Machine Learning

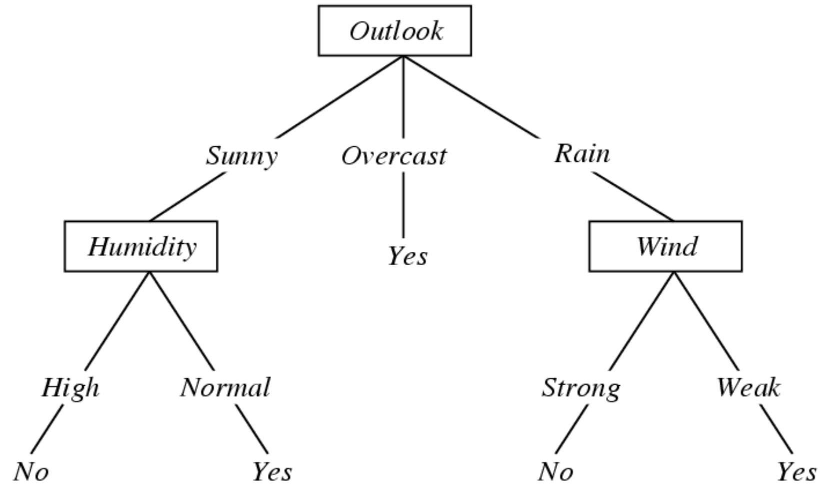
Decision Trees

Decision Trees

- Classifiers covered so far have been
  - Non-parametric (KNN)
  - Probabilistic with independence (Naïve Bayes)
  - Linear in features (Logistic regression, SVM)
- Decision trees use a different representation that is inherently non-linear
  - Hypothesis space contains logic sentences over boolean variables and feature functions (e.g.=, >)
    - Intuitive representation
    - Can be converted into rules relatively easily

Decision Trees

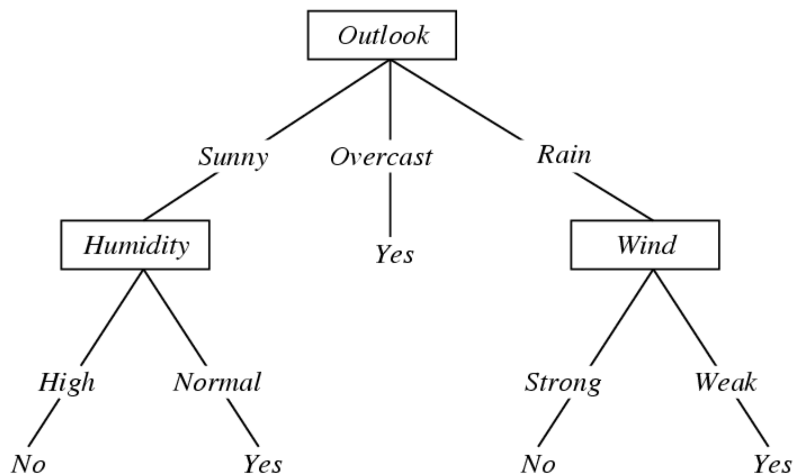
- Hypotheses are represented as trees
  - Nodes are variables (features)
  - Leaves are class predictions (or class probabilities)
    - Leaves can also contain subsets of the training set
  - Arcs represent node evaluations



