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Decision Trees

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Slide 1



Machine Learning Datasets

What is Classification?

Contingency Tables

OLAP (Online Analytical Processing)

What is Data Mining?

Searching for High Information Gain

Learning an unpruned decision tree recursively

Training Set Error

Test Set Error

Overfitting

Avoiding Overfitting

Information Gain of a real valued input

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Andrew's homebrewed hack: Binary Categorical Splits

Example Decision Trees

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Here is a dataset

age	employme	education	edun	marital		job	relation	race	gender	hour	country	wealth
39	State_gov	Bachelors	13	Never_mar		Adm_cleric	Not_in_fan	White	Male	40	United_St	poor
51	Self_emp_	Bachelors	13	Married		Exec_man	Husband	White	Male	13	United_St	poor
39	Private	HS_grad	9	Divorced		Handlers_d	Not_in_fan	White	Male	40	United_St	poor
54	Private	11th	7	Married		Handlers_d	Husband	Black	Male	40	United_St	poor
28	Private	Bachelors	13	Married		Prof_speci	Wife	Black	Female	40	Cuba	poor
38	Private	Masters	14	Married		Exec_man	Wife	White	Female	40	United_St	poor
50	Private	9th	5	Married_sr		Other_serv	Not_in_fan	Black	Female	16	Jamaica	poor
52	Self_emp_	HS_grad	9	Married		Exec_man	Husband	White	Male	45	United_St	rich
31	Private	Masters	14	Never_mar		Prof_speci	Not_in_fan	White	Female	50	United_St	rich
42	Private	Bachelors	13	Married		Exec_man	Husband	White	Male	40	United_St	rich
37	Private	Some_coll	10	Married		Exec_man	Husband	Black	Male	80	United_St	rich
30	State_gov	Bachelors	13	Married		Prof_speci	Husband	Asian	Male	40	India	rich
24	Private	Bachelors	13	Never_mar		Adm_cleric	Own_child	White	Female	30	United_St	poor
33	Private	Assoc_acc	12	Never_mar		Sales	Not_in_fan	Black	Male	50	United_St	poor
41	Private	Assoc_voc	11	Married		Craft_repai	Husband	Asian	Male	40	*MissingV	rich
34	Private	7th_8th	4	Married		Transport_	Husband	Amer_India	Male	45	Mexico	poor
26	Self_emp_	HS_grad	9	Never_mar		Farming_fi	Own_child	White	Male	35	United_St	poor
33	Private	HS_grad	9	Never_mar		Machine_c	Unmarried	White	Male	40	United_St	poor
38	Private	11th	7	Married		Sales	Husband	White	Male	50	United_St	poor
44	Self_emp_	Masters	14	Divorced		Exec_man	Unmarried	White	Female	45	United_St	rich
41	Private	Doctorate	16	Married		Prof_speci	Husband	White	Male	60	United_St	rich
_	:	:	:	:	:	:	:	:	:	:	:	:

48,000 records, 16 attributes [Kohavi 1995]

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Slide 3

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Example Decision Trees

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Classification

- A Major Data Mining Operation
- Give one attribute (e.g wealth), try to predict the value of new people's wealths by means of some of the other available attributes.
- · Applies to categorical outputs
 - Categorical attribute: an attribute which takes on two or more discrete values. Also known as a symbolic attribute.
 - · Real attribute: a column of real numbers

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Slide 5

Today's lecture

- Information Gain for measuring association between inputs and outputs
- Learning a decision tree classifier from data

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About this dataset

- It is a tiny subset of the 1990 US Census.
- It is publicly available online from the UCI Machine Learning Datasets repository

```
Used Attributes

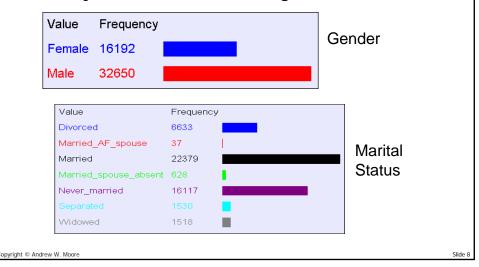
age edunum race hours_worked
employment marital gender country
taxweighting job capitalgain wealth
education relation capitalloss agegroup

This color = Real-valued This color = Symbol-valued

Successfully loaded a new dataset from the file \tadult.fds. It has 16
attributes and 48842 records.
```

What can you do with a dataset?

• Well, you can look at histograms...





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Slide 9

Contingency Tables

A better name for a histogram:

A One-dimensional Contingency Table

- Recipe for making a k-dimensional contingency table:
 - 1. Pick k attributes from your dataset. Call them $a_1, a_2, \dots a_k$.
 - 2. For every possible combination of values, $a_1, =x_1, a_2, =x_2, \dots a_k, =x_k$, record how frequently that combination occurs

Fun fact: A database person would call this a "k-dimensional datacube"

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lide 10

A 2-d Contingency Table

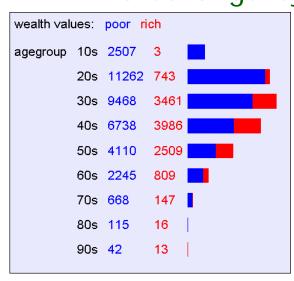
```
wealth values: poor rich
agegroup 10s 2507
         20s 11262 743
         30s 9468
                    3461
         40s 6738
                    3986
                    2509
         50s 4110
         60s 2245
                    809
         70s 668
                    147
         80s 115
                    16
         90s 42
                    13
```

 For each pair of values for attributes (agegroup, wealth) we can see how many records match.

