CS 1675 Introduction to Machine Learning
Lecture 14

Decision trees

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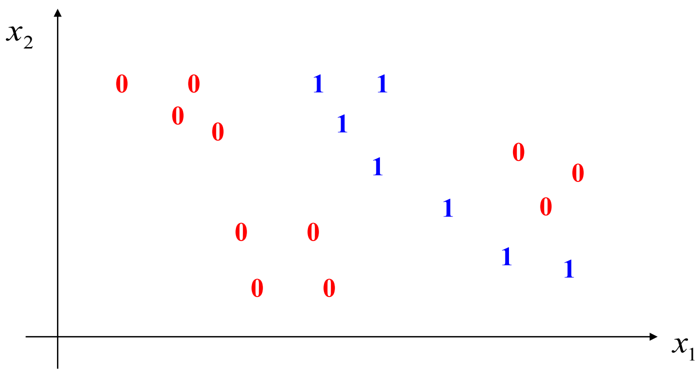
Decision tree classification

- An alternative approach to classification:
  - **Partition the input space to regions**
  - **Regress or classify independently in every region**



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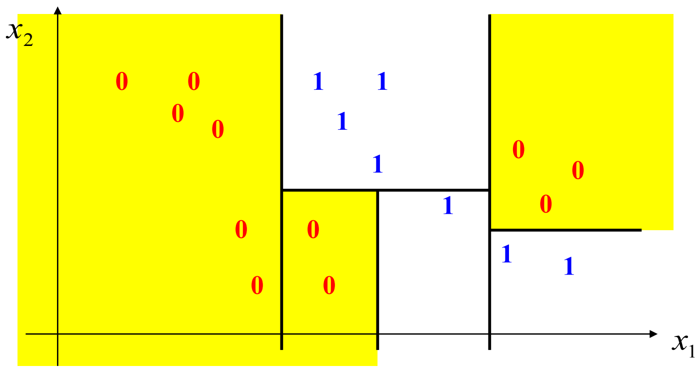


Decision tree classification

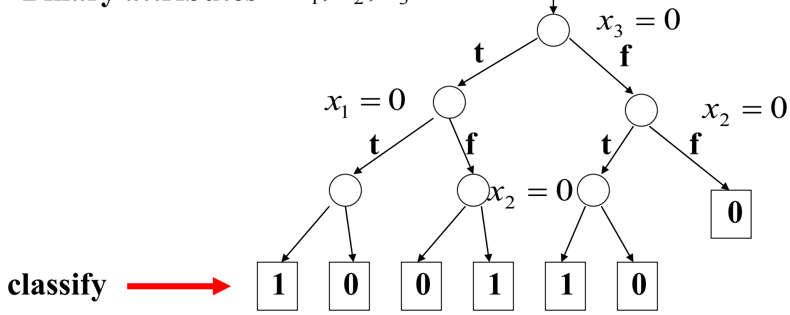
Decision tree model:

- Split recursively the input space **x** using simple conditions on x_i
- Classify at the bottom of the tree

Example:

Binary classification $\{0,1\}$

Binary attributes x_1, x_2, x_3



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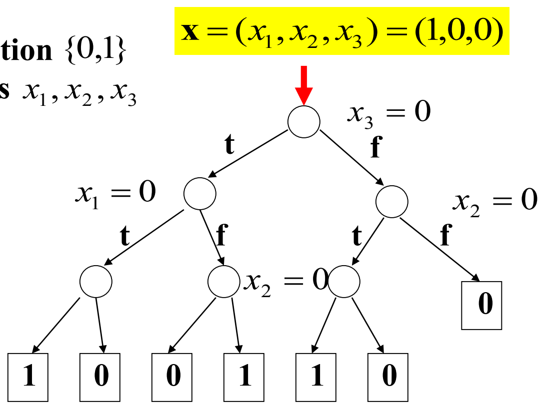

classify

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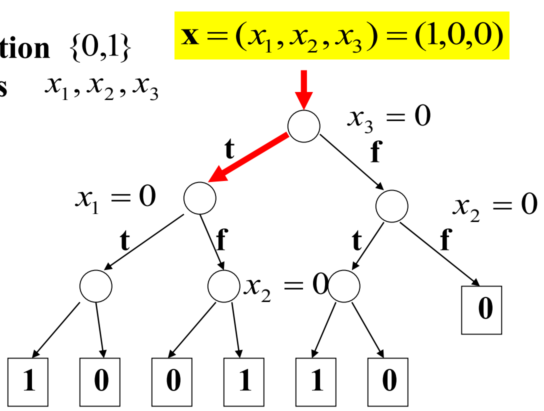