Example from Tom Mitchell

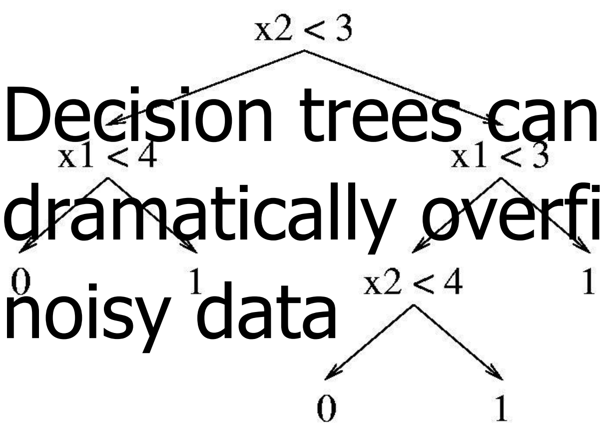
Decision Trees

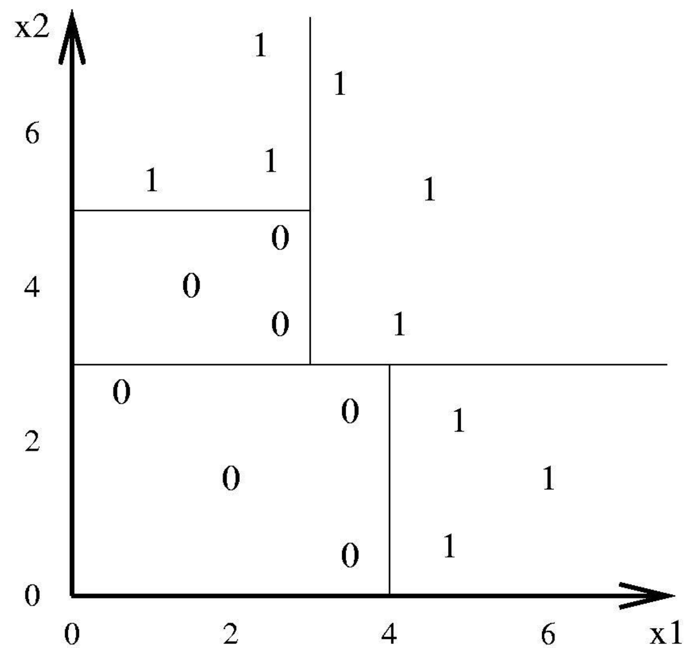
- Decision trees represent logical sentences in disjunctive normal form (DNF)
  - Consecutive elements in a branch form conjuncts
  - Branches with same leaf label form disjuncts
- Variables/features are assumed to be independent
- Can be co[r] ... the sentences into implic[...] ... hand side



Decision Trees

- Decision trees work with continuous and discrete variables and form complex decision boundaries
  - Non-continuous
  - Non-differentiable
- Decision trees can dramatically overfit noisy data





Decision Trees

- Variables can occur multiple times on a branch of the tree if they are non-boolean
  - Decision trees with "predicates" = , < represent all possible DNF sentences with arbitrary thresholds
    - Trees can have very different depths
    - Unlimited hypothesis space
    - Generally many decision trees for same classification
  - Decision trees can be extended
    - Use additional features
    - Including additional "predicates" for evaluation

Learning Decision Trees

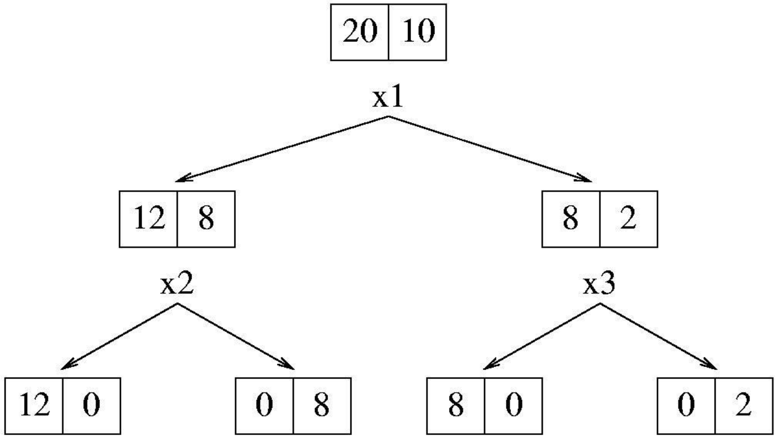
- There is no continuous interpretation of either the probability or the decision boundary
  - No derivative with respect to tree parameters
- To optimize performance, decision tree algorithms generally use search
  - Since the space of all trees is intractable they typically use greedy, fixed lookahead search
    - Each greedy search adds one node to the tree
    - The resulting tree is generally not optimal

Learning Decision Trees

- Performance function
  - Classification performance
    - "Purity" of the prediction
- Tree construction criterion
  - Tree simplicity
    - Usually in terms of number of nodes or depth of the tree
- Basic algorithms iterates as follows
  - Do lookahead search to find "best" feature node
    - Terminate if feature does not improve performance
  - Add node and split parent data set on node values

Learning Decision Trees

- How can we pick the best feature ?
  - Error in terms of number of misclassified data points
    - Does not consider whether the result of the split might allow for a better split later



Learning Decision Trees

- How can we pick the best feature ?
  - Information gain (reduction in the Entropy)
    - Performance function is entropy

      $$H_D(Y) = \sum_{y \in C} P_D(y) \log P_D(y)$$

    - Best feature is the one that reduces entropy the most (has the highest information gain)

$$Gain(D,A) = I_D(A,Y) = H_D(Y) - H_D(Y \mid A)$$
$$= H_D(Y) - \sum_{a \in range(A)} P_D(A=a) \log H_D(Y \mid A=a)$$