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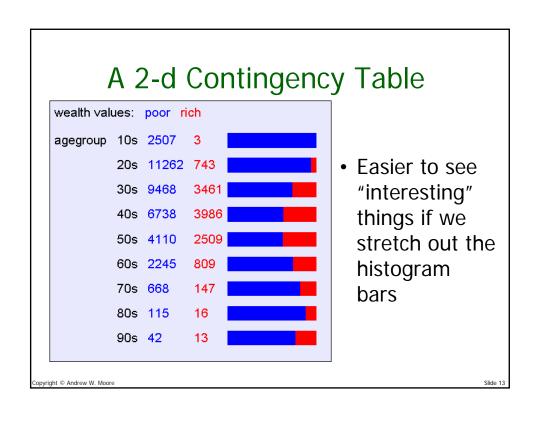
Slide 11

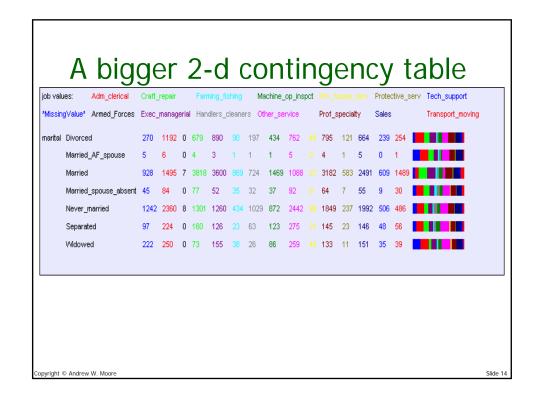
A 2-d Contingency Table



 Easier to appreciate graphically

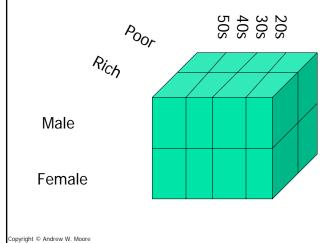
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3-d contingency tables

• These are harder to look at!



Machine Learning Datasets What is Classification? **Contingency Tables OLAP (Online Analytical Processing)** What is Data Mining? Searching for High Information Gain Learning an unpruned decision tree recursively Training Set Error Test Set Error Overfitting **Avoiding Overfitting** Information Gain of a real valued input **Building Decision Trees with real Valued Inputs** Andrew's homebrewed hack: Binary Categorical Splits **Example Decision Trees** opyright © Andrew W. Moore

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On-Line Analytical Processing (OLAP)

- Software packages and database add-ons to do this are known as OLAP tools
- They usually include point and click navigation to view slices and aggregates of contingency tables
- They usually include nice histogram visualization

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Time to stop and think

 Why would people want to look at contingency tables?

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Let's continue to think

- With 16 attributes, how many 1-d contingency tables are there?
- How many 2-d contingency tables?
- How many 3-d tables?
- With 100 attributes how many 3-d tables are there?

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Slide 19

Let's continue to think

- With 16 attributes, how many 1-d contingency tables are there? 16
- How many 2-d contingency tables? 16choose-2 = 16 * 15 / 2 = 120
- How many 3-d tables? 560
- With 100 attributes how many 3-d tables are there? 161,700

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lide 20

Manually looking at contingency tables

- Looking at one contingency table: can be as much fun as reading an interesting book
- Looking at ten tables: as much fun as watching CNN
- Looking at 100 tables: as much fun as watching an infomercial
- Looking at 100,000 tables: as much fun as a three-week November vacation in Duluth with a dying weasel.

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Example Decision Trees

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Data Mining

 Data Mining is all about automating the process of searching for patterns in the data.

Which patterns are interesting? Which might be mere illusions? And how can they be exploited?

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Slide 23

Data Mining

 Data Mining is all about automating the process of searching for patterns in the data.

Which patterns are interesting?

Which might be mere illusions? And how can they be exploited?

That's what we'll look at right now.

And the answer will turn out to be the engine that drives decision tree learning.

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Deciding whether a pattern is interesting

- We will use information theory
- A very large topic, originally used for compressing signals
- But more recently used for data mining...

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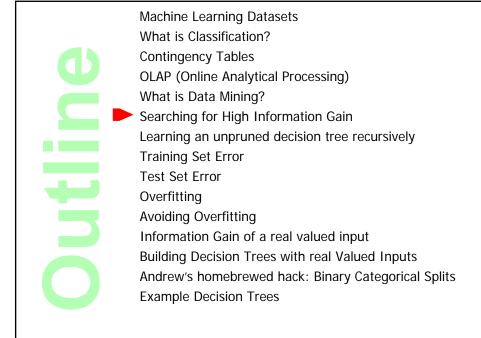
Slide 25

Deciding whether a pattern is interesting

- We will use information theory
- A very large topic, originally used for compressing signals
- But more recently used for data mining...

(The topic of Information Gain will now be discussed, but you will find it in a separate Andrew Handout)

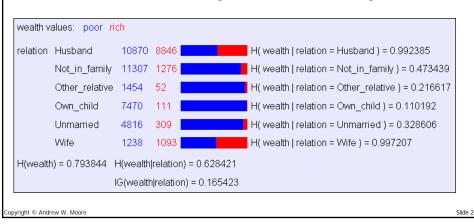
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Searching for High Info Gains

 Given something (e.g. wealth) you are trying to predict, it is easy to ask the computer to find which attribute has highest information gain for it.



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Example Decision Trees

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Slide 2

Learning Decision Trees

- A Decision Tree is a tree-structured plan of a set of attributes to test in order to predict the output.
- To decide which attribute should be tested first, simply find the one with the highest information gain.
- Then recurse...