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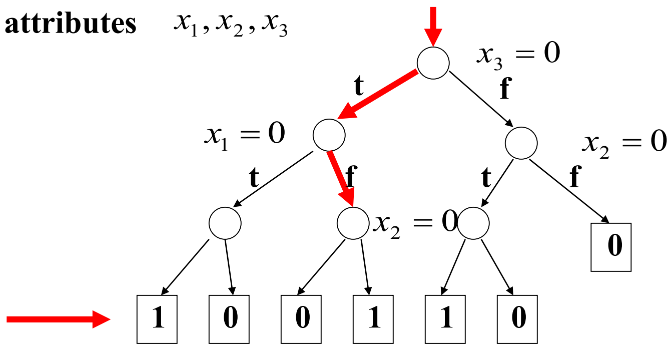
$\mathbf{x} = (x_1, x_2, x_3) = (1,0,0)$



classify

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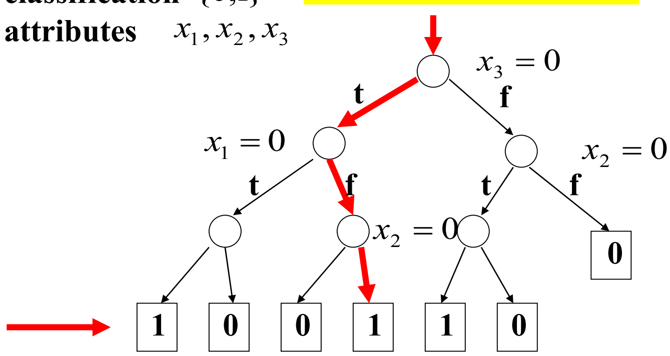
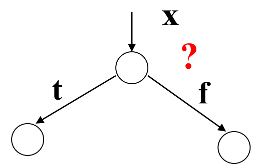


classify

Learning decision trees

How to construct /learn the decision tree?

- **Top-bottom algorithm**:
  - Find the best split condition (quantified based on the **impurity measure**)
  - Stops when no improvement possible



- **Impurity measure *I*(D)**:
  - measures the degree of mixing of the two classes in the subset of the training data D
  - Worst (maximum impurity) when # of 0s and 1s is the same
- Splits: **finite or continuous value attributes**

Continuous value attributes conditions: $x_3 \leq 0.5$

Impurity measure

Let $|D|$ **- Total number of data instances in D**

$|D_i|$ **- Number of data entries classified as *i***

$p_i = \frac{|D_i|}{|D|}$ **- ratio of instances classified as *i***

Impurity measure *I*(D)

- Measures the degree of mixing of the two classes in D
- The impurity measure should satisfy:
  - Largest when data are split evenly for attribute values

$$p_i = \frac{1}{\text{number of classes}}$$

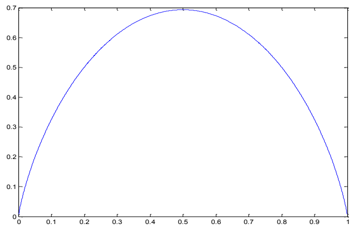
  - Should be 0 when all data belong to the same class

Impurity measures

- There are various impurity measures used in the literature
  - **Entropy based measure** **(Quinlan, C4.5)**

$$I(D) = Entropy(D) = -\sum_{i=1}^{k} p_i \log p_i$$

Example for k=2



  - **Gini measure** **(Breiman, CART)**

$$I(D) = Gini(D) = 1 - \sum_{i=1}^{k} p_i^{\,2}$$

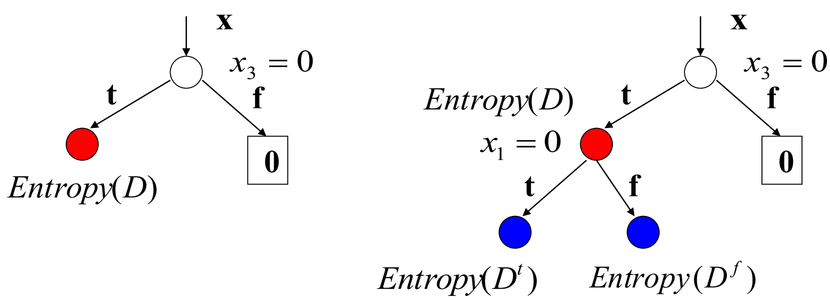
Impurity measures

- **Gain due to split** – expected reduction in the impurity measure (entropy example)

Split condition

$$Gain(D, A) = Entropy(D) - \sum_{v \in Values(A)} \frac{|D^v|}{|D|} Entropy(D^v)$$

$|D^v|$ **- a partition of *D* with the value of attribute A = *v***



Decision tree learning

- **Greedy learning algorithm:**
  - Builds the tree in the top-down fashion
  - Gradually expands the leaves of the partially built tree

Algorithm sketch:

Repeat until no or small improvement in the impurity

- Find the attribute with the highest gain
- Add the attribute to the tree and split the set accordingly

