Decision Trees

Off the shelf classifier

- A method that can be applied directly to the data without the need for preprocessing or tuning of learning algorithm
- So far
  - Perceptron – Directly learns the classifier
  - Logistic Regression – Discriminative
  - LDA - Generative

Criteria

- “Mixed” data types
- Missing values
  - Missing at random
  - Missing for a cause
- Robustness to outliers
- Insensitive to Monotone transformation of features
- Scalability
- Irrelevant inputs
- Interpretability
- Predictive power

Summary

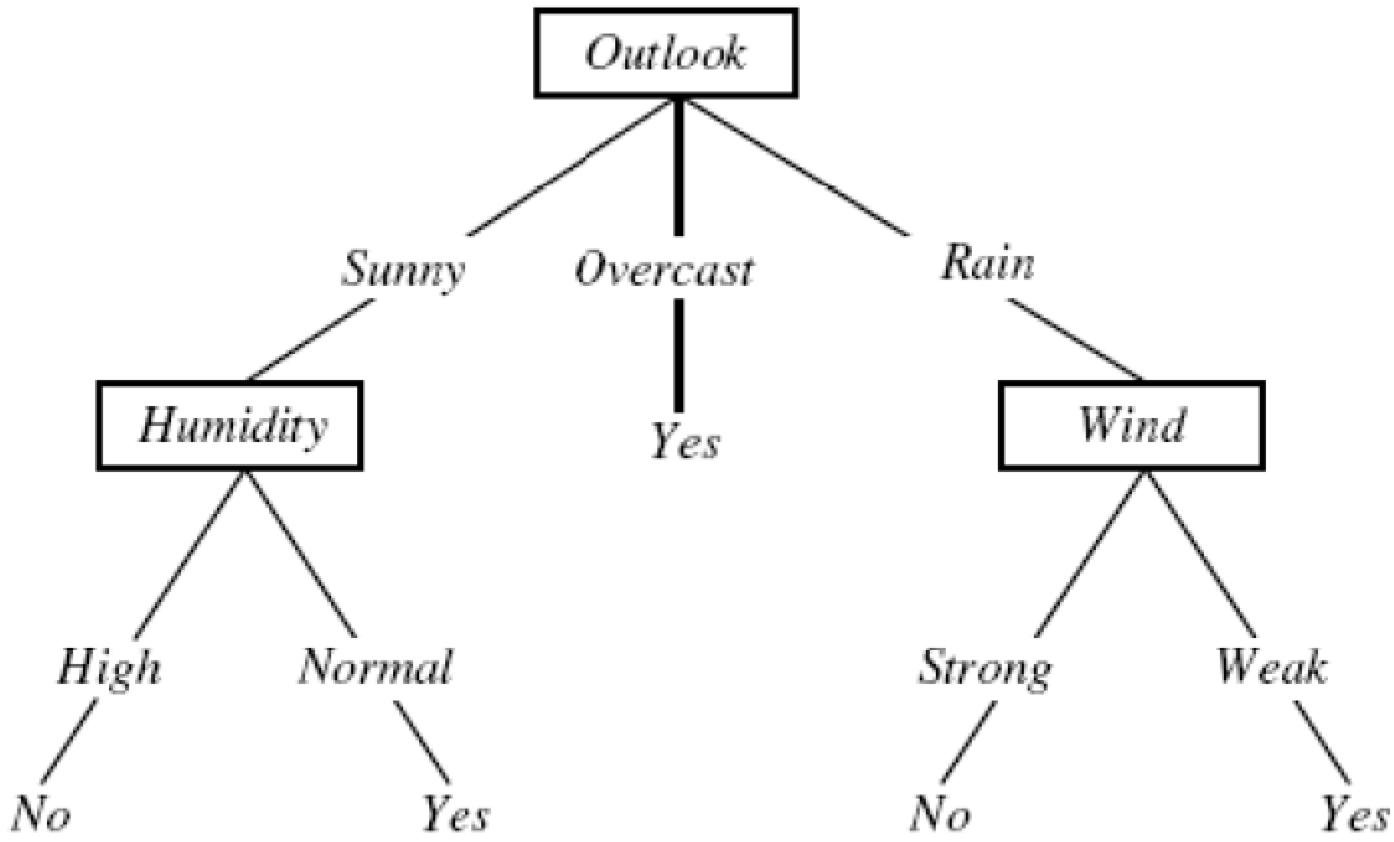
(This table will grow with the course)

Criterion	**Perceptron**	**Logistic**	**LDA**
Mixed data	N	N	N
Missing values	N	N	Y
Outliers	N	Y	N
Monotone	N	N	N
Scalability	Y	Y	Y
Irrelevant i/p	N	N	N
Interpretable	Y	Y	Y
Accurate	Y	Y	Y

