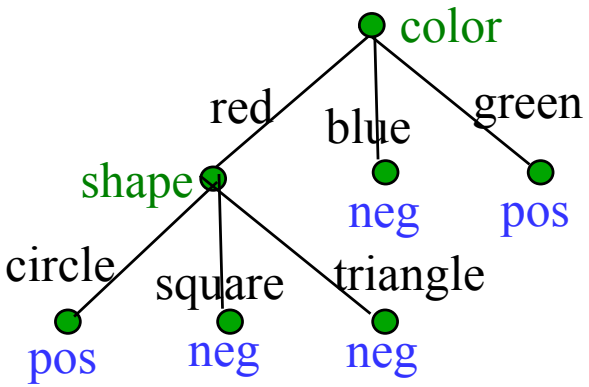
Decision Tree Learning

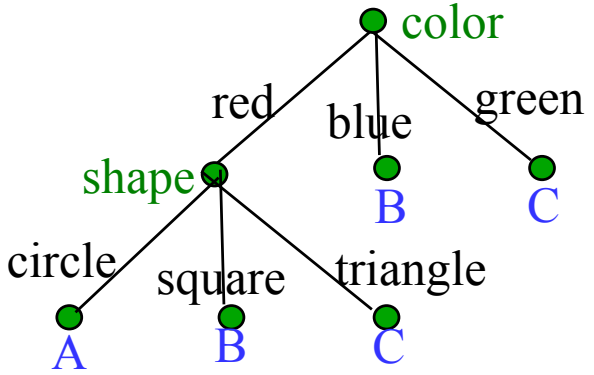
Based on the ML lecture by Raymond J. Mooney

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 ∧ circle → pos
  - red ∧ circle → A

    blue → B; red ∧ square → B

    green → C; red ∧ triangle → C

Properties of Decision Tree Learning

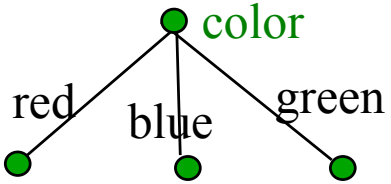
- Continuous (real-valued) features can be handled by allowing nodes to split a real valued feature into two ranges based on a threshold (e.g. length < 3 and length ≥ 3)
- Classification trees have discrete class labels at the leaves, ***regression trees*** allow real-valued outputs at the leaves.
- 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, square>: -

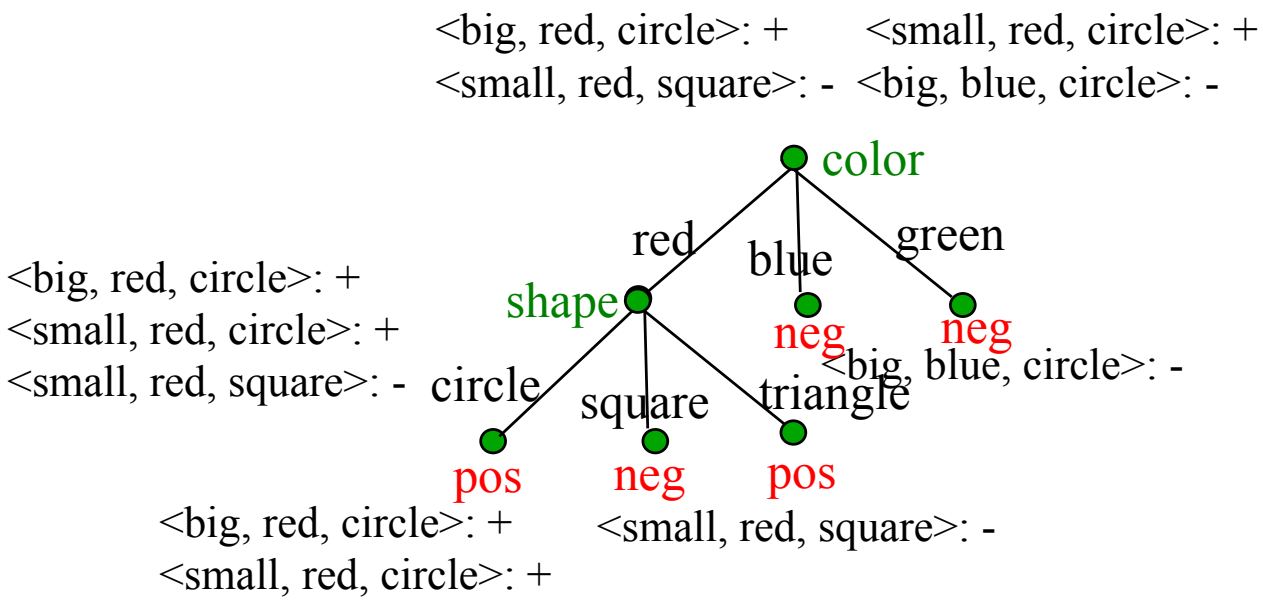
<small, red, circle>: +
<big, blue, circle>: -



