

# CS540 Introduction to Artificial Intelligence

## Lecture 6

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## Decision Tree Iteration

$$g(\mathbf{w}^T \mathbf{x} + b) \geq 0 \text{ or } 1$$

$\mathbf{x} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\mathbf{x} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$

$\mathbf{x} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$

$\mathbf{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

## Decision Tree

## Random Forrest

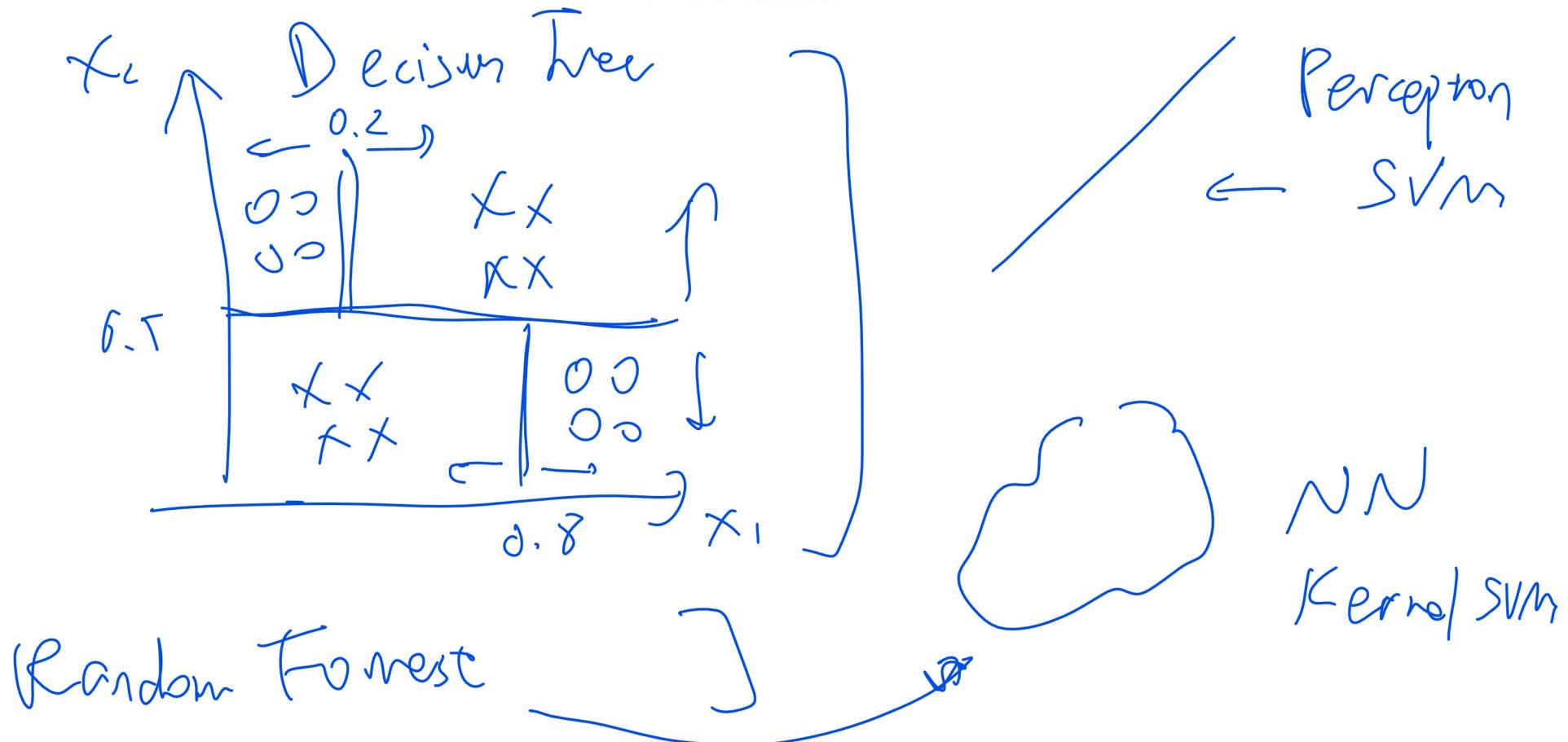
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## Nearest Neighbor

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## Axes Aligned Decision Boundary

## Motivation



# Decision Tree

## Description

- Find the feature that is the most informative.
- Split the training set into subsets according to this feature.
- Repeat on the subsets until all the labels in the subset are the same.