Linear Separability

- A data set is linearly separable if there exists a hyperplane that separates pos examples from neg examples
- Many data sets in real world are not linearly separable!
- Two options
  - Use non-linear features and learn a linear classifier on this non-linear feature space. We will see a few such methods later
  - Use non-linear classifiers (decision trees, neural nets, nearest neighbors etc)

Decision Tree for Playing Tennis

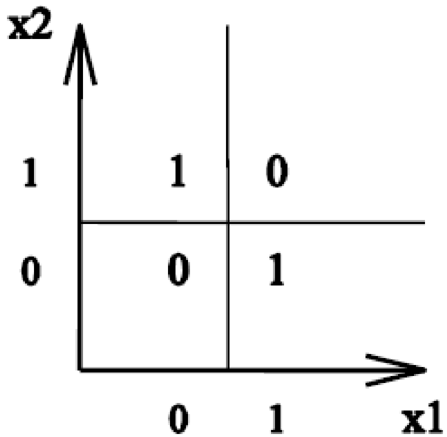


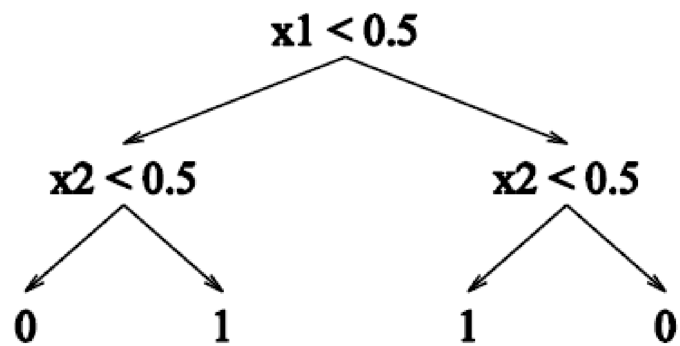
Decision Trees

- Decision tree representation:
  - Each internal node tests an attribute
  - Each branch corresponds to attribute value
  - Each leaf node assigns a classification
- How would we represent:
  - $\wedge$, $\vee$, XOR
  - $(A \wedge B) \vee (C \wedge \neg D \wedge E)$
  - M of N

Decision Trees Can Represent Any Boolean Function

XOR

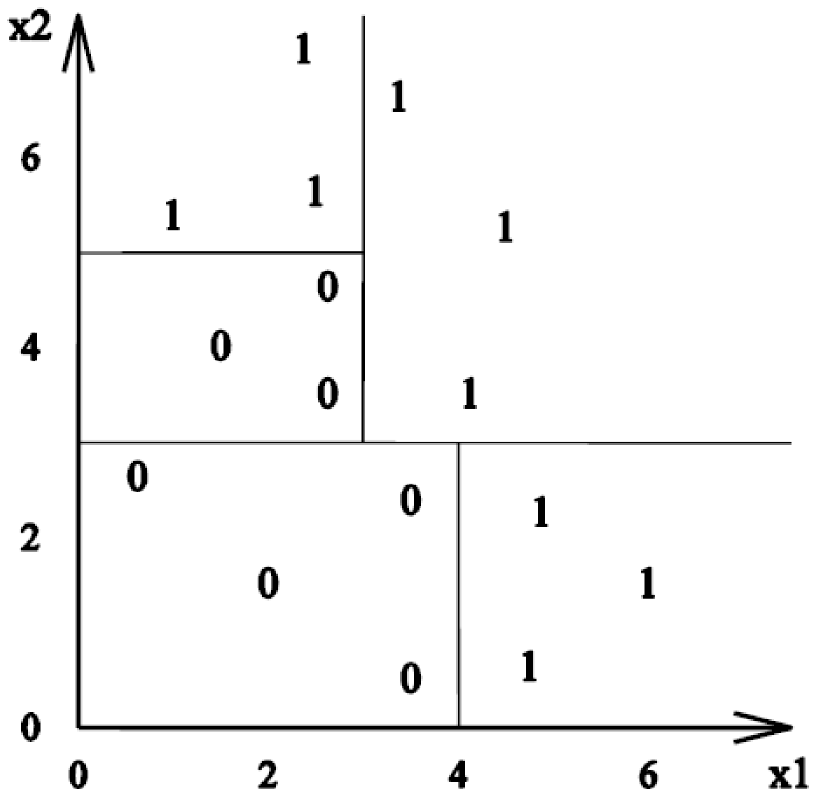


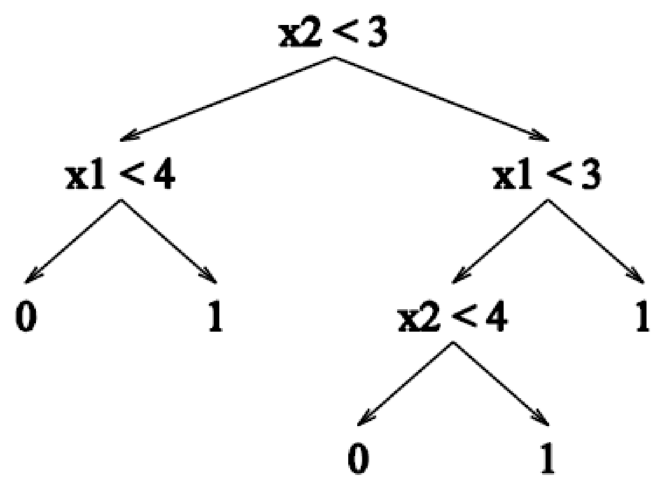


- If a target Boolean function has *n* inputs, there always exists a decision tree representing that target function.
- However, in the worst case, exponentially many nodes will be needed (why?)
  - 2^n possible inputs to the function
  - In the worst case, we need to use one leaf node to represent each possible input