<big, red, circle>: +
<small, red, circle>: +
<small, red, square>: -

Top-Down Decision Tree Induction

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



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

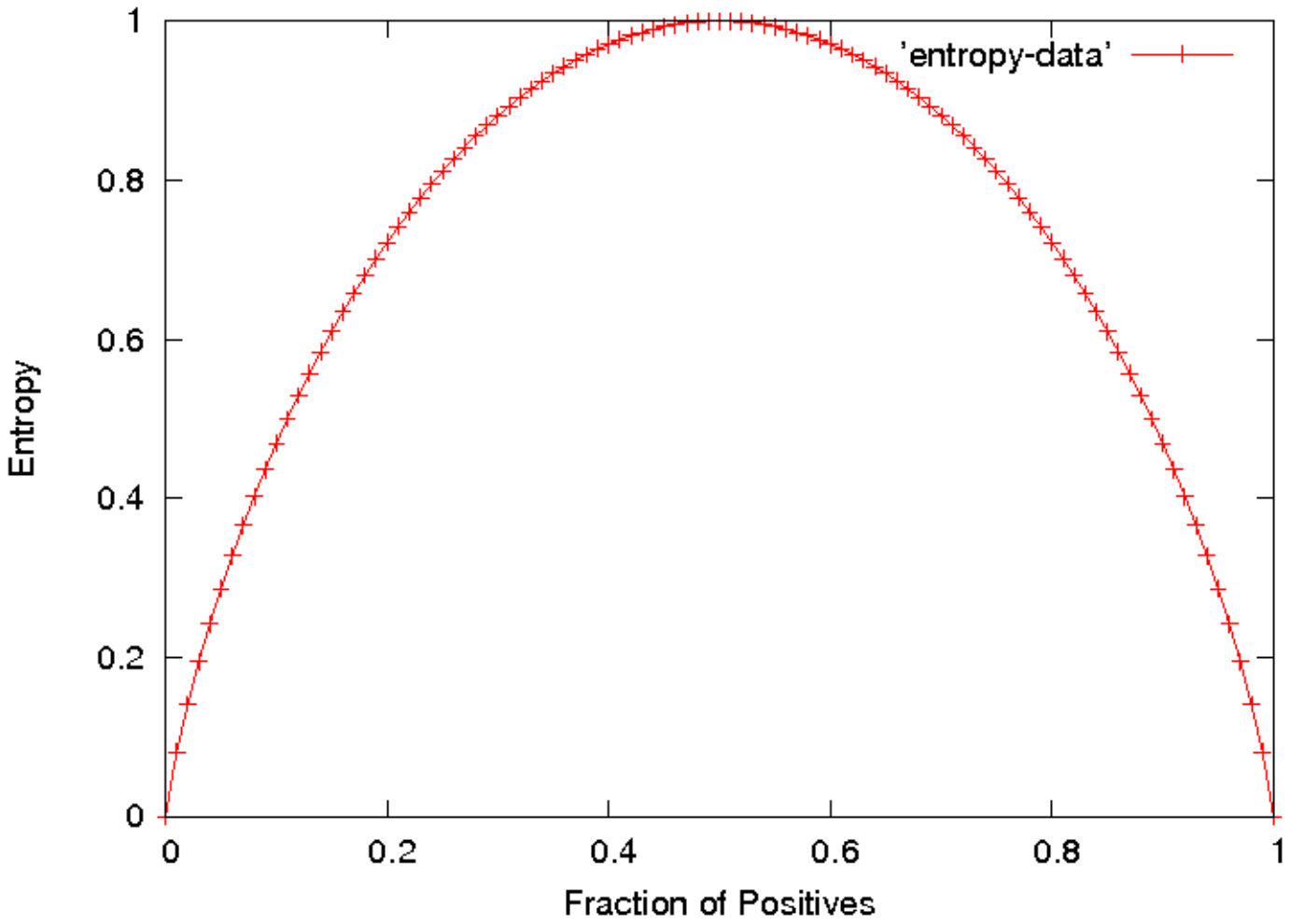
- Entropy (disorder, impurity) of a set of examples, S, relative to a binary classification is:

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

  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



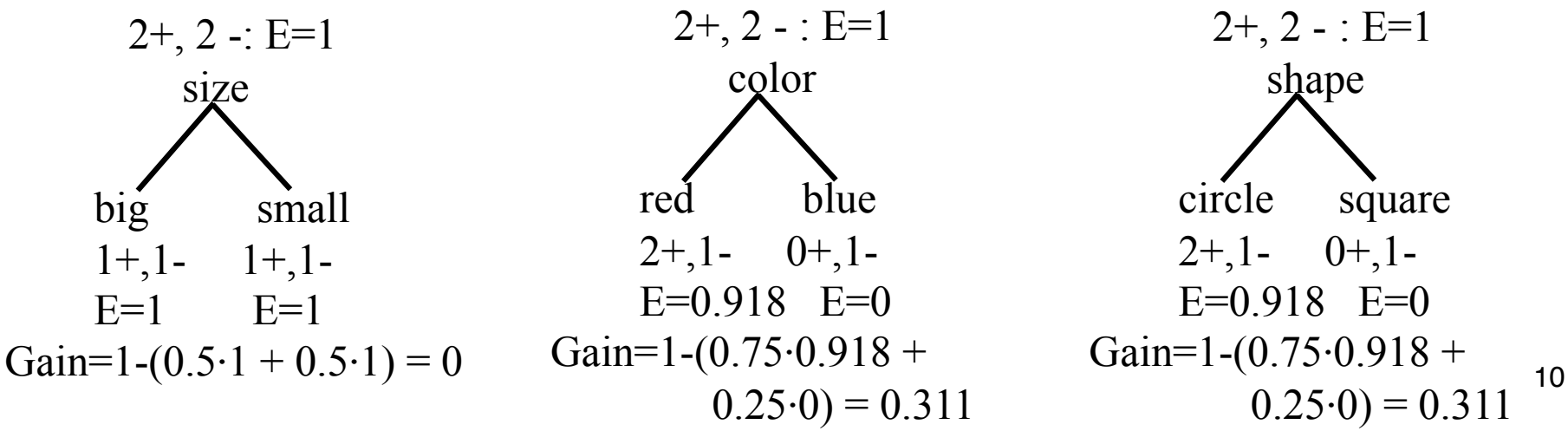
Information Gain

- 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>: -



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

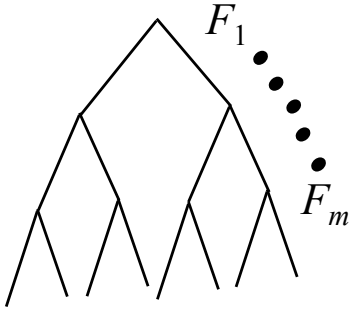
- Information-gain gives a bias for trees with minimal depth.
- Implements a search (preference) bias instead of a language (restriction) bias.