# Binary Entropy

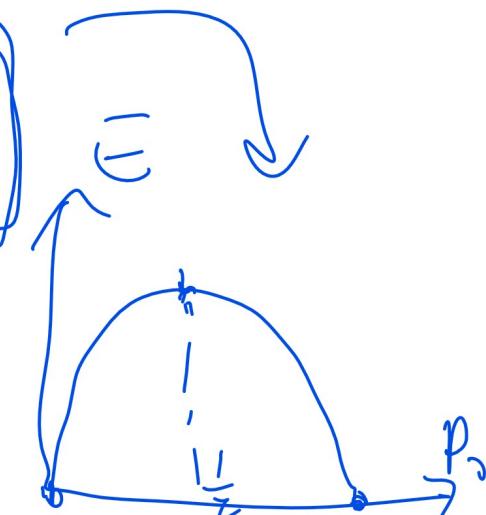
## Definition

- Entropy is the measure of uncertainty.
  - The value of something uncertain is more informative than the value of something certain.
  - For binary labels,  $y_i \in \{0, 1\}$ , suppose  $p_0$  fraction of labels are 0 and  $1 - p_0 = p_1$  fraction of the training set labels are 1, the entropy is:

$$H(Y) = p_0 \log_2 \left( \frac{1}{p_0} \right) + p_1 \log_2 \left( \frac{1}{p_1} \right)$$

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

Certain C  
most uncertain C



# Measure of Uncertainty

## Definition

- If  $p_0 = 0$  and  $p_1 = 1$ , the entropy is 0, the outcome is certain, so there is no uncertainty.
- If  $p_0 = 1$  and  $p_1 = 0$ , the entropy is 0, the outcome is also certain, so there is no uncertainty.
- If  $p_0 = \frac{1}{2}$  and  $p_1 = \frac{1}{2}$ , the entropy is the maximum 1, the outcome is the most uncertain.

# Entropy

## Definition

- If there are  $K$  classes and  $p_y$  fraction of the training set labels are in class  $y$ , with  $y \in \{1, 2, \dots, K\}$ , the entropy is:

$$H(Y) = \sum_{y=1}^K p_y \log_2 \left( \frac{1}{p_y} \right)$$

$$= - \sum_{y=1}^K p_y \underbrace{\log_2}_{\uparrow} \underbrace{(p_y)}_{\text{ }}$$

# Conditional Entropy

## Definition

- Conditional entropy is the entropy of the conditional distribution. Let  $K_X$  be the possible values of a feature  $X$  and  $K_Y$  be the possible labels  $Y$ . Define  $p_x$  as the fraction of the instances that is  $x$ , and  $p_{y|x}$  as the fraction of the labels that are  $y$  among the ones with instance  $x$ .

$$H(Y|X = x) = - \sum_{y=1}^{K_Y} p_{y|x} \log_2 (p_{y|x})$$

$$H(Y|X) = \sum_{x=1}^{K_X} p_x H(Y|X = x)$$

# Aside: Cross Entropy

## Definition

- Cross entropy measures the difference between two distributions.

$$H(Y, X) = - \sum_{z=1}^K p_{Y=z} \log_2 (p_{X=z})$$

- It is used in logistic regression to measure the difference between actual label  $Y_i$  and the predicted label  $A_i$  for instance  $i$ , and at the same time, to make the cost convex.

*min*

$$H(Y_i, A_i) = -y_i \log (a_i) - (1 - y_i) \log (1 - a_i)$$

*Uncertainty*

# Information Gain

## Definition

- The information gain is defined as the difference between the entropy and the conditional entropy.

$$I(Y|X) = H(Y) - H(Y|X).$$

- The larger than information gain, the larger the reduction in uncertainty, and the better predictor the feature is.

