Decision Trees: many possible refs., e.g.,

Mitchell, Chapter 3

Boosting: (Linked from class website)

Schapire '01

Decision Trees Boosting

Machine Learning – 10701/15781

Carlos Guestrin

Carnegie Mellon University

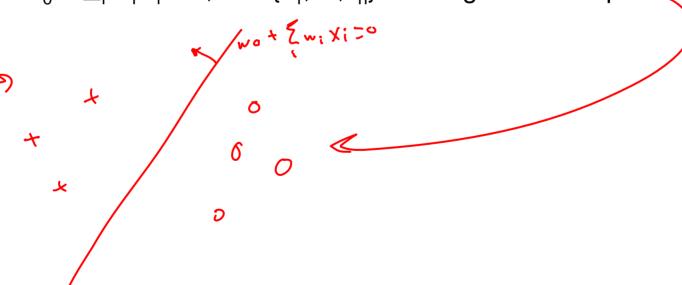
February 6th, 2006

Announcements

- Recitations stay on Thursdays
 - □ 5-6:30pm in Wean 5409
 - □ This week: Decision Trees and Boosting
- Pittsburgh won the Super Bowl !!

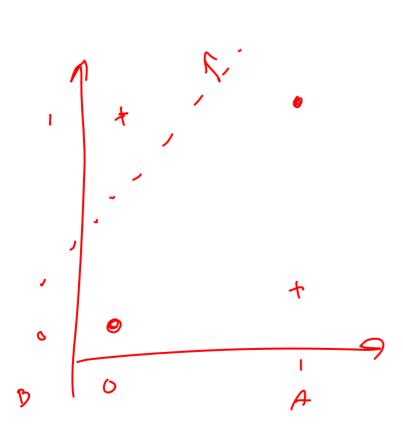
Linear separability

- A dataset is linearly separable iff ∃ a separating hyperplane:
 - □ ∃ w, such that:
 - $w_0 + \sum_i w_i x_i > 0$; if $\mathbf{x} = \{x_1, \dots, x_n\}$ is a positive example
 - $\mathbf{w}_0 + \sum_i \mathbf{w}_i \mathbf{x}_i < 0$; if $\mathbf{x} = \{x_1, \dots, x_n\}$ is a negative example



Not linearly separable data

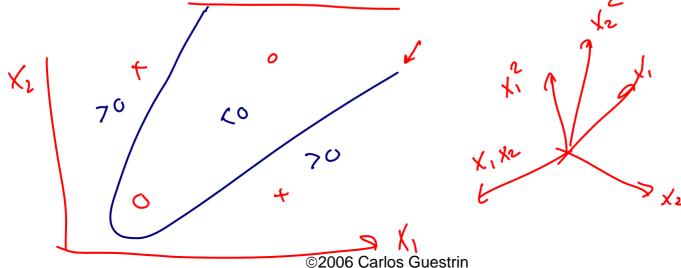
Some datasets are not linearly separable!



A xoa B no hyperplane!

Addressing non-linearly separable data — Option 1, non-linear features

- Choose non-linear features, e.g.,
 - □ Typical linear features: $w_0 + \sum_i w_i x_i$
 - Example of non-linear features: >
 - Degree 2 polynomials, $w_0 + \sum_i w_i x_i + \sum_{ij} w_{ij} x_i x_j$
- Classifier h_w(x) still linear in parameters w
 - □ Usually easy to learn (closed-form or convex/concave optimization)
 - Data is linearly separable in higher dimensional spaces
 - More discussion later this semester



Addressing non-linearly separable data – Option 2, non-linear classifier

- Choose a classifier $h_w(x)$ that is non-linear in parameters w, e.g.,
 - □ Decision trees, neural networks, nearest neighbor,...
- More general than linear classifiers
- But, can often be harder to learn (non-convex/concave optimization required)
- But, but, often very useful
- (BTW. Later this semester, we'll see that these options are not that different)

A small dataset: Miles Per Gallon

Suppose we want to predict MPG

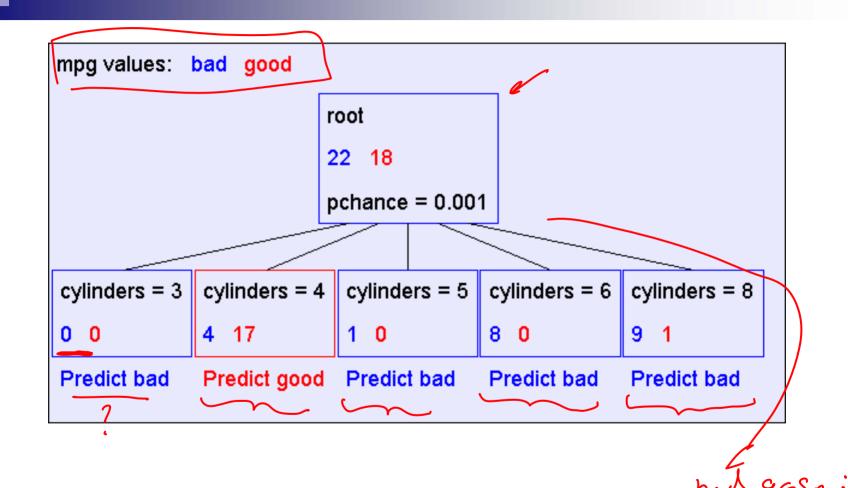
| | 1 | | | | | | | |
|-----|-----|-----------|--------------|------------|--------|--------------|-----------|---------|
| mn | `\ | ovlindoro | diaplacement | horoopowor | woight | acceleration | modelyeer | makar |
| mp | g | cylinders | displacement | horsepower | weight | acceleration | modelyear | ттакег |
| goo | od | 4 | low | low | low | high | 75to78 | asia |
| bad | _ | 6 | medium | medium | medium | medium | 70to74 | america |
| bad | i | 4 | medium | medium | medium | low | 75to78 | europe |
| bad | i | 8 | high | high | high | low | 70to74 | america |
| bad | | | medium | medium | medium | 70to74 | america | |
| bad | i | 4 | low | medium | low | medium | 70to74 | asia |
| bad | | 4 | low | medium | low | low | 70to74 | asia |
| bad | ł | 8 | high | high | high | low | 75to78 | america |
| | | | | | | | : | : |
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| : | | | : | : | : | : | : | : |
| bad | ł | 8 | high | high | high | low | 70to74 | america |
| goo | od | 8 | high | medium | high | high | 79to83 | america |
| bad | ł | 8 | high | high | high | low | 75to78 | america |
| goo | od | 4 | low | low | low | low | 79to83 | america |
| bad | ł | 6 | medium | medium | medium | high | 75to78 | america |
| goo | od | 4 | medium | low | low | low | 79to83 | america |
| goo | od | 4 | low | low | medium | high | 79to83 | america |
| bad | i | 8 | high | high | high | low | 70to74 | america |
| goo | od | | | medium | low | medium | 75to78 | europe |
| bad | 1 / | 5 | medium | medium | medium | medium | 75to78 | europe |

