Machine Learning: Decision Trees

CS540
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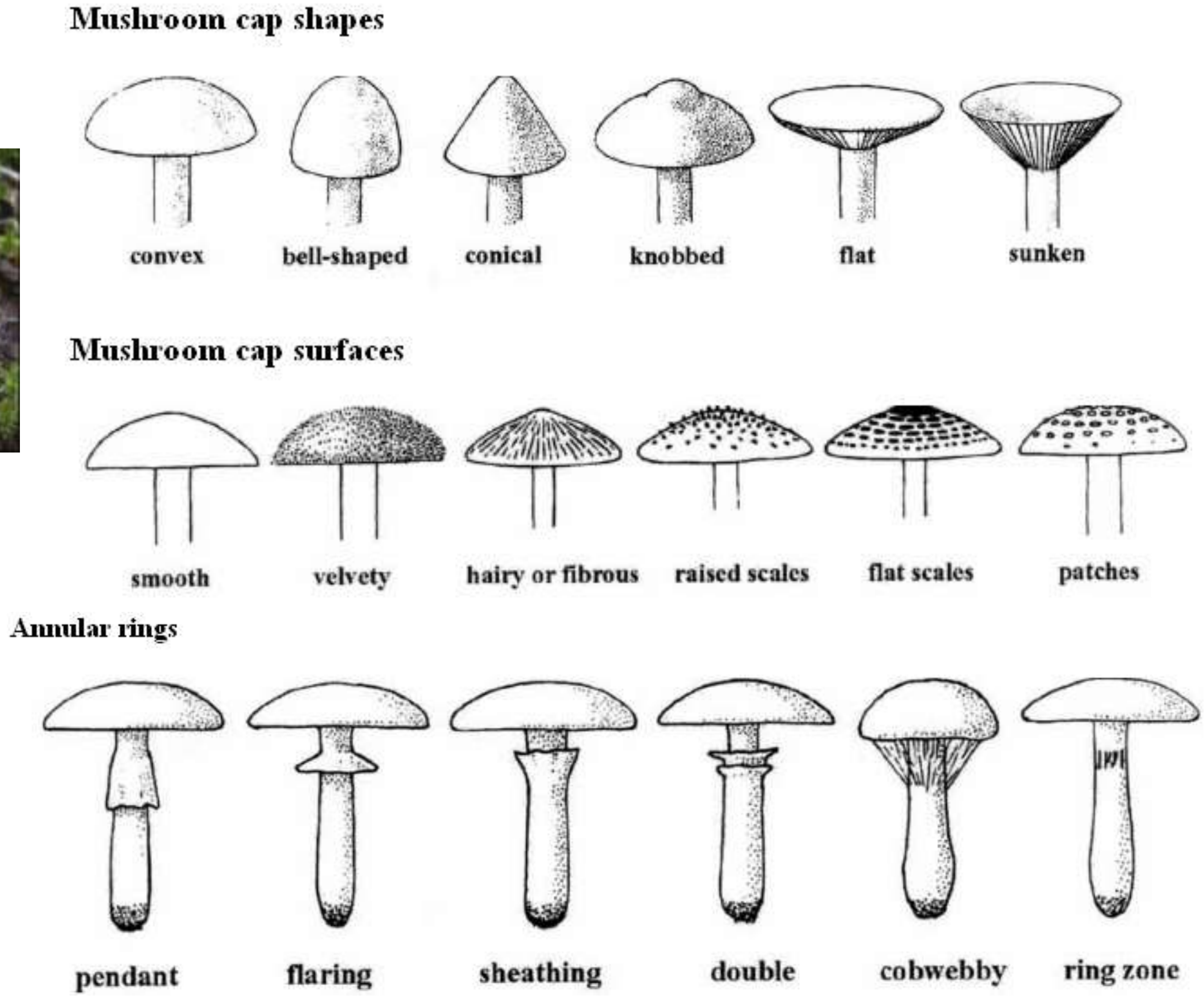
[Some slides from Andrew Moore http://www.cs.cmu.edu/~awm/tutorials and Chuck Dyer, with permission.]

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: $(x_1,y_1)\ldots(x_n,y_n)$
- A predictor (i.e., hypothesis: classifier, regression function) $f: x \rightarrow y$
- Hypothesis space: space of predictors, 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 $x_{n+1} \ldots x_{n+m}$, your classifier generates predicted labels $y'_{n+1} \ldots y'_{n+m}$
- Test set accuracy:
  - You need to know the true test labels $y_{n+1} \ldots y_{n+m}$
  - 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