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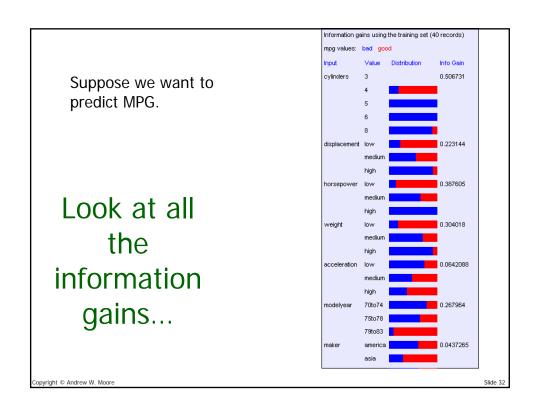
A small dataset: Miles Per Gallon

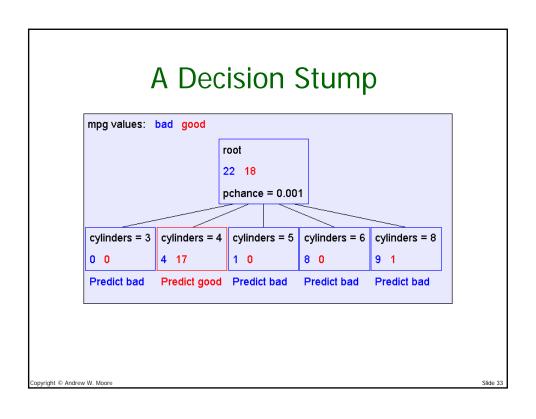
40 Records

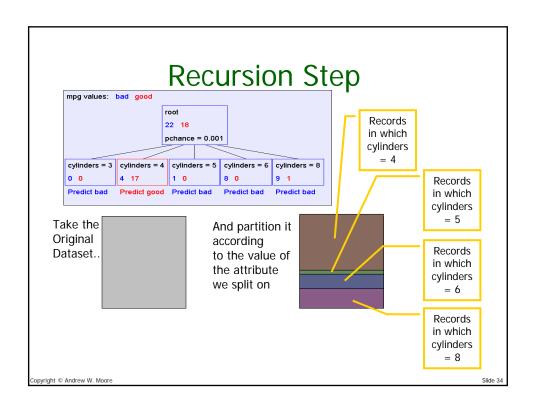
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low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

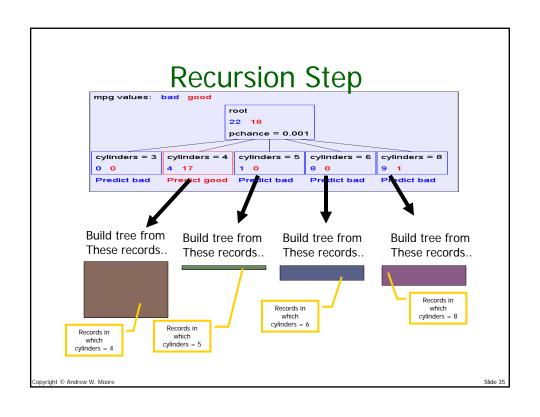
From the UCI repository (thanks to Ross Quinlan)

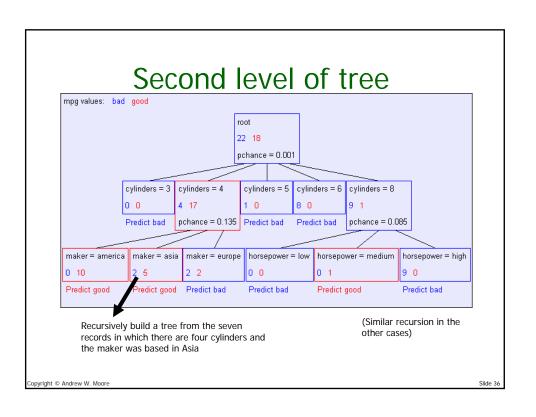
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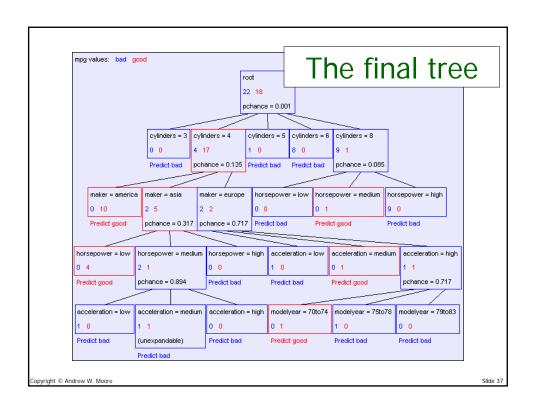


