INFO 251: Applied ML

Decision Trees

Should I do the laundry? A decision tree:



Course Outline

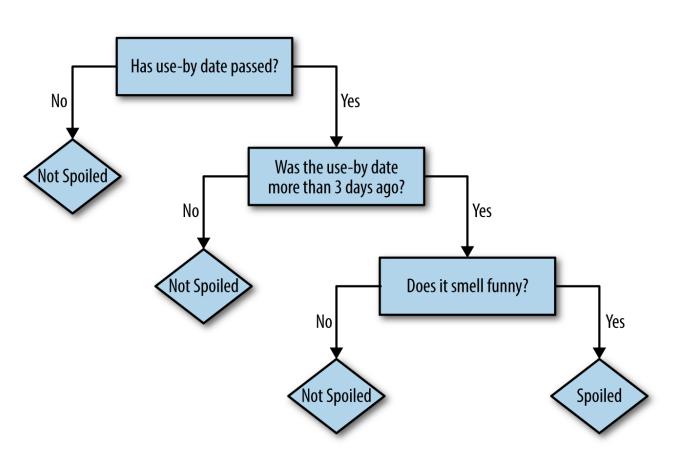
- Causal Inference and Research Design
 - Experimental methods
 - Non-experiment methods
- Machine Learning
 - Design of Machine Learning Experiments
 - Linear Models and Gradient Descent
 - Non-linear models
 - Neural models
 - Unsupervised Learning
 - Practicalities, Fairness, Bias
- Special topics

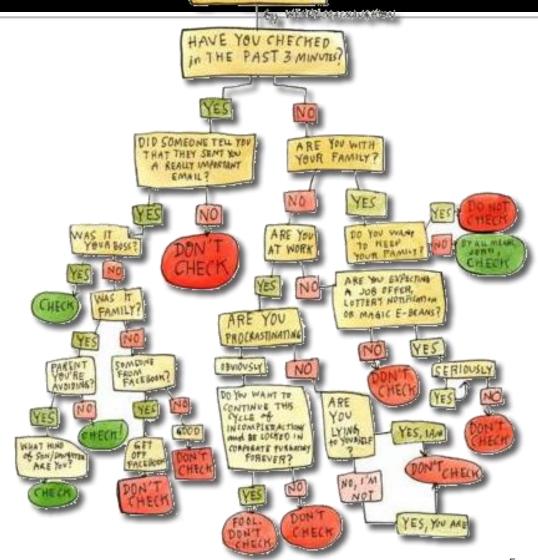
Outline

- Decision Trees
 - Introduction
 - Representation
 - Algorithms
 - Splitting
 - Extended example
 - Overfitting and Pruning
 - Extensions

Decision Trees





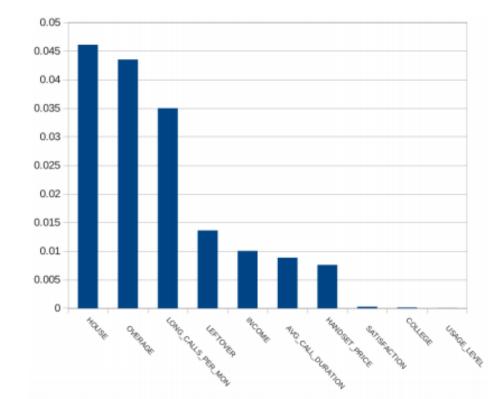


- Goal: reduce customer churn
 - E.g., target customers to encourage retention
 - Start by predicting who is likely to churn
 - What features to include?

Variable	Explanation
COLLEGE	Is the customer college educated?
INCOME	Annual income
OVERAGE	Average overcharges per month
LEFTOVER	Average number of leftover minutes per month
HOUSE	Estimated value of dwelling (from census tract)
HANDSET_PRICE	Cost of phone
LONG_CALLS_PER_MONTH	Average number of long calls (15 mins or over) per month
AVERAGE_CALL_DURATION	Average duration of a call
REPORTED_SATISFACTION	Reported level of satisfaction
REPORTED_USAGE_LEVEL	Self-reported usage level
LEAVE	Target variable: Did the customer stay or leave (churn)?

