*** Applied Machine Learning Fundamentals ***
Logistic Regression

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Find all slides on GitHub (DaWe1992/Applied_ML_Fundamentals)

Lecture Overview

Agenda for this Unit

1. Introduction
2. Model Architecture
3. Non-linear Data
4. Multi-Class Classification
5. Wrap-Up

Section:
Introduction

- What is logistic Regression?
- Why you should not use linear Regression

What is logistic Regression?

- Logistic regression is a learning algorithm for classification (!!!)
- In its standard form it is applicable to **binary classification problems only**
- **Class labels:**
  - The 'positive class' $\oplus$ is encoded as **1**
  - The 'negative class' $\ominus$ as **0**
- **Probabilistic interpretation:** The raw output of the algorithm is between 0 and 1 and can be interpreted as *the probability of the instance belonging to the positive class*

Why you should not use linear Regression...

- Linear regression:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{\theta}^{\intercal}\boldsymbol{x}$$

- We can turn linear regression into a classifier by putting a **threshold** at $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0.5$ (or any other value between 0 and 1)
  - If $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geqslant 0.5$, predict $y = 1$
  - If $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$, predict $y = 0$
- **Problems:**
  1. **Outliers heavily affect the decision boundary** (see example below)
  2. Furthermore, we only want $0 \leqslant h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leqslant 1$; Linear regression can output values $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \ll 0$ or $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \gg 1$

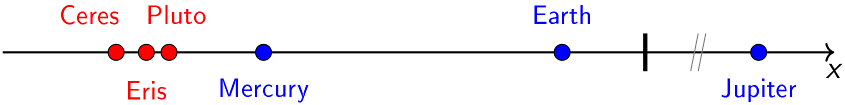
Why you should not use linear Regression... (Ctd.)

Consider the following dataset:

Row	Object	Radius ($\times 10^6$ m)	Label	Label encoded
1	Ceres	1.0	dwarf planet	0
2	Eris	2.3	dwarf planet	0
3	Pluto	2.4	dwarf planet	0
4	Mercury	4.9	planet	1
5	Earth	12.8	planet	1
6	Jupiter	143.0	planet	1

Why you should not use linear Regression... (Ctd.)

- Let us train a linear regression model for classification:



- Both, Mercury and Earth, are classified as dwarf planets due to Jupiter's massive radius!

Linear regression is sensitive to outliers! We need a better cost function!

Why you should not use linear Regression... (Ctd.)

- Logistic regression to the rescue:

- Logistic regression is less sensitive to outliers

(It is a valuable exercise to reproduce this result. See the exercise sheet!)

Section:

Model Architecture

Sigmoid Function
Probabilistic Interpretation
Model Training
Decision Boundary

Logistic Regression Model

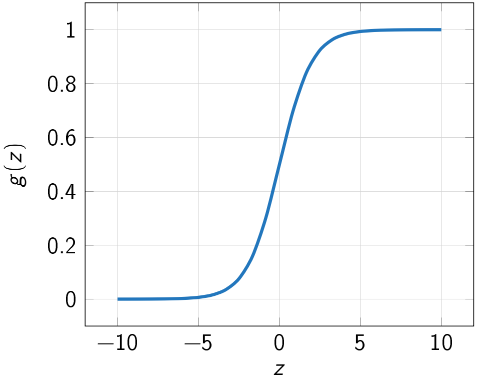
- Remember that we want: $0 \leqslant h_{\theta}(x) \leqslant 1$
- **Solution:** Logistic function / Sigmoid function:

$$g(z) := \frac{1}{1 + e^{-z}} \tag{1}$$

- We plug $\boldsymbol{\theta}^{\intercal}\boldsymbol{x}$ into the sigmoid function to obtain our new model function:

$$h_{\theta}(x) := g(\boldsymbol{\theta}^{\intercal}\boldsymbol{x}) = \frac{1}{1 + e^{-(\boldsymbol{\theta}^{\intercal}\boldsymbol{x})}} \tag{2}$$

Logistic/Sigmoid Function



- $g(z)$ is symmetric around $z = 0$
- $0 \leqslant g(z) \leqslant 1$ holds true

Where does the Sigmoid come from?