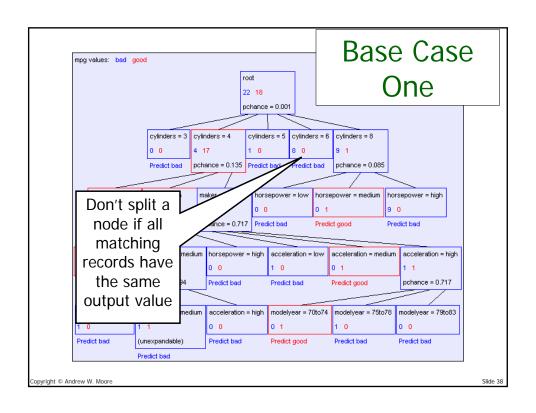


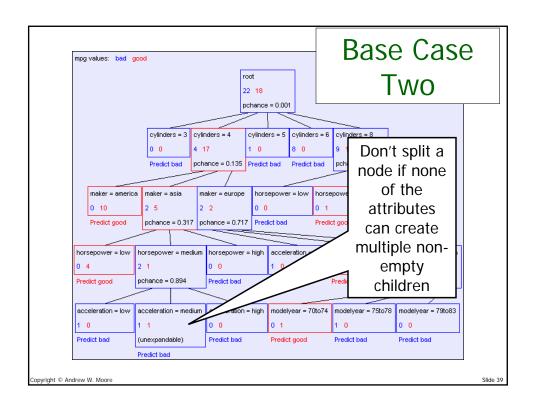


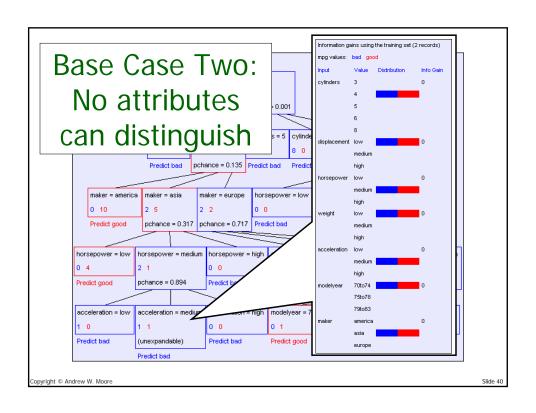












Base Cases

- 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

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Base Cases: An idea

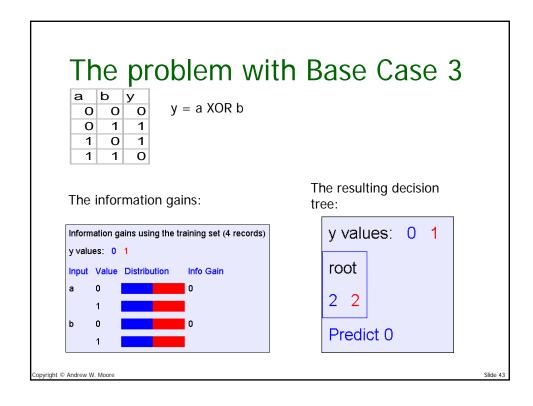
- Base Case One: If all records in current data subset have the same output then don't recurse
- Base Case Two: If all records have exactly the same set of input attributes then don't recurse

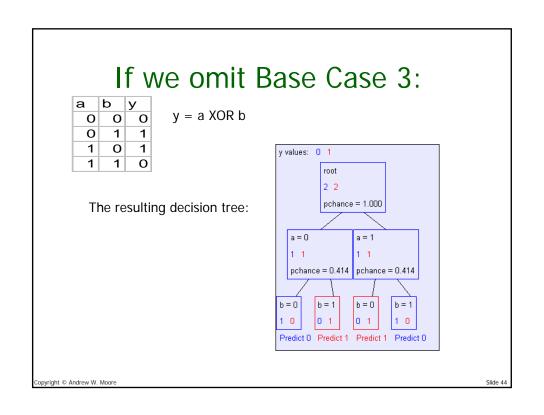
Proposed Base Case 3:

If all attributes have zero information gain then don't recurse

• Is this a good idea?

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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).
 - Create and return a non-leaf node with n_x children.
 - The /th child should be built by calling BuildTree(DS_i, Output)

Where DS_j built consists of all those records in DataSet for which $X = \hbar h$ distinct value of X.

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Example Decision Trees

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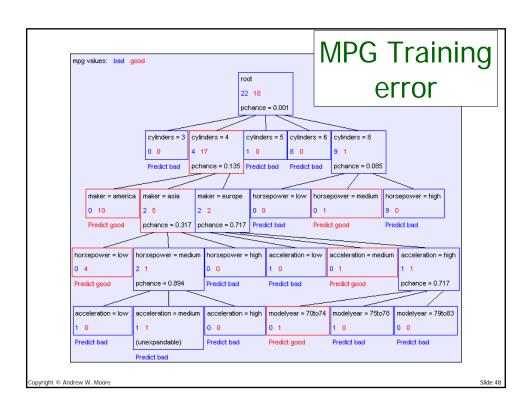
Training Set Error

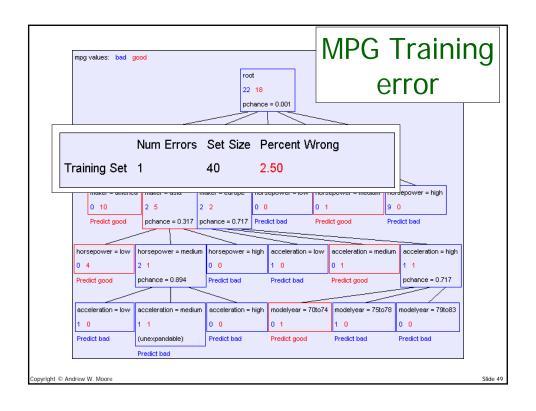
 For each record, follow the decision tree to see what it would predict

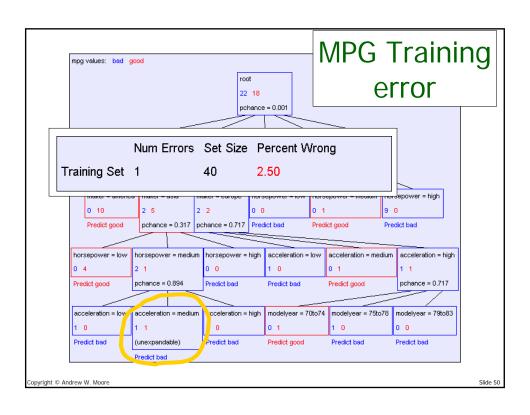
For what number of records does the decision tree's prediction disagree with the true value in the database?

• This quantity is called the *training set error*. The smaller the better.

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Stop and reflect: Why are we doing this learning anyway?

 It is not usually in order to predict the training data's output on data we have already seen.

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Slide 51

Stop and reflect: Why are we doing this learning anyway?

- It is not usually in order to predict the training data's output on data we have already seen.
- It is more commonly in order to predict the output value for future data we have not yet seen.

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Stop and reflect: Why are we doing this learning anyway?

- It is not usually in order to predict the training data's output on data we have already seen.
- It is more commonly in order to predict the output value for future data we have not yet seen.

Warning: A common data mining misperception is that the above two bullets are the only possible reasons for learning. There are at least a dozen others.

