Machine Learning (CS 567) Lecture 6

Fall 2008

Time: T-Th 5:00pm - 6:20pm
Location: GFS 118

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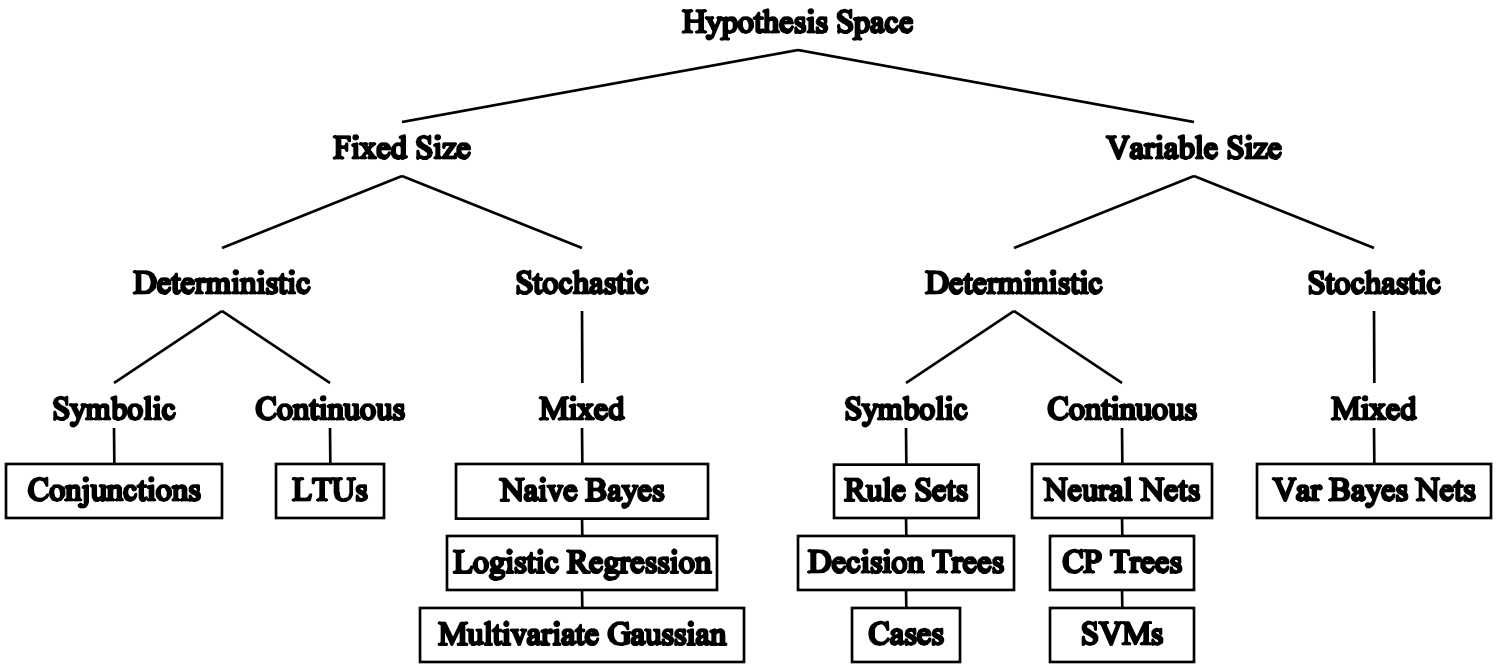
Class web page:
http://www-scf.usc.edu/~csci567/index.html

Lecture 6 Outline

- Off-the-shelf Classifiers
- Decision Trees, Part 1

Hypothesis Spaces, LTUs, etc.



This is representative and not comprehensive

Comparing Perceptron, Logistic Regression, and LDA

- How should we choose among these three algorithms?
- There is a big debate within the machine learning community!

Issues in the Debate

- Statistical Efficiency. If the generative model P(**x**,*y*) is correct, then LDA usually gives the highest accuracy, particularly when the amount of training data is small. If the model is correct, LDA requires 30% less data than Logistic Regression in theory
- Computational Efficiency. Generative models typically are the easiest to learn. In our example, LDA can be computed directly from the data without using gradient descent.

Issues in the Debate

- Robustness to changing loss functions. Both generative and conditional probability models allow the loss function to be changed at run time without re-learning. Perceptron requires re-training the classifier when the loss function changes.
- Robustness to model assumptions. The generative model usually performs poorly when the assumptions are violated. For example, if $P(\mathbf{x} \mid y)$ is very non-Gaussian, then LDA won't work well. Logistic Regression is more robust to model assumptions, and Perceptron is even more robust.
- Robustness to missing values and noise. In many applications, some of the features x_{ij} may be missing or corrupted in some of the training examples. Generative models typically provide better ways of handling this than non-generative models.