$$
\begin{aligned}
p(\mathcal{C}_1|\boldsymbol{x}) &= \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{x})} = \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{\sum_k^K p(\boldsymbol{x}, \mathcal{C}_k)} = \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{\sum_k^K p(\boldsymbol{x}|\mathcal{C}_k)p(\mathcal{C}_k)} \\
&= \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\boldsymbol{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\
&= \frac{1}{1 + p(\boldsymbol{x}|\mathcal{C}_2)p(\mathcal{C}_2)/(p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1))} \\
&= \frac{1}{1 + \exp\{-z\}} = g(z) \qquad \longrightarrow \textbf{logistic sigmoid}
\end{aligned}
$$

$$
z := \log \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \qquad \longrightarrow \textbf{log odds}
$$

Interpretation of Hypothesis Output

- $h_{\theta}(\boldsymbol{x})$ is interpreted as the probability of instance $\boldsymbol{x}$ belonging to class $y = 1$
- **Example:**

$$\boldsymbol{x} = \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = \begin{pmatrix} 1 \\ tumorSize \end{pmatrix} \tag{3}$$

- If $h_{\theta}(\boldsymbol{x}) = 0.7 = p(y = 1|\boldsymbol{x}, \boldsymbol{\theta})$, we have to tell the patient that there is a **70 % chance** of the tumor being malignant
- **Binary case:**

$$p(y = 0|\boldsymbol{x}, \boldsymbol{\theta}) = 1 - p(y = 1|\boldsymbol{x}, \boldsymbol{\theta})$$

Training Setup

- We have a labeled training set:

$$\mathcal{D} = \left\{ \left(\boldsymbol{x}^{(1)}, y^{(1)}\right), \left(\boldsymbol{x}^{(2)}, y^{(2)}\right), \dots, \left(\boldsymbol{x}^{(n)}, y^{(n)}\right) \right\} = \left\{ \left(\boldsymbol{x}^{(i)}, y^{(i)}\right) \right\}_{i=1}^{n} \tag{4}$$

- Each $y \in \{0, 1\}$ and each $\boldsymbol{x}$ is a vector of features:

$$\boldsymbol{x} = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_m \end{pmatrix} \in \mathbb{R}^{m+1} \tag{5}$$

Logistic Regression Cost Function

- We require a suitable cost function:

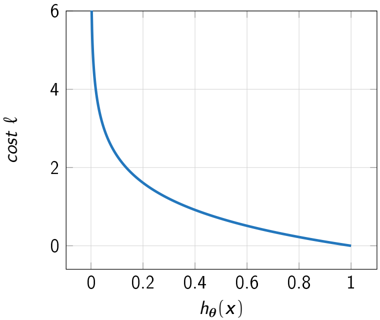
$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \ell\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)}\right) \tag{6}$$

- In our case, the cost function $\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y)$ is defined as follows:
  *(square loss would be **non-convex** due to the sigmoid non-linearity...)*

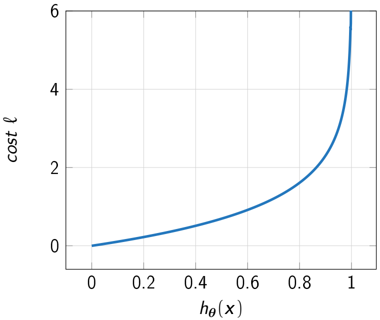
$$\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) := \begin{cases} -\log\left(h_{\boldsymbol{\theta}}(\boldsymbol{x})\right) & \text{if } y = 1 \\ -\log\left(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})\right) & \text{if } y = 0 \end{cases} \tag{7}$$

Logistic Regression Cost Function (Ctd.)

$y = 1$:



$y = 0$:



Logistic Regression Cost Function (Ctd.)

- $\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y)$ can be written in a more compact form:

$$\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) := -y \log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) - (1-y)\log(1-h_{\boldsymbol{\theta}}(\boldsymbol{x})) \tag{8}$$

  - If $y = 1$, we get: $\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x}))$ ✓
  - If $y = 0$, we get: $\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}))$ ✓
- This gives rise to the **(binary) cross entropy** cost function $\mathcal{J}(\boldsymbol{\theta})$:

$$\mathcal{J}(\boldsymbol{\theta}) := \frac{1}{n}\sum_{i=1}^{n}\left[-y^{(i)}\log(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) - (1-y^{(i)})\log(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}))\right] \tag{9}$$

Derivation of (binary) Cross Entropy using Maximum Likelihood

- The likelihood function for logistic regression can be written in the form:

$$p(\boldsymbol{y}|\boldsymbol{\theta}) := \prod_{i=1}^{n} h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})^{y^{(i)}} \cdot (1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}))^{1-y^{(i)}} \tag{10}$$

- The cost function is then given by the **negative log-likelihood**:

$$\mathcal{J}(\boldsymbol{\theta}) = -\frac{1}{n} \log p(\boldsymbol{y}|\boldsymbol{\theta}) \tag{11}$$

We consider the **negative** log-likelihood because – in machine learning – we prefer minimizing functions over maximizing them. This is allowed since $\max\{f(x)\} = \min\{-f(x)\}$.