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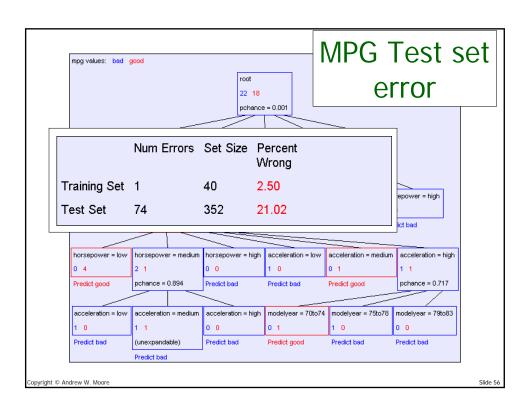
Example Decision Trees

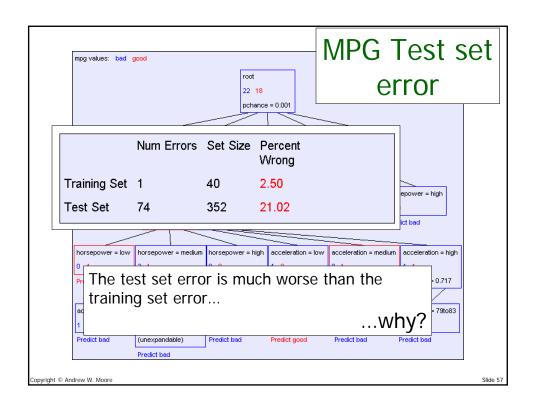
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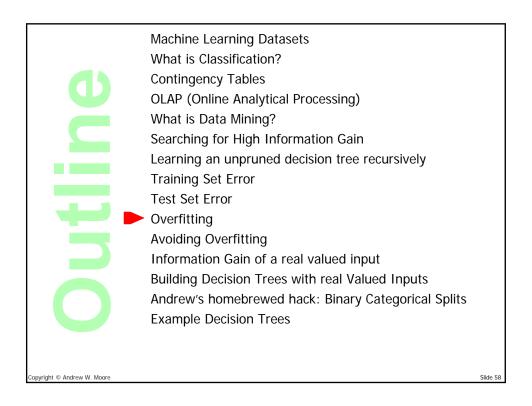
Test Set Error

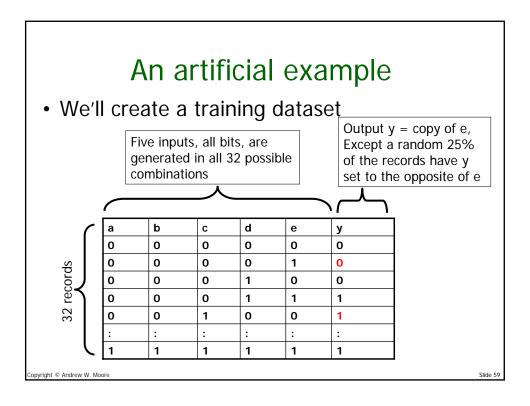
- Suppose we are forward thinking.
- We hide some data away when we learn the decision tree.
- But once learned, we see how well the tree predicts that data.
- This is a good simulation of what happens when we try to predict future data.
- And it is called Test Set Error.

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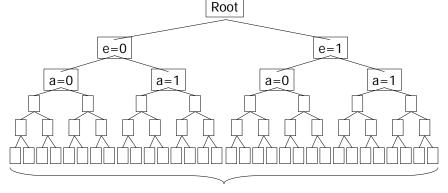
In our artificial example

- Suppose someone generates a test set according to the same method.
- The test set is identical, except that some of the y's will be different.
- Some y's that were corrupted in the training set will be uncorrupted in the testing set.
- Some y's that were uncorrupted in the training set will be corrupted in the test set.

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Building a tree with the artificial training set

Suppose we build a full tree (we <u>always</u> split until base case 2)



25% of these leaf node labels will be corrupted

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Training set error for our artificial tree

All the leaf nodes contain exactly one record and so...

We would have a training set error of zero

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Testing the tree with the test set

	1/4 of the tree nodes are corrupted	3/4 are fine
1/4 of the test set records are corrupted	1/16 of the test set will be correctly predicted for the wrong reasons	3/16 of the test set will be wrongly predicted because the test record is corrupted
3/4 are fine	3/16 of the test predictions will be wrong because the tree node is corrupted	9/16 of the test predictions will be fine

In total, we expect to be wrong on 3/8 of the test set predictions

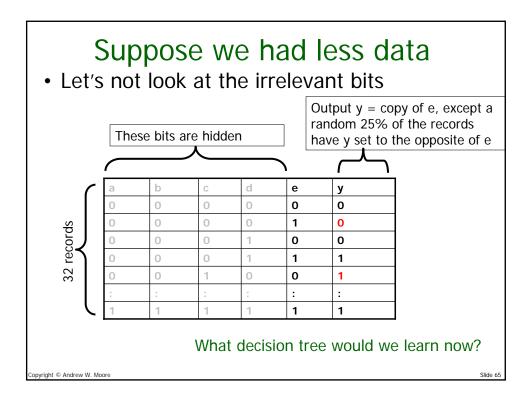
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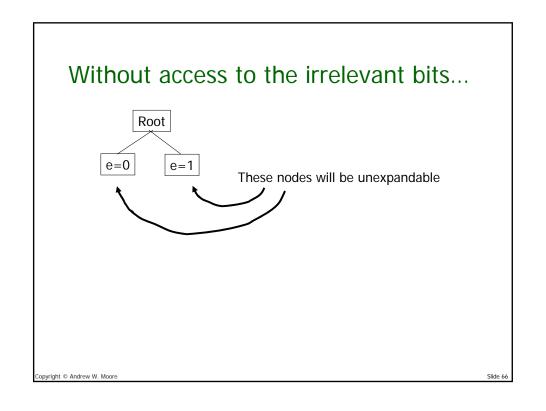
Slide 6

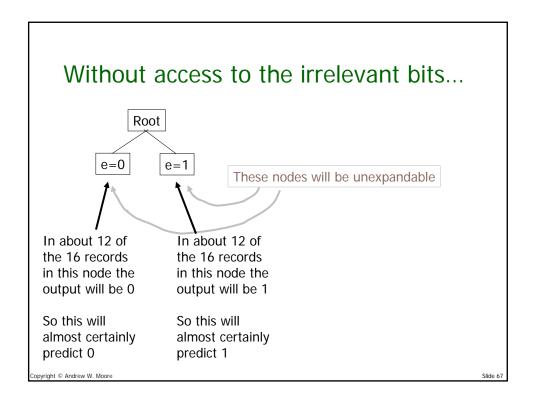
What's this example shown us?