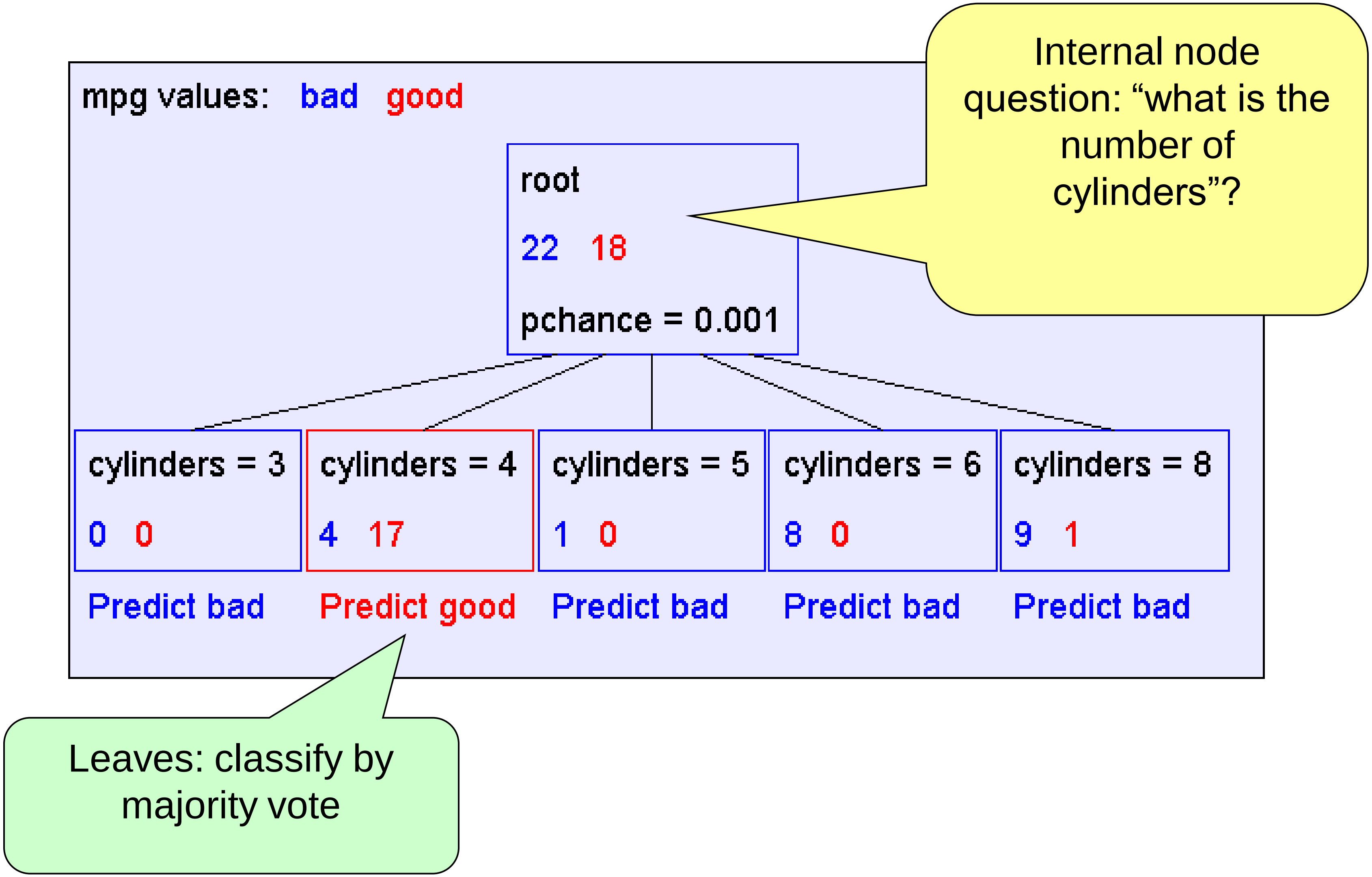
A Decision Tree

- 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.