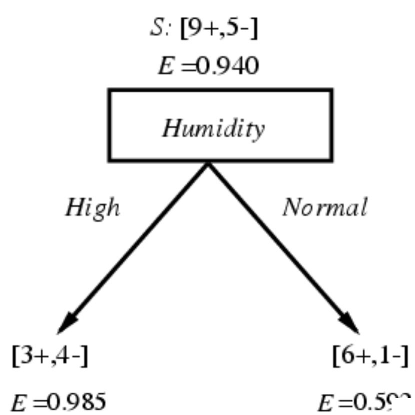
      - Prefer "purer" sets

Example

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

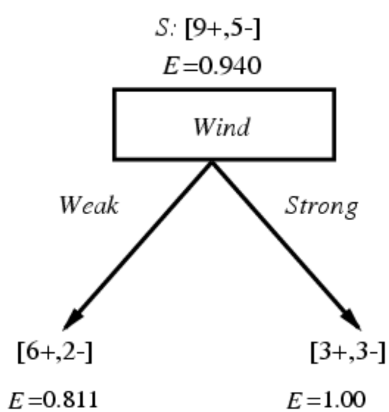
Example form Tom Mitchell

Example



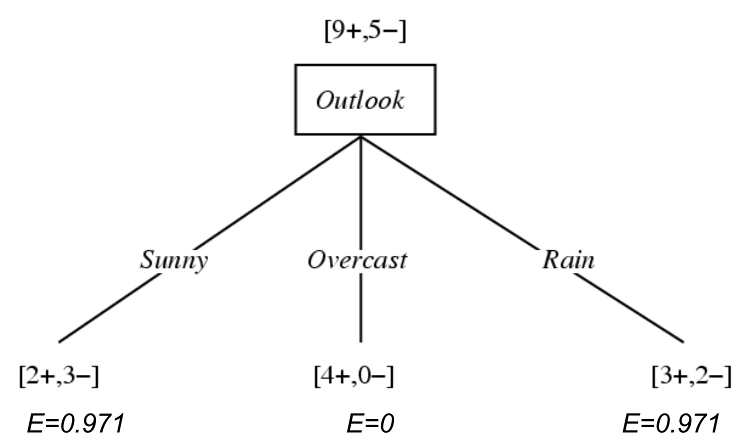
Gain (S, Humidity)

= .940 - (7/14).985 - (7/14).592
= .151



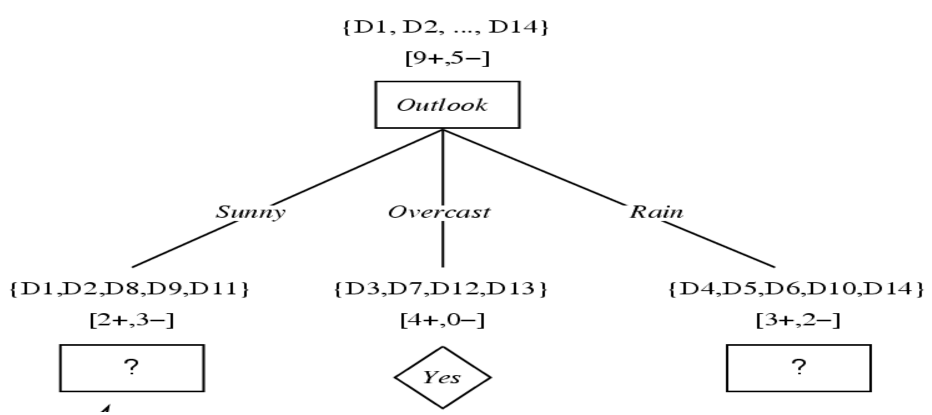
Gain (S, Wind)

= .940 - (8/14).811 - (6/14)1.0
= .048



Gain(S, Outlook)

=.940 - (5/14).971 – (4/14)0 – (5/14).971
= 0.246



Multi-Valued Features

- Features with multiple values have to be treated differently
  - Many-way splits result in very small sets and thus unreliable estimates of the entropy
    - Gain ratio provides one possible way to overcome this
      - Gain ratio looks at the information gain relative to the intrinsic information of the feature

$$GainRatio(D,A) = \frac{Gain(D,A)}{-\sum_{a \in range(A)} \frac{|D_a|}{|D|} \log \frac{|D_a|}{|D|}}$$