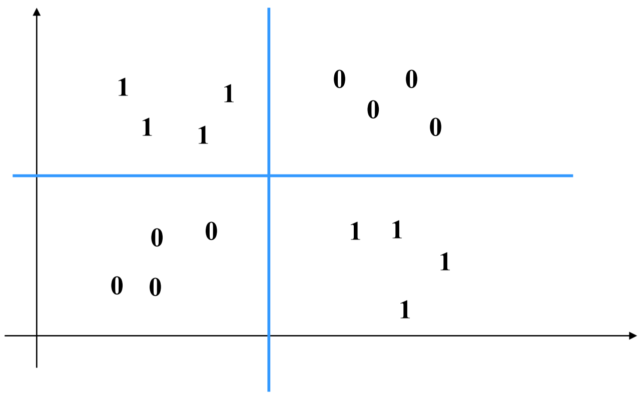
The method is greedy:

- It looks at a single attribute and gain in each step
- May fail when the combination of attributes is needed to improve the purity (parity functions)

Decision tree learning

- **Limitations of greedy methods**

  Cases in which only a combination of two or more attributes improves the impurity



Decision tree learning

By reducing the impurity measure we can grow **very large trees**

Problem: Overfitting

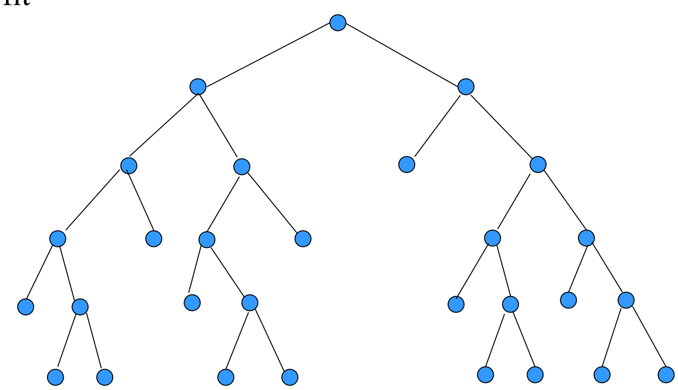
- We may split and classify very well the training set, but we may do worse in terms of the generalization error

Solutions to the overfitting problem:

- **Solution 1. Build the tree then prune the branches**
  - Build the tree, then eliminate leaves that overfit
  - Use **validation set** to test for the overfit
- **Solution 2. Prune while building the tree**
  - Test for the overfit in the tree building phase
  - Stop building the tree when performance on the **validation set** deteriorates

Decision tree learning

Backpruning: Prune branches of the tree built in the first phase in the botton-up fashion by using the validation set to test for the overfit



Decision tree learning

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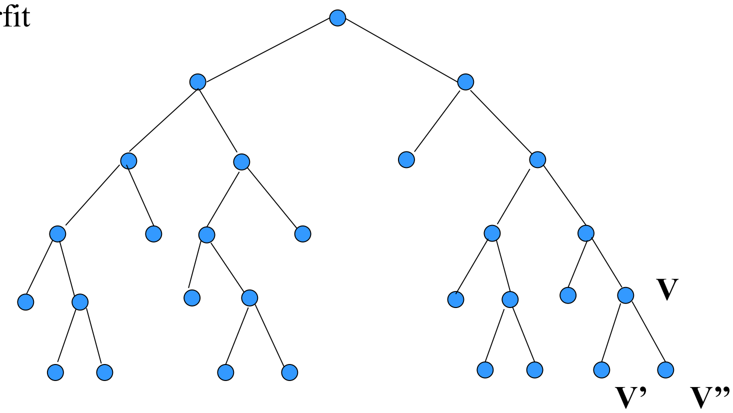

Compare: #Errors (V) vs #Error (V') + # Errors(V'')

Decision tree learning

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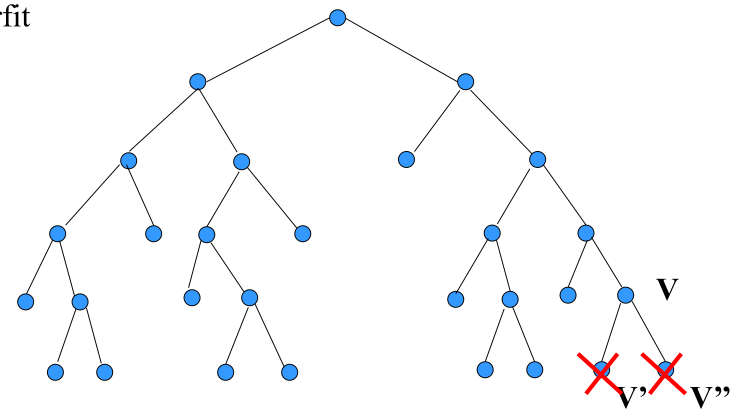

Compare: #Errors (V) < #Error (V') + # Errors(V'')