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

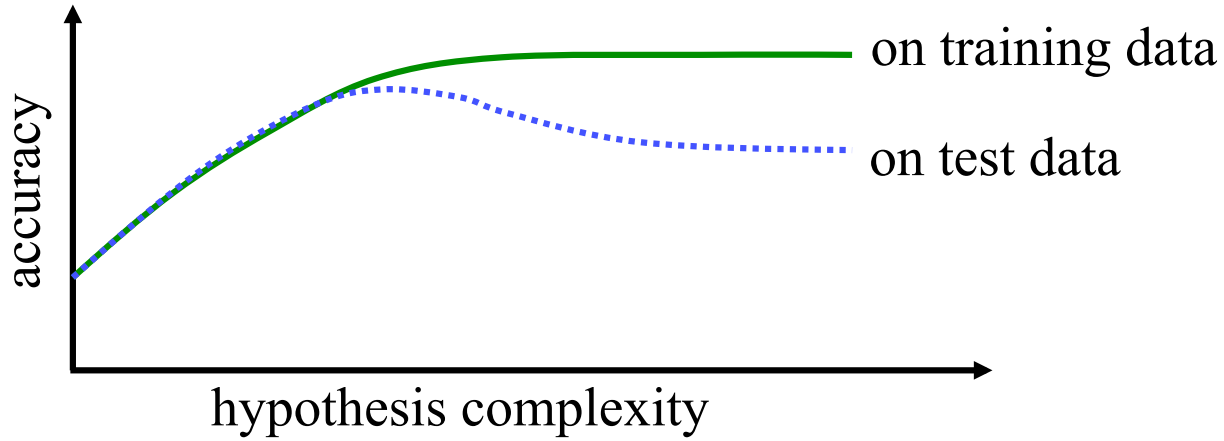
- At each level, *i*, in the tree, must examine the remaining *m-i* features for each instance at the level to calculate info gains.

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

- 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.

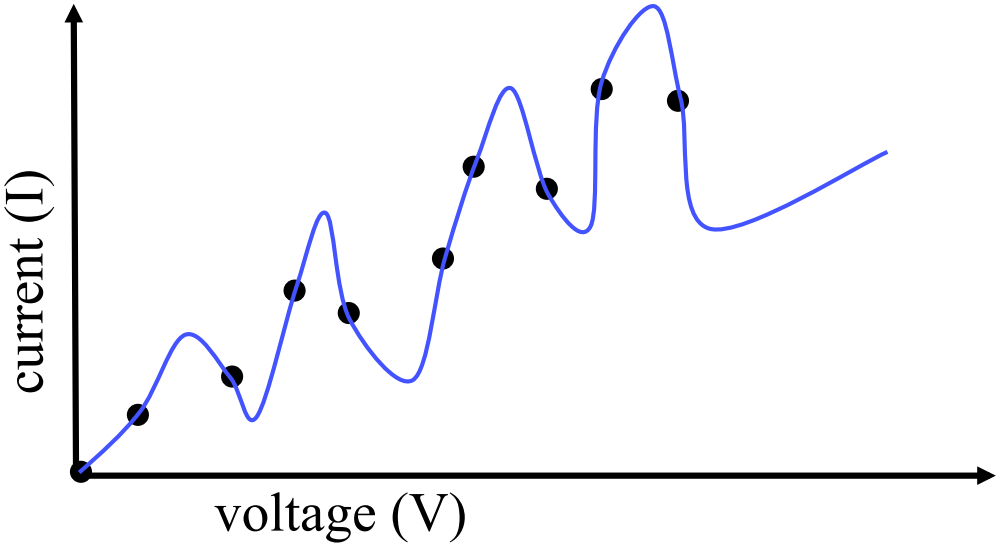


Overfitting Example

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

Experimentally measure 10 points

Fit a curve to the Resulting data.