- A simple approach: "Forward Selection"
 - Add features to a model (e.g., kNN, logistic regression, Naïve Bayes) one at a time, based on the relevance of that feature
 - How to define "relevance"?
 - Unconditional correlation
 - Information gain (we'll define this soon)

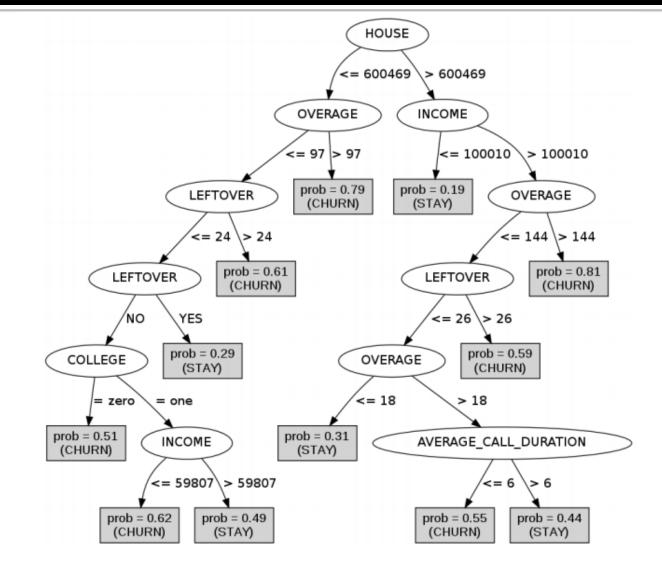
Rank	Info. Gain	Attribute name
1	0.0461296	HOUSE
2	0.0435518	OVERAGE
3	0.0350337	LONG_CALLS_PER_MON
4	0.013648	LEFTOVER
5	0.0100534	INCOME
6	0.0088899	AVG_CALL_DURATION
7	0.007624	HANDSET_PRICE
8	0.0003062	SATISFACTION
9	0.0001553	COLLEGE
10	0.0000388	USAGE_LEVEL



- Decision Tree
 - Idea: Build tree from training data to explain labeled examples
 - Progressively add features that are most informative
 - Keep tree as small and as simple as possible (Occam's razor)
- Different from forward selection
 - Decisions are made conditional on existing tree
 - E.g., second variable not necessarily OVERAGE

Rank	Info. Gain	Attribute name
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The final tree (churn dataset)



Decision trees

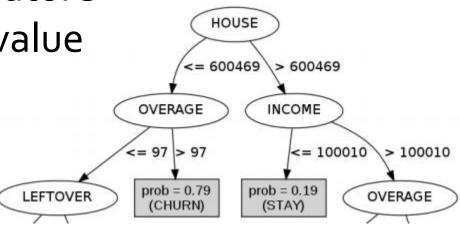
- Very popular, easy to interpret
- Reflects the logic of decision-making
- Arbitrarily complex (non-linear functions)
- Can be used for classification or regression
- Simple, fast algorithms for generating compact trees from data

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Representation

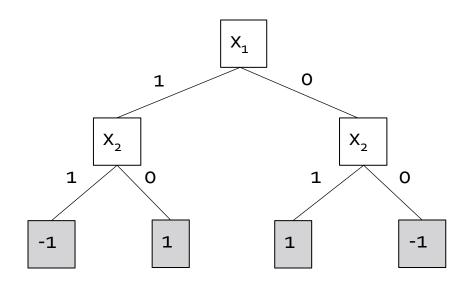
- Internal nodes test the value of a feature
 - Categorical
 - Binary
 - Continuous
- Branches indicate possible values for feature
- Leaf nodes output a predicted class or value



Simple Example: XOR

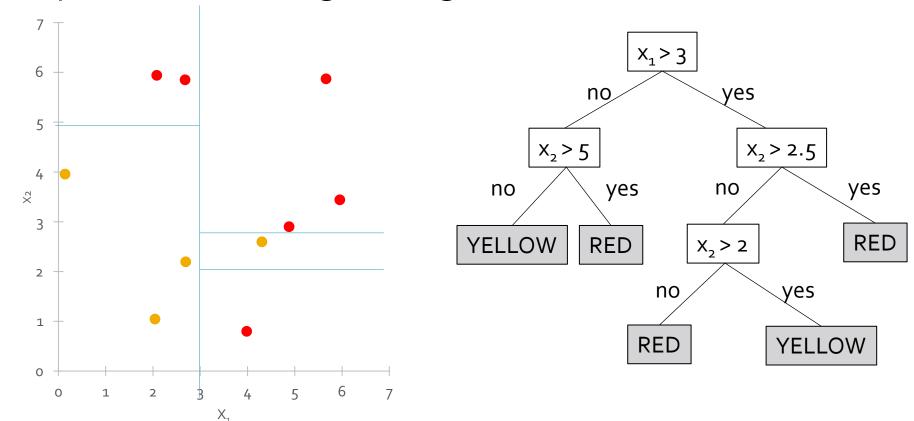
- Expressiveness
 - Any logical function that can be encoded in a truth table can be expressed in a decision tree!
 - Why? For any truth table, use each variables as a split