- This explains the discrepancy between training and test set error
- But more importantly... ...it indicates there's something we should do about it if we want to predict well on future data.

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Without access to the irrelevant bits... almost certainly almost certainly all Root none of the tree are fine nodes are corrupted e=0e=11/4 of the test 1/4 of the test set n/a set records will be wrongly are corrupted predicted because the test record is corrupted 3/4 are fine n/a 3/4 of the test predictions will be fine In total, we expect to be wrong on only 1/4 of the test set predictions opyright © Andrew W. Moore

Overfitting

- · Definition: If your machine learning algorithm fits noise (i.e. pays attention to parts of the data that are irrelevant) it is overfitting.
- Fact (theoretical and empirical): If your machine learning algorithm is overfitting then it may perform less well on test set data.

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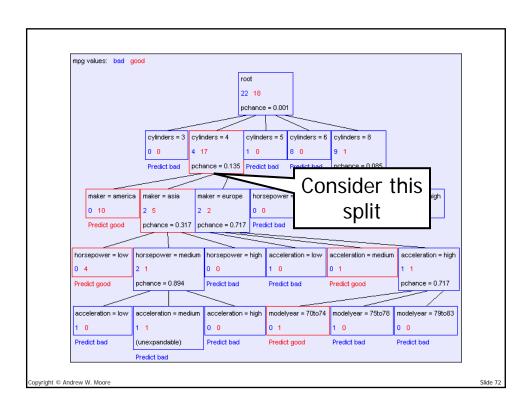
Avoiding overfitting

- Usually we do not know in advance which are the irrelevant variables
- ...and it may depend on the context

For example, if y = a AND b then b is an irrelevant variable only in the portion of the tree in which a=0

But we can use simple statistics to warn us that we might be overfitting.

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A chi-squared 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?

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A chi-squared 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-squared test, the answer is 13.5%.

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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.

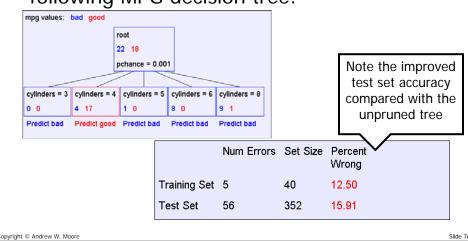
MaxPchance is a magic parameter you must specify to the decision tree, indicating your willingness to risk fitting noise.

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Pruning example

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



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MaxPchance

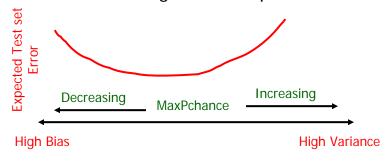
- Good news: The decision tree can automatically adjust its pruning decisions according to the amount of apparent noise and data.
- Bad news: The user must come up with a good value of MaxPchance. (Note, Andrew usually uses 0.05, which is his favorite value for any magic parameter).
- Good news: But with extra work, the best MaxPchance value can be estimated automatically by a technique called cross-validation.

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MaxPchance

• Technical note (dealt with in other lectures): MaxPchance is a regularization parameter.



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The simplest tree

 Note that this pruning is heuristically trying to find

The simplest tree structure for which all within-leafnode disagreements can be explained by chance

- This is not the same as saying "the simplest classification scheme for which..."
- Decision trees are biased to prefer classifiers that can be expressed as trees.

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Expressiveness of Decision Trees

- Assume all inputs are Boolean and all outputs are Boolean.
- What is the class of Boolean functions that are possible to represent by decision trees?
- Answer: All Boolean functions.

Simple proof:

- 1. Take any Boolean function
- Convert it into a truth table
- 3. Construct a decision tree in which each row of the truth table corresponds to one path through the decision tree.

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Machine Learning Datasets

What is Classification?

Contingency Tables

OLAP (Online Analytical Processing)

What is Data Mining?

Searching for High Information Gain

Learning an unpruned decision tree recursively

Training Set Error

Test Set Error

Overfitting

Avoiding Overfitting

Information Gain of a real valued input

Building Decision Trees with real Valued Inputs

Andrew's homebrewed hack: Binary Categorical Splits

Example Decision Trees

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Real-Valued inputs

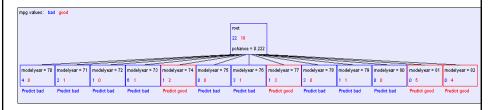
 What should we do if some of the inputs are real-valued?

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

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 over fit

Note pchance is 0.222 in the above...if MaxPchance was 0.05 that would end up pruning away to a single root node.

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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

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Computational Issues

- You can compute $IG^*(Y|X)$ in time $R \log R + 2R n_y$
- Where

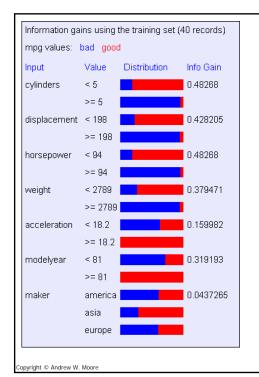
R is the number of records in the node under consideration n_v is the arity (number of distinct values of) Y

How?