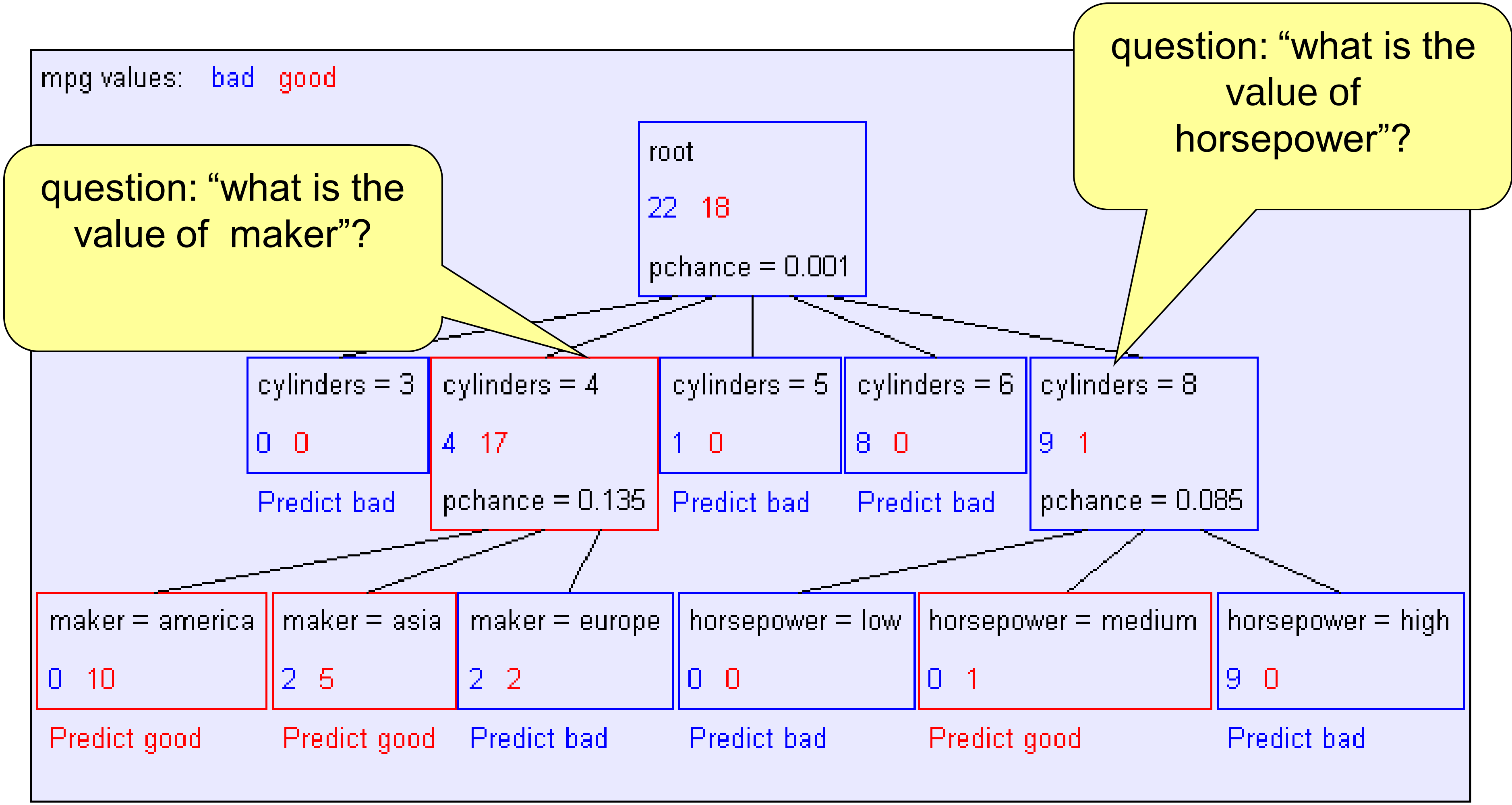
Automobile Miles-per-gallon prediction

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

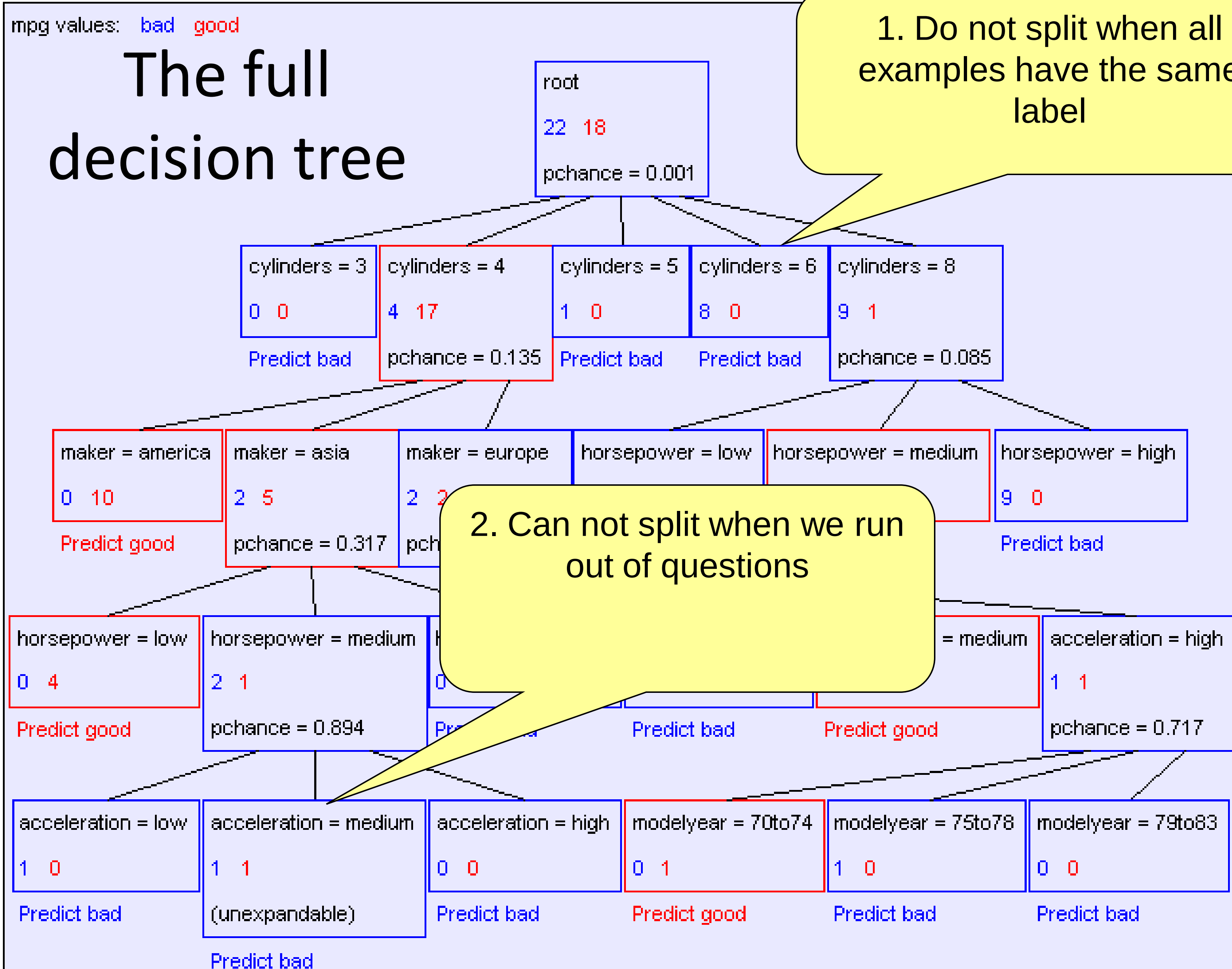
A very small decision tree



A bigger decision tree



The full decision tree



1. Do not split when all examples have the same label

2. Can not split when we run out of questions

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
(a.k.a. 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

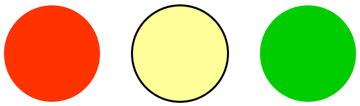