Off-The-Shelf Classifiers

- A method that can be applied directly to data without requiring a great deal of time-consuming data preprocessing or careful tuning of the learning procedure

- Let's compare Perceptron, Logistic Regression, and LDA to ask which algorithms can serve as good off-the-shelf classifiers

Off-The-Shelf Criteria

- Natural handling of "mixed" data types
  - continuous, ordered-discrete, unordered-discrete
- Handling of missing values
- Robustness to outliers in input space
- Insensitive to monotone transformations of input features
- Computational scalability for large data sets
- Ability to deal with irrelevant inputs
- Ability to extract linear combinations of features
- Interpretability
- Predictive power

Handling Mixed Data Types with Numerical Classifiers

- Indicator Variables
  - sex: Convert to 0/1 variable
  - county-of-residence: Introduce a 0/1 variable for each county
- Ordered-discrete variables
  - example: {small, medium, large}
  - Treat as unordered
  - Treat as real-valued
    - Sometimes it is possible to measure the "distance" between discrete terms. For example, how often is one value mistaken for another? These distances can then be combined via multi-dimensional scaling to assign real values

Missing Values

- Two basic causes of missing values
  - Missing at random: independent errors cause features to be missing. Examples:
    - clouds prevent satellite from seeing the ground.
    - data transmission (wireless network) is lost from time-to-time
  - Missing for cause:
    - Results of a medical test are missing because physician decided not to perform it.
    - Very large or very small values fail to be recorded
    - Human subjects refuse to answer personal questions

Dealing with Missing Values

- Missing at Random
  - P(**x**,*y*) methods can still learn a model of P(**x**), even when some features are not measured.
  - The EM algorithm can be applied to fill in the missing features with the most likely values for those features
  - A simpler approach is to replace each missing value by its average value or its most likely value
  - There are specialized methods for decision trees
- Missing for cause
  - The "first principles" approach is to model the causes of the missing data as additional hidden variables and then try to fit the combined model to the available data.
  - Another approach is to treat "missing" as a separate value for the feature
    - For discrete features, this is easy
    - For continuous features, we typically introduce an indicator feature that is 1 if the associated real-valued feature was observed and 0 if not.

Robust to Outliers in the Input Space

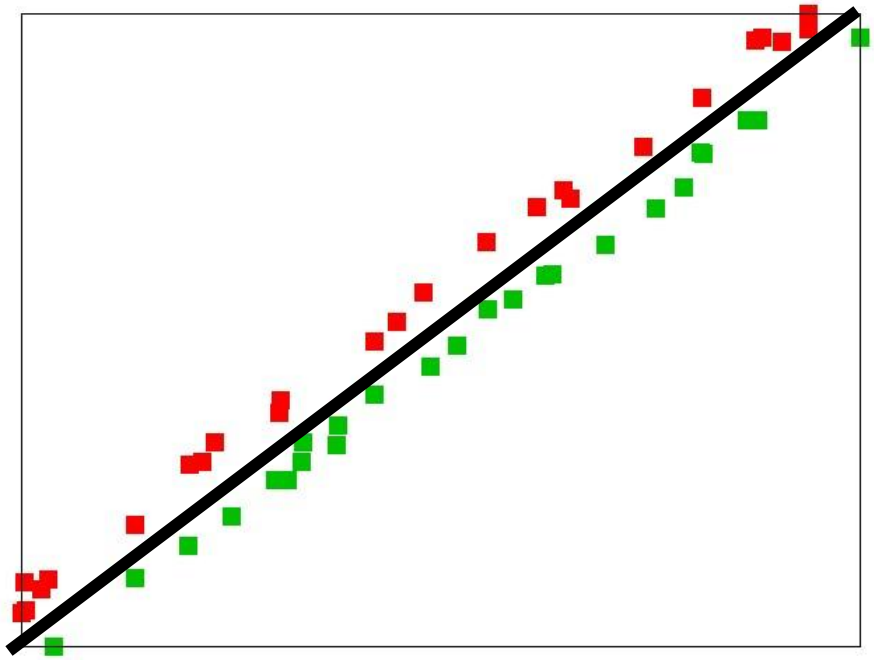
- Perceptron: Outliers can cause the algorithm to loop forever
- Logistic Regression: Outliers far from the decision boundary have little impact – robust!
- LDA/QDA: Outliers have a strong impact on the models of $P(\mathbf{x}|y)$ – not robust!

Remaining Criteria

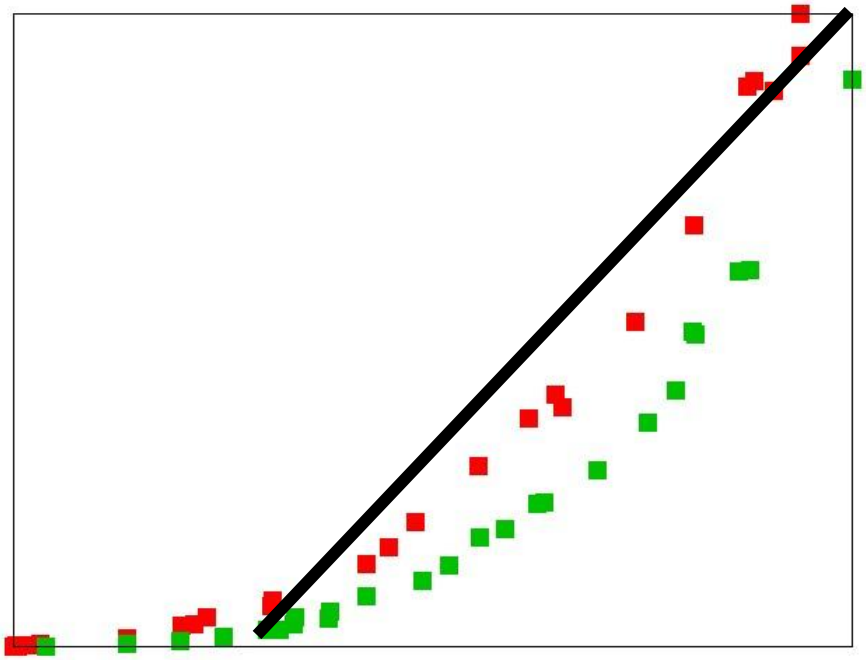
- Monotone Scaling: All linear classifiers are sensitive to non-linear transformations of the inputs, because this may make the data less linearly separable
- Computational Scaling: All three methods scale well to large data sets.
- Irrelevant Inputs: In theory, all three methods will assign smalll weights to irrelevant inputs. In practice, LDA can crash because the Σ matrix becomes singular and cannot be inverted. This can be solved through a technique known as regularization (later!)
- Extract linear combinations of features: All three algorithms learn LTUs, which are linear combinations!
- Interpretability: All three models are fairly easy to interpret
- Predictive power: For small data sets, LDA and QDA often perform best. All three methods give good results.