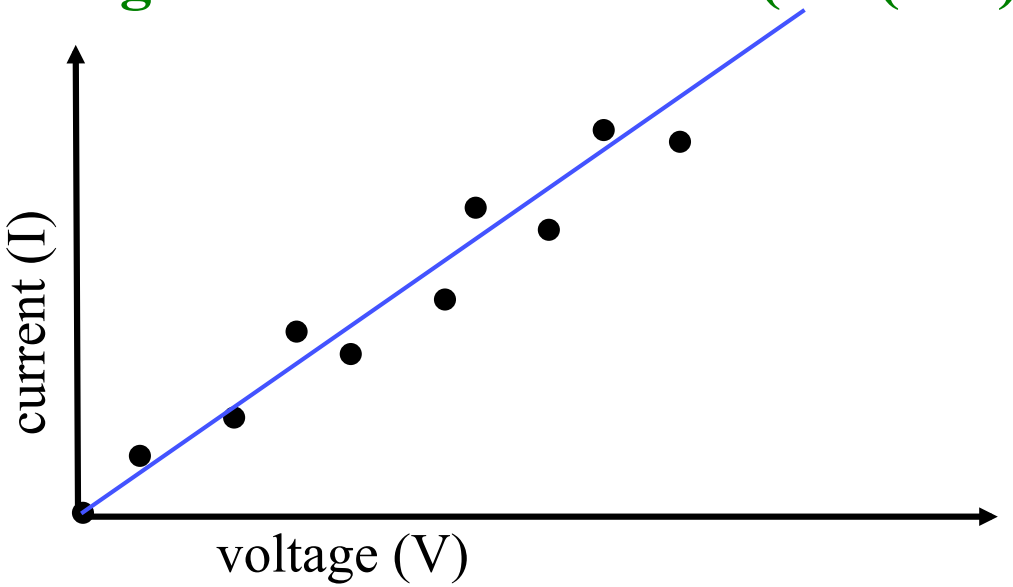


Perfect fit to training data with an 9th degree polynomial
(can fit *n* points exactly with an *n*-1 degree polynomial)

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

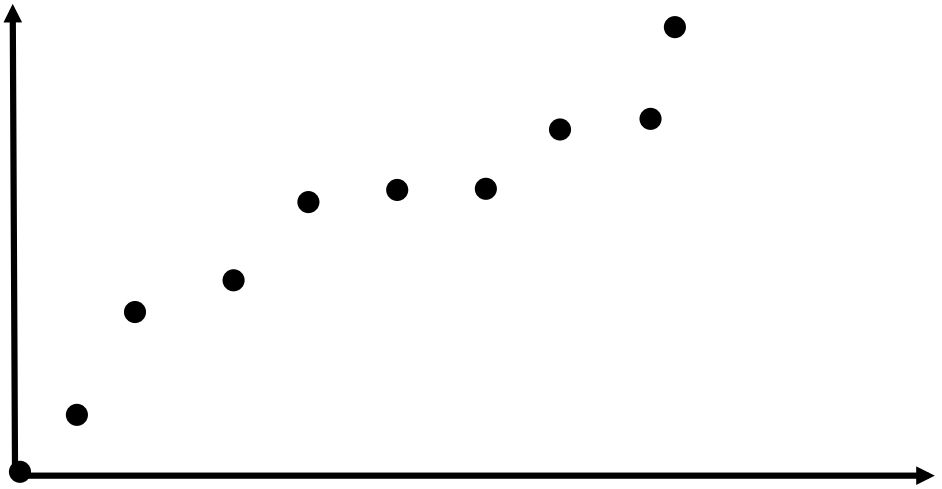
Overfitting Example

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



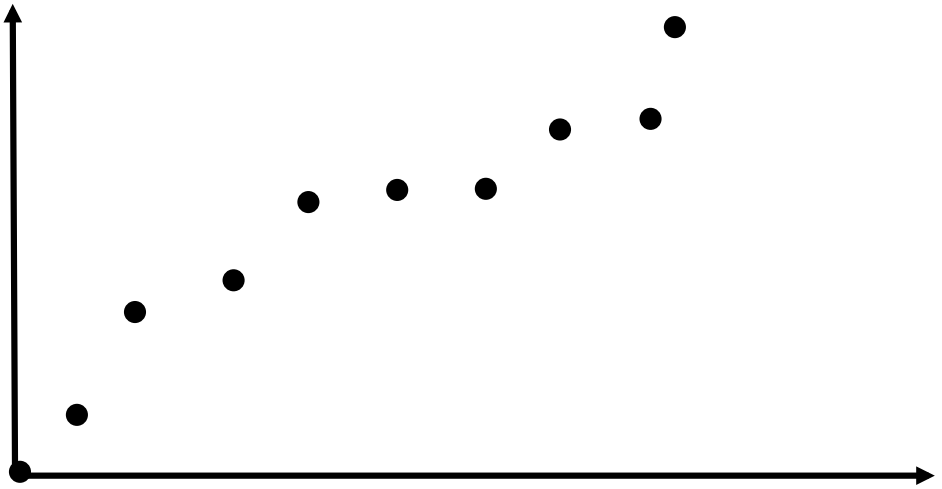
Better generalization with a linear function that fits training data less accurately.