- Probability estimated from samples:
  - with probability $p_1=n_1/n$ the example has label y_1
  - with probability $p_2=n_2/n$ the example has label y_2
  - …
  - with probability $p_k=n_k/n$ the example has label y_k
- $p_1+p_2+\ldots+p_k=1$
- The "outcome" of the draw is a random variable y with probability $(p_1, p_2, \ldots, p_k)$
- 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

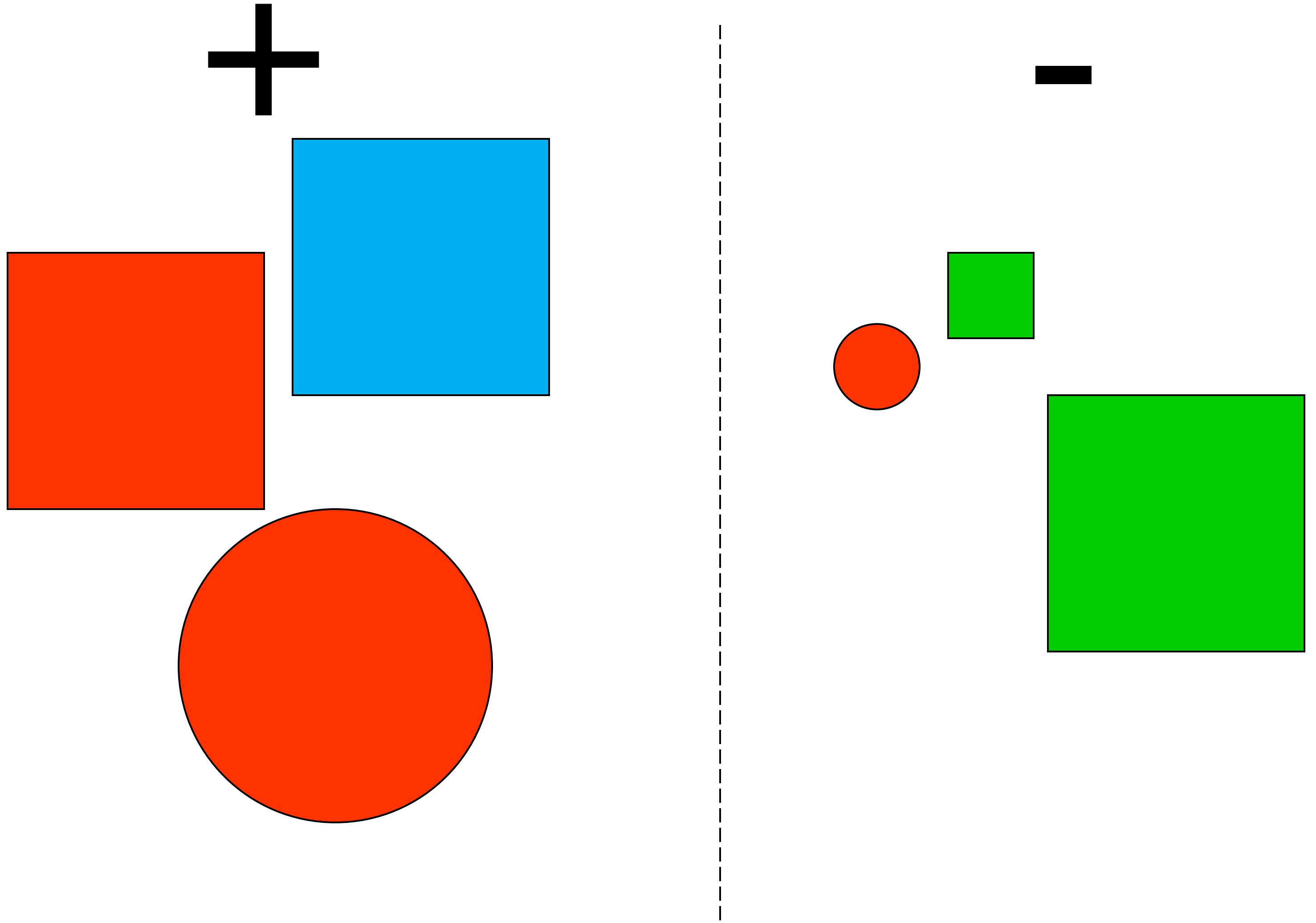
- Information gain, or mutual information