Sensitivity to monotone transformations

linearly separable



After $y=y^4$ transform
not linearly separable



Summary So Far
(we will add to this later)

Criterion	Perc	Logistic	LDA
Mixed data	no	no	no
Missing values	no	no	yes
Outliers	no	yes	no
Monotone transformations	no	no	no
Scalability	yes	yes	yes
Irrelevant inputs	no	no	no
Linear combinations	yes	yes	yes
Interpretable	yes	yes	yes
Accurate	yes	yes	yes

The Top Five Algorithms

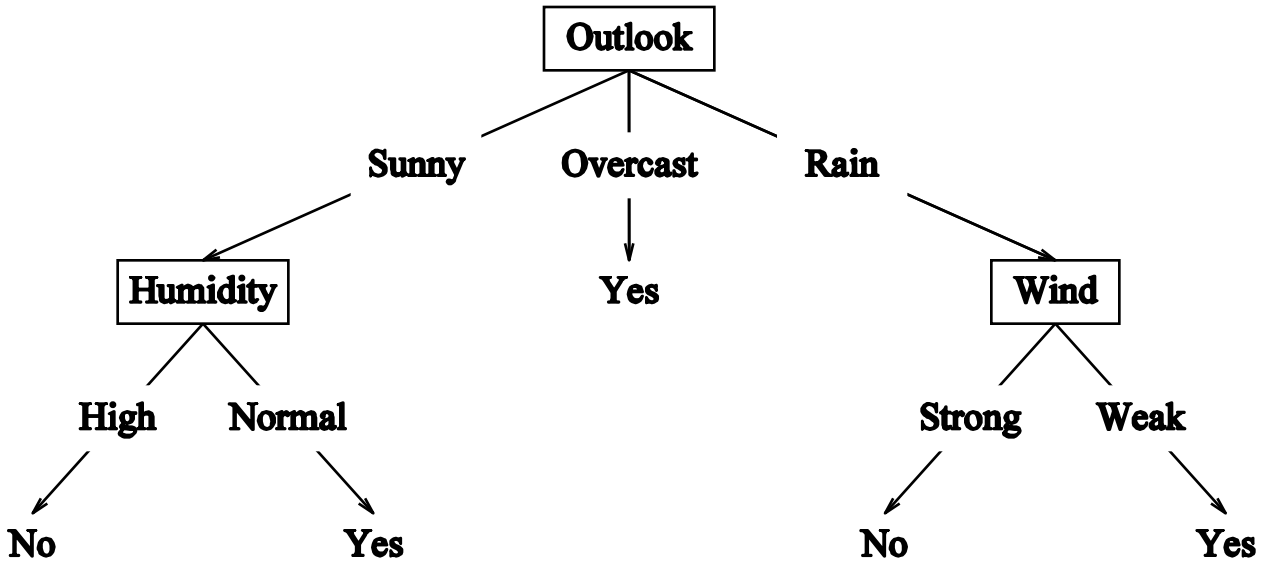
- Decision trees (C4.5)
- Nearest Neighbor Method
- Neural networks (backpropagation)
- Probabilistic networks (Naïve Bayes; Mixture models)
- Support Vector Machines (SVMs)

Learning Decision Trees

- Decision trees provide a very popular and efficient hypothesis space
  - Variable size: any boolean function can be represented
  - Deterministic
  - Discrete and Continuous Parameters
- Learning algorithms for decision trees can be described as
  - Constructive Search: The tree is built by adding nodes
  - Eager
  - Batch (although online algorithms do exist)

