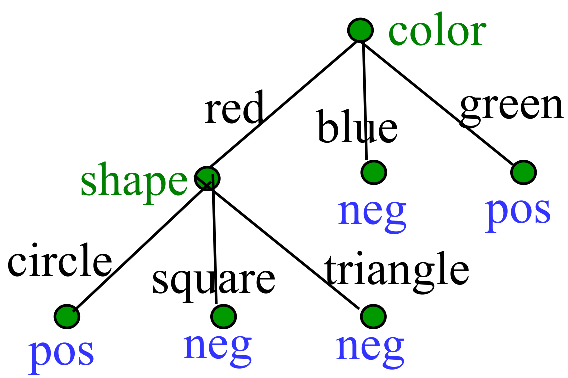
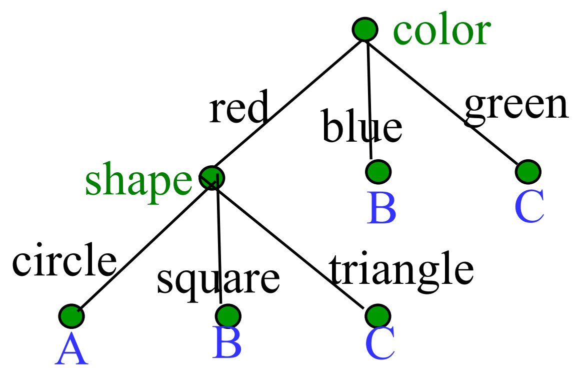
Decision Tree Learning

Based on the ML lecture by Raymond J. Mooney
University of Texas at Austin

Decision Trees

- Tree-based classifiers for instances represented as feature-vectors. Nodes test features, there is one branch for each value of the feature, and leaves specify the category.





- Can represent arbitrary conjunction and disjunction. Can represent any classification function over discrete feature vectors.
- Can be rewritten as a set of rules, i.e. disjunctive normal form (DNF).
  - red $\wedge$ circle $\rightarrow$ pos
  - red $\wedge$ circle $\rightarrow$ A
    blue $\rightarrow$ B; red $\wedge$ square $\rightarrow$ B
    green $\rightarrow$ C; red $\wedge$ triangle $\rightarrow$ C

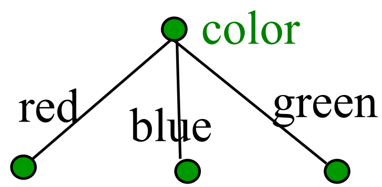
Properties of Decision Tree Learning

- Continuous (real-valued) features can be handled by allowing nodes to split a real valued feature into two ranges based on a threshold (e.g. length < 3 and length ≥3)
- Classification trees have discrete class labels at the leaves, ***regression trees*** allow real-valued outputs at the leaves.
- Algorithms for finding consistent trees are efficient for processing large amounts of training data for data mining tasks.
- Methods developed for handling noisy training data (both class and feature noise).
- Methods developed for handling missing feature values.

Top-Down Decision Tree Induction

- Recursively build a tree top-down by divide and conquer.

<big, red, circle>: + <small, red, circle>: +
<small, red, square>: – <big, blue, circle>: –



