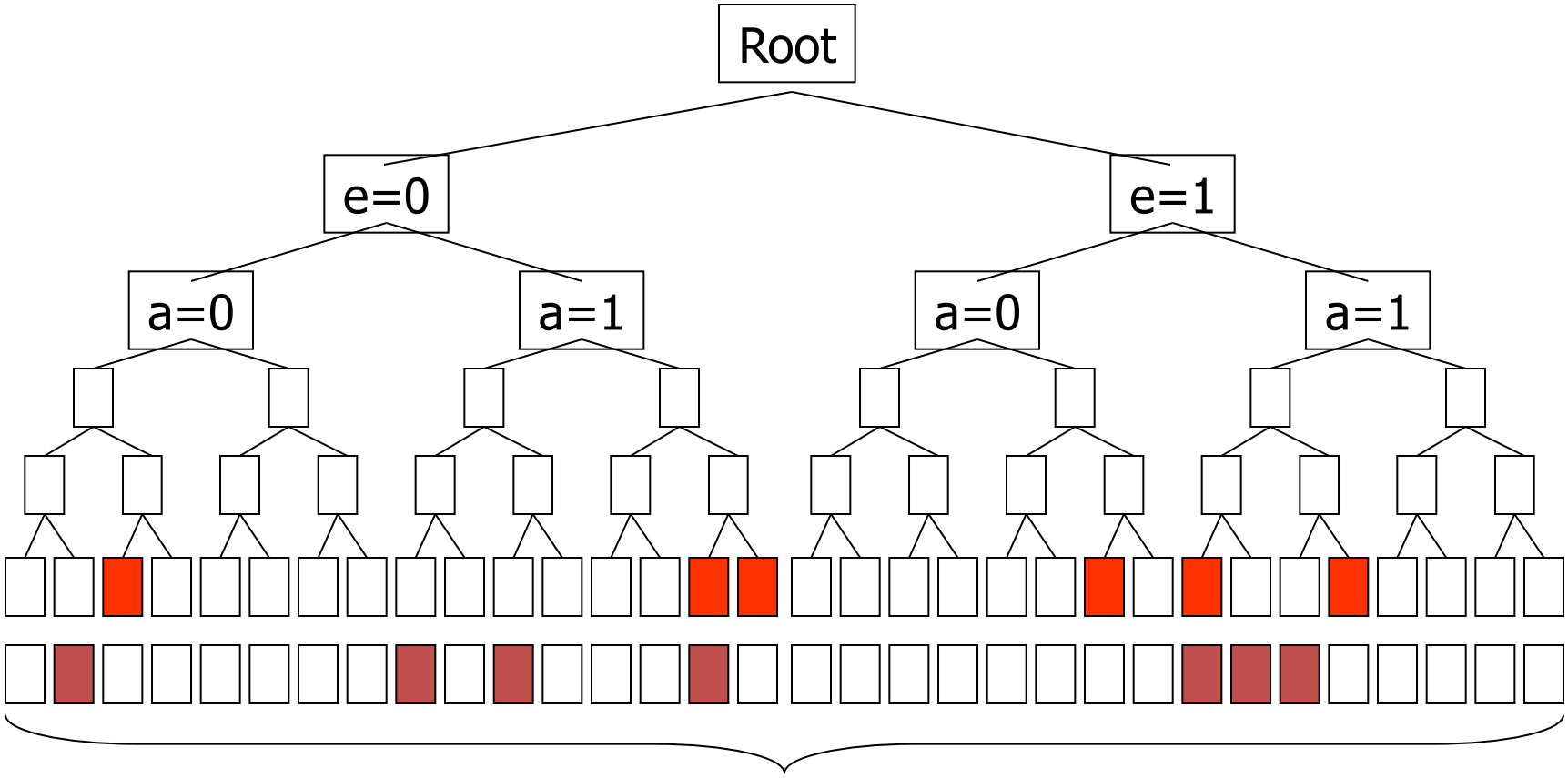


Training set accuracy = 100%

25% of these training leaf node labels will be corrupted ($\neq$e)

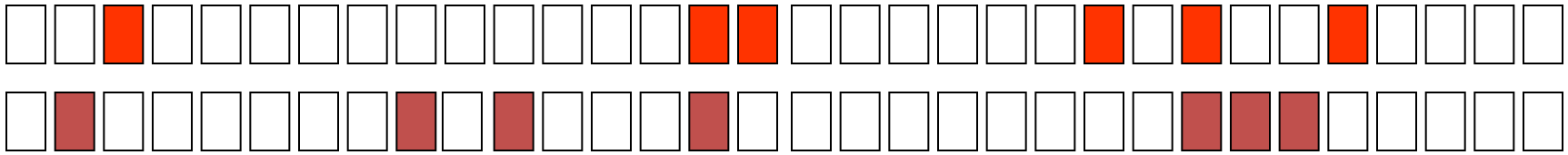
Overfit a decision tree

- And classify the test data with the tree



25% of the test examples are corrupted – independent of training data

Overfit a decision tree



On average:

- ¾ training data uncorrupted
  - ¾ of these are uncorrupted in test – correct labels
  - ¼ of these are corrupted in test – wrong
- ¼ training data corrupted
  - ¾ of these are uncorrupted in test – wrong
  - ¼ of these are also corrupted in test – correct labels
- Test accuracy = ¾ * ¾ + ¼ * ¼ = 5/8 = 62.5%

Overfit a decision tree

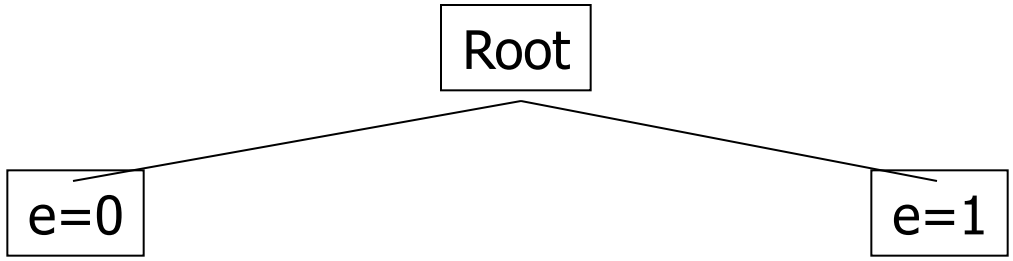
- But if we knew a,b,c,d are irrelevant features and don't use them in the tree…

Pretend they don't exist

a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

Overfit a decision tree

- The tree would be



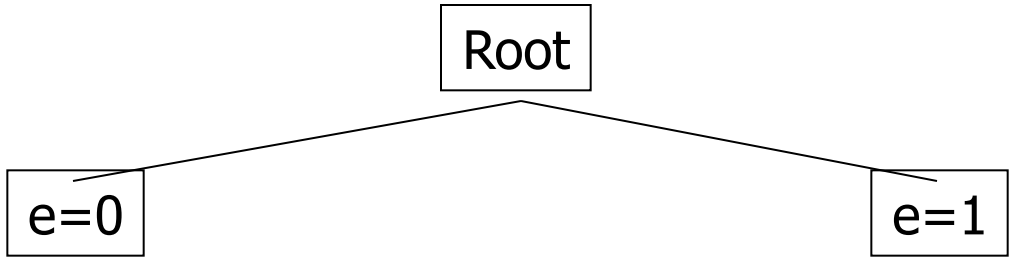
In training data, about ¾ y's are 0 here. Majority vote predicts y=0

In training data, about ¾ y's are 1 here. Majority vote predicts y=1

In test data, ¼ y's are different from e.
test accuracy = ?