X ₁	X ₂	У
1	1	-1
1	0	1
0	1	1
0	0	-1



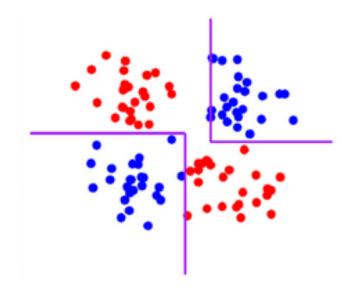
Decision boundaries

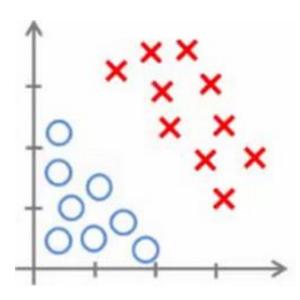
- What does the decision boundary of a decision tree look like?
 - Compare to k-NN? Logistic regression?



Decision boundaries

- "Hyper-rectangles" partition high-dimensional space
- Diagonal lines approximated as step function





Hypothesis space

- How many possible decision trees over N binary variables?
 - \blacksquare = number of distinct truth tables with 2^N rows
 - $= 2^{(2^N)}$
 - e.g. 6 attributes: 18,446,744,073,709,551,616 possible trees
 - Be careful!
- More expressive hypothesis spaces...
 - Increases chance that target function can be expressed
 - Increases hypotheses consistent with training data
 - Means we can get better predictions
 - But we may fail to generalize

Good vs. bad trees

- Many trees perfectly classify all training examples
 - A trivial model has a leaf for every training example
 - Doesn't matter what the root feature is
- But we want our tree to generalize
 - i.e., we want the smallest tree that explains the data
 - Will need methods to reduce overfitting (pruning, forests, ...)

Intuition check

 True or False: A decision tree is able to recover non-linear decision boundary

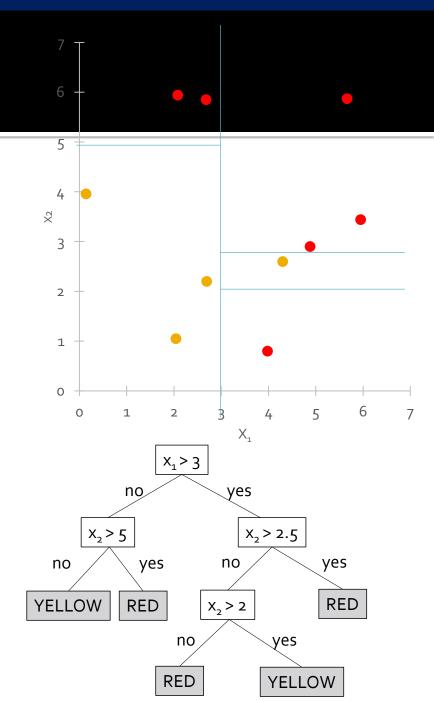
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Building a tree (recursively)

- Goal: find a tree consistent with training examples
- Strategy: (recursively) choose the most significant attribute as the root of the (sub)tree
- Binary tree example

```
GrowTree(S):
    if y==0 for all <x,y> in S:
        return new leaf(0)
    else if y==1 for all <x,y> in S:
        return new leaf(1)
    else:
        choose best attribute x;
        S0 = all <x,y> in S with x;==0
        S1 = all <x,y> in S with x;==1
        return new node(x;,
GrowTree(S0), GrowTree(S1))
```



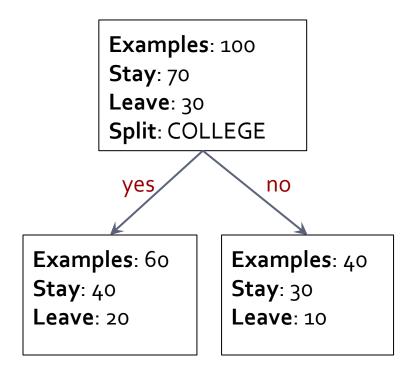
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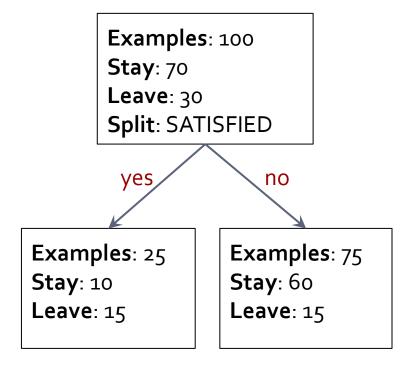
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What is the "best" attribute?