40 Records

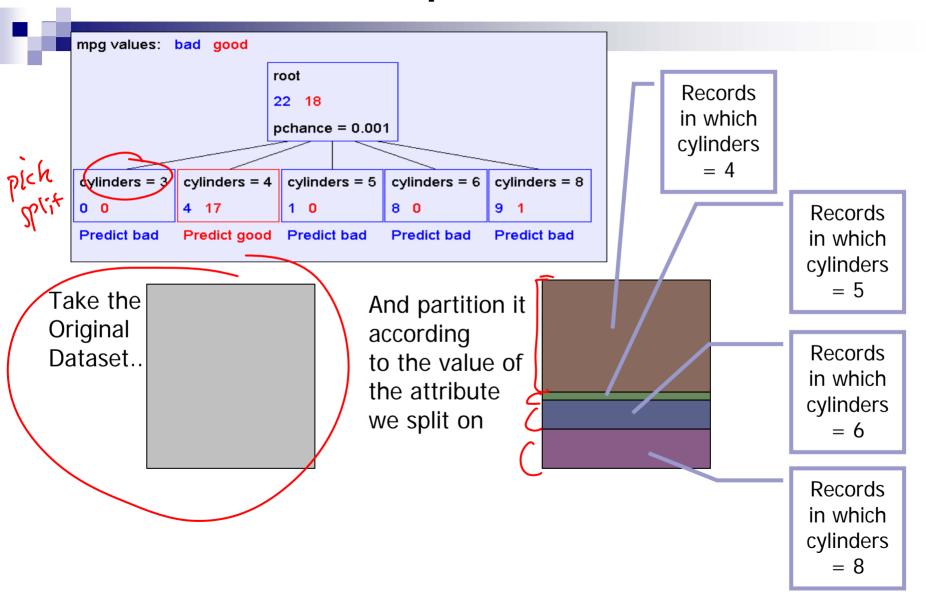
From the UCI repository (thanks to Ross Quinlan)

A Decision Stump

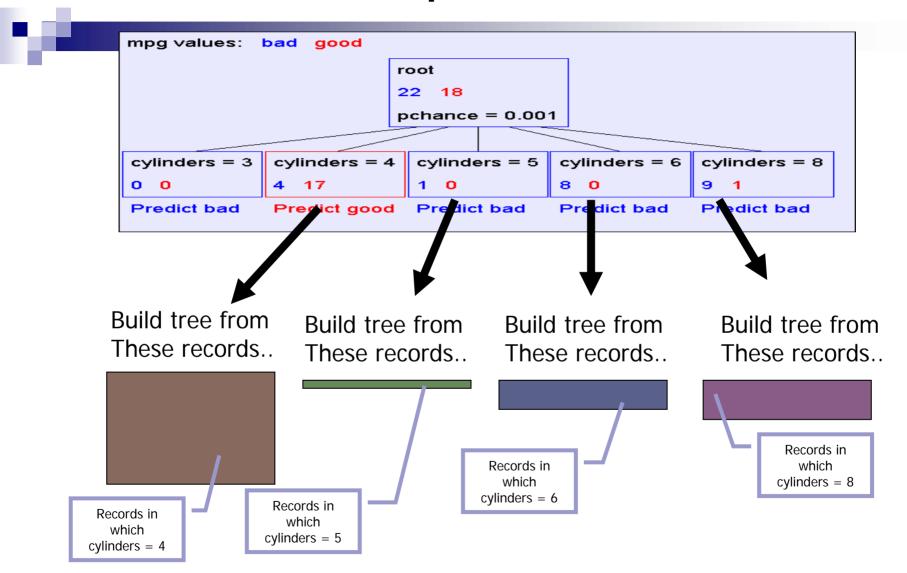




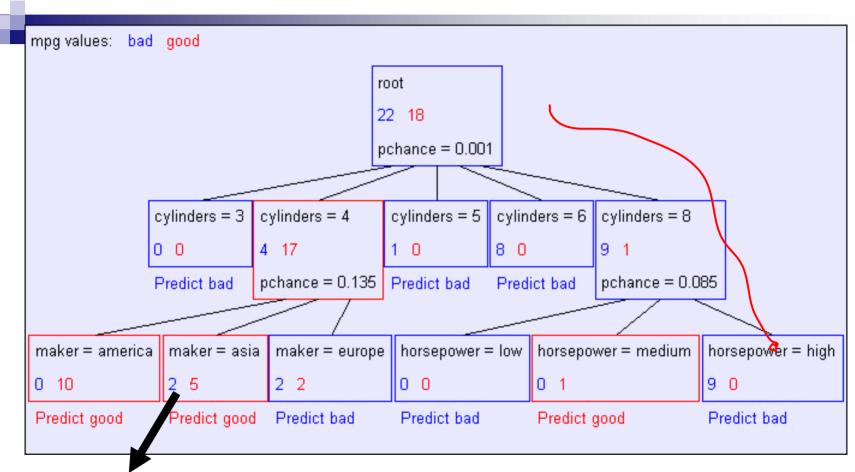
Recursion Step



Recursion Step

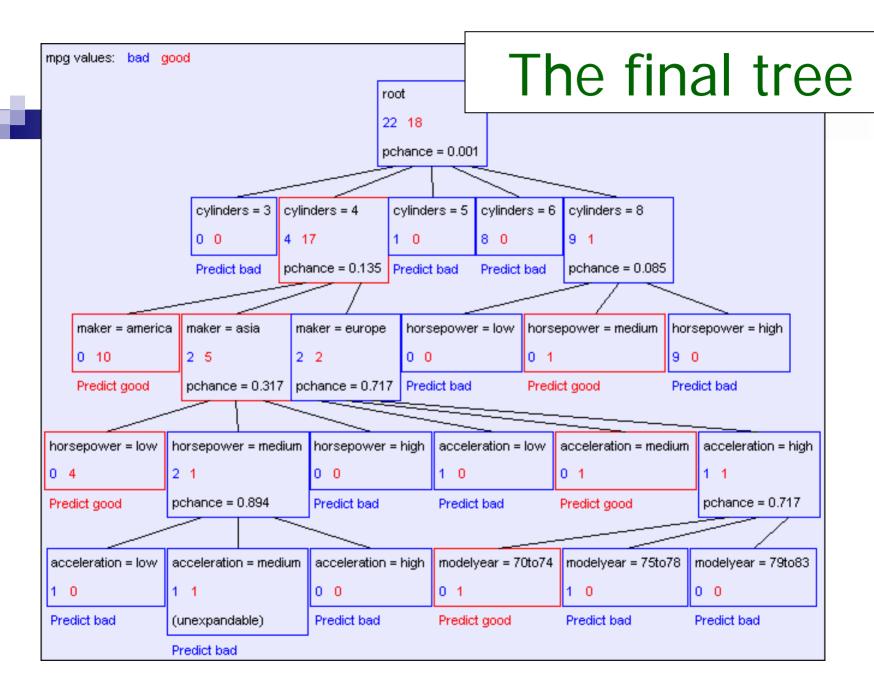


Second level of tree



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

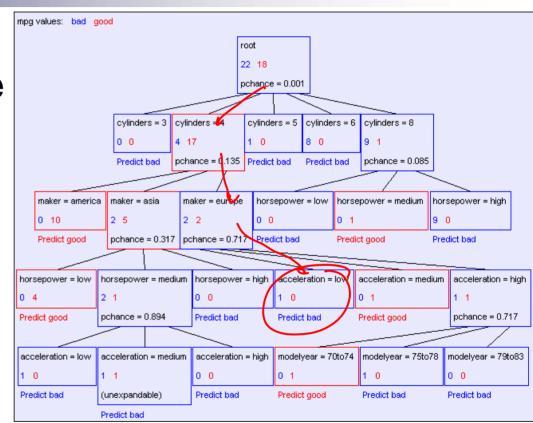
(Similar recursion in the other cases)