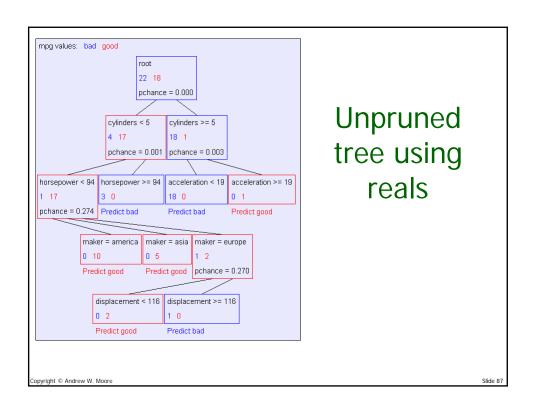
Sort records according to increasing values of X. Then create a $2xn_y$ contingency table corresponding to computation of $IG(Y|X:x_{min})$. Then iterate through the records, testing for each threshold between adjacent values of X, incrementally updating the contingency table as you go. For a minor additional speedup, only test between values of Y that differ.

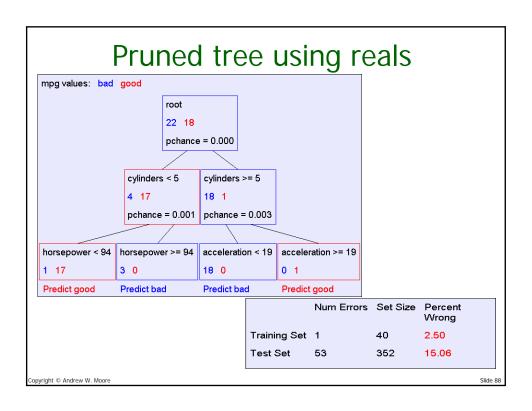
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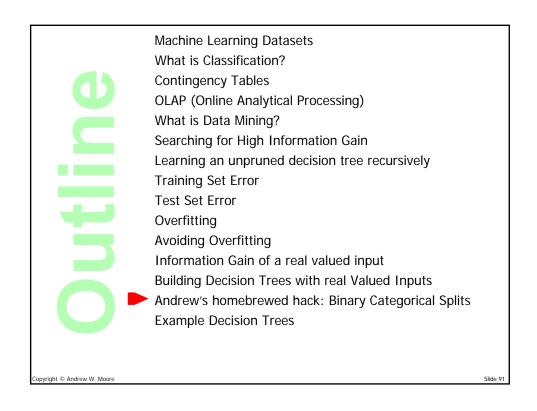
Example with MPG

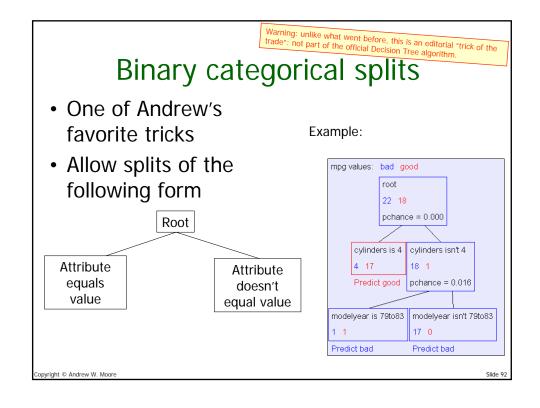


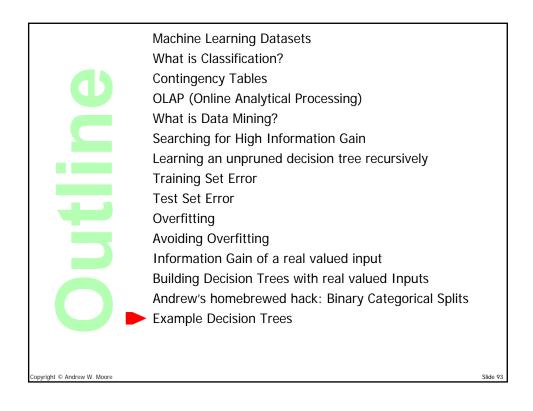


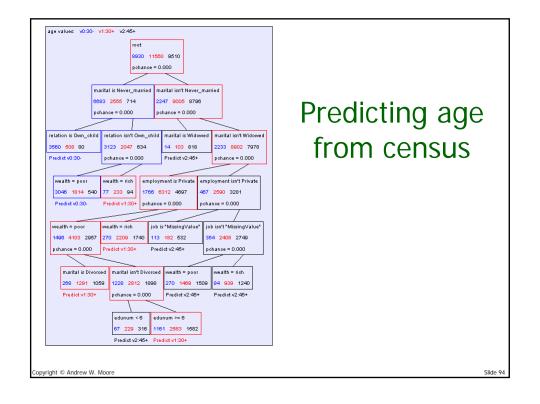
```
LearnUnprunedTree(X,Y)
        Input: X a matrix of R rows and M columns where X<sub>ij</sub> = the value of the j'th attribute in the i'th input datapoint. Each column consists of either all real values or all categorical values.
         Input: Y a vector of R elements, where Y_i = the output class of the i'th datapoint. The Y_i values are categorical.
         Output: An Unpruned decision tree
         If all records in X have identical values in all their attributes (this includes the case where R<2), return a Leaf Node
             predicting the majority output, breaking ties randomly. This case also includes
         If all values in Y are the same, return a Leaf Node predicting this value as the output
         Flse
                For j = 1 ... M
                        If j'th attribute is categorical
                               IG_i = IG(Y|X_i)
                        Else (j'th attribute is real-valued)
                               IG_i = IG^*(Y|X_i) from about four slides back
                Let j^* = \operatorname{argmax}_{i} \operatorname{IG}_{i} (this is the splitting attribute we'll use)
                If j* is categorical then
                        For each value v of the j'th attribute
                               Let X^v = subset of rows of X in which X_{ij} = v. Let Y^v = corresponding subset of Y
                               Let Child^v = LearnUnprunedTree(X^v, Y^v)
                        Return a decision tree node, splitting on j'th attribute. The number of children equals the number of
                            values of the j'th attribute, and the v'th child is Childy
                Else i* is real-valued and let t be the best split threshold
                        Let X^{LO} = subset of rows of X in which X_{ij} <= t. Let Y^{LO} = corresponding subset of Y
                        Let Child^{LO} = LearnUnprunedTree(X^{LO}, Y^{LO})
                        Let X^{HI} = subset of rows of X in which X_{ii} > t. Let Y^{HI} = corresponding subset of Y
                        Let ChildHI = LearnUnprunedTree(XHI,YHI)
                        Return a decision tree node, splitting on j'th attribute. It has two children corresponding to whether the
                           j'th attribute is above or below the given threshold.
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                                                                                                                                              Slide 89
```