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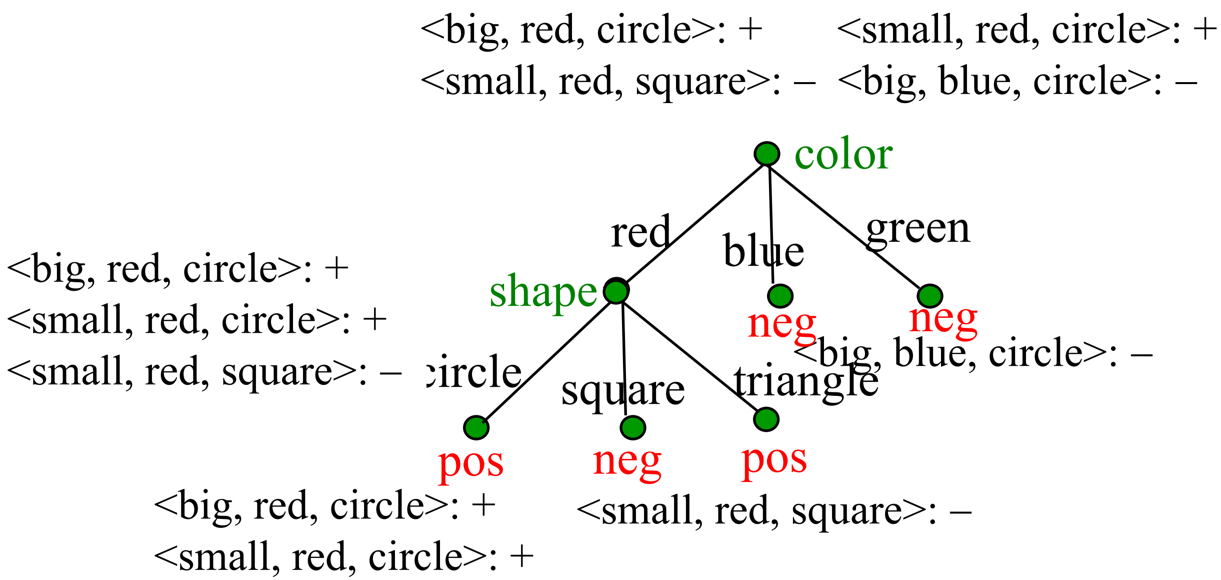


Decision Tree Induction Pseudocode

DTree(*examples*, *features*) returns a tree
  If all *examples* are in one category, return a leaf node with that category label.
  Else if the set of *features* is empty, return a leaf node with the category label that
    is the most common in examples.
  Else pick a feature F and create a node R for it
    For each possible value v_i of F:
      Let $examples_i$ be the subset of examples that have value v_i for F
      Add an out-going edge E to node R labeled with the value v_i.
      If $examples_i$ is empty
        then attach a leaf node to edge E labeled with the category that
          is the most common in *examples*.
        else call DTree($examples_i$, $features - \{F\}$) and attach the resulting
          tree as the subtree under edge E.
    Return the subtree rooted at R.

Picking a Good Split Feature

- Goal is to have the resulting tree be as small as possible, per Occam's razor.
- Finding a minimal decision tree (nodes, leaves, or depth) is an NP-hard optimization problem.
- Top-down divide-and-conquer method does a greedy search for a simple tree but does not guarantee to find the smallest.
  - General lesson in ML: "Greed is good."
- Want to pick a feature that creates subsets of examples that are relatively "pure" in a single class so they are "closer" to being leaf nodes.
- There are a variety of heuristics for picking a good test, a popular one is based on information gain that originated with the ID3 system of Quinlan (1979).