Classification of a new example

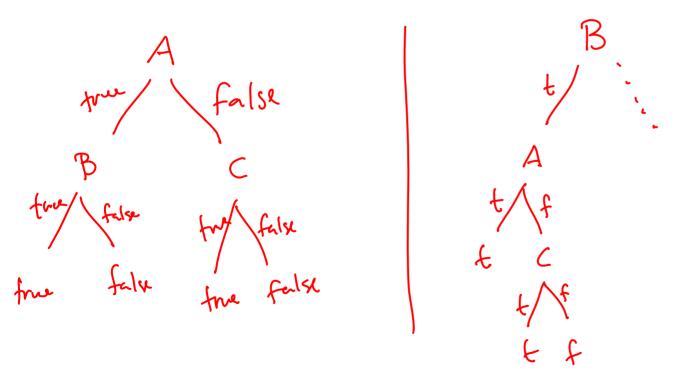
Classifying a test
 example – traverse tree
 and report leaf label

(Cy=4, Europe, acc=low7 => predict bad |}



Are all decision trees equal?

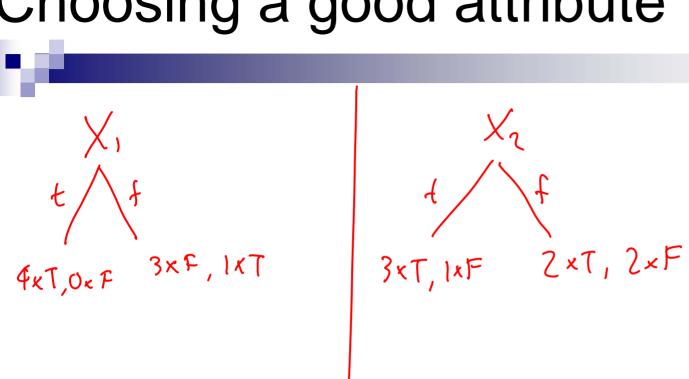
- Many trees can represent the same concept
- But, not all trees will have the same size!
 - \square e.g., $\phi = A \land B \lor \neg A \land C$ ((A and B) or (not A and C))



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

Choosing a good attribute



| X ₁ | X_2 | Υ |
|----------------|-------|---|
| Т | Т | Т |
| Т | F | Т |
| Т | Т | Т |
| Т | F | Т |
| F | Т | Т |
| Ŧ | F | F |
| F | Т | F |
| F | F | F |

Measuring uncertainty

- Good split if we are more certain about classification after split
 - Deterministic good (all true or all false)
 - Uniform distribution bad

Less uncertainty

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

Entropy

def:

Entropy H(X) of a random variable Y

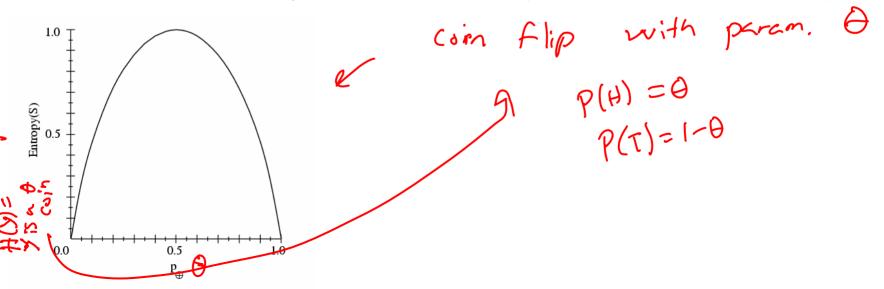
$$0 \log 0 = 0$$

$$\lim_{x \to 0^+} x \ln x = 0$$

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

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)



Andrew Moore's Entropy in a nutshell

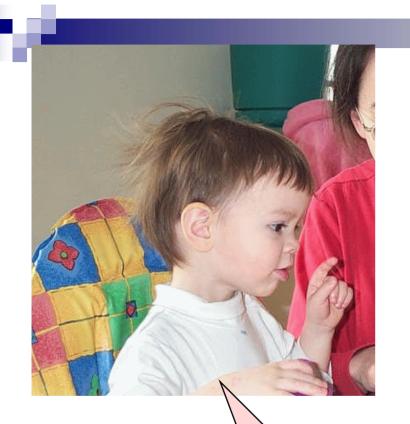




Low Entropy

High Entropy

Andrew Moore's Entropy in a nutshell





Low Entropy

High Entropy

..the values (locations of soup) sampled entirely from within the soup bowl

..the values (locations of soup) unpredictable... almost uniformly sampled throughout our dining room

Information gain

- Advantage of attribute decrease in uncertainty
 - H(Y)Entropy of Y before you split
 - H(X|X)Entropy after split 6 x X
 - Weight by probability of following each branch, i.e., normalized number of records

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

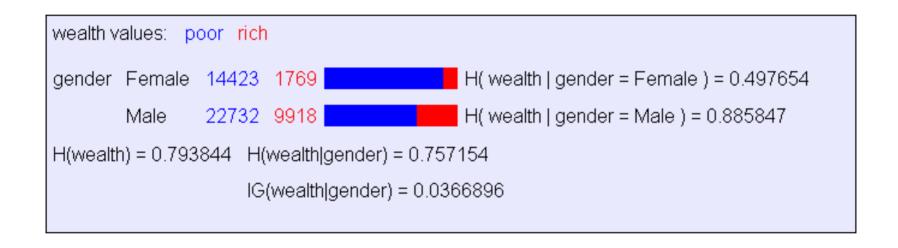
 $IG(X) = H(Y) - H(Y \mid X)$ Information gain is difference

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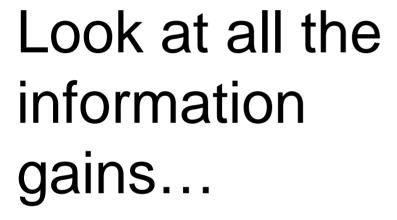
Learning decision trees

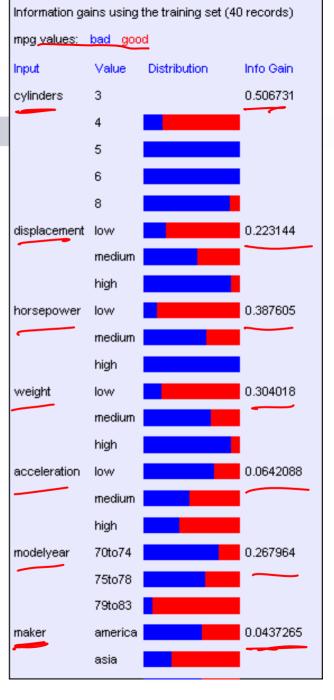
- Start from empty decision tree
- Split on next best attribute (feature)
- Use, for example, information gain to select attribute
 - □ Split on $\underset{i}{\operatorname{arg max}} IG(X_i) = \underset{i}{\operatorname{arg max}} H(Y) H(Y \mid X_i)$
 - Recurse