Decision tree learning

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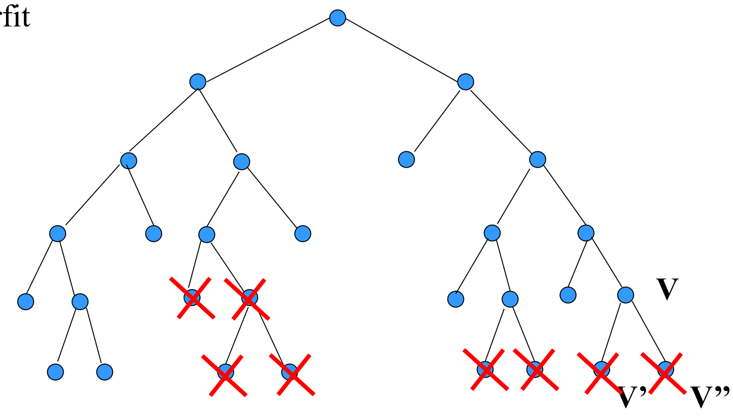


Compare: #Errors (V) < #Error (V') + # Errors(V'')

Nonparametric classification models

We have covered multiple non-parametric density estimation approaches

How can we use them in classification?

Nonparametric classification models

We have a set D of <**x**,y> pairs

We have a new data point **x** and want to assign it a class y

How ?

Algorithm 1. Generative model

Step 1: Estimate p(y=1) and p(y=0)

Step 2: Estimate p(**x** |y=1) and p(**x** |y=0) using nonparametric estimation methods and labels

Step 3: choose a class by comparing

p(**x** |y=1) p(y=1) with p(**x** |y=0) p(y=1)

Nonparametric classification models

We have a set D of <**x**,y> pairs

We have a new data point **x** and want to assign it a class y

Algorithm 2 (K nearest neighbors)

Recall:

Step 1: Find the closest K examples to x

Step 2: choose a class by considering the majority of the class labels

A special case: **the nearest neighbour algorithm**

Multiclass classification

Multiclass classification

- **Binary classification** $Y = \{0,1\}$
  - Learn: $f : X \rightarrow \{0,1\}$
- **Multiclass classification**
  - **K classes** $Y = \{0,1,\ldots,K-1\}$
  - **Goal:** learn to classify correctly K classes
  - Or **learn K discriminant functions**

$$f : X \rightarrow \{0,1,\ldots,K-1\}$$

Multiclass classification

Approaches:

- **Generative model approach**
  - Generative model of the distribution p(**x**,y)
  - Learns the parameters of the model through density estimation techniques
  - Discriminant functions are based on the model
    - "Indirect" learning of a classifier
- **Discriminative approach**
  - Parametric discriminant functions
  - Learns discriminant functions **directly**
    - A logistic regression model

Generative model approach

Indirect:

1. **Represent and learn the distribution** $p(\mathbf{x}, y)$
2. **Define and use probabilistic discriminant functions**

$$g_i(\mathbf{x}) = \log p(y = i \mid \mathbf{x})$$

Model $p(\mathbf{x}, y) = p(\mathbf{x} \mid y)p(y)$

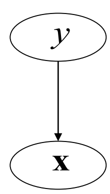
- $p(\mathbf{x} \mid y)$ = **Class-conditional distributions (densities)**

  k class-conditional distributions

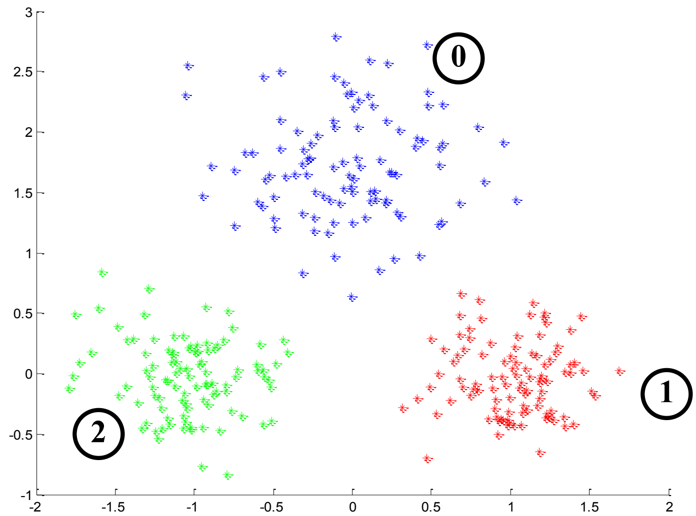
$$p(\mathbf{x} \mid y = i) \qquad \forall i \quad 0 \le i \le K - 1$$

- $p(y)$ = **Priors on classes**
- **-** probability of class y

$$\sum_{i=1}^{K-1} p(y = i) = 1$$



Multi-way classification. Example



Making class decision

Discriminant functions:

- **Posterior of a class** – choose the class with the highest posterior probability

Choice: $i = \arg\max_{i=0,\dots k-1} p(y = i \mid \mathbf{x}, \boldsymbol{\theta}_i)$

$$p(y = i \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \Theta_i) p(y = i)}{\sum_{j=0}^{k-1} p(\mathbf{x} \mid \Theta_j) p(y = j)}$$

Discriminative approach

- **Parametric model** of discriminant functions:
  - $g_0(x), g_1(x), .. g_{K-1}(x)$
- Learn the discriminant functions directly

Key issues:

- How to design the discriminant functions?
- How to train them?