Decision Tree Hypothesis Space

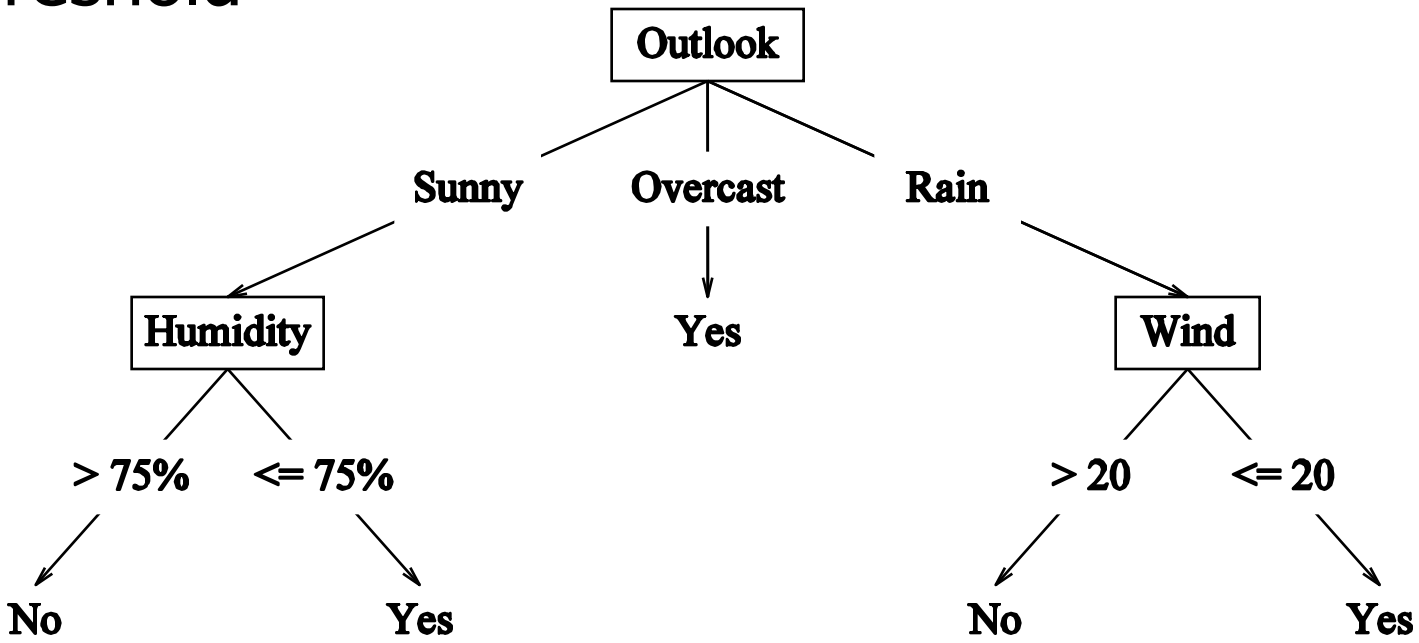
- Internal nodes: test the value of particular features x_j and branch according to the results of the test
- Leaf nodes: specify the class f(**x**)



- Features: Outlook (x_1), Temperature (x_2), Humidity (x_3), and Wind (x_4)
- **x** = (sunny, hot, high, strong) will be classified as No.

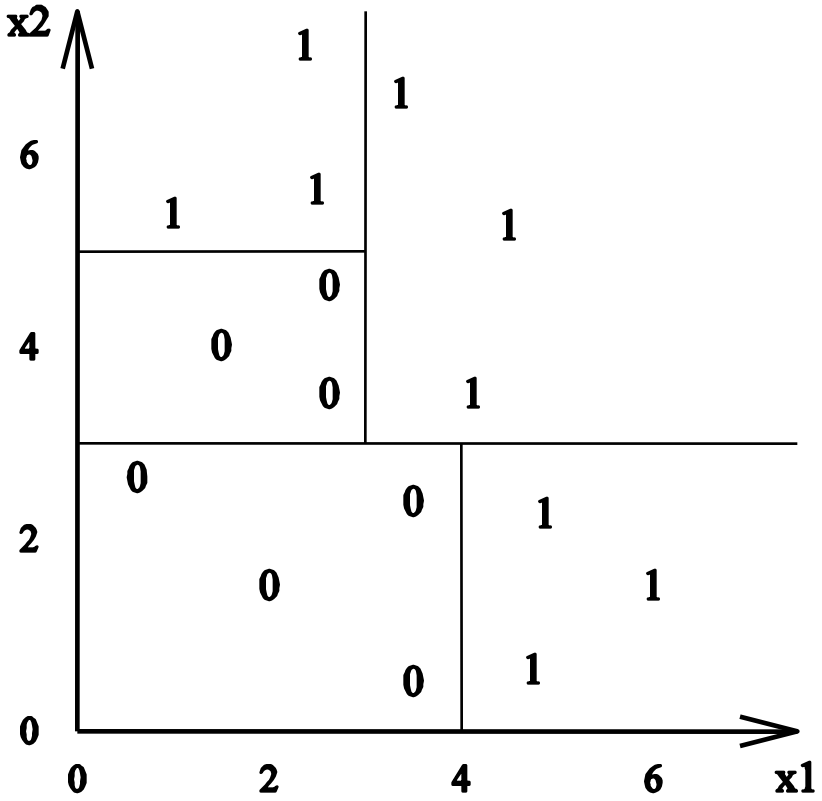
Decision Tree Hypothesis Space (2)

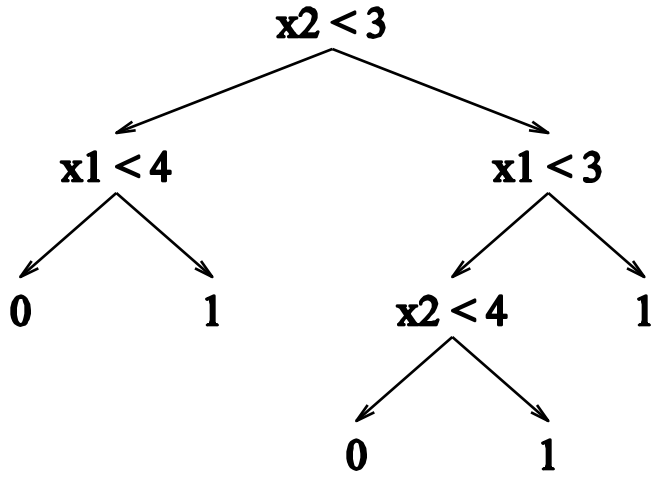
- If the features are continuous, internal nodes may test the value of a feature against a threshold