Entropy

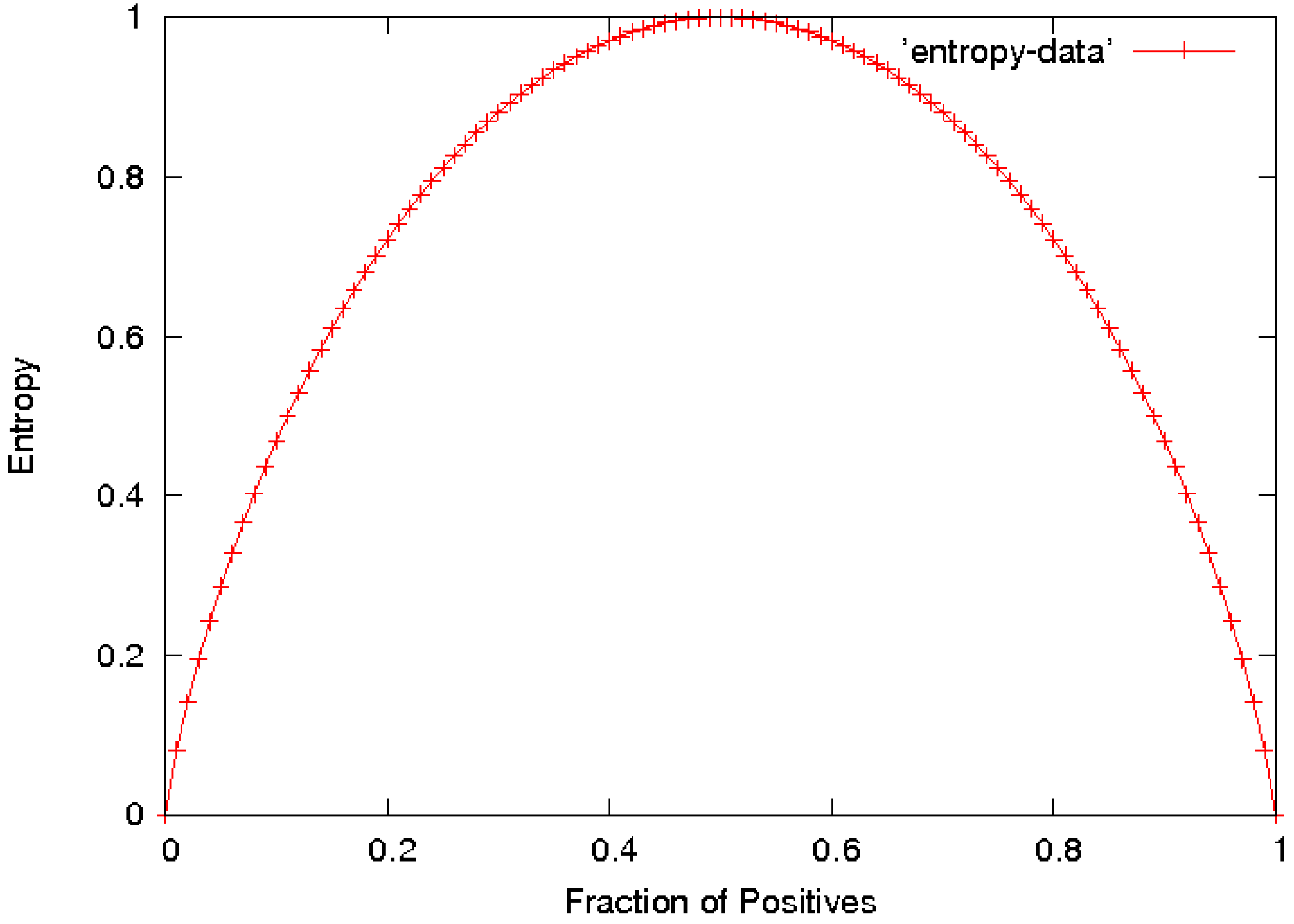
- Entropy (disorder, impurity) of a set of examples, S, relative to a binary classification is:

$$Entropy(S) = -p_1 \log_2(p_1) - p_0 \log_2(p_0)$$

  where p_1 is the fraction of positive examples in S and p_0 is the fraction of negatives.
- If all examples are in one category, entropy is zero (we define $0 \cdot \log(0) = 0$)
- If examples are equally mixed ($p_1 = p_0 = 0.5$), entropy is a maximum of 1.
- Entropy can be viewed as the number of bits required on average to encode the class of an example in *S* where data compression (e.g. Huffman coding) is used to give shorter codes to more likely cases.
- For multi-class problems with c categories, entropy generalizes to:

$$Entropy(S) = \sum_{i=1}^{c} -p_i \log_2(p_i)$$

Entropy Plot for Binary Classification



Information Gain

- The information gain of a feature F is the expected reduction in entropy resulting from splitting on this feature.

$$Gain(S,F) = Entropy(S) - \sum_{v \in Values(F)} \frac{|S_v|}{|S|} Entropy(S_v)$$

where S_v is the subset of S having value v for feature F.