Information Gain Example

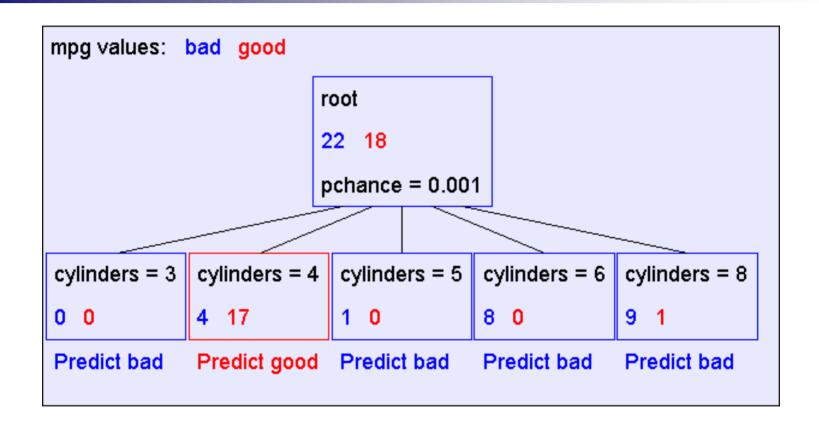


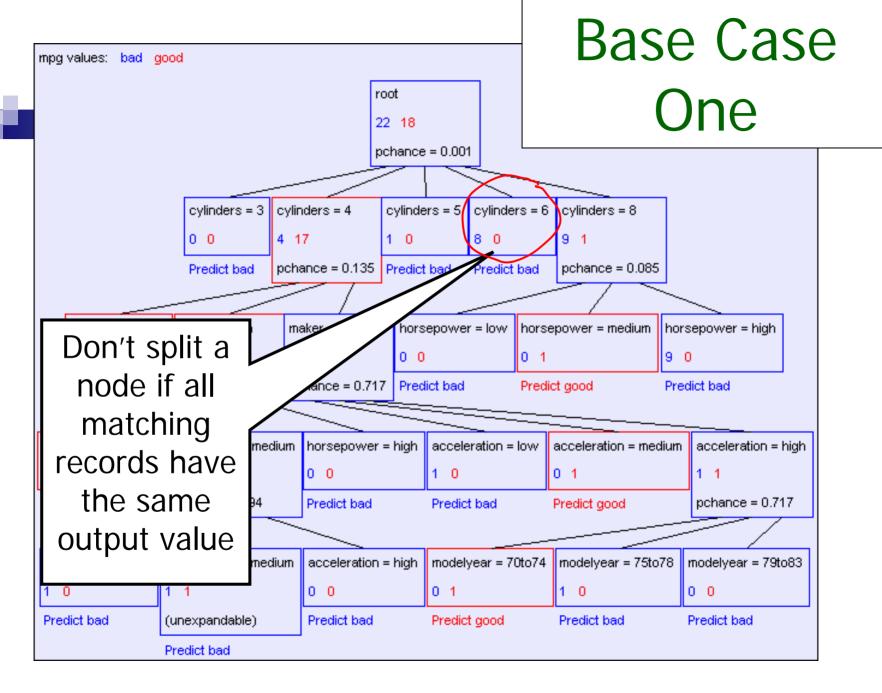
Suppose we want to predict MPG

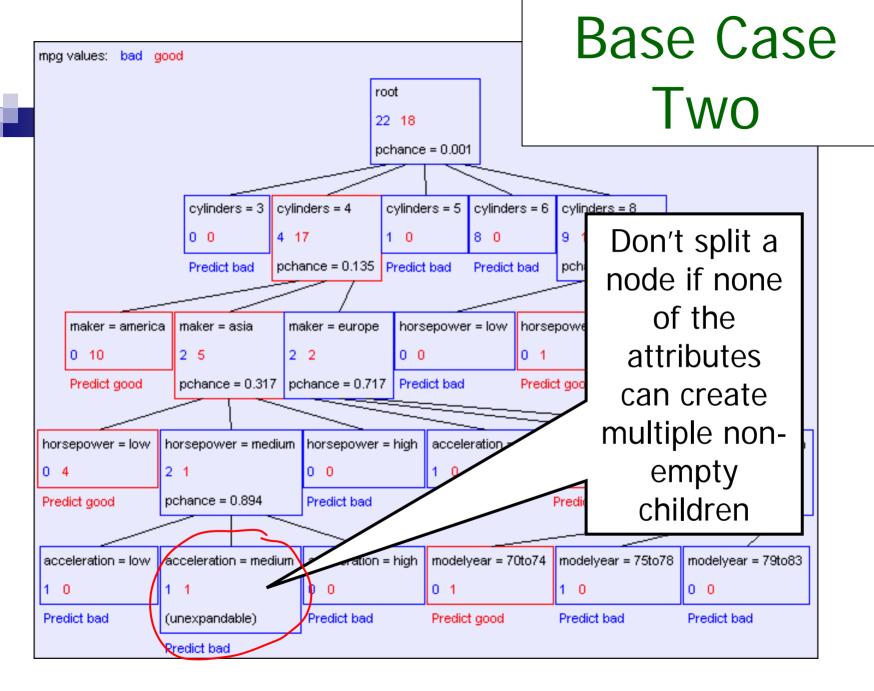


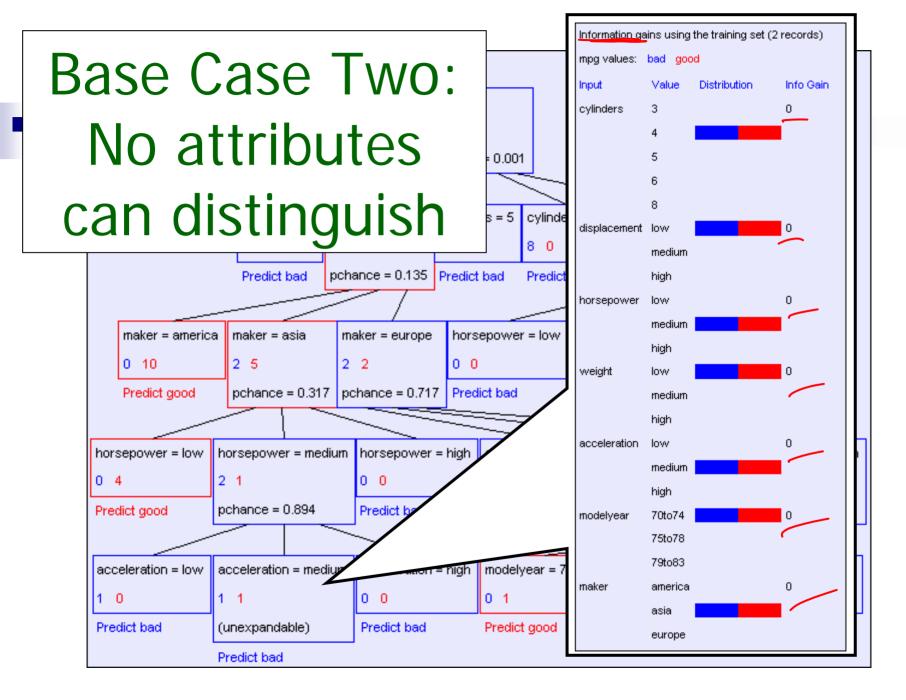


A Decision Stump







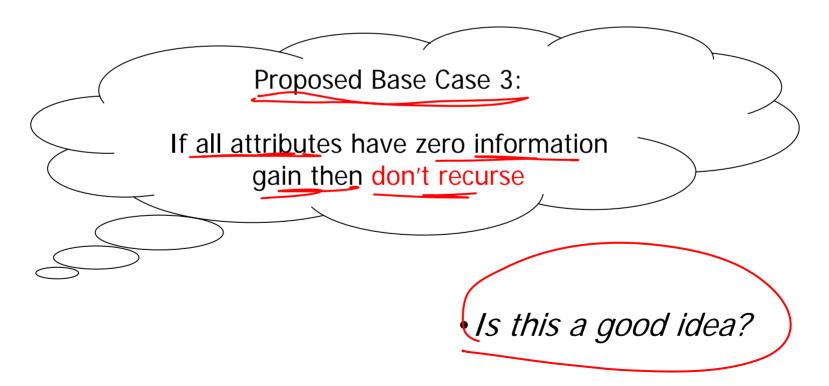


Base Cases

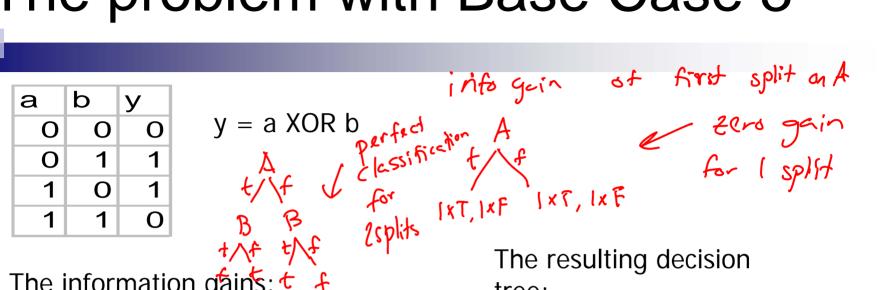
- Base Case One: If all records in current data subset have the same output then don't recurse
- Base Case Two: If all records have exactly the same set of input attributes then don't recurse

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



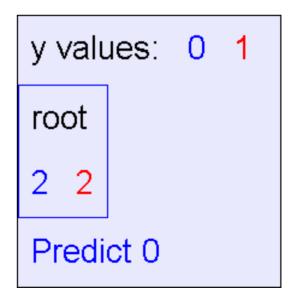
The problem with Base Case 3



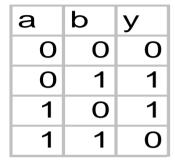
The information gains: t

Information gains using the training set (4 records) y values: 0 1 Input Value Distribution Info Gain 0 а 0

tree:



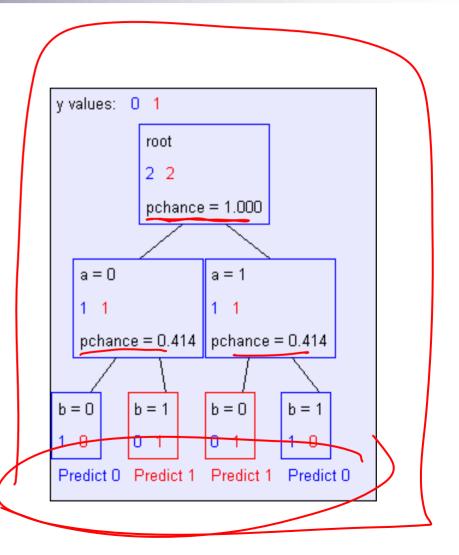
If we omit Base Case 3:



$$y = a XOR b$$

The resulting decision tree:





Basic Decision Tree Building Summarized

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).
 - \square Create and return a non-leaf node with n_X children.
 - ☐ The *i*th child should be built by calling

BuildTree(DS,, Output)

Where DS_i built consists of all those records in DataSet for which X = ith distinct value of X.

Real-Valued inputs

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

| mpg | cylinders | disp | lacemen | hor | sepower | w | eight/ | ac | celeration | modelyear | maker |