Decision Tree Decision Boundaries

- Decision Trees divide the feature space into axis-parallel rectangles and label each rectangle with one of the K classes





When do you want Decision trees?

- Instances describable by attribute-value pairs
- Target function is discrete valued
- Disjunctive hypothesis may be required
- Possibly noisy training data
- Need for interpretable model

Examples:

- Equipment or medical diagnosis
- Credit risk analysis
- Modeling calendar scheduling preferences

Learning Decision Trees

- Goal: Find a decision tree **h** that achieves minimum misclassification errors on the training data
- A trivial solution: just create a decision tree with one path from root to leaf for each training example
  - Bug: Such a tree would just memorize the training data. It would not generalize to new data points
- Solution 2: Find the <u>smallest</u> tree *h* that minimizes error
  - Bug: This is NP-Hard

Top Down Induction

There are different ways to construct these trees. We will now look at a top-down, greedy search approach

High-level Idea:

1. Choose the best feature f^* for the root of the tree.
2. Separate the training set into subsets $\{S_1, S_2, \ldots, S_k\}$ where each subset S_i contains examples that have the same value for f^*
3. Recursively apply the algorithm on each new subset until all examples have the same class label

Growing Trees

How to choose next feature to place in decision tree?

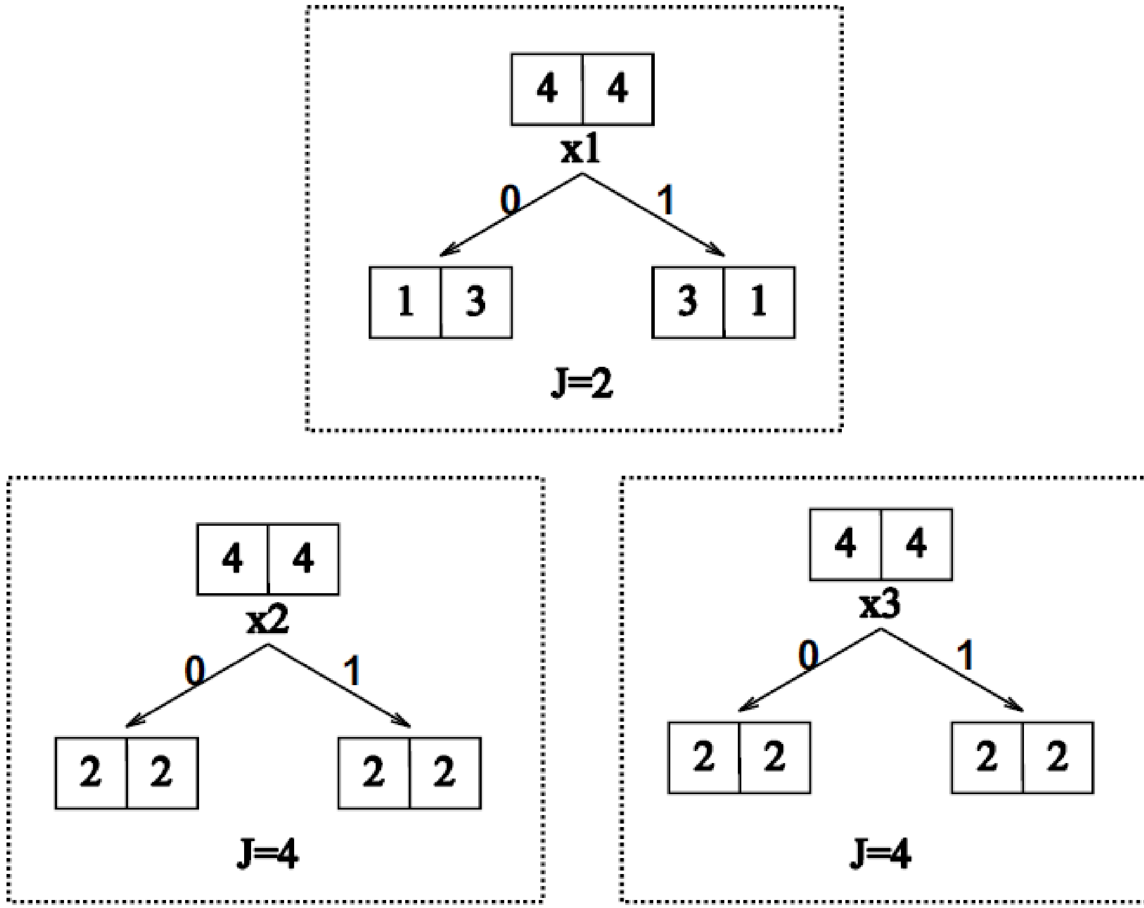
- Random choice?
- Feature with largest number of values?
- Feature with fewest?
- Lowest classification error?
- <u>Information theoretic</u> measure (Quinlan's approach)