Bias-variance tradeoff



Another example

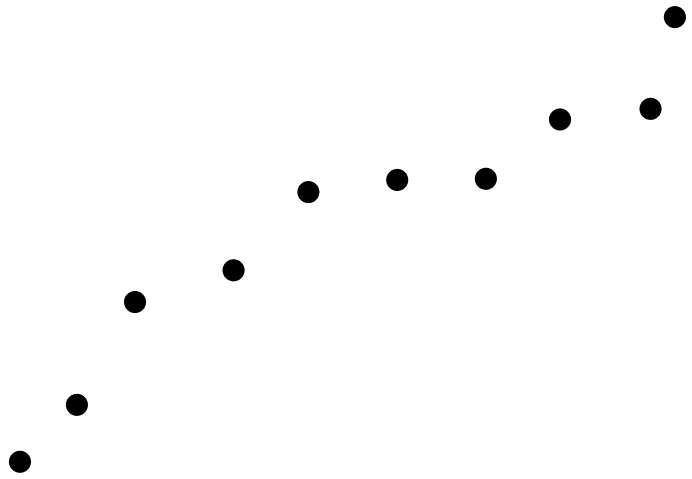
Bias-variance tradeoff



Linear function works well but
Cubic seems better

Is there any general view to the problem,
preferably with a theoretical background?