# Splitting Discrete Features

## Definition

- The most informative feature is the one with the largest information gain.

$$\arg \max_j I(Y|X_j)$$

- Splitting means dividing the training set into  $K_{X_j}$  subsets.

$$\{(x_i, y_i) : x_{ij} = 1\}, \{(x_i, y_i) : x_{ij} = 2\}, \dots, \{(x_i, y_i) : x_{ij} = K_{X_j}\}$$

# Splitting Continuous Features

## Definition

- Continuous features can be (arbitrarily) uniformly split into  $K_X$  categories.
- To construct binary splits, all possible splits of the continuous feature can be constructed, and the one that yields the highest information gain is used.

$$\mathbb{1}_{\{X_j \leq x_{1j}\}}, \mathbb{1}_{\{X_j \leq x_{2j}\}}, \dots, \mathbb{1}_{\{X_j \leq x_{nj}\}}$$

- One of the above binary features is used in place of the original continuous feature  $X_j$ .

# Choice of Thresholds

## Definition

- In practice, the efficient way to create the binary splits uses the midpoint between instances of different classes.
- The instances in the training set are sorted by  $X_j$ , say  $x_{(1)j}, x_{(2)j}, \dots, x_{(n)j}$ , and suppose  $x_{(i)j}$  and  $x_{(i+1)j}$  have different labels, then  $\frac{1}{2}(x_{(i)j} + x_{(i+1)j})$  is considered as a possible binary split.

$$\mathbb{1}_{\left\{X_j \leq \frac{1}{2}(x_{(i)j} + x_{(i+1)j})\right\}}$$

Decision Tree

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Random Forrest

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Nearest Neighbor

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# Splitting Continuous Variables Diagram

## Definition

# ID3 Algorithm (Iterative Dichotomiser 3), Part I

## Algorithm

- Input: instances:  $\{x_i\}_{i=1}^n$  and  $\{y_i\}_{i=1}^n$ , feature  $j$  is split into  $K_j$  categories and  $y$  has  $K$  categories
- Output: a decision tree
- Start with the complete set of instances  $\{x_i\}_{i=1}^n$ .
- Suppose the current subset of instances is  $\{x_i\}_{i \in S}$ , find the information gain from each feature.

$$I(Y|X_j) = H(Y) - H(Y|X_j)$$

# ID3 Algorithm (Iterative Dichotomiser 3), Part II

## Algorithm

$$H(Y) = - \sum_{y=1}^K \frac{\#(Y = y)}{\#(Y)} \log \left( \frac{\#(Y = y)}{\#(Y)} \right)$$

$$H(Y|X_j) = - \sum_{x=1}^{K_j} \sum_{y=1}^K \frac{\#(Y = y, X_j = x)}{\#(Y)} \log \left( \frac{\#(Y = y, X_j = x)}{\#(X_j = x)} \right)$$

- Find the more informative feature  $j^*$ .

$$j^* = \arg \max_j I(Y|X_j)$$

# ID3 Algorithm (Iterative Dichotomiser 3), Part III

## Algorithm

- Split the subset  $S$  into  $K_{j^*}$  subsets.

$$S_1 = \{(x_i, y_i) \in S : x_{ij^*} = 1\}$$

$$S_2 = \{(x_i, y_i) \in S : x_{ij^*} = 2\}$$

...

$$S_{K_{X_{j^*}}} = \left\{ (x_i, y_i) \in S : x_{ij^*} = K_{X_{j^*}} \right\}$$

- Recurse over the subsets until  $p_y = 1$  for some  $y$  on the subset.

Decision Tree

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Random Forrest

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# Pruning Diagram

## Disucssion

# Pruning

## Discussion

- Use the validation set to prune subtrees by making them a leaf. The leaf created by pruning a subtree has label equal to the majority of the training examples reaching this subtree.
- If making a subtree a leaf does not decrease the accuracy on the validation set, then the subtree is pruned.
- This is one of the simplest ways to prune a decision tree, called Reduced Error Pruning.