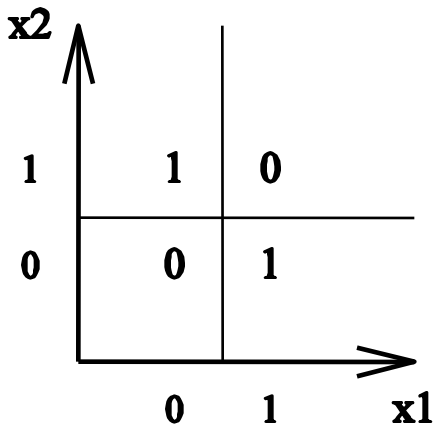
Decision Tree Decision Boundaries

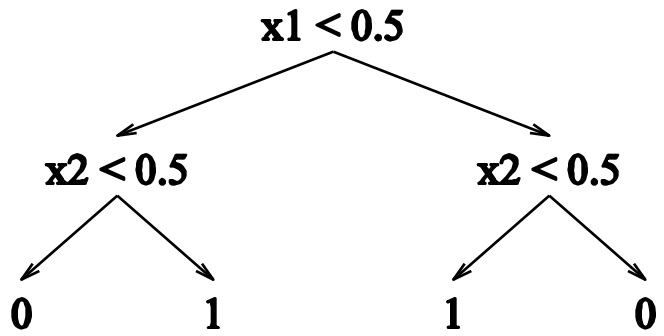
- Decision Trees divide the feature space into axis-parallel rectangles and label each rectangle with one of the K classes





Decision Trees Can Represent Any Boolean Function





- In the worst case, exponentially many nodes will be needed, however

Decision Trees Provide Variable-Sized Hypothesis Space

- As the number of nodes (or depth) of tree increases, the hypothesis space grows
  - Depth 1 ("decision stump") can represent any boolean function of one feature
  - Depth 2: Any boolean function of two features and some boolean functions involving three features:
    - $(x_1 \wedge x_2) \vee (\neg x_1 \wedge \neg x_2)$

Objective Function

- Let h be a decision tree
- Define our objective function to be the number of misclassification errors on the training data:

$$J(h) = |\{ (\mathbf{x},y) \in S : h(\mathbf{x}) \neq y \}|$$

(what is the name of this loss function?)

- Find h that minimizes $J(h)$
  - 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 smallest tree h that minimizes $J(h)$.
  - Bug 2: This is NP-Hard
  - Solution 3: Use a greedy approximation

Learning Algorithm for Decision Trees

GrowTree(S)

for $c \in \{0, 1\}$

    if ($y = c$ for all $\langle \mathbf{x}, y \rangle \in S$) return new leaf(c);

choose best attribute x_j;

for $c \in \{0, 1\}$

    $S_c :=$ all $\langle \mathbf{x}, y \rangle \in S$ with $x_j = c$;

    if ($S_c = \emptyset$) return new leaf(majority(S));

return new node(x_j, GrowTree(S_0), GrowTree(S_1));

Choosing the Best Attribute (Method 1)

- Perform 1-step lookahead search and choose the attribute that gives the lowest error rate on the training data

ChooseBestAttribute(S)

choose j to minimize J_j, computed as follows:

for $c \in \{0, 1\}$

$S_c :=$ all $\langle \mathbf{x}, y \rangle \in S$ with $x_j = c$;

$y_c :=$ the most common value of y in S_c;

$J_c :=$ number of examples $\langle \mathbf{x}, y \rangle \in S_c$ with $y \neq y_c$;

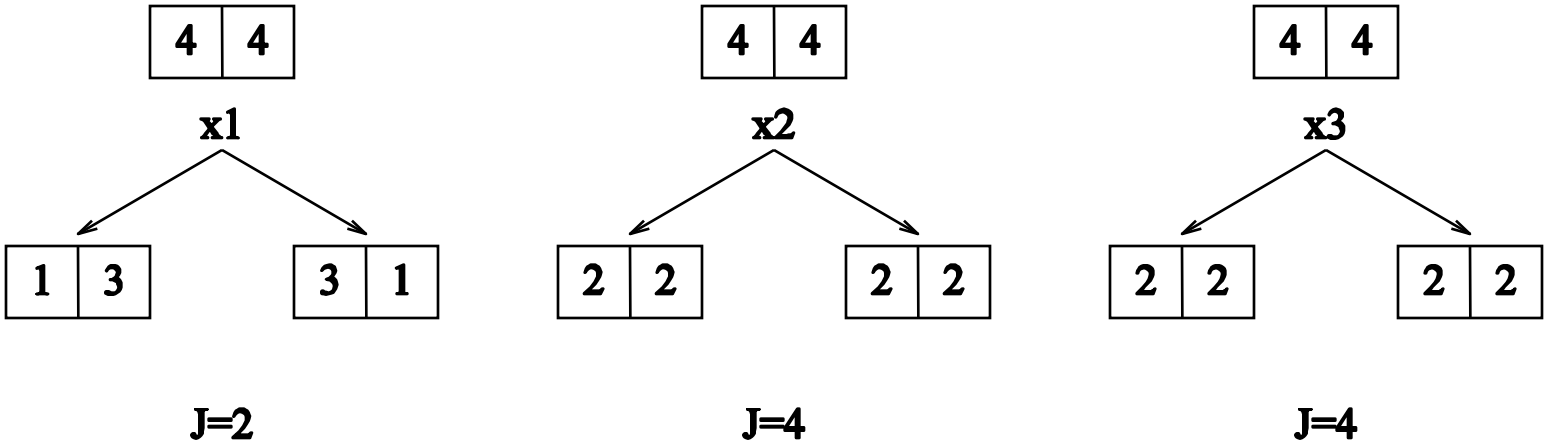
$J_j := J_0 + J_1$; (total errors if we split on this feature)

return j;