|------|-----------|------|---------|-----|---------|----|--------|----|------------|-----------|---------|
| | | | | | | | | | | | |
| good | 4 | | 97 | - 1 | 75 | / | 2265 | | 18.2 | 77 | asia |
| bad | 6 | | 199 | | 90 | | 2648 | | 15 | 70 | america |
| bad | 4 | | 121 | | 110 | 1 | 2600 | | 12.8 | 77 | europe |
| bad | 8 | | 350 | | 175 | П | 4100 | | 13 | 73 | america |
| bad | 6 | | 198 | | 95 | П | 3102 | 7 | 16.5 | 74 | america |
| bad | 4 | | 108 | | 94 | П | 2379 | 1 | 16.5 | 73 | asia |
| bad | 4 | | 113 | | 95 | П | 2228 | T | 14 | 71 | asia |
| bad | 8 | | 302 | | 139 | | 3570 | | 12.8 | 78 | america |
| : | : | : | | : | | H | | 1 | | : | : |
| : | : | : | | : | | 1: | | : | | : | : |
| : | : | : | | : | | : | | : | | : | : |
| good | 4 | | 120 | | 79 | П | 2625 | | 18.6 | 82 | america |
| bad | 8 | | 455 | | 225 | J | 4425 | Г | 10 | 70 | america |
| good | 4 | | 107 | | 86 | / | 2464 | | 15.5 | 76 | europe |
| bad | 5 | | 131 | | 103 | ١ | 2830 | | 15.9 | 78 | europe |
| | | | | | | 1 | | | | | |
| | • | | | | | | | | | | |

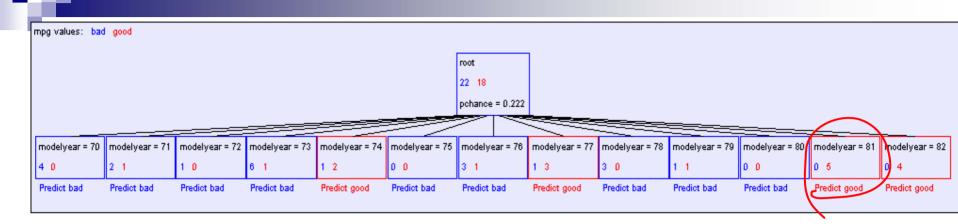
Infinite number of possible split values!!!

Finite dataset, only finite number of relevant splits!

Idea One: Branch on each possible real value

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"One branch for each numeric value" idea:



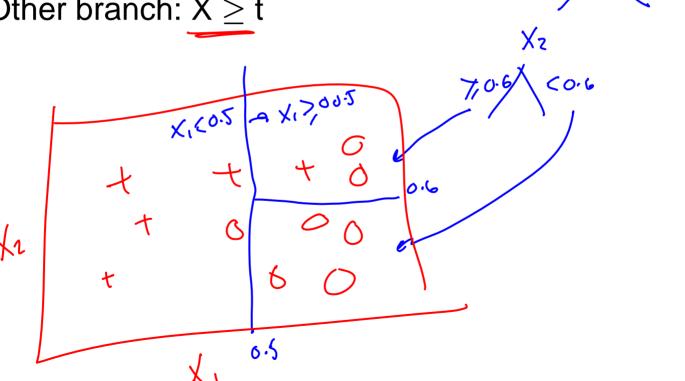
Hopeless: with such high branching factor will shatter the dataset and overfit 5 dec.