Overfit a decision tree

- The tree would be



In training data, about ¾ y's are 0 here. Majority vote predicts y=0

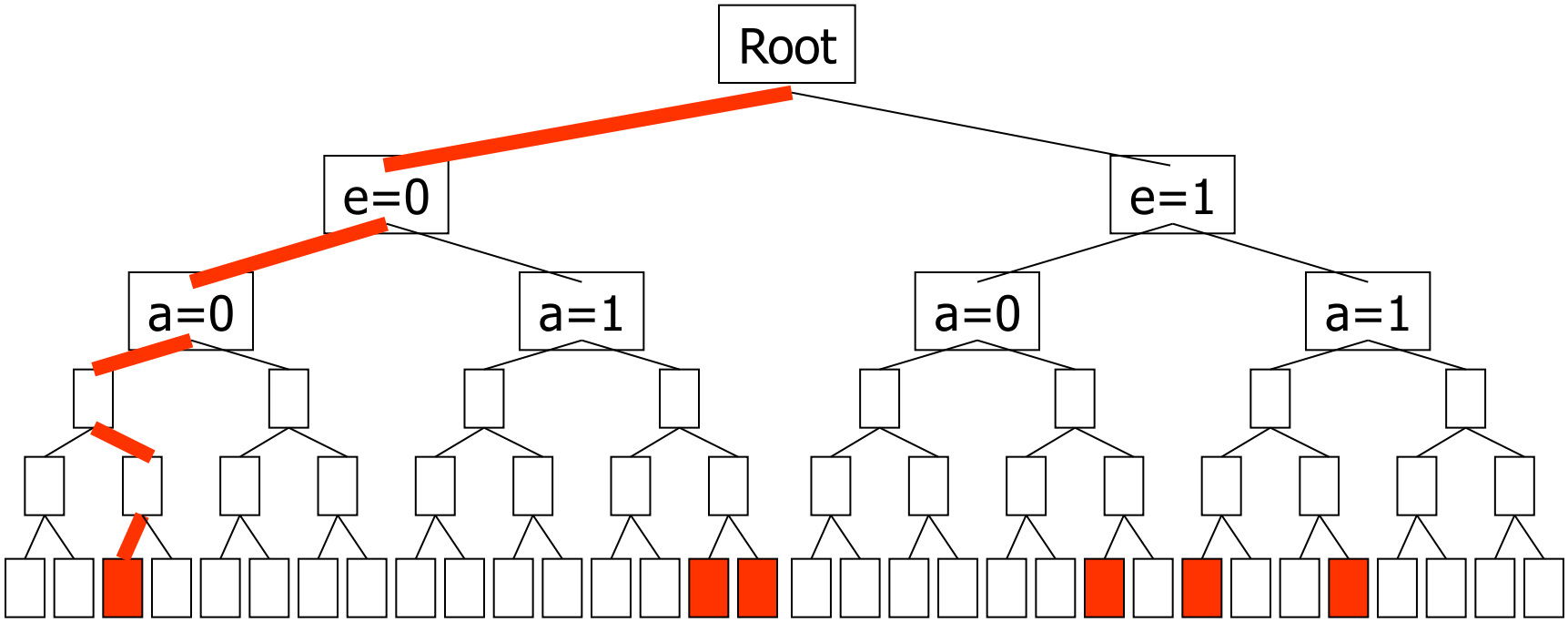
In training data, about ¾ y's are 1 here. Majority vote predicts y=1

In test data, ¼ y's are different from e.
test accuracy = ¾ = 75% (better!)

Full tree test accuracy = ¾ * ¾ + ¼ * ¼ = 5/8 = 62.5%

Overfit a decision tree

- In the full tree, we overfit by learning non-existent relations (noise)



Avoid overfitting: pruning

Pruning with a tuning set

1. Randomly split data into TRAIN and TUNE, say 70% and 30%
2. Build a full tree using only TRAIN
3. Prune the tree down on the TUNE set. On the next page you'll see a greedy version.

Pruning

Prune(tree T, TUNE set)

1. Compute T's accuracy on TUNE, call it A(T)
2. For every internal node N in T:
   a) New tree T_N = copy of T, but prune (delete) the subtree under N.
   b) N becomes a leaf node in T_N. The label is the majority vote of TRAIN examples reaching N.
   c) $A(T_N)$ = T_N's accuracy on TUNE
3. Let T* be the tree (among the T_N's and T) with the largest A(). Set T←T^* /* prune */
4. Repeat from step 1 until no more improvement available. Return T.

Real-valued features

- What if some (or all) of the features x1, x2, …, xk are real-valued?
- Example: x1=height (in inches)
- Idea 1: branch on each possible numerical value.

Real-valued features

- What if some (or all) of the features x1, x2, …, xk are real-valued?
- Example: x1=height (in inches)
- Idea 1: branch on each possible numerical value. (fragments the training data and prone to overfitting)
- Idea 2: use questions in the form of (x1>t?), where t is a threshold. There are fast ways to try all(?) t.

$$H(y \mid x_i > t?) = p(x_i > t)H(y \mid x_i > t) + p(x_i \leq t)H(y \mid x_i \leq t)$$

$$I(y \mid x_i > t?) = H(y) - H(y \mid x_i > t?)$$

What does the feature space look like?

Axis-parallel cuts

Tree → Rules

- Each path, from the root to a leaf, corresponds to a rule where all of the decisions leading to the leaf define the antecedent to the rule, and the consequent is the classification at the leaf node.
- For example, from the tree in the color/shape/size example, we could generate the rule:

if color = red and size = big then +

Conclusions

- Decision trees are popular tools for data mining
  - Easy to understand
  - Easy to implement
  - Easy to use
  - Computationally cheap
- Overfitting might happen
- We used decision trees for classification (predicting a categorical output from categorical or real inputs)

What you should know

- Trees for classification
- Top-down tree construction algorithm
- Information gain
- Overfitting
- Pruning
- Real-valued features