Choosing the Best Attribute
An Example

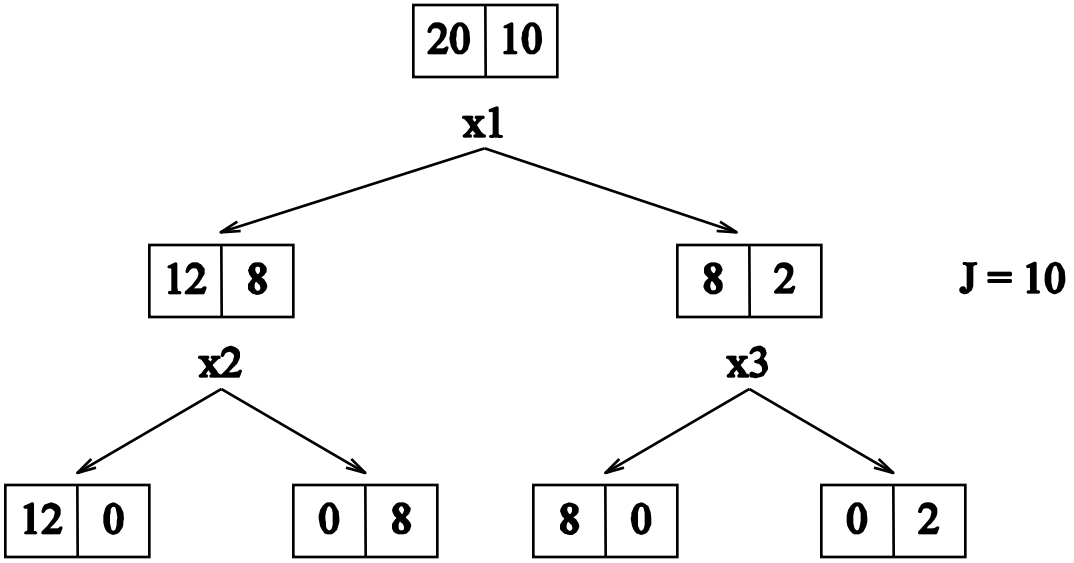
Training Examples

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



Choosing the Best Attribute (3)

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



A Better Heuristic from Information Theory

- Let V be a random variable with the following probability distribution

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

- The surprise $S(V=v)$ of each value of V is defined to be

$$S(V=v) = -\log_2 P(V = v)$$

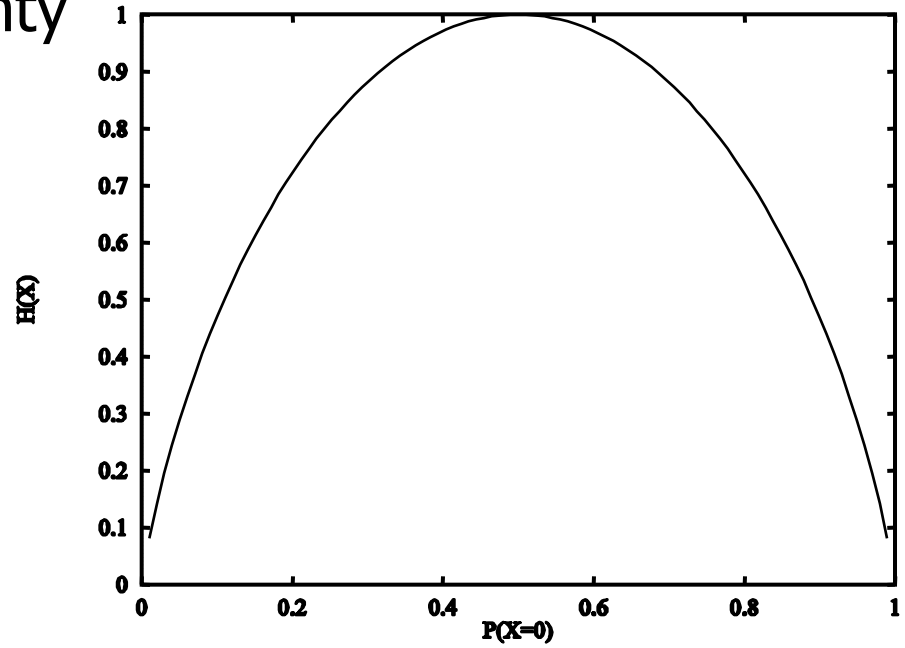
- An event with probability 1 has zero surprise
- An event with probability 0 has infinite surprise
- The surprise is equal to the asymptotic number of bits of information that need to be transmitted to a recipient who knows the probabilities of the results. Hence, this is also called the description length of V.