Criteria: Classification Error

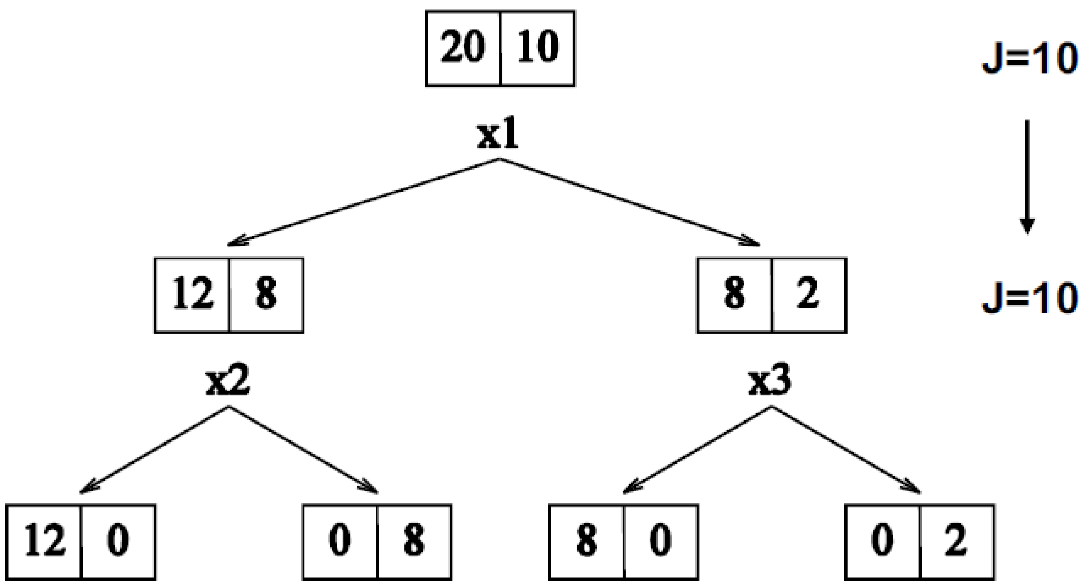
- Choose the feature for split as the one that has the lowest error on the training data

x_1	x_2	x_3	y
0	0	0	1
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	0
1	1	1	0

Training examples



Unfortunately, this measure does not always work well, because it does not detect cases where we are making "progress" toward a good tree



Information Theory to the rescue

- Let X be a random variable with the distribution

$P(X = 0)$	$P(X = 1)$
0.2	0.8

- The surprise S(X=x) of each example of V is defined to be $S(V = v) = -logP(V = v)$
- An event with probability 1 has zero surprise
- An event with probability 0 has infinite surprise
- The surprise is the asymptotic number of bits of information that need to be transmitted to a recipient who knows the probabilities of the results. This is also called as description length of X.

Entropy

- The entropy of ***X***, denoted *H(**X**)*, is defined as

$$H(X) = -\sum_{x} P_X(x) \log_2 P_X(x)$$

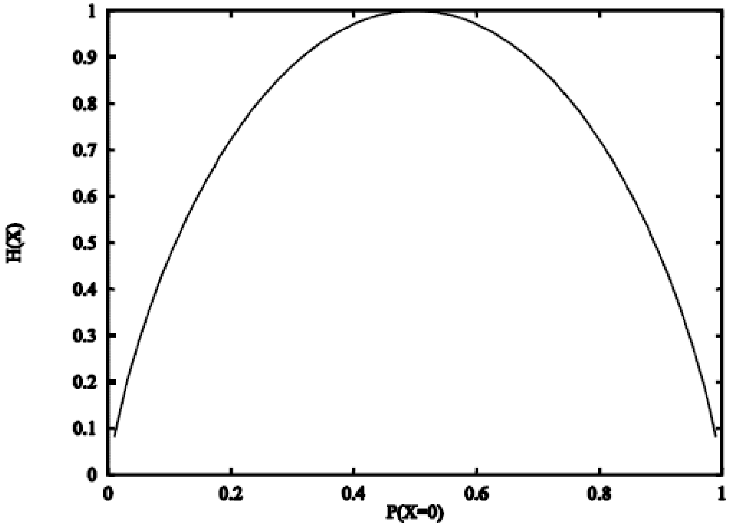
- **Entropy** measures the uncertainty of a random variable
- The larger the entropy, the more uncertain we are about the value of *X*
- If P(X=0)=0 (or 1), there is no uncertainty about the value of X, entropy = 0
- If P(X=0)=P(X=1)=0.5, the uncertainty is maximized, entropy = 1