- Entropy of each resulting subset weighted by its relative size.
- Example:
  - <big, red, circle>: + <small, red, circle>: +
  - <small, red, square>: – <big, blue, circle>: –

2+, 2 –: E=1
size
big: 1+,1– E=1
small: 1+,1– E=1
Gain=1–(0.5·1 + 0.5·1) = 0

2+, 2 – : E=1
color
red: 2+,1– E=0.918
blue: 0+,1– E=0
Gain=1–(0.75·0.918 + 0.25·0) = 0.311

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Gain=1–(0.75·0.918 + 0.25·0) = 0.311

Hypothesis Space Search

- Performs ***batch learning*** that processes all training instances at once rather than ***incremental learning*** that updates a hypothesis after each example.
- Performs hill-climbing (greedy search) that may only find a locally-optimal solution. Guaranteed to find a tree consistent with any conflict-free training set (i.e. identical feature vectors always assigned the same class), but not necessarily the simplest tree.
- Finds a single discrete hypothesis, so there is no way to provide confidences or create useful queries.

Bias in Decision-Tree Induction

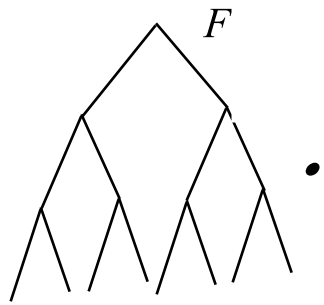
- Information-gain gives a bias for trees with minimal depth.
- Implements a search (preference) bias instead of a language (restriction) bias.

History of Decision-Tree Research

- Hunt and colleagues use exhaustive search decision-tree methods (CLS) to model human concept learning in the 1960's.
- In the late 70's, Quinlan developed ID3 with the information gain heuristic to learn expert systems from examples.
- Simulataneously, Breiman and Friedman and colleagues develop CART (Classification and Regression Trees), similar to ID3.
- In the 1980's a variety of improvements are introduced to handle noise, continuous features, missing features, and improved splitting criteria. Various expert-system development tools results.
- Quinlan's updated decision-tree package (C4.5) released in 1993.
- Weka includes Java version of C4.5 called J48.

Computational Complexity

- Worst case builds a complete tree where every path test every feature. Assume *n* examples and *m* features.



Maximum of *n* examples spread across all nodes at each of the *m* levels

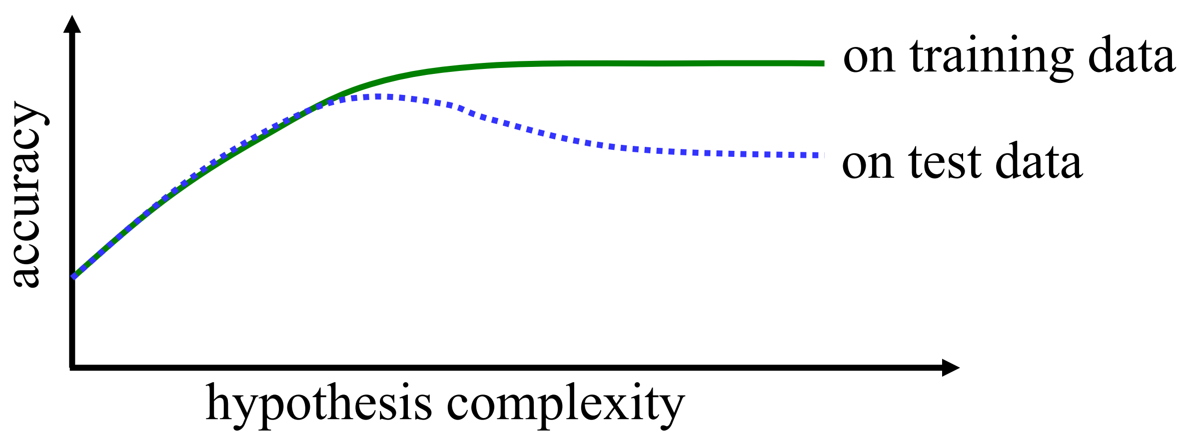
- At each level, *i*, in the tree, must examine the remaining $m-i$ features for each instance at the level to calculate info gains.

$$\sum_{i=1}^{m} i \cdot n = O(nm^2)$$

- However, learned tree is rarely complete (number of leaves is ≤ *n*). In practice, complexity is linear in both number of features (*m*) and number of training examples (*n*).