Entropy

- The entropy if *V*, denoted *H(V)*, is defined as

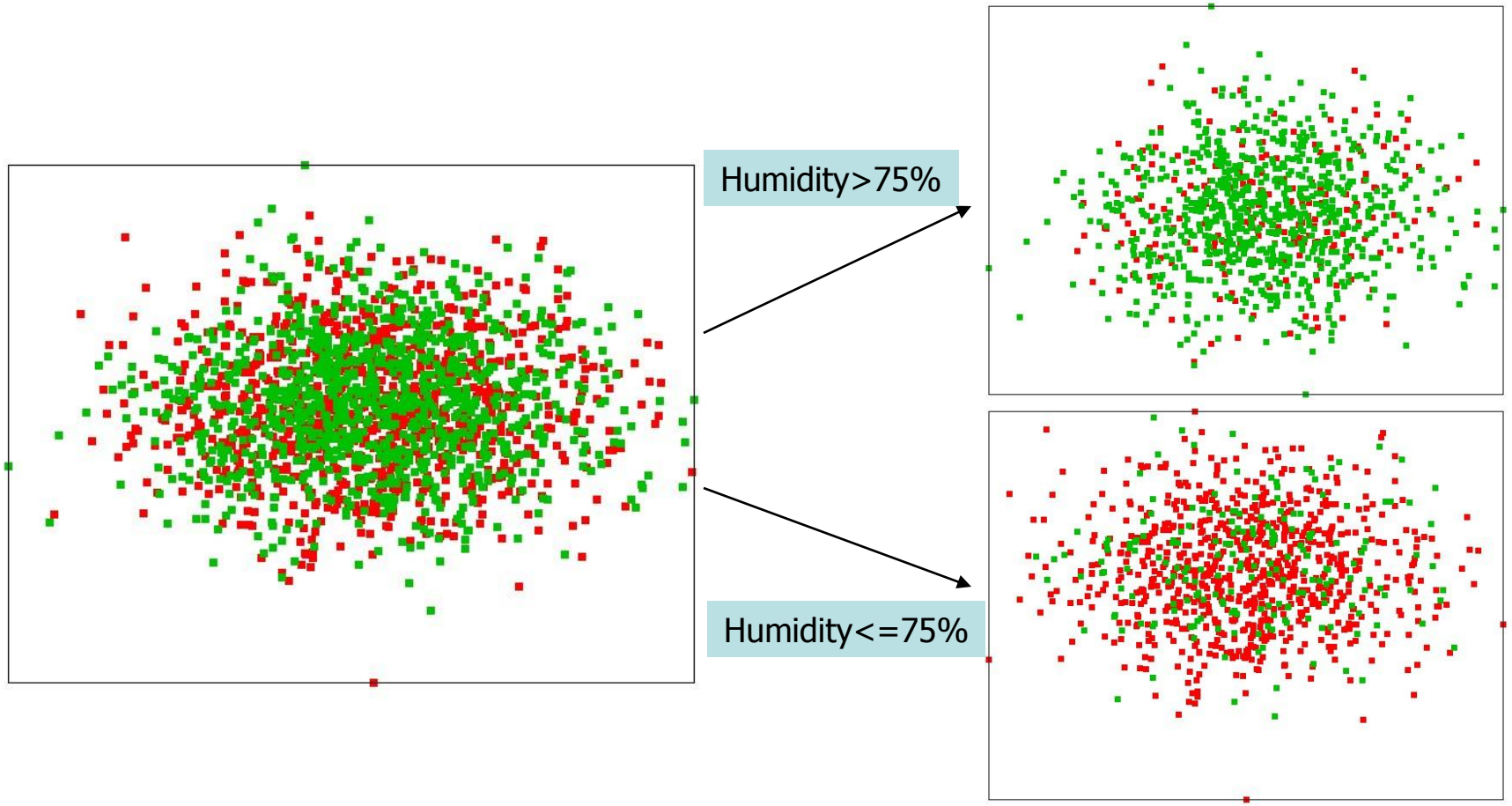
$$H(V) = \sum_{v=0}^{1} -P(V = v) log_2 P(V = v)$$

- This is the average surprise describing the result of one trial of *V* (one coin toss). It can be viewed as a measure of uncertainty



Entropy and Information Gain

- Purpose of decision-tree split is to have each subset be "cleaner" than the original data set.



Entropy and Information Gain

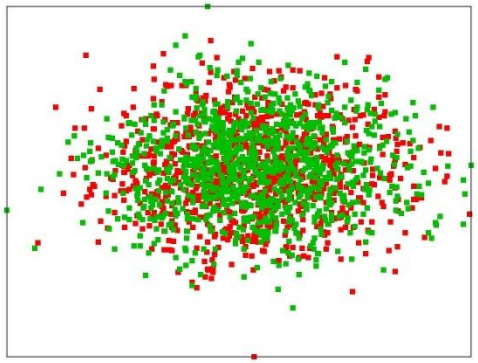
- Purpose of decision-tree split is to have each subset be "cleaner" than the original data set.
  - Entropy measures 'cleanliness' of a set of points with respect to a particular attribute (e.g. target label)
  - Take 'outlook' attribute. It has 3 possible values:

$$H(V) = -\sum_{v \in \mathbf{V}} P(V = v) log_2 P(V = v)$$

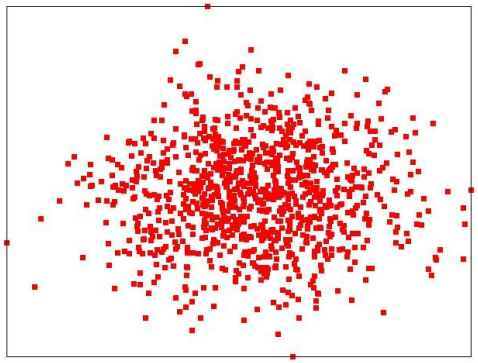
$$\begin{aligned}
p_{\text{sunny}} &= 0.1 \\
p_{\text{rain}} &= 0.2 \\
p_{\text{overcast}} &= 0.7 \\
H(\text{outlook}) &= -[p_{\text{sunny}} \cdot \log_2(p_{\text{sunny}}) + \\
&\quad p_{\text{rain}} \cdot \log_2(p_{\text{rain}}) + \\
&\quad p_{\text{overcast}} \cdot \log_2(p_{\text{overcast}})] \\
&= -[\ (.1) \cdot \log_2(.1) + (.2) \cdot \log_2(.2) + (.7) \cdot \log_2(.7)\ ] \\
&= \boxed{1.157}
\end{aligned}$$

Entropy and Information Gain

- Purpose of decision-tree split is to have each subset be "cleaner" than the original data set.
  - Entropy measures 'cleanliness' of a set of points with respect to a particular attribute (e.g. target label)
  - Maximum entropy is when all values are equally likely (boring uniform distribution).