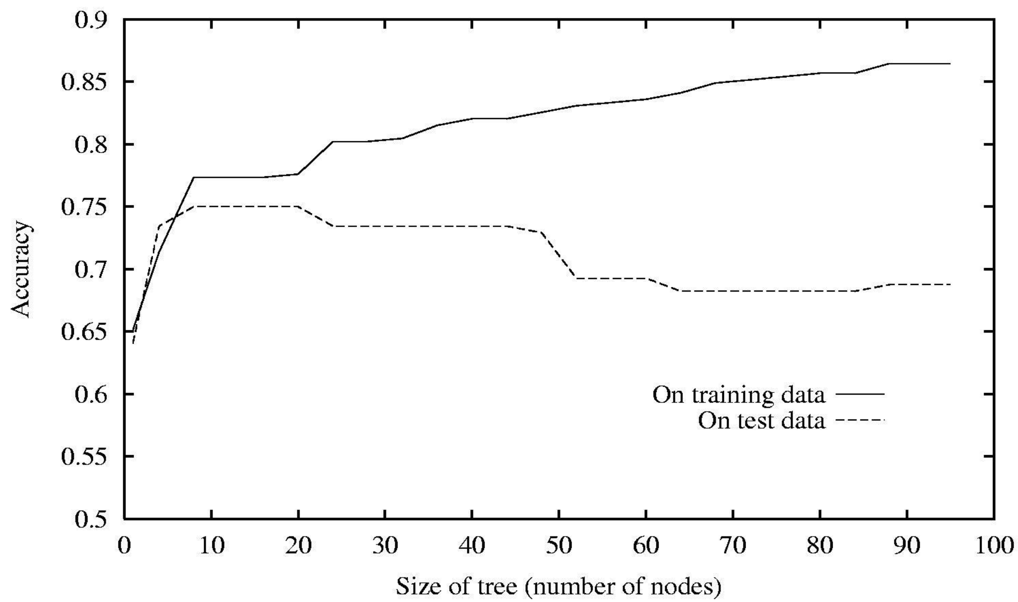
      - Tries to compensate for the benefits of multiple options

Continuous features

- Continuous Features have to be converted into boolean (or multi-valued)
  - For continuous variables a threshold for the < "predicate" has to be picked
    - Sort data elements and evaluate every possible threshold at which the classification changes
      - Other points can not result in maximum
    - Use the threshold with the highest gain

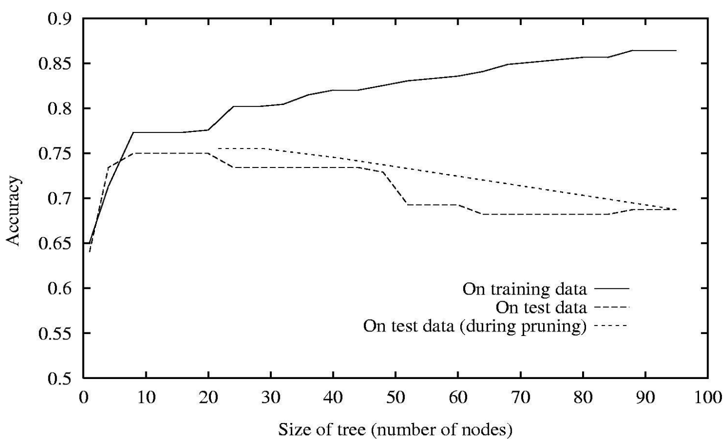
Overfitting in Decision Trees

- If there is noise in the data, decision trees can significantly overfit
  - To determine overfitting, we need to use test data that was not used for training



Overfitting in Decision Trees

- There are two basic mechanisms to address overfitting
  - Early stopping when split is not significant
  - Post-pruning after complete learning
    - Evaluate benefit of pruning on accuracy in test set and remove the node (branch) with highest accuracy gain



Decision Trees and Rules

- Decision trees can be easily converted into a set of rules (one rule per branch)

IF $(Outlook = Sunny)\ AND\ (Humidity = High)$
THEN $PlayTennis = No$

IF $(Outlook = Sunny)\ AND\ (Humidity = Normal)$
THEN $PlayTennis = Yes$

  - In C4.5 (and a number of other decision tree algorithms) pruning is performed on the rules
    - Prune each rule individually
    - Sort rules into desired sequence for faster use

Decision Trees

- Decision trees are a very frequently used type of classifier in particular when discrete features are present
  - Can represent highly non-linear classes
  - Can be translated into rules
  - Result is easy to understand and interpret
  - Does not represent continuous relationships
    - Can be augmented by including logistic regression "predicates" and multi-variate feature functions
- Many practical algorithms: ID3, C4.5, …