Bias-variance tradeoff

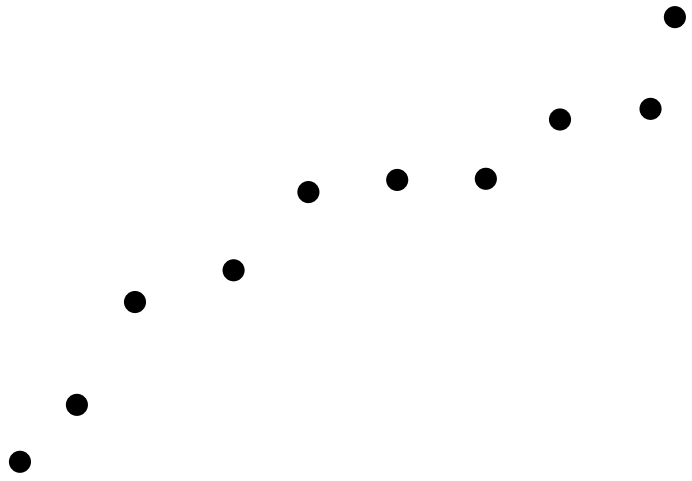


$y = f(x) + e, \quad E[e] = 0, \mathrm{Var}[e] = s^2$

f'() … estimate of f() learned by a classifier

$E[\,(y-f'(x))^2\,] = \mathrm{Bias}[\,f'(x)\,] + \mathrm{Var}[\,f'(x)\,] + s^2$

Bias-variance tradeoff

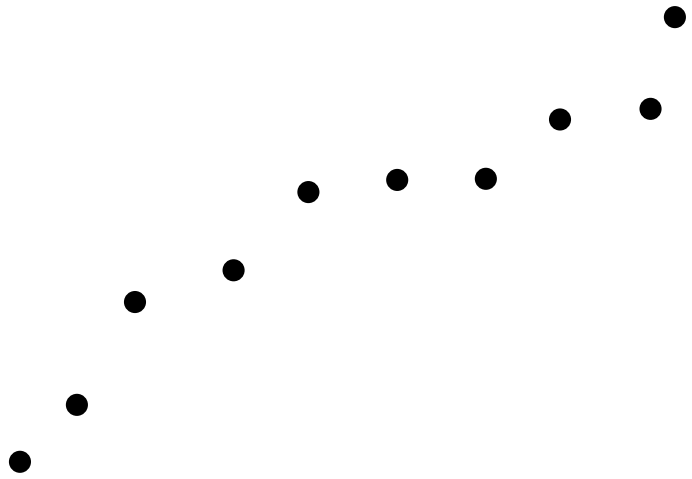


$y = f(x) + e, \quad E[e] = 0, \mathrm{Var}[e] = s^2$

f'() … estimate of f() learned by a classifier

$E[\,(y-f'(x))^2\,] = \mathrm{Bias}[\,f'(x)\,] + \mathrm{Var}[\,f'(x)\,] + s^2$

Bias-variance tradeoff

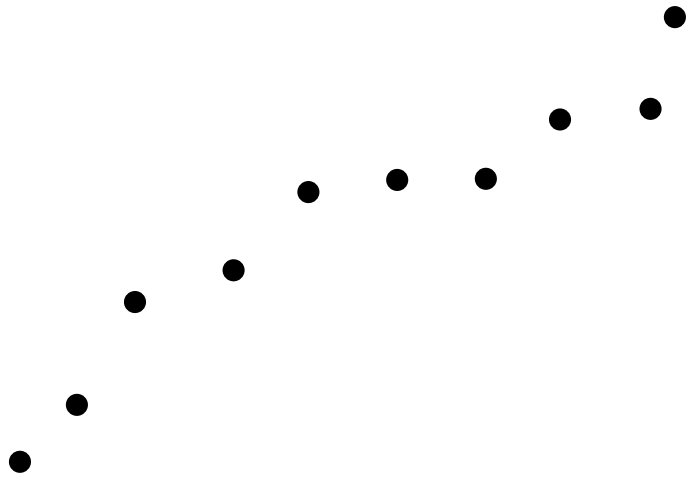


$y = f(x) + e, \quad E[e] = 0, \mathrm{Var}[e] = s^2$

f'() … estimate of f() learned by a classifier

$E[\,(y-f'(x))^2\,] = \mathrm{Bias}[\,f'(x)\,] + \mathrm{Var}[\,f'(x)\,] + s^2$

Bias-variance tradeoff

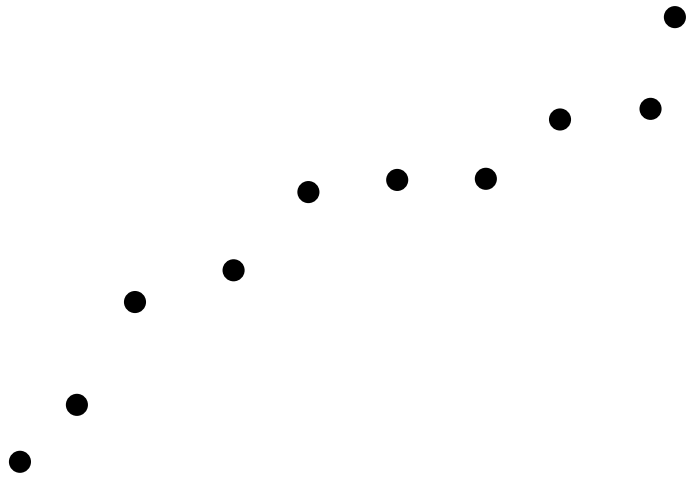


$y = f(x) + e, \quad E[e] = 0, \mathrm{Var}[e] = s^2$

f'() … estimate of f() learned by a classifier

$E[\,(y-f'(x))^2\,] = \mathrm{Bias}[\,f'(x)\,] + \mathrm{Var}[\,f'(x)\,] + s^2$

Bias-variance tradeoff

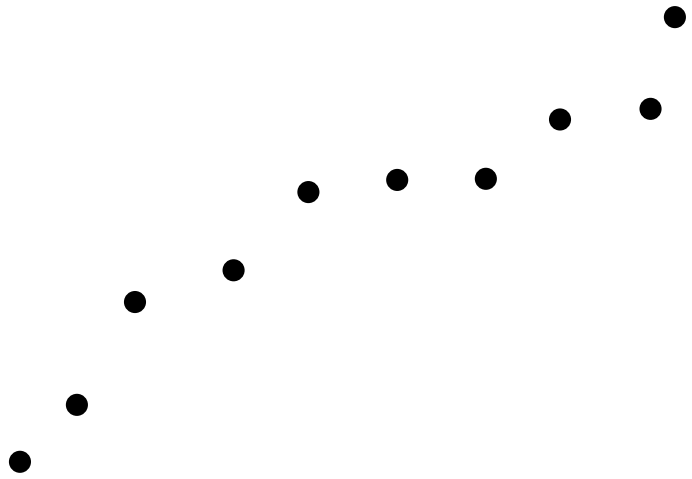