  - Minimum entropy is when only one value is present.



Entropy and Information Gain

- Purpose of decision-tree split is to have each subset be "cleaner" than the original data set.
- If we split on 'outlook', we can measure the *specific conditional entropy* of the target label with respect to each possible value of outlook:

$$H(\text{rain}|\text{outlook} = \text{sunny})$$
$$H(\text{rain}|\text{outlook} = \text{rain})$$
$$H(\text{rain}|\text{outlook} = \text{overcast})$$

Entropy and Information Gain

- Purpose of decision-tree split is to have each subset be "cleaner" than the original data set.
- *Conditional Entropy* is the average specific conditional entropy of splitting on an attribute:

$$H(\text{target}|A) = \sum_a P(A = a) * H(\text{target}|A = a)$$

v	**P(v)**	**P(rain|outlook=v)**	**H(rain|outlook=v)**
sunny	0.1	0.1	0.469
rain	0.2	0.8	0.722
overcast	0.7	0.5	1.000

$$\begin{aligned} H(\text{rain}|\text{outlook}) &= 0.1 \cdot 0.469 + 0.2 \cdot 0.722 + 0.7 \cdot 1 \\ &= \boxed{0.893} \end{aligned}$$

Entropy and Information Gain

- Purpose of decision-tree split is to have each subset be "cleaner" than the original data set.
- *Information Gain* is how much we improve, on average, the "cleanliness" of the data by splitting on an attribute.
  - i.e., how much do we decrease the entropy

$$I(\text{target}|A) = H(\text{target}) - H(\text{target}|A)$$

$$I(\text{rain}|\text{outlook}) = H(\text{rain}) - H(\text{rain}|\text{outlook})$$

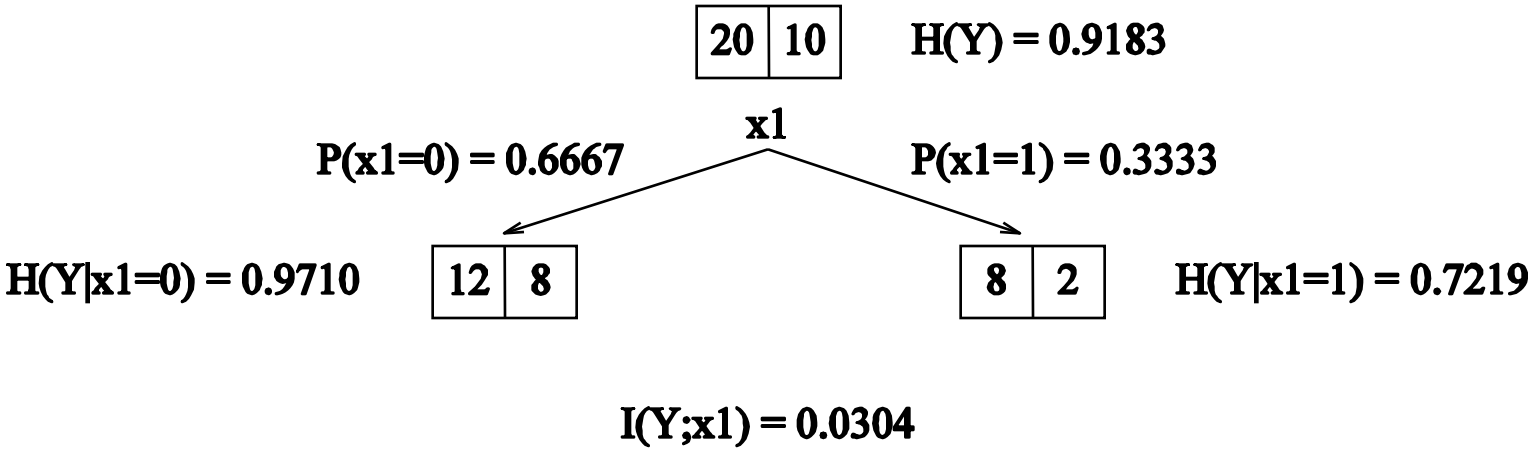
$$\begin{aligned} P(\text{rain}) &= 0.52 \\ H(\text{rain}) &= 0.999 \\ I(\text{rain}|\text{outlook}) &= 0.999 - 0.893 = \boxed{0.106} \end{aligned}$$

Mutual Information

- Consider two random variables *A* and *B* that are not necessarily independent. The mutual information between *A* and *B* is the amount of information we learn about *B* by knowing the value of *A* (and vice versa – it is symmetric). It is computed as follows:

$$I(A;B) = H(B) - \sum_a P(A=a) \cdot H(B|A=a)$$

- 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 Attribute (Method 2)

- Choose the attribute x_j that has the highest mutual information with y.

$$\begin{aligned} \operatorname{argmax}_j I(x_j; y) &= H(y) - \sum_v P(x_j = v) H(y|x_j = v) \\ &= \operatorname{argmin}_j \sum_v P(x_j = v) H(y|x_j = v) \end{aligned}$$

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

$$\tilde{J}(j) = \sum_v P(x_j = v) H(y|x_j = v)$$