Overfitting

- Learning a tree that classifies the training data perfectly may not lead to the tree with the best generalization to unseen data.
  - There may be noise in the training data that the tree is erroneously fitting.
  - The algorithm may be making poor decisions towards the leaves of the tree that are based on very little data and may not reflect reliable trends.
- A hypothesis, *h*, is said to overfit the training data is there exists another hypothesis which, *h* , such that *h* has less error than *h* on the training data but greater error on independent test data.

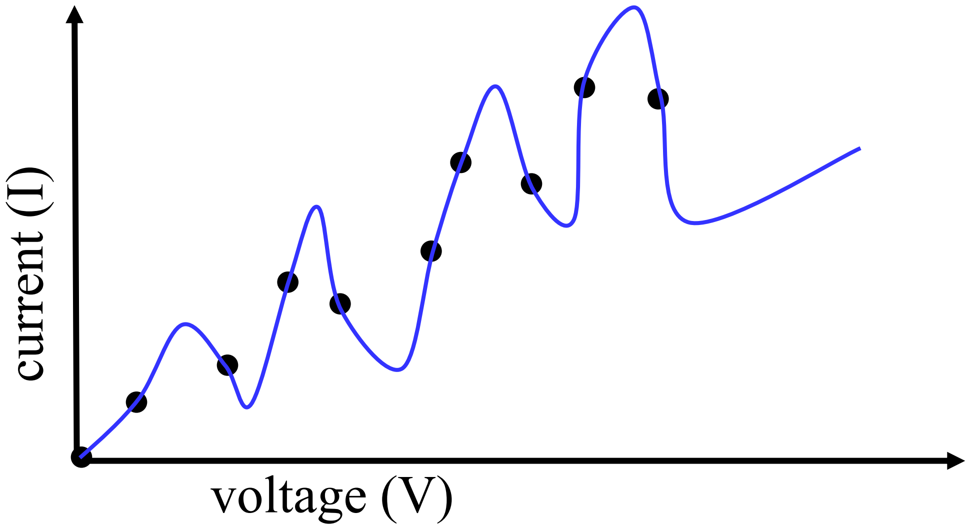


Overfitting Example

Testing Ohms Law: V = IR   (I = (1/R)V)

Experimentally measure 10 points

Fit a curve to the Resulting data.

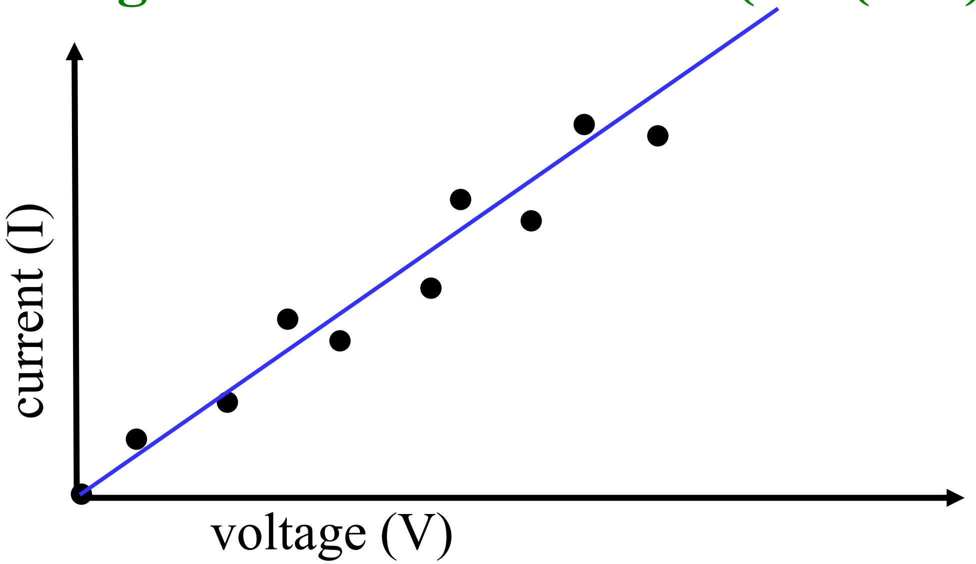


Perfect fit to training data with an 9th degree polynomial
(can fit *n* points exactly with an *n*-1 degree polynomial)

Ohm was wrong, we have found a more accurate function!