Another question:

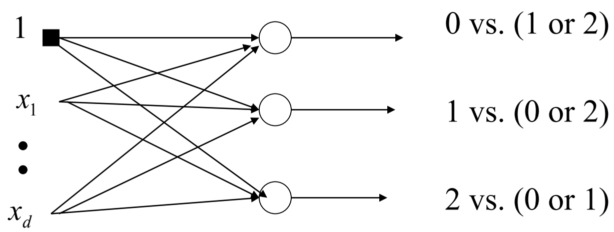
- Can we use binary classifiers to build the multi-class models?

One versus the rest (OVR)

Methods based on binary classification methods

- **Assume:** we have 3 classes labeled 0,1,2
- **Approach 1:**

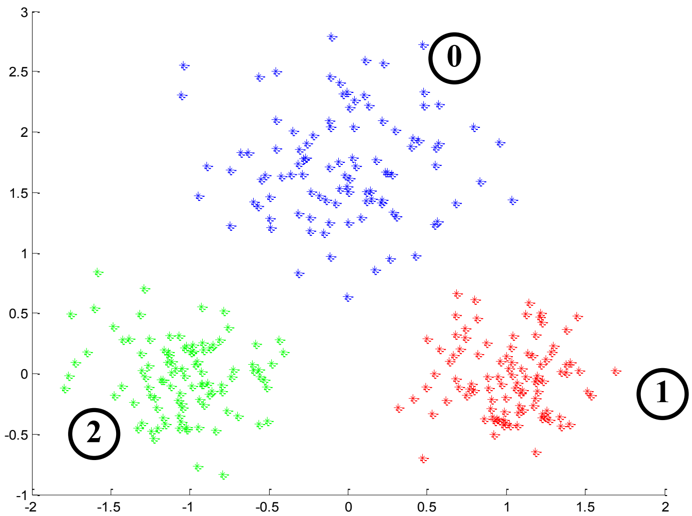
  A binary logistic regression on every class versus the rest (OvR)



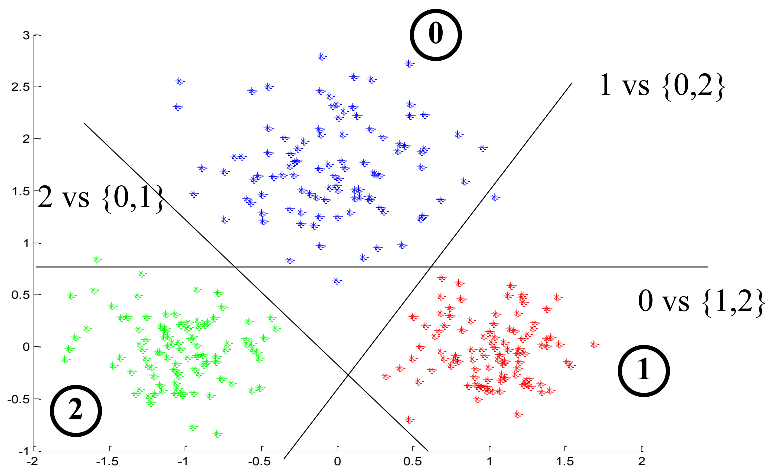
Class decision: class label for a 'singleton' class

– Does not work all the time

Multiclass classification. Example



Multiclass classification. Approach 1.



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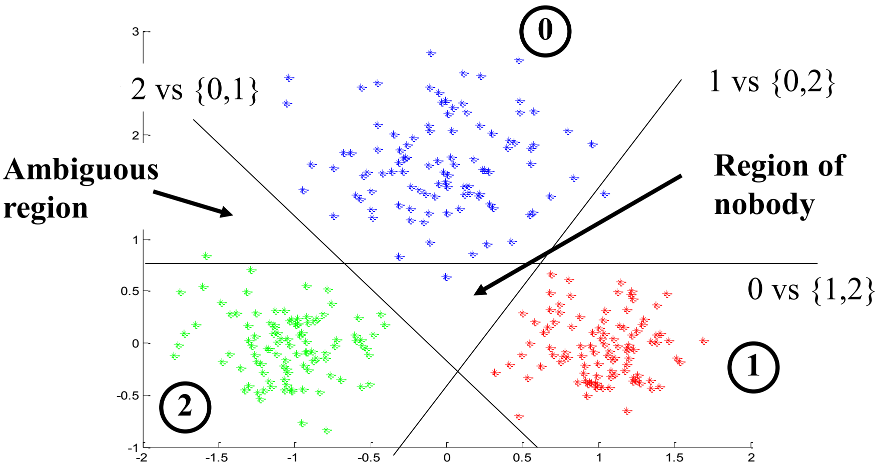