- Good attributes split examples into pure subsets
- Should we split on COLLEGE or SATISFIED?
 - How to measure subset purity?





Information Theory

Shannon's Game: predict the character

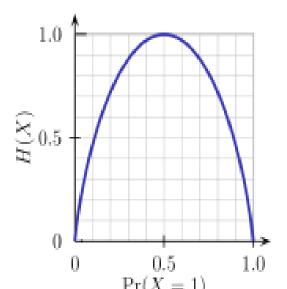
- Explores mathematics of encoded messages
- How much information is conveyed by a single letter?
 - If the alphabet contains only one letter: o bits
 - With 27 equiprobable letters: 4.8 bits
 - Shannon's estimate of English characters: ~1 bit
- "Information" is the expected code length to convey a message



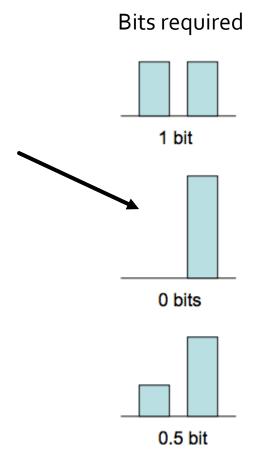
Claude Shannon

Entropy

- Entropy is a measure of uncertainty
 - More uncertainty requires longer codes
 - A distribution where one value has P(1) has no entropy
 - Uniform distribution maximizes entropy

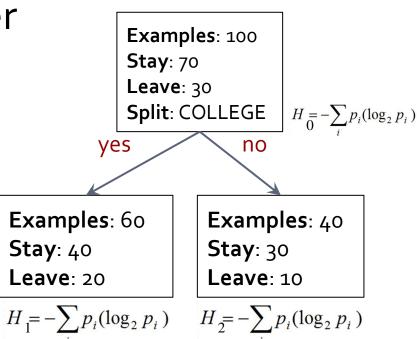


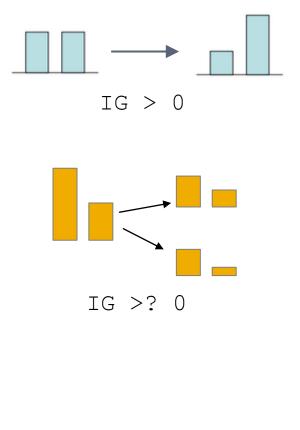
$$H = -\sum_{i} p_{i} (\log_{2} p_{i})$$



Information gain

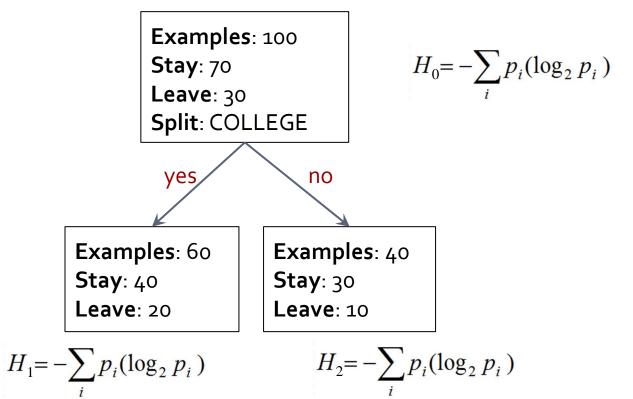
- Information Gain: describes a change in entropy
 - Entropy before Entropy after
- Example with positive information gain:
- Our example is trickier
 - Requires a calculator



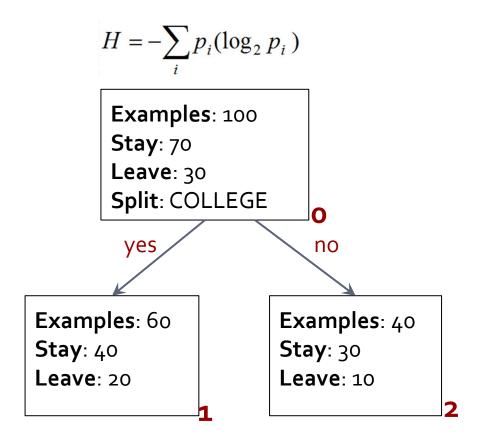


Information gain

- Before we calculate information gain, notice that the split produces branches of different sizes (60 vs. 40)
 - Solution: weight by the number of examples