Measuring Entropy

- S is a sample of training examples
- $p_{\oplus}$ is the proportion of positive examples in S
- $p_{\otimes}$ is the proportion of negative examples in S

Entropy measures the impurity of S

$$Entropy(S) = -p_{\oplus} \log p_{\oplus} - p_{\otimes} \log p_{\otimes}$$



More About Entropy

- Joint Entropy

$$H(X,Y) = -\sum_{x}\sum_{y} P(X=x,Y=y)\log P(X=x,Y=y)$$

- Conditional Entropy is defined as

$$H(Y|X) = \sum_{x} P(X=x) H(Y|X=x)$$
$$= -\sum_{x} P(X=x) \sum_{y} P(Y=y|X=x)\log P(Y=y|X=x)$$

  – The average surprise of Y when we know the value of X

- Entropy is additive

$$H(X,Y) = H(X) + H(Y|X)$$

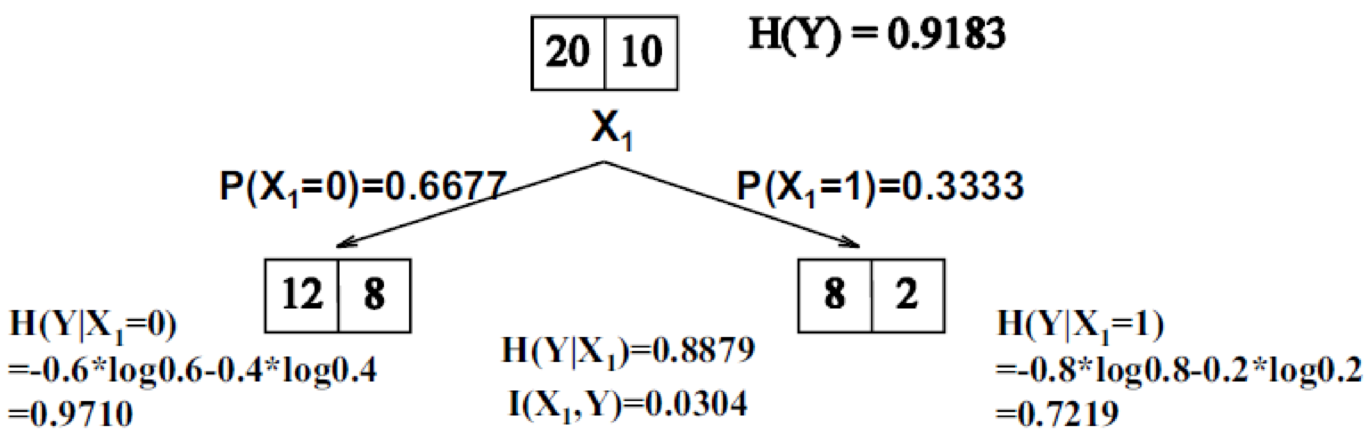
Mutual Information

- The <u>mutual information</u> between two random variables *X* and *Y* is defined as:

$$I(X,Y) = H(Y) - H(Y \mid X)$$

  - the amount of information we learn about *Y* by knowing the value of *X* (and vice versa – it is symmetric).

- Consider the class *Y* of each training example and the value of feature X_1 to be random variables. The mutual information quantifies how much X_1 tells us about *Y*.



Choosing the Best Feature

- Choose the feature X_j that has the highest mutual information with Y - often referred to as the **information gain** criterion

$$\arg\max_j I(X_j;Y) = \arg\max_j H(Y) - H(Y \mid X_j)$$
$$= \arg\min_j H(Y \mid X_j)$$

- Define $\tilde{J}(j)$ to be the expected remaining uncertainty about y after testing x_j

$$\tilde{J}(j) = H(Y \mid X_j) = \sum_x P(X_j = x) H(Y \mid X_j = x)$$

Non-Boolean Features

- Multiple discrete values
  - Method 1: Construct multiway split
  - Method 2: Test for one value versus all of the others
  - Method 3: Group the values into two disjoint sets and test one set against the other
- Real-valued variables
  - Test the variable against a threshold
- In all the cases, mutual information can be computed to choose the split