Threshold splits



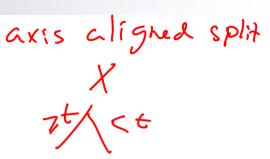
One branch: X < t

Other branch: $X \ge t$

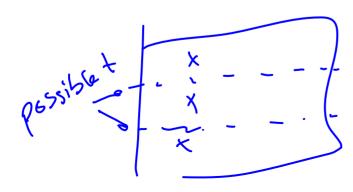


Choosing threshold split

- Binary tree, split on attribute X
 - □ One branch: X < t</p>
 - \square Other branch: $X \ge t$
- Search through possible values of t
 - □ Seems hard!!!
- But only finite number of t's are important
 - □ Sort data according to X into $\{x_1,...,x_m\}$
 - \Box Consider split points of the form $x_i + (x_{i+1} x_i)/2$

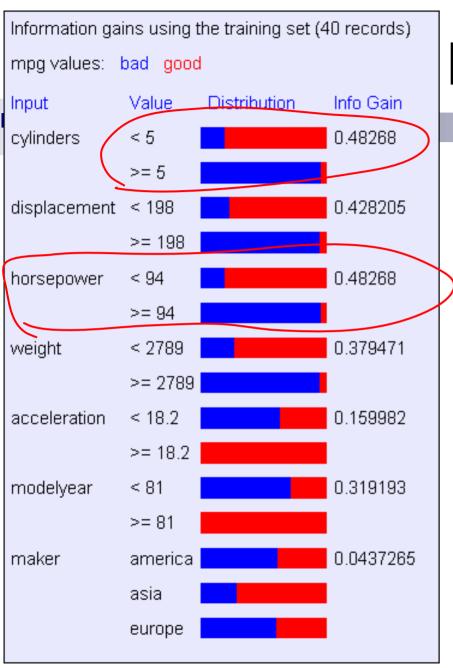


non axis alignele



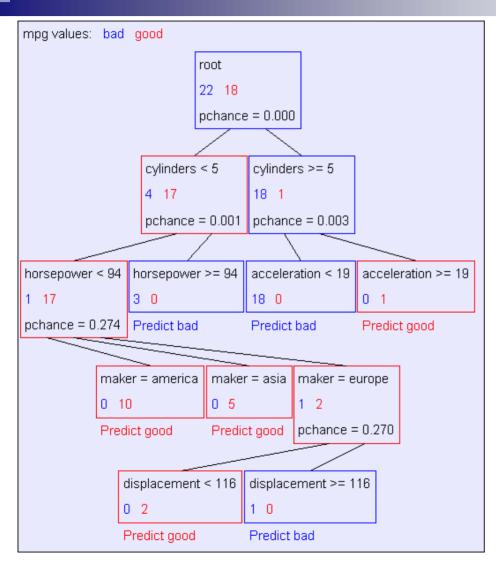
A better idea: thresholded splits

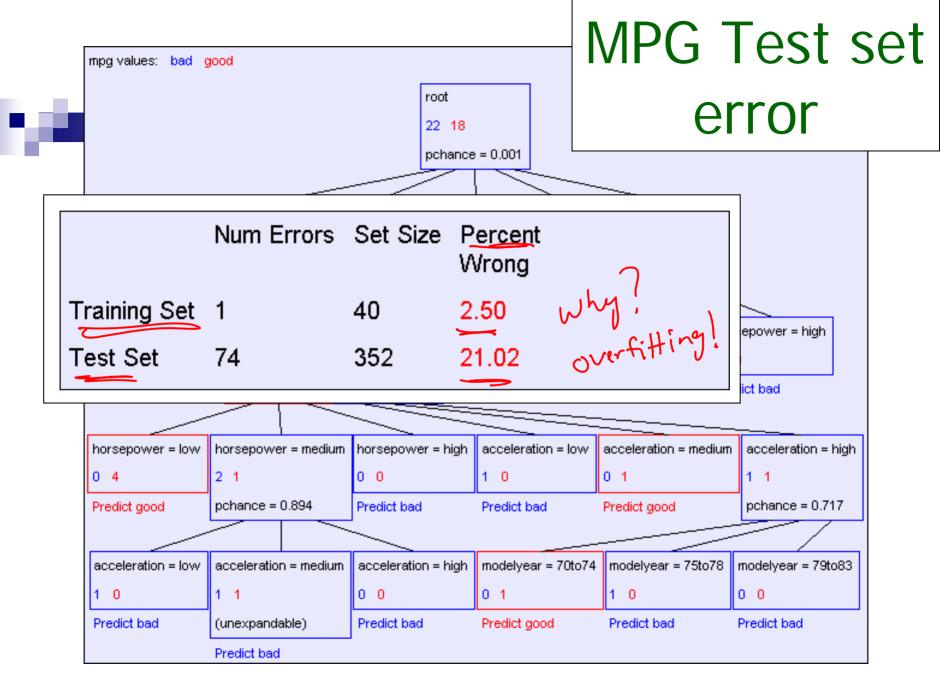
- Suppose X is real valued
- Define IG(Y|X:t) as H(Y) H(Y|X:t)
- Define H(Y|X:t) = H(Y|X < t) P(X < t) + H(Y|X >= t) P(X >= t)
 - IG(Y|X:t) is the information gain for predicting Y if all you know is whether X is greater than or less than t
- Then define $IG^*(Y|X) = max_t IG(Y|X:t)$
- For each real-valued attribute, use IG*(Y|X) for assessing its suitability as a split

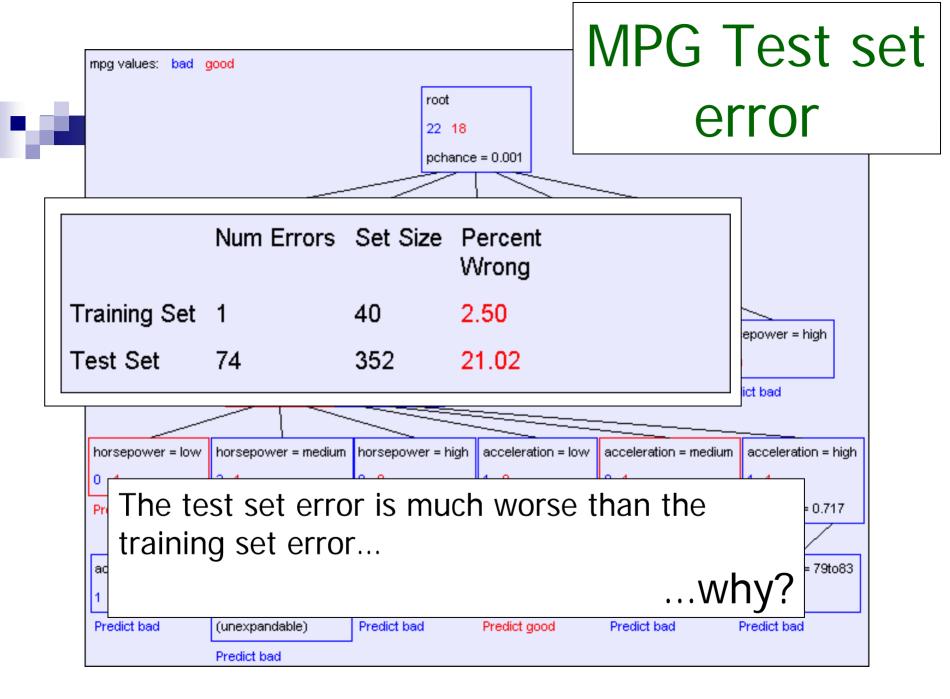


Example with MPG

Example tree using reals







Decision trees & Learning Bias

Any "separable data
no examples with
some attrib. values
have diff. labels

| 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 |
| : | : | : | : | : | : | : | : |
| : | : | : | : | : | 1: | : | : |
| : | : | : | : | : | : | : | : |
| 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 |