Information gain: example



```
H_0 = -.7 \log(.7) -.3 \log(.3) = .881
H_1 = -.66 \log(.66) -.33 \log(.33) = .92
H_2 = -.75 \log(.75) -.25 \log(.25) = .81
IG(COLLEGE) = .881 - [.6(.92) + .4(.81)]
             = .881 - .875
             = .006
             (= small gain)
IG(SATISFIED) = .88 - [.25(.97) + .75(.72)]
              = .09
             (= larger gain)
```

Outline

Decision Trees

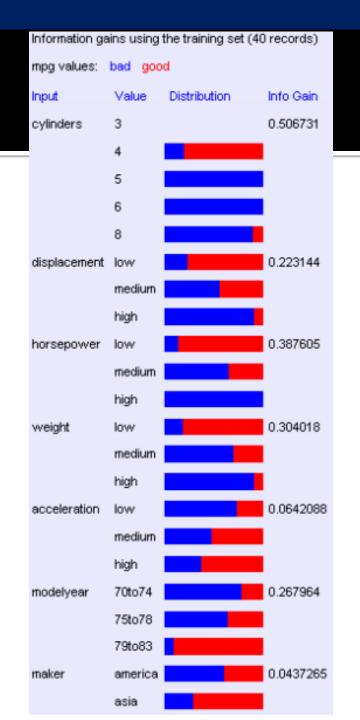
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Extended Example: Predicting MPG

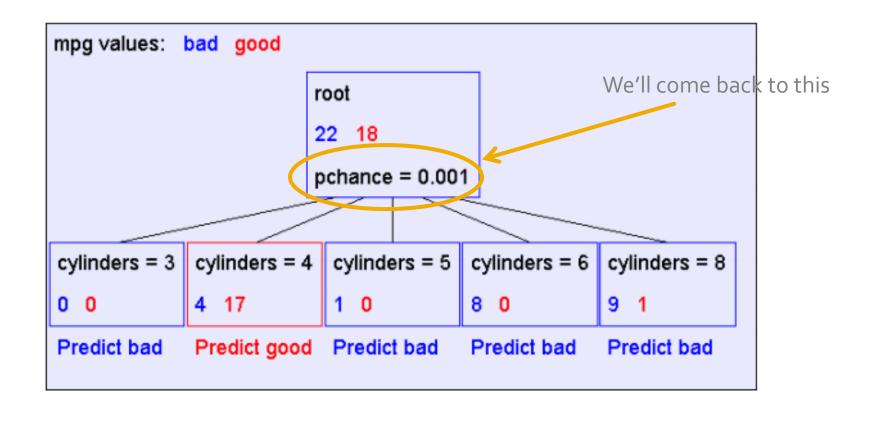
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low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

The first split

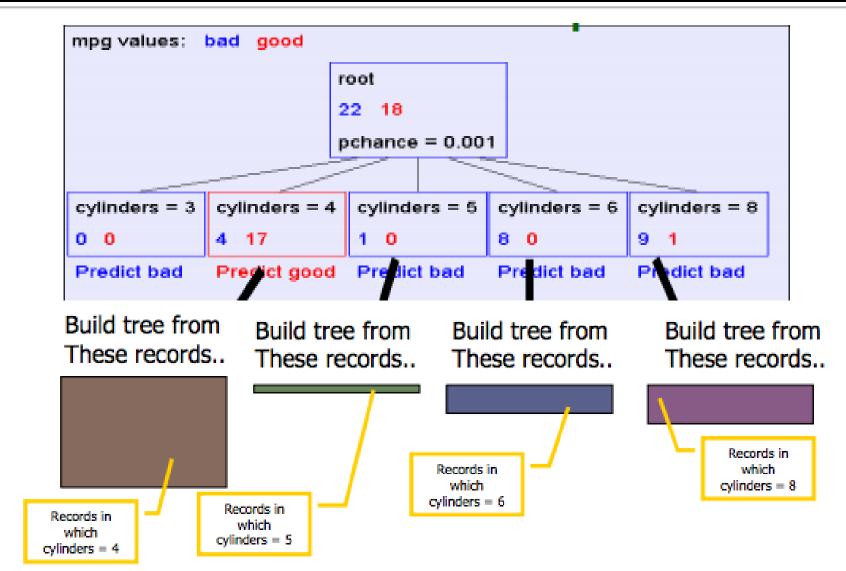
- Each attribute is correlated with the target
- Calculate information gain for each possible split
 - (Note that attributes don't have to be binary)
- Choose the split that maximizes information gain