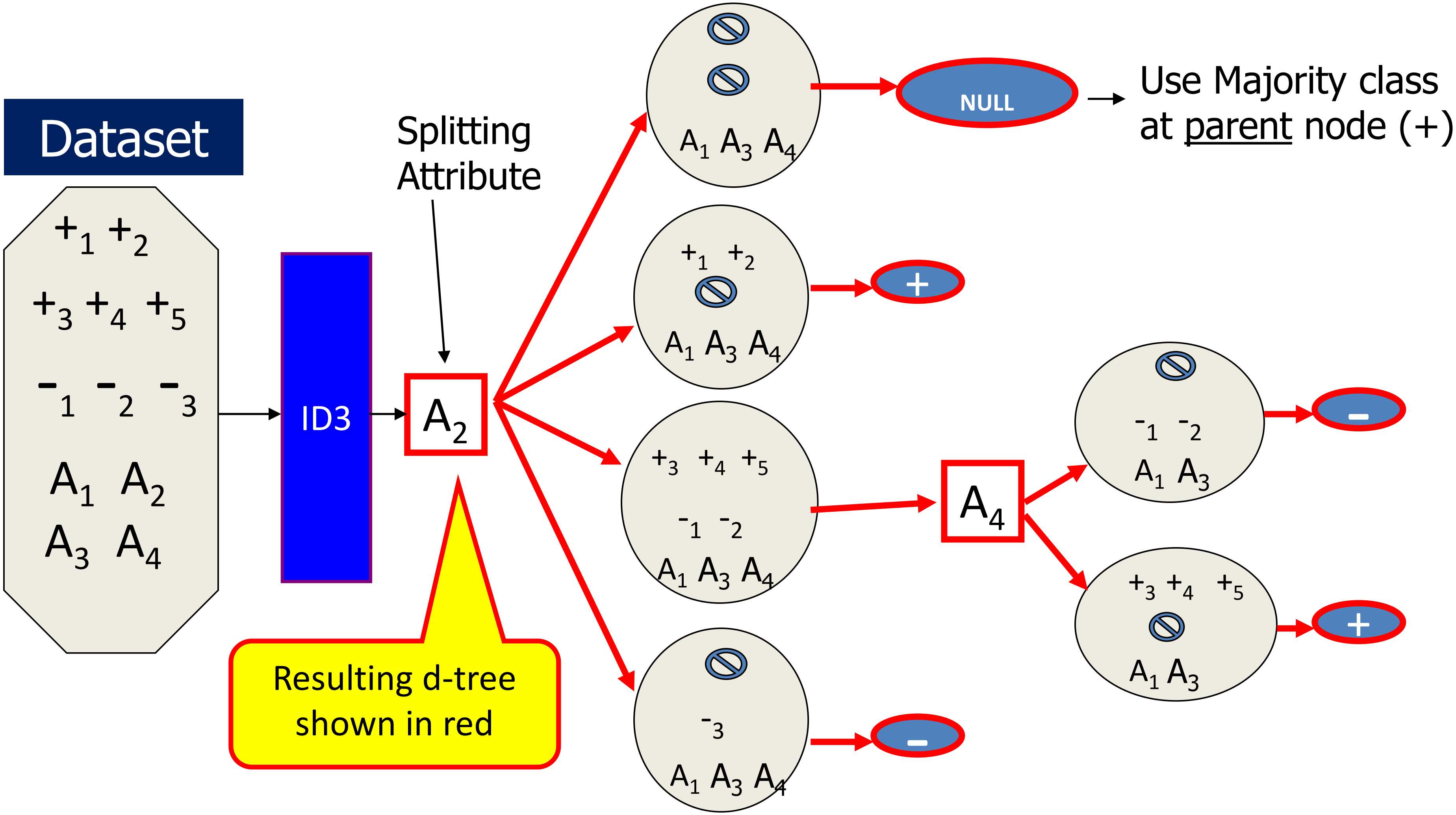
Top Down Induction

There are different ways to construct these trees. We will now look at a top-down, greedy search approach

High-level Idea:

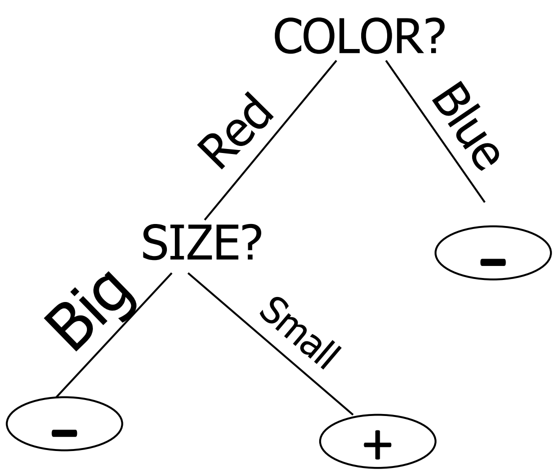
1. Choose the best feature f^* for the root of the tree.
2. Separate the training set into subsets $\{S_1, S_2, \ldots, S_k\}$ where each subset S_i contains examples that have the same value for f^*
3. Recursively apply the algorithm on each new subset until all examples have the same class label

Overview of ID3

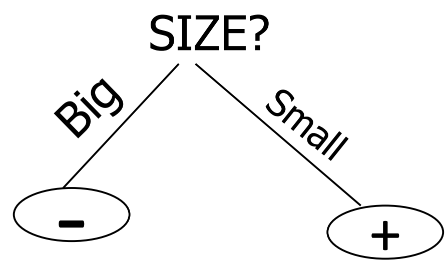


Main Hypothesis of ID3

The simplest tree that classifies training examples will work best on future examples (Occam's Razor)[1]



VS.