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

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

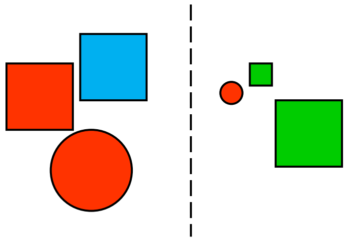
Example

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



The training set

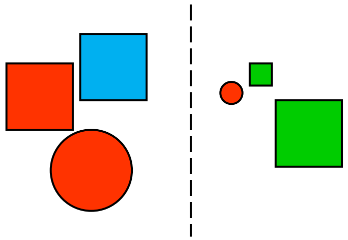
Example	Color	Shape	Size	Class
1	Red	Square	Big	+
2	Blue	Square	Big	+
3	Red	Circle	Big	+
4	Red	Circle	Small	-
5	Green	Square	Small	-
6	Green	Square	Big	-



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 +

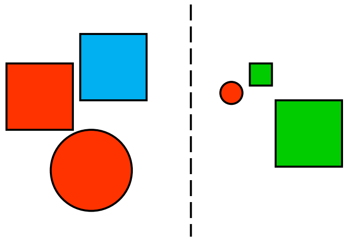
1 out of 6 is blue

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	-

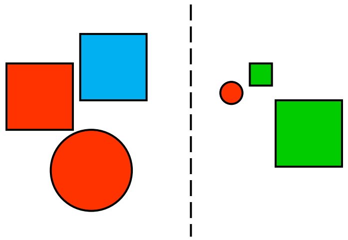


H(class)= H(3/6,3/6) = 1

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	-



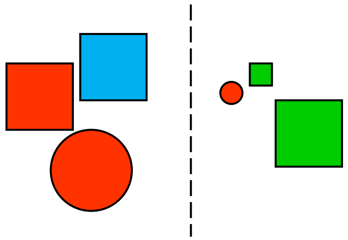
H(class)= H(3/6,3/6) = 1

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	-

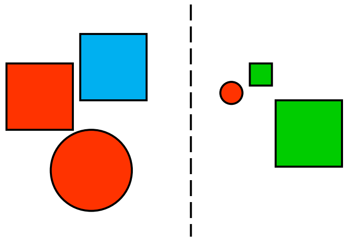


H(class)= H(3/6,3/6) = 1

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 (regression): 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

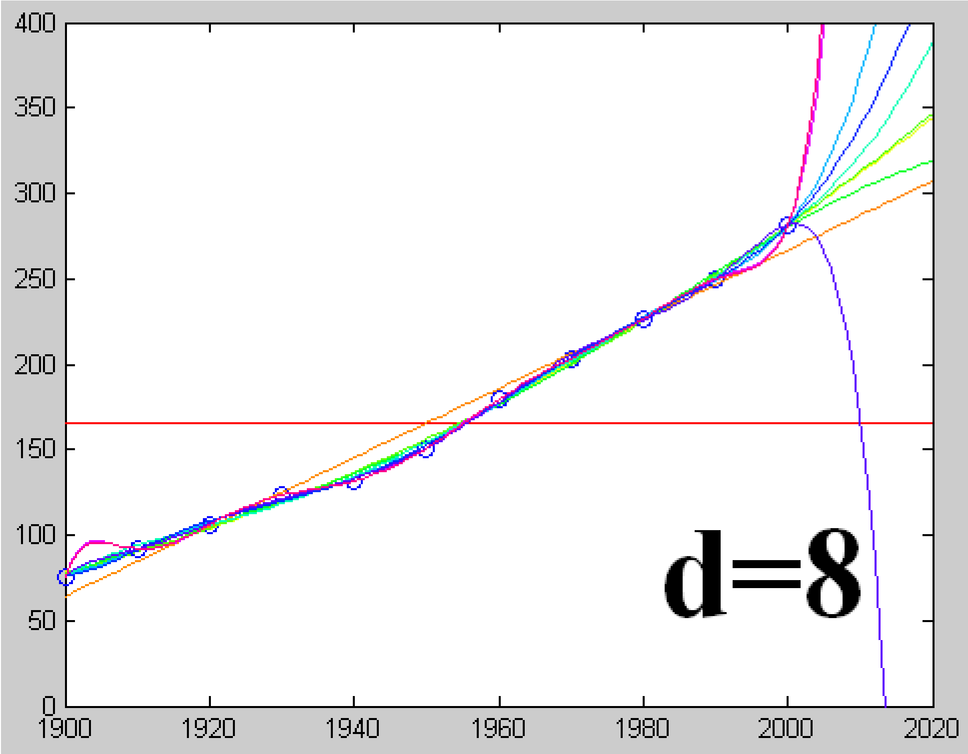
$$MSE = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2$$