One versus the rest (OVR)

Unclear how to decide on class in some regions

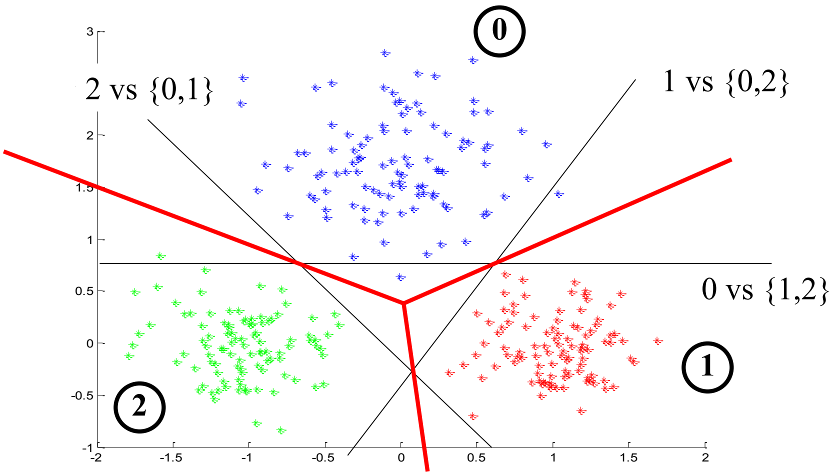
- **Ambigous region:**
  - 0 vs. (1 or 2) classifier says 0
  - 1 vs. (0 or 2) classifier says 1
- **Region of nobody:**
  - 0 vs. (1 or 2) classifier says (1 or 2)
  - 1 vs. (0 or 2) classifier says (0 or 2)
  - 2 vs (1 or 2) classifier says (1 or 2)

- **One solution:** compare discriminant functions defined on binary classifiers for single option:

  $g_i(\mathbf{x}) = g_{i \text{ vs rest}}(\mathbf{w}^T\mathbf{x})$

  – discriminant function for i trained on i vs. rest

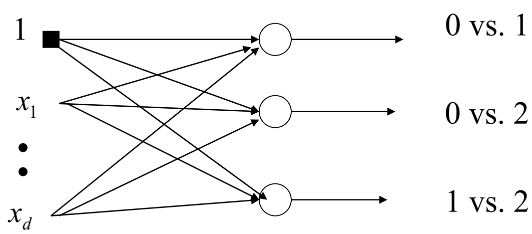
Multiclass classification. Approach 1.



One vs One (OVO)

Methods based on binary classification methods

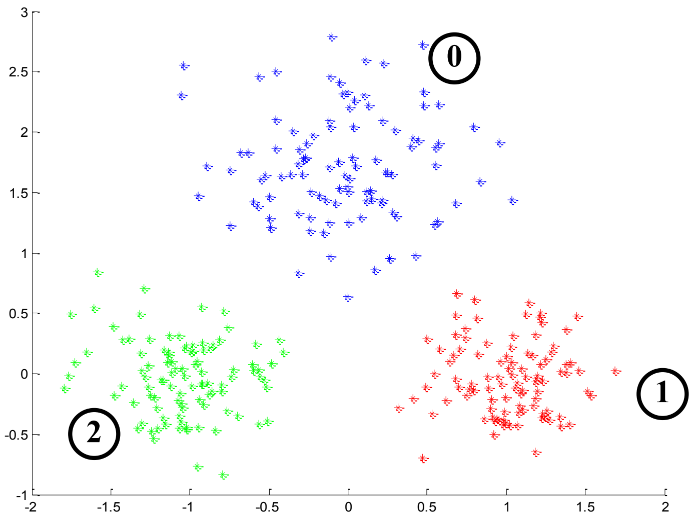
- **Assume:** we have 3 classes labeled 0,1,2
- **Approach 2:**
  - A binary logistic regression on all pairs



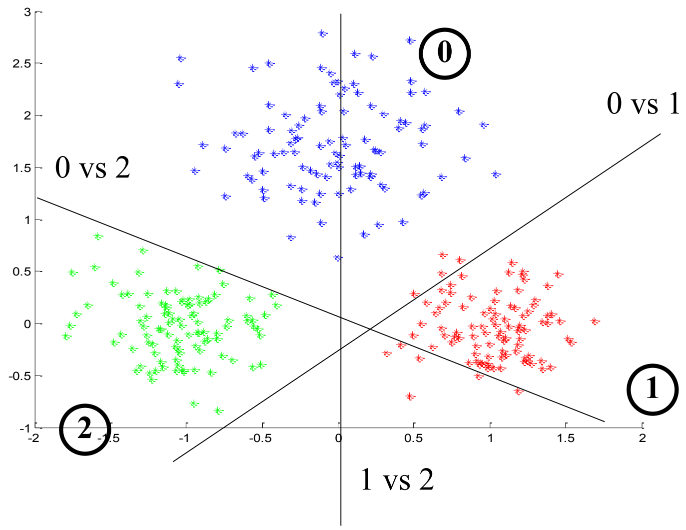
Class decision: class label based on who gets the majority