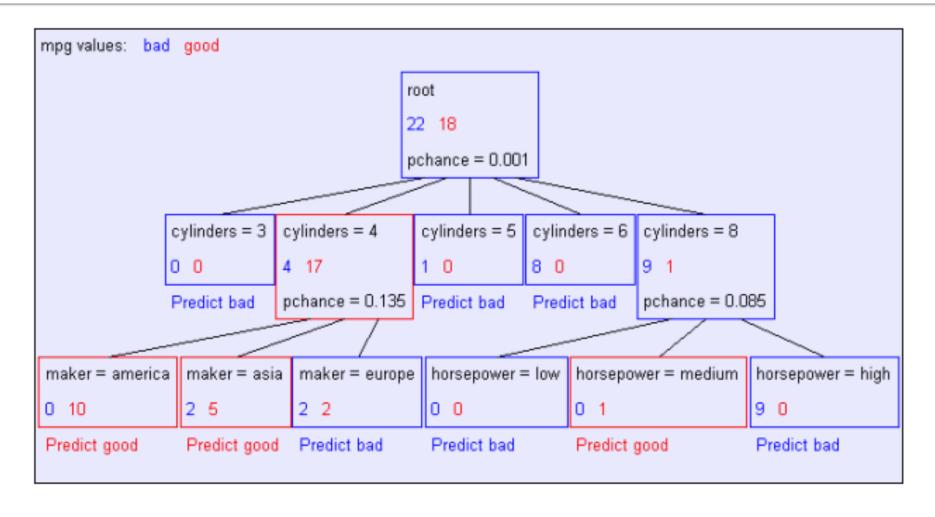
Depth-1 tree: "decision stump"



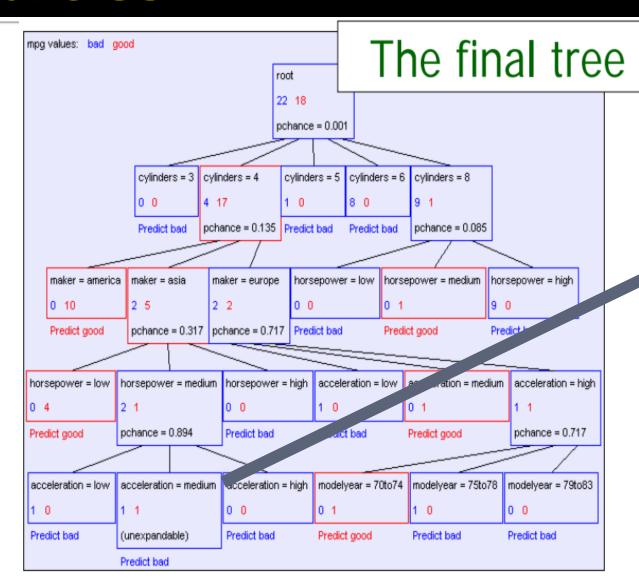
Recursive tree building

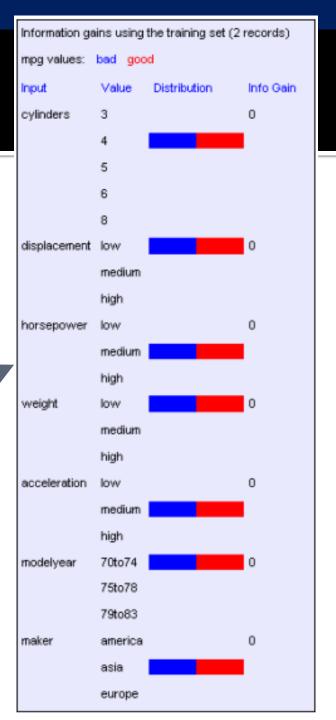


Second level (depth-2 tree)