- 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

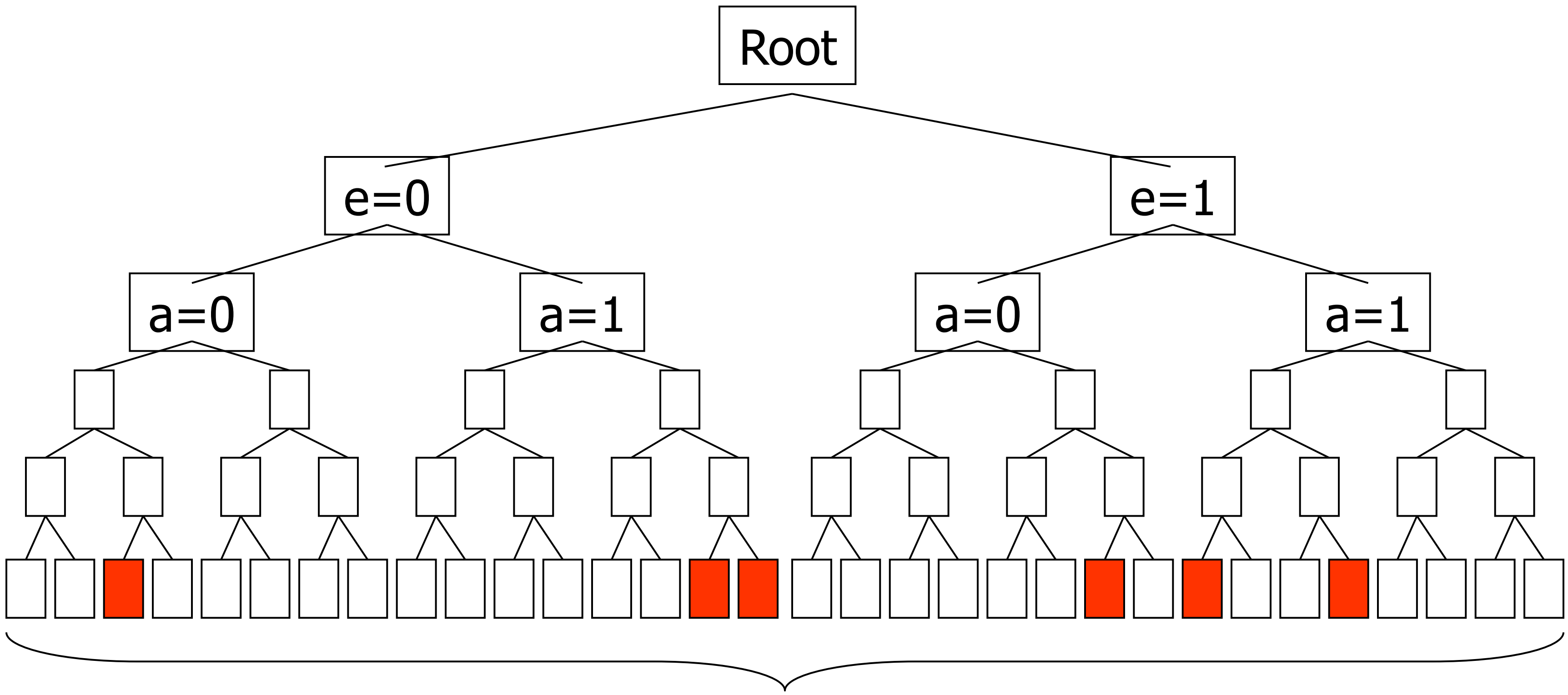
a	b	c	d	e	y
0	0	0	0	0	0
0	0	0	0	1	0
0	0	0	1	0	0
0	0	0	1	1	1
0	0	1	0	0	1
:	:	:	:	:	:
1	1	1	1	1	1

Overfit a decision tree

- The test set is constructed similarly
  - $y=e$, but 25% the time we corrupt it by $y=\neg e$
  - 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