– Does not work all the time

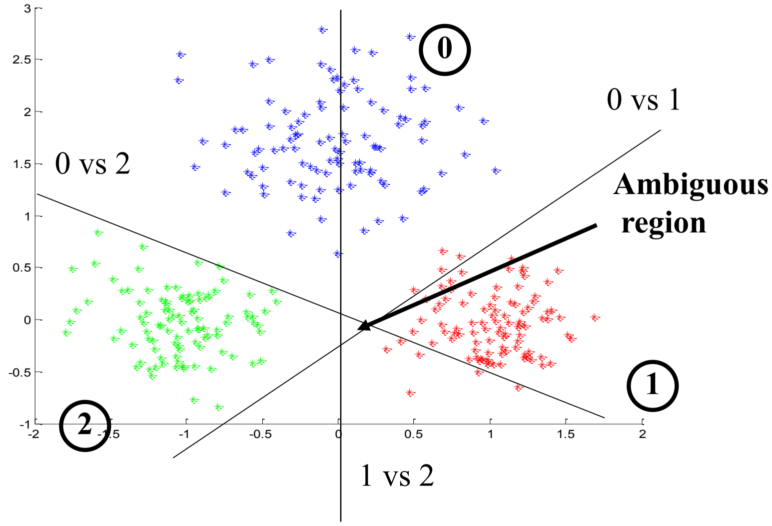
Multiclass classification. Example



Multiclass classification (OVO)



Multiclass classification OVO



One vs one (OVO) model

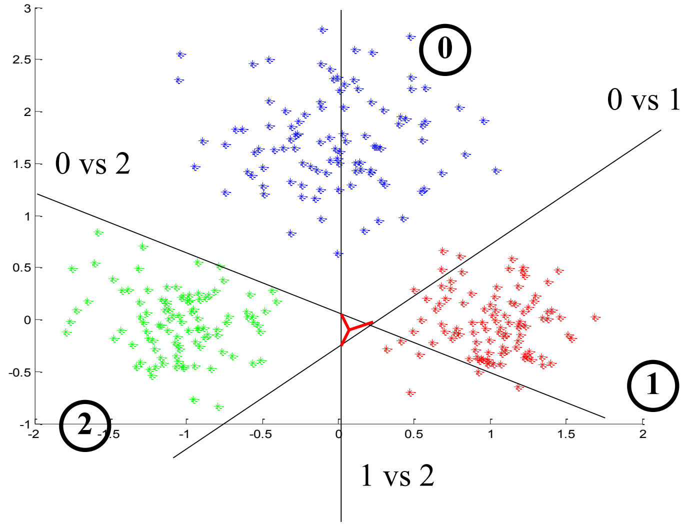
Unclear how to decide on class in some regions

- **Ambigous region:**
  - 0 vs. 1 classifier says 0
  - 1 vs. 2 classifier says 1
  - 2 vs. 0 classifier says 2

- **One solution:** define a new discriminant function by adding the discriminant functions for pairwise classifiers

  $g_i(\mathbf{x}) = \text{sum\_j}\,(\, g_{i \text{ vs } j}(\mathbf{w}^T\mathbf{x}))$

Multiclass classification.



Multiclass classification

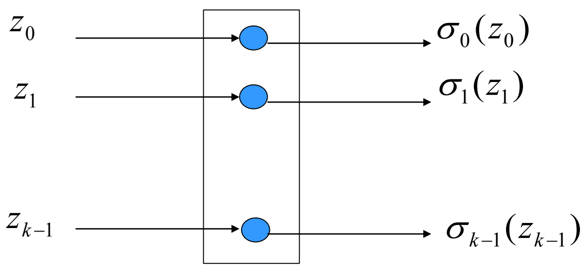
OVR and OVO:
- learn the discriminant functions for binary classification problems
- combine them to define the multiclass discriminant functions

Issues:
- calibration of the discriminant functions

Question:
- can we learn the discriminant function for the multiclass problem jointly

Softmax function

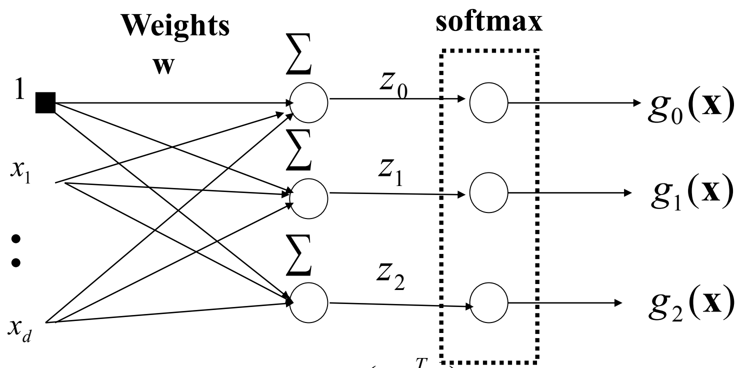
- **Multiple inputs → outputs probabilities**



$$\sigma_i(z_i) = \frac{\exp(z_i)}{\sum_{j=0}^{k-1} \exp(z_j)} \qquad \sum_{i=0}^{k-1} \sigma_i(z_i) = 1$$