# Bagging

## Discussion

- Create many smaller training sets by sampling with replacement from the complete training set.
- Train different decision trees using the smaller training sets.
- Predict the label of new instances by majority vote from the decision trees.
- This is called bootstrap aggregating (bagging).

# Random Forrest

## Discussion

- When training the decision trees on the smaller training sets, only a random subset of the features are used. The decision trees are created without pruning.
- This algorithm is called random forests.

# Boosting

## Discussion

- The idea of boosting is to combine many weak decision trees, for example, decision stumps, into a strong one.
- Decision trees are trained sequentially. The instances that are classified incorrectly by previous trees are made more important for the next tree.

# Adaptive Boosting, Part I

## Discussion

- The weights  $w$  for the instances are initialized uniformly.

$$w = \left( \frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n} \right)$$

- In each iteration, a decision tree  $f_k$  is trained on the training instances weighted by  $w$ .

$$f_k = \arg \min_f \sum_{i=1}^n w_i \mathbb{1}_{\{f(x_i) \neq y_i\}}$$

$$\varepsilon_k = \min_f \sum_{i=1}^n w_i \mathbb{1}_{\{f_k(x_i) \neq y_i\}}$$

# Adaptive Boosting, Part II

## Discussion

- The weights for the tree  $f_k$  is computed.

$$\alpha_k = \log \left( \frac{1 - \varepsilon_k}{\varepsilon_k} \right)$$

- The weights are updated according to the error  $\varepsilon$  made by  $f_k$ , and normalized so that the sum is 1.

$$w_i = w_i e^{-\alpha_k (2 \cdot \mathbb{1}_{\{f_k(x_i) = y_i\}} - 1)}$$

# Adaptive Boosting, Part II

## Discussion

- The label of a new test instance  $x_i$  is the  $\alpha$  weighted majority of the labels produced by all  $K$  trees:  
 $f_1(x_i), f_2(x_i), \dots, f_K(x_i)$ .
- For example, if there are only two classes  $\{0, 1\}$ , and  $\alpha$  is normalized so that the sum is 1, then the prediction is the following.

$$\hat{y}_i = \mathbb{1} \left\{ \sum_{k=1}^K \alpha_k f_k(x_i) \geq 0.5 \right\}$$

# K Nearest Neighbor

## Description

- Given a new instance, find the  $K$  instances in the training set that are the closest.
- Predict the label of the new instance by the majority of the labels of the  $K$  instances.

# Distance Function

## Definition

- Many distance functions can be used in place of the Euclidean distance.

$$\rho(x, x') = \|x - x'\|_2 = \sqrt{\sum_{j=1}^m (x_j - x'_j)^2}$$

- An example is Manhattan distance.

$$\rho(x, x') = \sum_{j=1}^m |x_j - x'_j|$$

Decision Tree

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Random Forrest

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Nearest Neighbor

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# Manhattan Distance Diagram

## Definition

# P Norms

## Definition

- Another group of examples is the  $p$  norms.

$$\rho(x, x') = \left( \sum_{j=1}^m |x_j - x'_j|^p \right)^{\frac{1}{p}}$$

- $p = 1$  is the Manhattan distance.
- $p = 2$  is the Euclidean distance.
- $p = \infty$  is the sup distance,  $\rho(x, x') = \max_{i=1,2,\dots,m} \{|x_i - x'_i|\}$ .
- $p$  cannot be less than 1.

# K Nearest Neighbor Algorithm

- Input: instances:  $\{x_i\}_{i=1}^n$  and  $\{y_i\}_{i=1}^n$ , and a new instance  $\hat{x}$ .
- Output: new label  $\hat{y}$ .
- Order the training instances according to the distance to  $\hat{x}$ .

$$\rho(\hat{x}, x_{(i)}) \leq \rho(\hat{x}, x_{(i+1)}), i = 1, 2, \dots, n-1$$

- Assign the majority label of the closest  $k$  instances.

$$\hat{y} = \text{mode } \{y_{(1)}, y_{(2)}, \dots, y_{(k)}\}$$