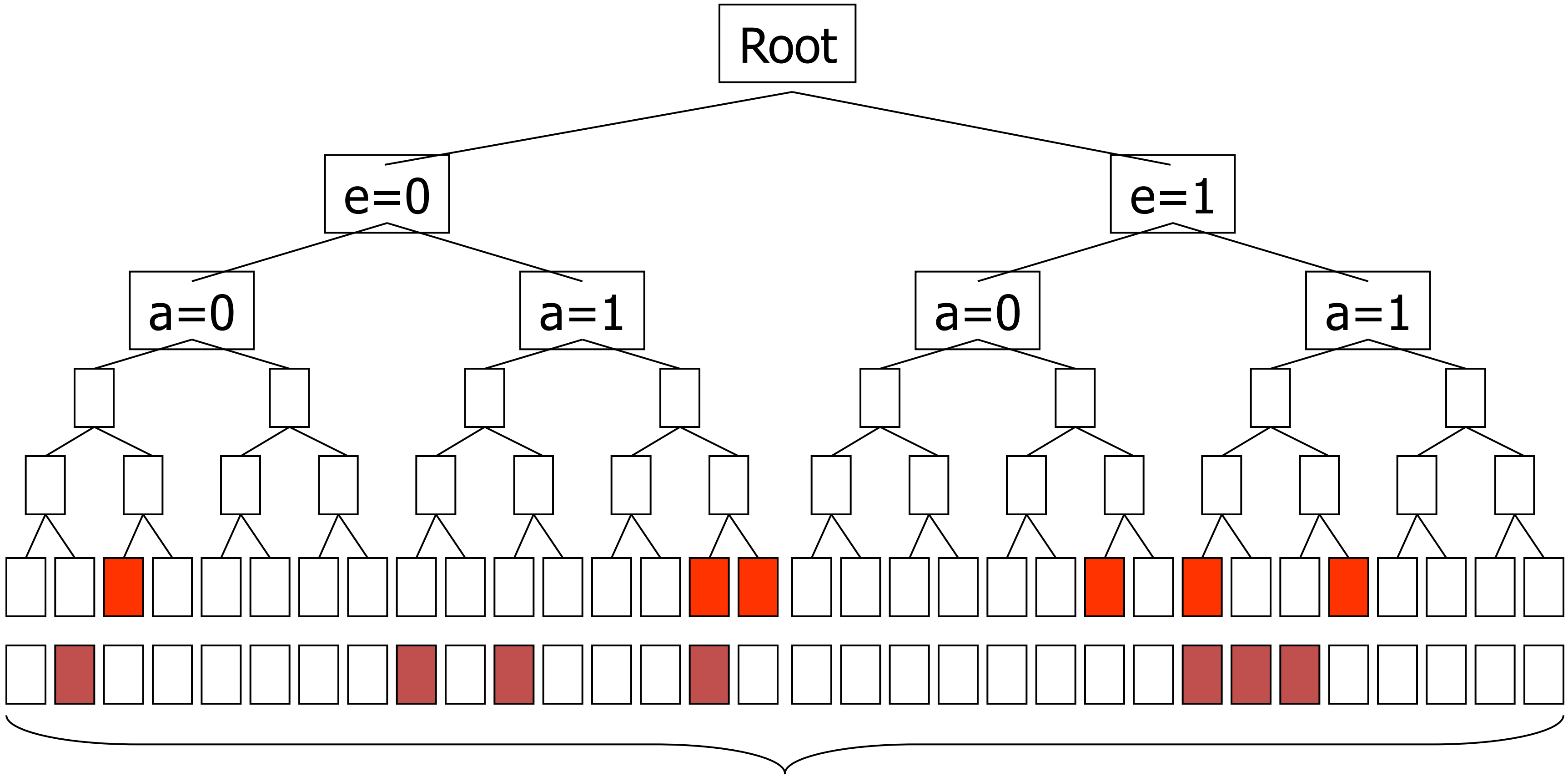
- We build a full tree on the training set



Training set accuracy = 100%
25% of these training leaf node labels will be corrupted (≠e)

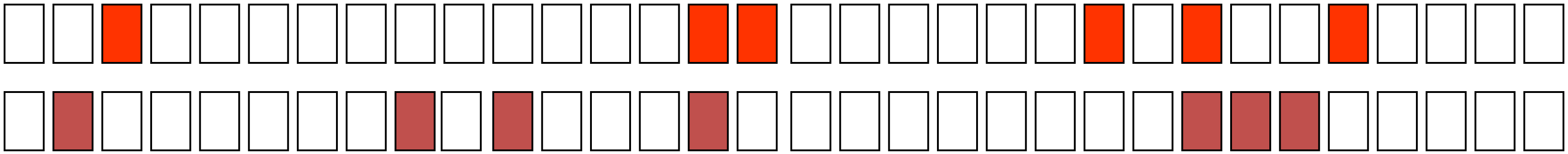
Overfit a decision tree

- 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

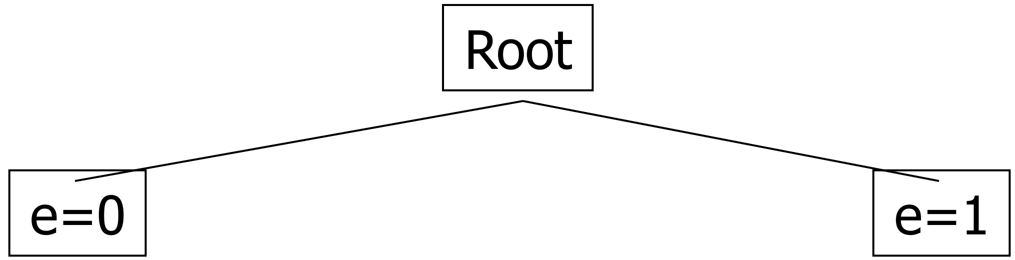
- But if we knew a,b,c,d are irrelevant features and don’t use them in the tree…