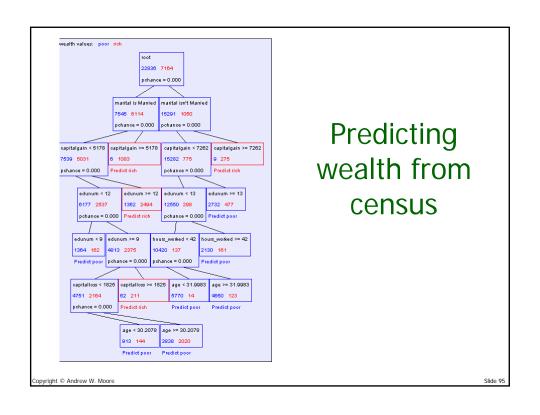
```
LearnUnprunedTree(X,Y)
       Input: X a matrix of R rows and M columns where X_{ij} = the value of the j'th attribute in the i'th input datapoint. Each
           column consists of eithe
                                   Things to note:
       Input: Y a vector of R eleme
                                                                                            lues are categorical.
       Output: An Unpruned decision
                                   Below the root node, there is no point
                                   testing categorical attributes that have
       If all records in X have ide
                                                                                           R<2), return a Leaf Node
                                  already been split upon further up the tree.
           predicting the majority
                                  This is because all the values of that
       If all values in Y are the sa
                                 attribute will be the same and IG must
              For j = 1 .. M
                                  therefore be zero.
                    If i'th attribu
                                 But it's worth retesting real-valued
                          IG<sub>i</sub> =
                                 attributes, since they may have different
                    Else (j'th att
                                 values below the binary split, and may
                          IG<sub>i</sub> =
             Let j* = argmax<sub>j</sub> I
                                benefit from splitting further.
              If j* is categorical
                                To achieve the above optimization, you
                    For each va
                                should pass down through the recursion a
                          Let X
                                                                                        na subset of Y
                               current active set of attributes.
                          Let
                                                                                        ildren equals the number of
                    Return a d
                               Pedantic detail: a third termination
                       values
                               condition should occur if the best split
              Else j* is real-valu
                               attribute puts all its records in exactly one
                    Let XLO =
                                                                                        subset of Y
                              child (note that this means it and all other
                    Let Child<sup>LC</sup>
                    Let XHI =
                                                                                       ubset of Y
                               attributes have IG=0).
                    Let Child<sup>1</sup>
                                                                                      en corresponding to whether the
                    Return a
                       j'th att
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                                                                                                                    Slide 90
```

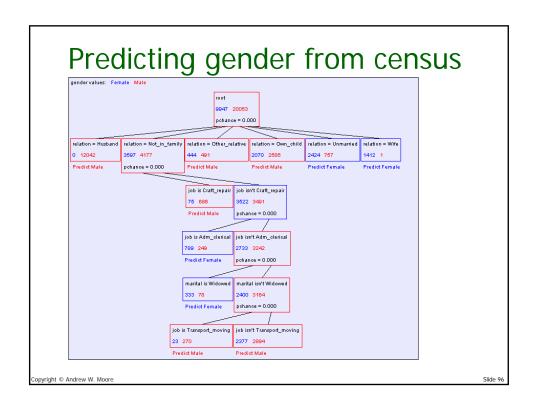












Conclusions

- Decision trees are the single most popular data mining tool
 - · Easy to understand
 - · Easy to implement
 - · Easy to use
 - Computationally cheap
- It's possible to get in trouble with overfitting
- They do classification: predict a categorical output from categorical and/or real inputs

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What you should know

- What's a contingency table?
- · What's information gain, and why we use it
- The recursive algorithm for building an unpruned decision tree
- What are training and test set errors
- Why test set errors can be bigger than training set
- Why pruning can reduce test set error
- How to exploit real-valued inputs

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What we haven't discussed

- It's easy to have real-valued outputs too---these are called Regression Trees*
- Bayesian Decision Trees can take a different approach to preventing overfitting
- Computational complexity (straightforward and cheap) *
- Alternatives to Information Gain for splitting nodes
- How to choose MaxPchance automatically *
- The details of Chi-Squared testing *
- Boosting---a simple way to improve accuracy *

* = discussed in other Andrew lectures

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For more information

- Two nice books
 - L. Breiman, J. H. Friedman, R. A. Olshen, and C. J. Stone. Classification and Regression Trees. Wadsworth, Belmont, CA, 1984.
 - C4.5 : Programs for Machine Learning (Morgan Kaufmann Series in Machine Learning) by J. Ross Quinlan
- Dozens of nice papers, including
 - Learning Classification Trees, Wray Buntine, Statistics and Computation (1992), Vol 2, pages 63-73
 - Kearns and Mansour, On the Boosting Ability of Top-Down Decision Tree Learning Algorithms, STOC: ACM Symposium on Theory of Computing, 1996"
- Dozens of software implementations available on the web for free and commercially for prices ranging between \$50 - \$300,000

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Discussion

- Instead of using information gain, why not choose the splitting attribute to be the one with the highest prediction accuracy?
- Instead of greedily, heuristically, building the tree, why not do a combinatorial search for the optimal tree?
- If you build a decision tree to predict wealth, and marital status, age and gender are chosen as attributes near the top of the tree, is it reasonable to conclude that those three inputs are the major causes of wealth?
- ..would it be reasonable to assume that attributes not mentioned in the tree are not causes of wealth?
- ..would it be reasonable to assume that attributes not mentioned in the tree are not correlated with wealth?

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