NP-Hard to find the smallest tree
(Hyafil +Rivest, 1976)

Some empirical evidence calls this assumption into question
(Mingers MLJ, Murphy+Pazzani JAIR)

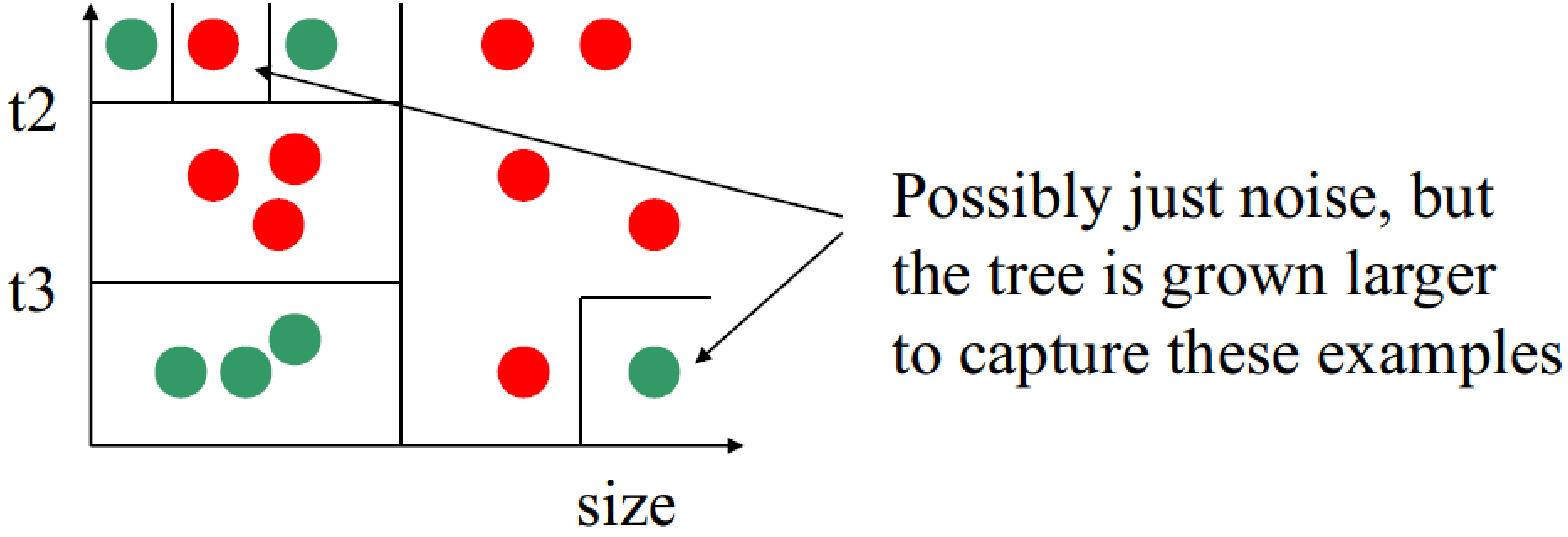
Why Occam's Razor?

(Occam lived 1285 – 1349)