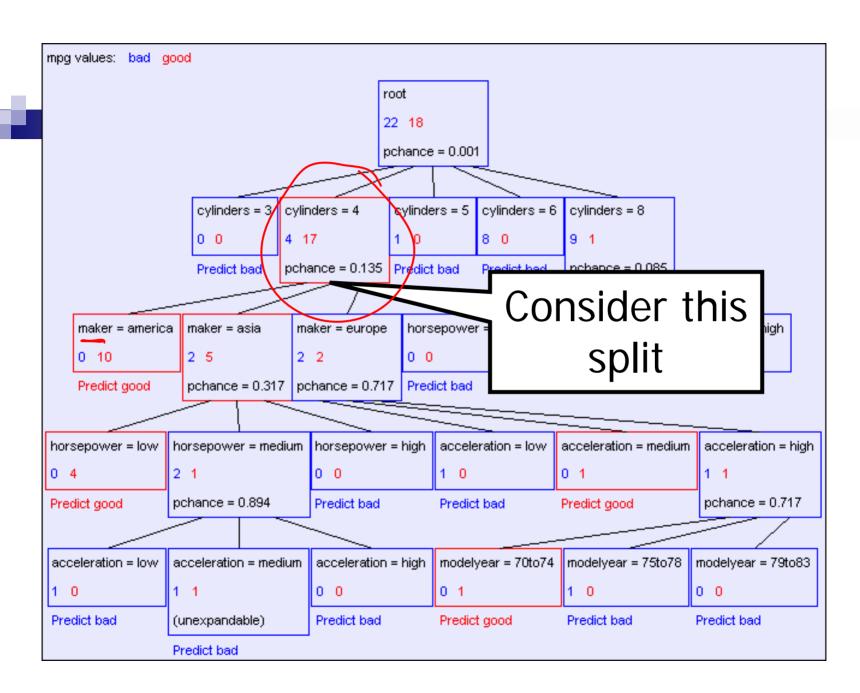
con classified exactly with a d. true

almost) zero byas!

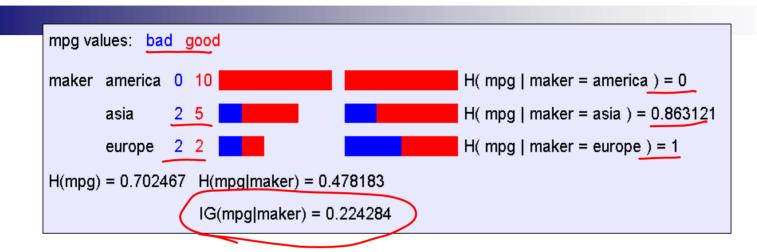
Decision trees will overfit

- Standard decision trees are have no learning biased
 - □ Training set error is always zero!
 - Lots of variance
 - □ Will definitely overfit!!!
 - Must bias towards simpler trees
- Many strategies for picking simpler trees:
 - □ Fixed depth 5 d. tres
 - □ Fixed number of leaves
 - □ Or something smarter...

1000 leaves

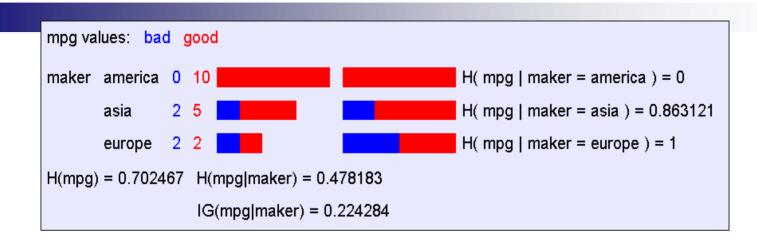


A chi-square test



- Suppose that mpg was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

A chi-square test



- Suppose that mpg was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

By using a particular kind of chi-square test, the answer is 13.5%

(Such simple hypothesis tests are very easy to compute, unfortunately, not enough time to cover in the lecture)

Using Chi-squared to avoid overfitting

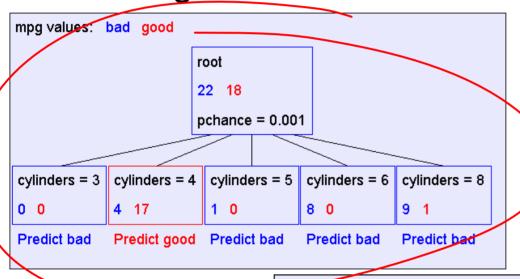
- Build the full decision tree as before
- But when you can grow it no more, start to prune:
 - □ Beginning at the bottom of the tree, delete splits in which $p_{chance} > MaxPchance$
 - □ Continue working you way up until there are no more prunable nodes

MaxPchance is a magic parameter you must specify to the decision tree, indicating your willingness to risk fitting noise

Pruning example

■ With MaxPchance = 0.1, you will see the following MPG decision tree:

| MaxPchance = 0.1, you will see the following MPG decision tree: | Set a decision tree: | Set a decision tree | Set a decisi

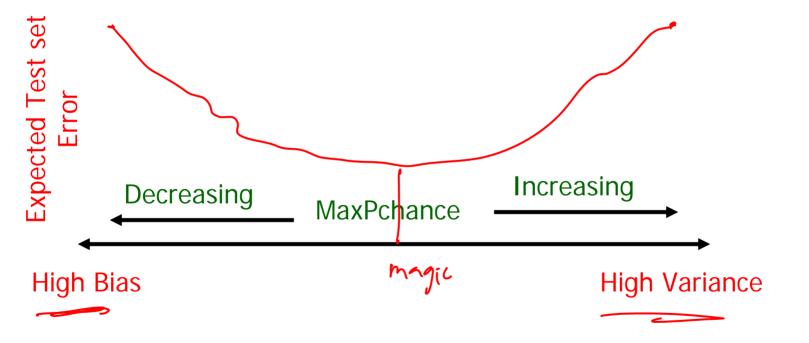


Note the improved test set accuracy compared with the unpruned tree

| | Num Errors | Set Size | Wrong |
|--------------|------------|----------|--------------|
| Training Set | 5 | 40 | 12.50 higher |
| Test Set | 56 | 352 | 15.91 lower |

MaxPchance

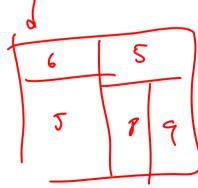
 Technical note MaxPchance is a regularization parameter that helps us bias towards simpler models



We'll learn to choose the value of these magic parameters soon!

What you need to know about decision trees

- Decision trees are one of the most popular data mining tools
 - Easy to understand
 - □ Easy to implement
 - □ Easy to 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!!!
 - □ Zero bias classifier → Lots of variance
 - □ Must use tricks to find "simple trees", e.g.,
 - Fixed depth/Early stopping
 - Pruning
 - Hypothesis testing



Fighting the bias-variance tradeoff

- Simple (a.k.a. weak) learners are good
 - □ e.g., naïve Bayes, logistic regression, decision stumps (or shallow decision trees)
 - □ Low variance, don't usually overfit
- Simple (a.k.a. weak) learners are bad
 - □ High bias, can't solve hard learning problems
- Can we make weak learners always good???
 - □ No!!!
 - But often yes…

Boosting [Schapire, 1989]

- Idea: given a weak learner, run it multiple times on (reweighted) training data, then let learned classifiers vote
- On each iteration t.
 - weight each training example by how incorrectly it was classified
 - □ Learn a hypothesis h_t
 - \square A strength for this hypothesis α_t
- Final classifier:

- Practically useful
- Theoretically interesting

Learning from weighted data

- Sometimes not all data points are equal
 - □ Some data points are more equal than others
- Consider a weighted dataset
 - \square D(i) weight of *i*th training example ($\mathbf{x}^i, \mathbf{y}^i$)
- Now, in all calculations, whenever used, ith training example counts as D(i) "examples"
 - □ e.g., MLE for Naïve Bayes, redefine Count(Y=y) to be weighted count

Given: $(x_1, y_1), ..., (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$ Initialize $D_1(i) = 1/m$.