Final tree





Recap: Decision Tree algorithm

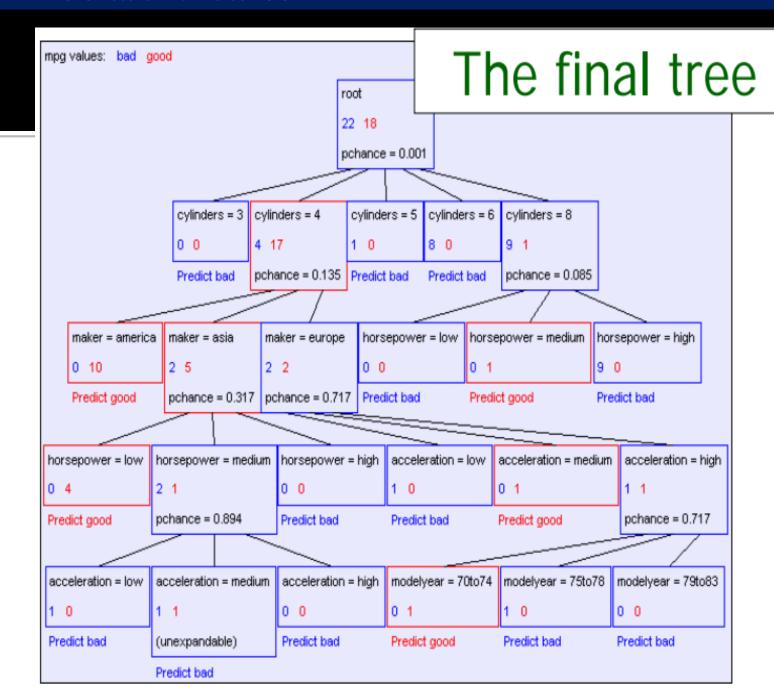
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     if y==0 for all \langle x,y \rangle in S:
            return new leaf(0)
     else if y==1 for all \langle x,y \rangle in S:
            return new leaf(1)
     else:
            x_i = max info gain(S)
            S0 = all \langle x, y \rangle in S with x_i == 0
            S1 = all < x, y > in S with <math>x_i == 1
            return new node (x_i, GrowTree(S0), GrowTree(S1))
```

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Overfitting



Overfitting

Overfitting strikes again:

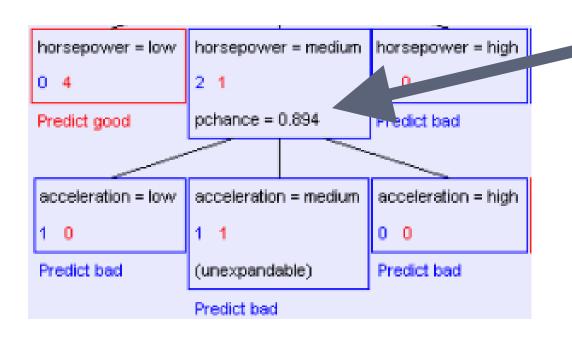
	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

- How to deal with overfitting in Regression?
 - Regularization
- K-Nearest Neighbors?
 - Increasing K
- Naïve Bayes?
 - Smoothing

Overfitting in Decision Trees

- Three common solutions:
 - Stop growing tree when split is not statistically significant
 - 2. Grow tree, then prune afterwards
 - 3. Set maximum depth

Example: Over-splitting



- Should we really split here?
- Only 3 relevant training examples
- The resulting distributions are likely due to chance

- One solution: compute the value/ significance of each split
 - For instance, a chi-squared test, or info gain
- Only split if value exceeds some threshold

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i - E_i)^2}{E_i}$$

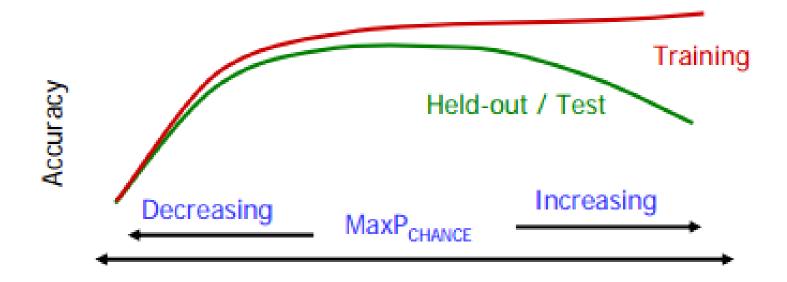
Pruning

- Build the full decision tree
- Starting with the deepest nodes, delete splits where value of split does not exceed some threshold T
- Continue upward until no more prunable nodes