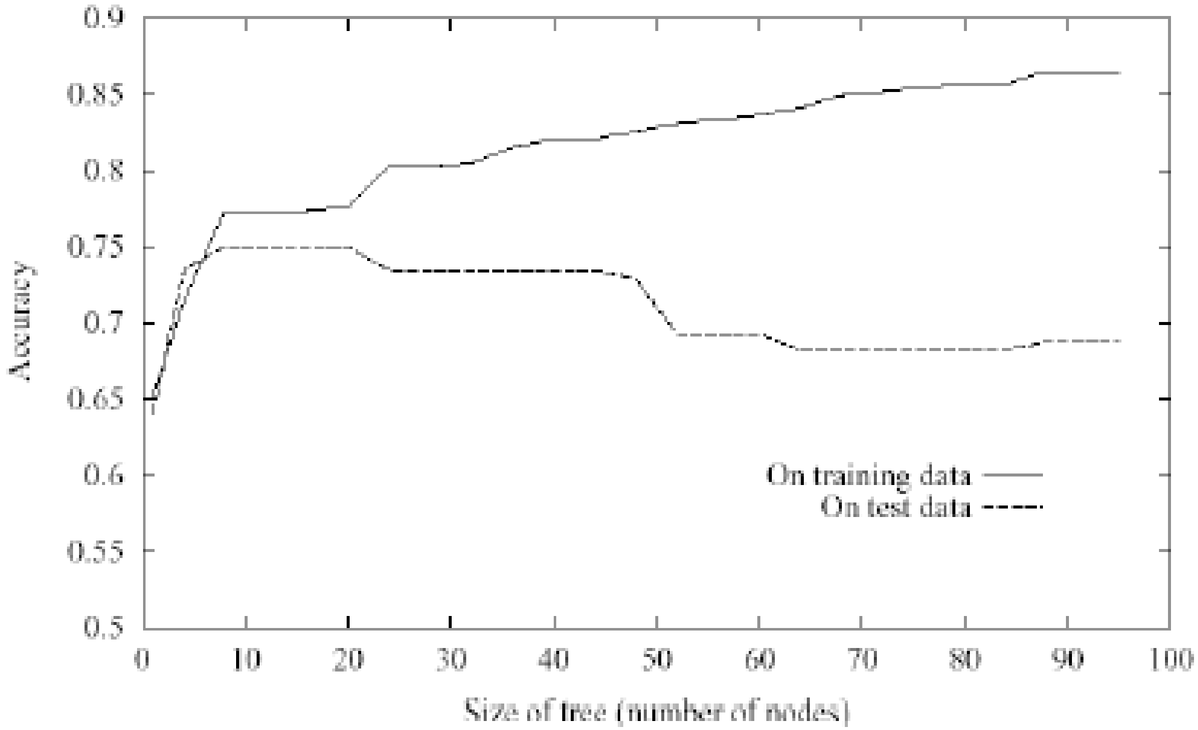
- There are fewer short hypotheses (trees in ID3) than long ones
- Short hypothesis that fits training data unlikely to be coincidence
- Long hypothesis that fits training data might be (since many more possibilities)
- COLT community formally addresses these issues (see Chapter 7 of Mitchell)
- **Arguments against**
  - There are many different ways to define small sets of hypotheses
  - E.g, All trees with a prime number of nodes that use attributes beginning with "Z"
  - What is so special about small sets based on size of hypothesis?

Over-fitting

- Decision tree has a very flexible hypothesis space
- As the nodes increase, we can represent arbitrarily complex decision boundaries – training set error is always zero
- This can lead to over-fitting

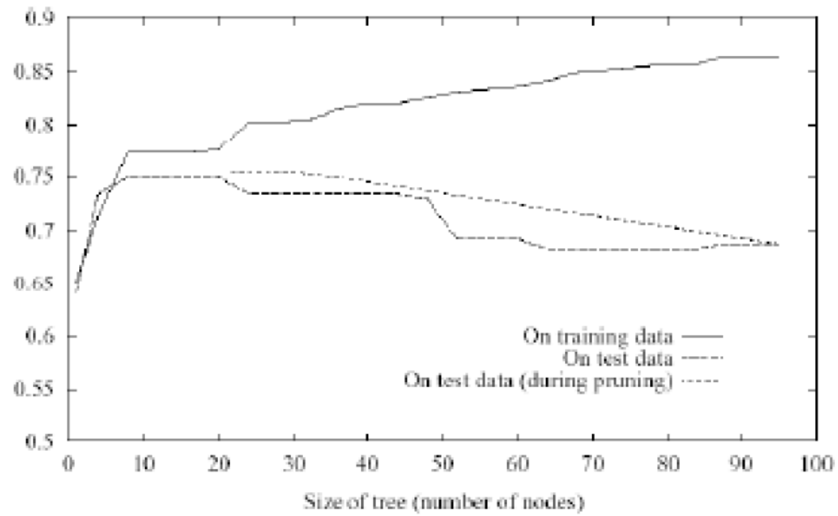


Over-fitting in Learning



Avoiding Overfitting

- Stop growing when data split is not statistically significant
- Grow a full tree, then post-prune
  - Separate training data into training set and validation set
  - Evaluate impact on validation set when a node is "pruned"
  - Greedily remove the one that improves the performance the most
  - Produces the smallest version of most accurate subtree
  - What if the data is limited?



Attributes with Costs

- Consider
  - Medical diagnosis, BloodTest costs $150
  - Robotics, Width_from_1ft has cost 23 sec
- How to learn a consistent tree with low expected cost? Find min cost tree.
- Another approach – Replace gain when you split by
- $Gain^2(S,A)/Cost(A)$ Tan and Schimmer (1990)
- $(2^{Gain(S,A)} - 1)/(Cost(A)+1)^w$ where w in [0,1] reflects the importance – Nunez (1998)

Decision Trees

- Decision Trees – Popular and a very efficient hypothesis space
  - Variable size: Any boolean function can be represented
  - Deterministic (can be extended)
  - Discrete and continuous paramters
- Constructive search: Built by adding nodes
- Eager
- Batch (now online algorithms are popular as well)

Criterion	Perceptron	Logistic	LDA	DT
Mixed data	N	N	N	Y
Missing values	N	N	Y	Y
Outliers	N	Y	N	Y
Monotone	N	N	N	Y
Scalability	Y	Y	Y	Y
Irrelevant i/p	N	N	N	Some what
Interpretable	Y	Y	Y	Y
Accurate	Y	Y	Y	N