Multiclass classification
+ Decision trees

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Multiclass classification

- **Binary classification:**
  - Number of classes = 2
  - A special case of multiclass classification

- **Multiclass classification**
  - Number of classes is > 2

**Discriminative approach**
- Parametric discriminant functions $g_i(x, w)$
- Learns discriminant functions for each class $i$ **directly** using a loss function
  - A logistic regression model

**Generative model approach**
- Generative model of the distribution $p(x, y) = p(x|y).p(y)$
- Learns the parameters $\Theta$ of the models $p(x|y)$ and $p(y)$ using the density estimation techniques
- Discriminant functions are based on the model
  \[ g_i(x, \Theta) = p(y = i | x, \Theta) \]

\[ y^* = \text{arg max}_i \ g_i(x) \]
Generative model approach

Indirect:
1. Represent and learn the distribution \( p(x, y) \)
2. Define and use probabilistic discriminant functions \( g_i(x) = \log p(y = i | x) \)

Model \( p(x, y) = p(x | y) p(y) \)
- \( p(x | y) = \text{Class-conditional distributions (densities)} \)
  k class-conditional distributions
  \( p(x | y = i) \quad \forall i \quad 0 \leq i \leq K - 1 \)
- \( p(y) = \text{Priors on classes} \)
- \( \text{- probability of class } y \)
  \( \sum_{i=1}^{K-1} p(y = i) = 1 \)

Multi-way classification. Example
Making class decision

**Discriminant functions:**

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

\[
\text{Choice: } i = \arg \max_{i=0,...,k-1} p(y = i \mid x, \Theta_i)
\]

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

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**Discriminative approach**

- **Parametric model** of discriminant functions:
  - \(g_0(x), g_1(x), \ldots g_{K-1}(x)\)
- 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.

0 vs \{1,2\}

1 vs \{0,2\}

2 vs \{0,1\}

0 vs \{1,2\}

Ambiguous region

Region of nobody
One versus the rest (OVR)

Unclear how to decide on class in some regions

- **Ambiguous 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:
  \[ g_i(x) = g_{i \text{ vs rest}}(w^Tx) \]
  - 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

  \[
  1 \quad 0 \text{ vs. } 1
  \]

  \[
  x_1 \quad 0 \text{ vs. } 2
  \]

  \[
  \vdots
  \]

  \[
  x_d \quad 1 \text{ vs. } 2
  \]

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

CS 2750 Machine Learning
One vs one (OVO) model

Unclear how to decide on class in some regions

- Ambiguous 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

\[ g_i(x) = \sum_j (g_{i \text{ vs } j}(w^T x)) \]
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

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**Softmax function**

- **Multiple inputs → outputs probabilities**

\[
\sigma_i(z_i) = \frac{\exp(z_i)}{\sum_{j=0}^{k-1} \exp(z_j)}
\]

\[
\sum_{i=0}^{k-1} \sigma_i(z_i) = 1
\]
Multiclass classification with softmax

- Multiclass discriminant functions (they are related via softmax)

\[ g_i(x) = p(y = i | x) = \frac{\exp(w_i^T x)}{\sum_{j=0}^{k-1} \exp(w_j^T x)} \]

\[ \sum_{i} g_i(x) = 1 \]
Learning of the softmax model

• Learning of parameters \( \mathbf{w} \): statistical view

\[
\begin{align*}
g_0(x) &= P(y = 0 \mid x) \\
g_{k-1}(x) &= P(y = k - 1 \mid x)
\end{align*}
\]

Assume outputs \( y \) are transformed to one hot vectors:

\[
y \in \{ 0, 1, \ldots, k-1 \} \quad \rightarrow \quad y \in \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}
\]

Learning of the softmax model

• Learning of the parameters \( \mathbf{w} \): statistical view

• Likelihood of outputs

\[
L(D, \mathbf{w}) = p(Y \mid X, \mathbf{w}) = \prod_{i=1}^{n} p(y_i \mid x_i, \mathbf{w})
\]

• We want parameters \( \mathbf{w} \) that maximize the likelihood

• Log-likelihood trick

  – Optimize log-likelihood of outputs instead:

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

\[
= \sum_{i=1}^{n} \sum_{j=0}^{k-1} \log g_j(x_i)^{y_{i,j}} = \sum_{i=1}^{n} \sum_{j=0}^{k-1} y_{i,j} \log g_j(x_i)
\]

• Corresponding error (negative log likelihood)

\[
J(D, \mathbf{w}) = -\sum_{i=1}^{n} \sum_{j=0}^{k-1} y_{i,j} \log g_j(x_i)
\]
Learning of the softmax model

• Error to optimize:

\[ J(D, w) = -\sum_{i=1}^{n} \sum_{j=0}^{k-1} y_{i,j} \log g_j(x_i) \]

• Gradient

\[ \frac{\partial}{\partial w_{ju}} J(D, w) = \sum_{i=1}^{n} x_{i,u} (y_{i,j} - g_j(x_i)) \]

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

\[ w_j \leftarrow w_j + \alpha \sum_{i=1}^{n} (y_{i,j} - g_j(x_i))x_i \]

• We have to update the weights of k networks

Decision trees
Decision tree classification

• An alternative approach to classification:
  – Partition the input space to regions
  – Regress or classify independently in every region
Decision tree classification

**Decision tree model:**
- Split recursively the input space \( \mathbf{x} \) using simple conditions on \( x_i \)
- Classify at the bottom of the tree

**Example:**
- Binary classification \( \{0,1\} \)
- Binary attributes \( x_1, x_2, x_3 \)

```
\begin{array}{c}
\text{classify} \\
1 & 0 & 0 & 1 & 1 & 0
\end{array}
```

Decision trees

**Decision tree model:**
- Split recursively the input space \( \mathbf{x} \) using simple conditions on \( x_i \)
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**Example:**
- Binary classification \( \{0,1\} \)
- Binary attributes \( x_1, x_2, x_3 \)

```
\begin{array}{c}
\text{classify} \\
1 & 0 & 0 & 1 & 1 & 0
\end{array}
```

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

Decision tree model:
• Split recursively the input space \( \mathbf{x} \) using simple conditions on \( x_i \)
• Classify at the bottom of the tree

Example:
Binary classification \{0,1\} \( x = (x_1, x_2, x_3) = (1,0,0) \)
Binary attributes \( x_1, x_2, x_3 \)

\[
\begin{array}{cccc}
\text{classify} & 1 & 0 & 0 & 1 & 1 & 0 \\
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**Decision trees**

**Decision tree model:**
- Split recursively the input space $\mathbf{x}$ using simple conditions on $x_i$
- Classify at the bottom of the tree

**Example:**
- Binary classification $\{0,1\}$
- Binary attributes $x_1, x_2, x_3$

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)
    \[ I(D) = \text{Entropy}(D) = -\sum_{i=1}^{k} p_i \log p_i \]
    *Example for k=2*

  - **Gini measure** (Breiman, CART)
    \[ I(D) = \text{Gini}(D) = 1 - \sum_{i=1}^{k} p_i^2 \]
**Impurity measures**

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

  **Split condition**

  \[
  \text{Gain}(D, A) = \text{Entropy}(D) - \sum_{v \in \text{Value}(A)} \frac{|D^v|}{|D|} \text{Entropy}(D^v)
  \]

  where \(D^v\) is 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 example](image)

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 bottom-up fashion by using the validation set to test for the overfit.

**Compare:** \#Errors (V) vs \#Error (V') + \# Errors(V'')
Decision tree learning

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

\[
\text{Compare: } \#\text{Errors (V)} < \#\text{Error (V')} + \#\text{Errors(V'')}
\]