Overfitting Example

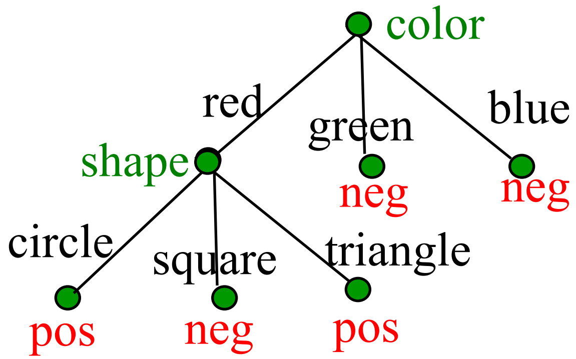
Testing Ohms Law: V = IR (I = (1/R)V)



Better generalization with a linear function that fits training data less accurately.

Overfitting Noise in Decision Trees

- Category or feature noise can easily cause overfitting.
  - Add noisy instance <medium, blue, circle>: pos (but really neg)



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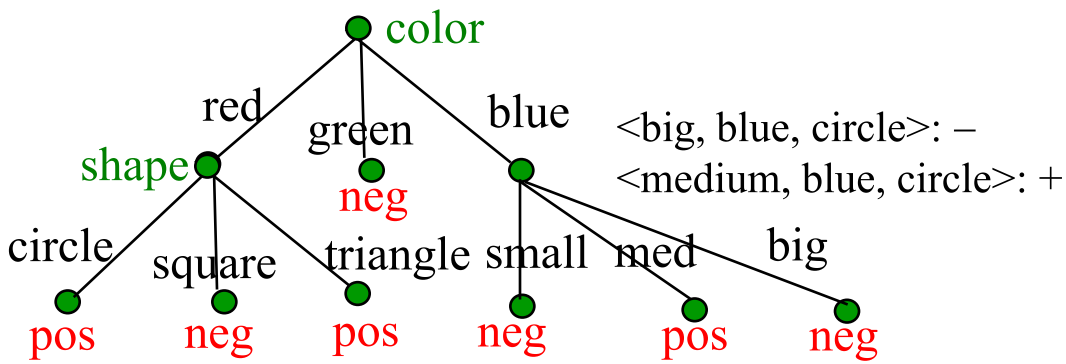

- Noise can also cause different instances of the same feature vector to have different classes. Impossible to fit this data and must label leaf with the majority class.
  - <big, red, circle>: neg (but really pos)
- Conflicting examples can also arise if the features are incomplete and inadequate to determine the class or if the target concept is non-deterministic.

Overfitting Prevention (Pruning) Methods

- Two basic approaches for decision trees
  - Prepruning: Stop growing tree as some point during top-down construction when there is no longer sufficient data to make reliable decisions.
  - Postpruning: Grow the full tree, then remove subtrees that do not have sufficient evidence.
- Label leaf resulting from pruning with the majority class of the remaining data, or a class probability distribution.
- Method for determining which subtrees to prune:
  - Cross-validation: Reserve some training data as a hold-out set (***validation set***, ***tuning set***) to evaluate utility of subtrees.
  - Statistical test: Use a statistical test on the training data to determine if any observed regularity can be dismisses as likely due to random chance.
  - Minimum description length (MDL): Determine if the additional complexity of the hypothesis is less complex than just explicitly remembering any exceptions resulting from pruning.

Additional Decision Tree Issues

- Better splitting criteria
  - Information gain prefers features with many values.
- Continuous features
- Predicting a real-valued function (regression trees)
- Missing feature values
- Features with costs
- Misclassification costs
- Incremental learning
- Mining large databases that do not fit in main memory

C4.5

- Based on ID3 algorithm, author Ross Quinlan
- In all (or most of) non-commercial and commercial data mining tools
- Weka Trees -> j48

C4.5 Algorithms

- B

AQ

- Riszard Michalski
- Bottom up

Regression trees

- Linear and multinomial regression
- Regression tree
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CART

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