	Num Errors	Set Size	Percent Wrong		Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50	Training Set	5	40	12.50
Test Set	74	352	21.02	Test Set	56	352	15.91

Regularization

- T is a regularization (hyper-)parameter
 - How to determine value?
- Cross-Validation!



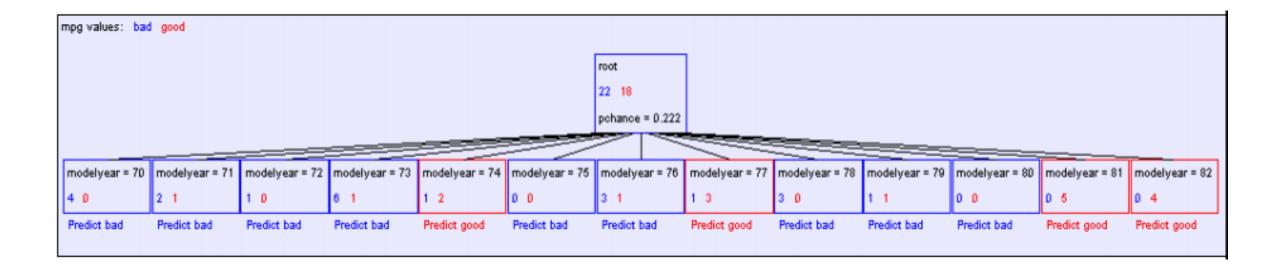
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Multi-valued features

- Features with many discrete values:
 - Splits with many children (comparing Info Gain?)
 - Can produce degenerate cases
 - Common solution: One vs. all other values

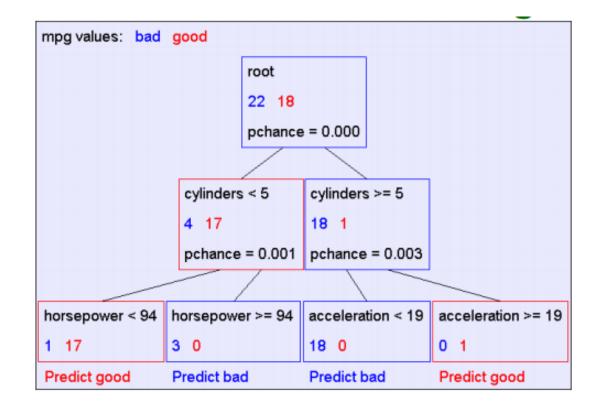


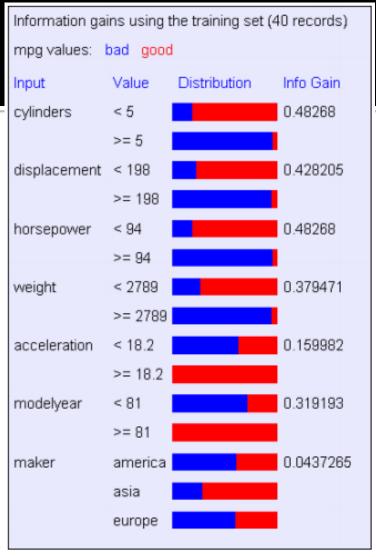
Continuous features

- Continuous features
 - Common solution: Bucket or threshold values
 - E.g., model years <1970, 1970-1980, >1980
- How to choose the buckets/thresholds?
 - Sort instances based on value of an attribute (e.g. year)
 - Identify adjacent examples that differ in their label
 - This generates a set of candidate thresholds splitting thresholds for that feature
 - Use information gain to decide appropriate threshold

Thresholded splits

- Bucketing example:
 - Creates deeper, denser tree



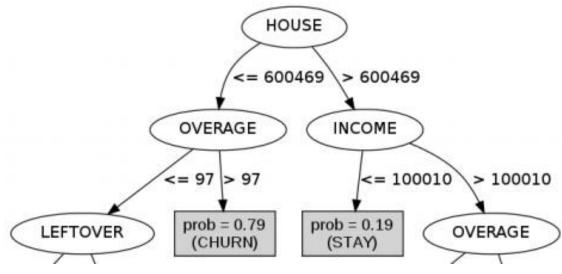


	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	53	352	15.06

Output probabilities

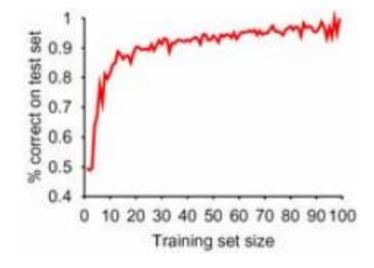
- How to do better than predicting majority class?
- Estimate probabilities from the relevant examples at each node

Can use smoothing to improve estimates (e.g., Laplace smoothing)



Scaling up

More data is almost always better



- Scaling up with standard recursive algorithms can be hard
- New algorithms make single pass through data
 - E.g. Very Fast Decision Trees (VFTD)