$y = f(x) + e, \quad E[e] = 0, \mathrm{Var}[e] = s^2$

f'() … estimate of f() learned by a classifier

$E[\,(y-f'(x))^2\,] = \mathrm{Bias}[\,f'(x)\,] + \mathrm{Var}[\,f'(x)\,] + s^2$

Bias-variance tradeoff



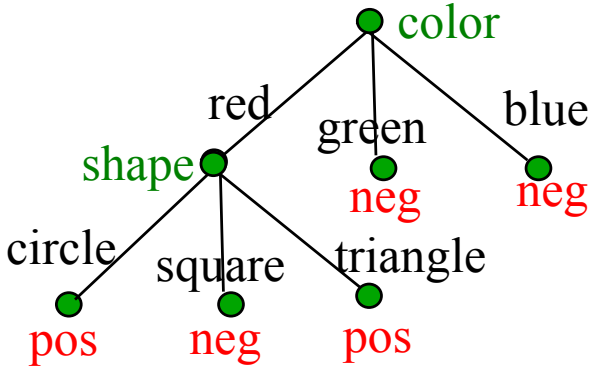
$y = f(x) + e, \quad E[e] = 0, \mathrm{Var}[e] = s^2$

f'() … estimate of f() learned by a classifier

$E[\,(y-f'(x))^2\,] = \mathrm{Bias}[\,f'(x)\,] + \mathrm{Var}[\,f'(x)\,] + s^2$

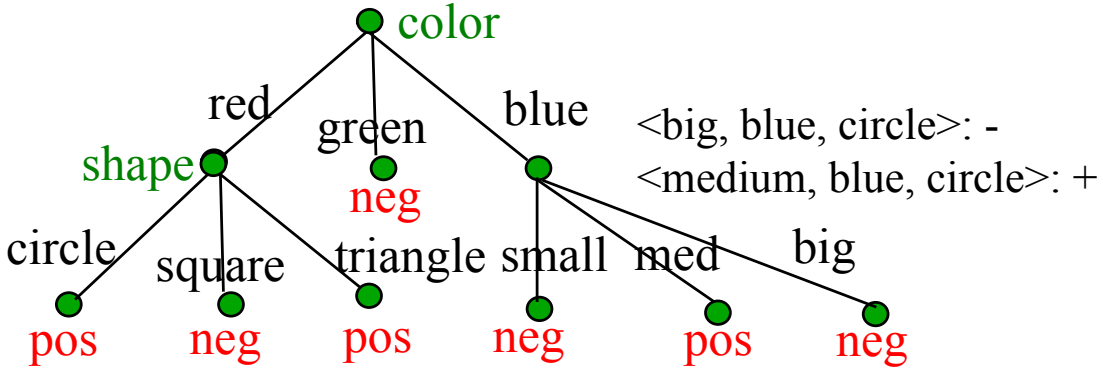
Overfitting Noise in Decision Trees

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



Overfitting Noise in Decision Trees

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



- 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: C4.5 ver.8 -> j48

Scheme of C4.5 algorithm:

Run several time and choose the best tree

Inner:Take L% of learning data randomly

Call ID3 (pre-pruning, see –m parameter)

Prune the tree (post-pruning, -cf)

Take T% of unseen learning data for validation

If validation criterion holds, exit

Otherwise add Lcrement to L and go to Inner