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



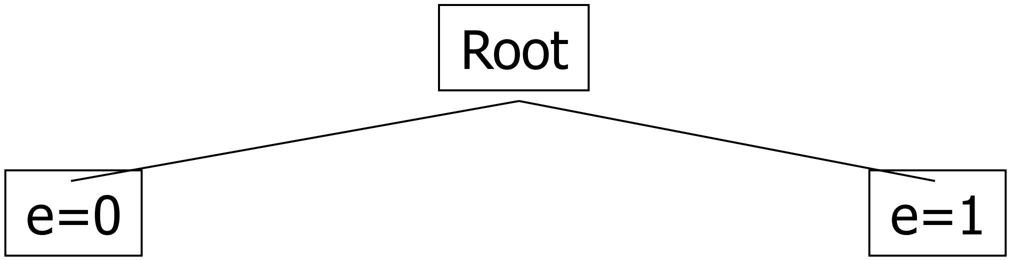
In training data, about ¾ y's are 0 here. Majority vote predicts y=0

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

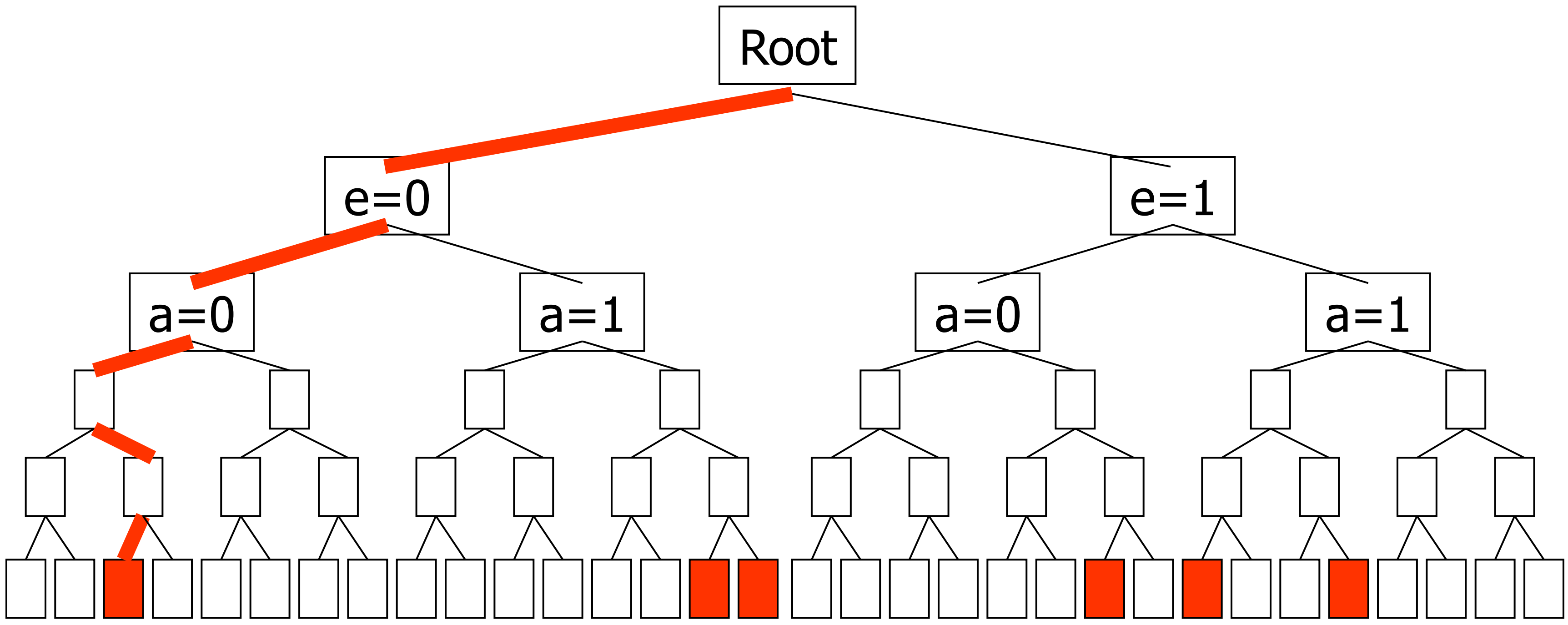
In training data, about ¾ y's are 1 here. Majority vote predicts y=1

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 $T \leftarrow T^*$ /* 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.

$$\boxed{\begin{gathered} H(y \mid x_i > t?) = p(x_i > t) H(y \mid x_i > t) + p(x_i \le t) H(y \mid x_i \le t) \\ I(y \mid x_i > t?) = H(y) - H(y \mid x_i > t?) \end{gathered}}$$

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