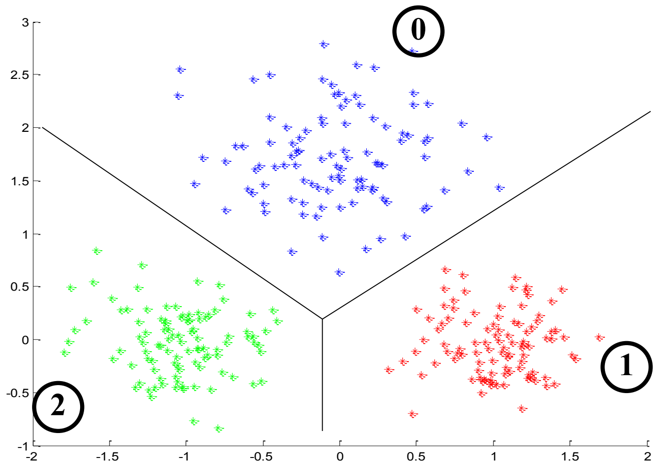
Multiclass classification with softmax

- learns the multiclass discriminant functions jointly



$$g_i(\mathbf{x}) = p(y = i \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_i^T \mathbf{x})}{\sum_{j=0}^{k-1} \exp(\mathbf{w}_j^T \mathbf{x})} \qquad \sum_i g_i(\mathbf{x}) = 1$$

Multiclass classification with softmax



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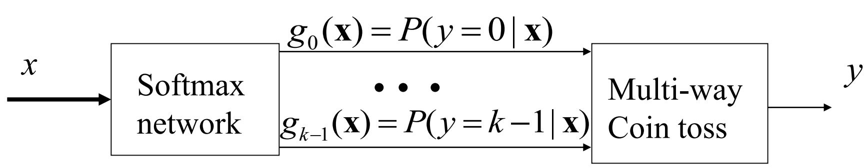
Learning of the softmax model

- Learning of parameters **w**: statistical view



Assume outputs y are transformed as follows

$$y \in \{0 \quad 1 \quad .. \quad k-1\} \quad \Rightarrow \quad y \in \left\{ \begin{pmatrix} 1 \\ 0 \\ .. \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ .. \\ 0 \end{pmatrix} \; .. \; \begin{pmatrix} 0 \\ 0 \\ .. \\ 1 \end{pmatrix} \right\}$$

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Learning of the softmax model

- Learning of the parameters **w**: statistical view
- **Likelihood of outputs**

$$L(D,\mathbf{w}) = p(\mathbf{Y} \mid \mathbf{X}, w) = \prod_{i=1,..n} p(y_i \mid \mathbf{x}_i, \mathbf{w})$$

- We want parameters **w** that maximize the likelihood
- **Log-likelihood trick**
  - Optimize log-likelihood of outputs instead:

$$l(D,\mathbf{w}) = \log \prod_{i=1,..n} p(y_i \mid \mathbf{x},\mathbf{w}) = \sum_{i=1,..n} \log p(y_i \mid \mathbf{x},\mathbf{w})$$

$$= \sum_{i=1,..n} \sum_{j=0}^{k-1} \log g_j(\mathbf{x}_i)^{y_{i,j}} = \sum_{i=1,..n} \sum_{j=0}^{k-1} y_{i,j} \log g_j(\mathbf{x}_i)$$

- **Objective to optimize** $J(D,\mathbf{w}) = -\sum_{i=1}^{n} \sum_{j=0}^{k-1} y_{i,j} \log g_j(\mathbf{x}_i)$

Learning of the softmax model

- **Error to optimize:**

$$J(D,\mathbf{w}) = -\sum_{i=1}^{n} \sum_{j=0}^{k-1} y_{i,j} \log g_j(\mathbf{x}_i)$$

- **Gradient**

$$\frac{\partial}{\partial w_{ju}} J(D\ ,\mathbf{w}) = \sum_{i=1}^{n} -x_{i,u}(y_{i,j} - g_j(\mathbf{x}_i))$$

- The same very easy **gradient update** as used for the binary logistic regression

$$\mathbf{w}_j \leftarrow \mathbf{w}_j + \alpha \sum_{i=1}^{n} (y_{i,j} - g_j(\mathbf{x}_i))\mathbf{x}_i$$

- We have to update the weights of k networks