For t = 1, ..., T:

- Train base learner using distribution D_t .
- Get base classifier $h_t: X \to \mathbb{R}$.
- Choose $\alpha_t \in \mathbb{R}$.
- Update:

$$D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

where Z_t is a normalization factor

$$Z_t = \sum_{i=1}^m D_t(i) \exp(-\alpha_t y_i h_t(x_i))$$

Output the final classifier:

$$H(x) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right).$$

Figure 1: The boosting algorithm AdaBoost. ©2006 Carlos Guestrin

Given: $(x_1, y_1), ..., (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$ Initialize $D_1(i) = 1/m$.

For t = 1, ..., T:

- Train base learner using distribution D_t .
- Get base classifier $h_t: X \to \mathbb{R}$.
- Choose $\alpha_t \in \mathbb{R}$.
- Update:

$$\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

$$D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

$$\epsilon_t = P_{i \sim D_i} [\mathbf{x}^i \neq y^i]$$

$$\epsilon_t = \frac{1}{\sum_{i=1}^n D_t(i)} \sum_{i=1}^m D_t(i) \delta(h_t(x_i) \neq y_i)$$



$$\frac{1}{m} \sum_{i=1}^{m} \delta(H(x_i) \neq y_i) \leq \frac{1}{m} \sum_{i=1}^{m} \exp(-y_i f(x_i))$$

Where
$$f(x) = \sum_{t} \alpha_t h_t(x)$$
; $H(x) = sign(f(x))$



$$\frac{1}{m} \sum_{i=1}^{m} \delta(H(x_i) \neq y_i) \leq \frac{1}{m} \sum_{i=1}^{m} \exp(-y_i f(x_i)) = \prod_{t} Z_t$$

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Where
$$f(x) = \sum_{t} \alpha_t h_t(x)$$
; $H(x) = sign(f(x))$

If we minimize $\prod_{t} \mathbf{Z}_{t}$, we minimize our training error

We can tighten this bound by choosing α_t and h_t on each iteration to minimize Z_t

$$Z_t = \sum_{i=1}^m D_t(i) \exp(-\alpha_t y_i h_t(x_i))$$



$$Z_t = \sum_{i=1}^m D_t(i) \exp(-\alpha_t y_i h_t(x_i))$$

For boolean target function, this is accomplished by [Freund & Schapire '97]:

$$\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

Strong, weak classifiers

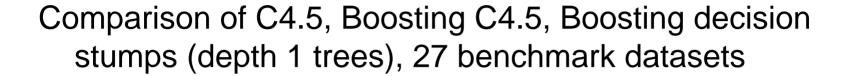
- If each classifier is (at least slightly) better than random
 - \square $\varepsilon_{\rm t} < 0.5$
- AdaBoost will achieve zero training error (exponentially fast):

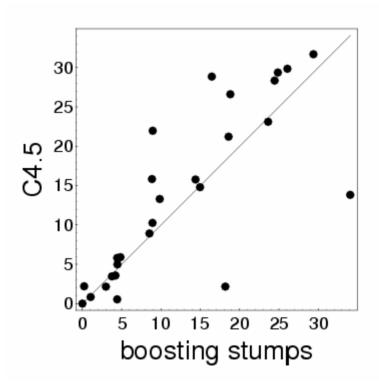
$$\frac{1}{m} \sum_{i=1}^{m} \delta(H(x_i) \neq y_i) \leq \prod_{t} Z_t \leq \exp\left(-2\sum_{t=1}^{T} (1/2 - \epsilon_t)^2\right)$$

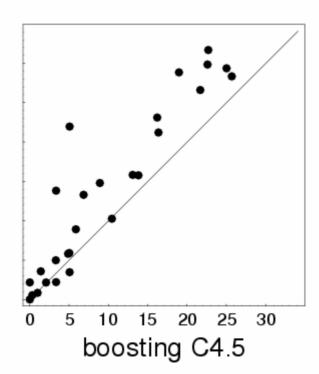
Is it hard to achieve better than random training error?

Boosting: Experimental Results

[Freund & Schapire, 1996]







AdaBoost and AdaBoost.MH on Train (left) and Test (right) data from Irvine repository. [Schapire and Singer, ML 1999] 20 ----labor labor promoters promoters 15 -10 -20 -15 -4 -5 -2 . 10 -0 -25 20 -hepatitis hepatitis sonar sonar 19 -5 -ο. io nosphere ionosphere cleve cleve 24 -22 -12 -10 -5 -18 -4.5 5.5 house-votes-84 house-votes-84 votes t votes 1 3.5 -5 -3 . 2.5 4.5 11 -1.5 -10 -1 -0.5 -0 -17.5 -14 breast-cancer-wiscons in breast-cancer-wiscons in CIX 17 -CIX 12 -16.5 -16 -10 -7 -15.5 -15 -6 -14.5 13.5 -1000 1 1000 1

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Boosting and Logistic Regression



$$P(Y = 1|X) = \frac{1}{1 + \exp(f(x))}$$

And tries to maximize data likelihood:

$$P(data|H) = \prod_{i=1}^{m} \frac{1}{1 + \exp(-y_i f(x_i))}$$

Equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i)))$$

Boosting and Logistic Regression



$$\sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i)))$$

Boosting minimizes similar loss function!!

$$\frac{1}{m}\sum_{i}\exp(-y_{i}f(x_{i})) = \prod_{t}Z_{t}$$

Both smooth approximations of 0/1 loss!

Logistic regression and Boosting

Logistic regression:

Minimize loss fn

$$\sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i)))$$

Define

$$f(x) = \sum_{j} w_j x_j$$

where x_i predefined

Boosting:

Minimize loss fn

$$\sum_{i=1}^{m} \exp(-y_i f(x_i))$$

Define

$$f(x) = \sum_{t} \alpha_t h_t(x)$$

where $h(x_i)$ defined dynamically to fit data

Weights α_j learned incrementally

What you need to know about Boosting

- Combine weak classifiers to obtain very strong classifier
 - □ Weak classifier slightly better than random on training data
 - Resulting very strong classifier can eventually provide zero training error
- AdaBoost algorithm
- Boosting v. Logistic Regression
 - □ Similar loss functions
 - □ Single optimization (LR) v. Incrementally improving classification (B)
- Most popular application of Boosting:
 - □ Boosted decision stumps!
 - Very simple to implement, very effective classifier

Acknowledgements

- Much of the decision trees material in the presentation is courtesy of Andrew Moore, from his excellent collection of ML tutorials:
 - □ http://www.cs.cmu.edu/~awm/tutorials
- Much of the boosting material in the presentation is courtesy of Tom Mitchell