Derivation of (binary) Cross Entropy (Ctd.)

$$\log p(\boldsymbol{y}|\boldsymbol{\theta}) = \log \left(\prod_{i=1}^{n} h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})^{y^{(i)}} \cdot (1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}))^{1-y^{(i)}} \right)$$

$$= \sum_{i=1}^{n} \log \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})^{y^{(i)}} \cdot (1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}))^{1-y^{(i)}} \right)$$

$$= \sum_{i=1}^{n} \left[\log \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})^{y^{(i)}} \right) + \log \left(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) \right)^{1-y^{(i)}} \right]$$

$$= \sum_{i=1}^{n} \left[y^{(i)} \cdot \log(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) + (1 - y^{(i)}) \cdot \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) \right]$$

Remember the rules:

$$\log(ab) = \log a + \log b$$

$$\log(a^b) = b \log a$$

Where have we used which rule?

Optimization of (binary) Cross Entropy

- Unfortunately, there is **no closed-form solution** to logistic regression *(due to the sigmoid non-linearity in the model function)*
- We have to resort to an iterative method like **gradient descent**

The partial derivative of $\mathcal{J}(\boldsymbol{\theta})$ (based on a single example) with respect to the j-th model parameter θ_j is given by:

$$\frac{\partial}{\partial \theta_j}\mathcal{J}(\boldsymbol{\theta}) = \big(h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y\big) \cdot x_j \tag{12}$$

Important

Optimization of (binary) Cross Entropy (Ctd.)

- The **stochastic gradient** of the binary cross entropy cost function is:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) = \begin{pmatrix} \left(g(\boldsymbol{\theta}^\intercal \boldsymbol{x}) - y\right) \cdot x_1 \\ \vdots \\ \left(g(\boldsymbol{\theta}^\intercal \boldsymbol{x}) - y\right) \cdot x_m \end{pmatrix} = \left(g(\boldsymbol{\theta}^\intercal \boldsymbol{x}) - y\right)\boldsymbol{x} \tag{13}$$

- The **batch gradient** for logistic regression is given by the expression:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) = \frac{1}{n}\boldsymbol{X}^\intercal\left(\boldsymbol{g}(\boldsymbol{X\theta}) - \boldsymbol{y}\right) \tag{14}$$

Derivation of the Gradient based on a single Example $(\boldsymbol{x}, y)$

- We give a proof of equation (12)
- In the derivation we will need the derivative of the sigmoid function:

$$\frac{\mathrm{d}}{\mathrm{d}z} g(z) = g(z) \cdot (1 - g(z)) \tag{15}$$

(You will be asked to proof this in the exercises!)

- Please find the derivation $\Rightarrow$ here

Gradient Descent

- The goal is to minimize the cost function $\mathcal{J}(\boldsymbol{\theta})$:

$$\boldsymbol{\theta}^\star = \arg\min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$$

- `Repeat until convergence`

$$\left\{\boldsymbol{\theta}_{t+1} \longleftarrow \boldsymbol{\theta}_t - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}_t)\right\}$$

- The gradient $\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$ is given by equation (14)

The algorithm looks identical to linear regression, but the model function is different due to the sigmoid function!

Decision Boundary

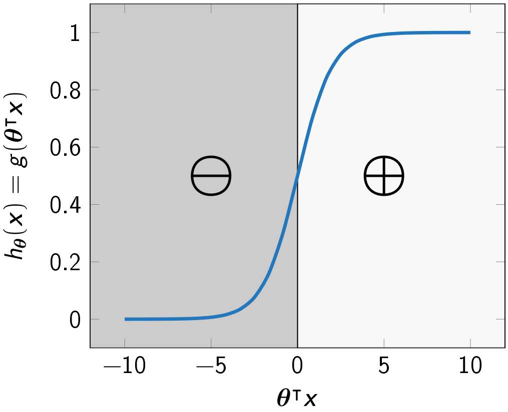
- Our trained model **outputs probabilities**
- To obtain a classifier, we have to **apply a threshold** ρ to the raw outputs
- Setting the threshold to $\rho := 0.5$ means:
  - Predict the positive class $\oplus$, if

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geqslant 0.5 \iff \boldsymbol{\theta}^\intercal \boldsymbol{x} \geqslant 0$$

  - Predict the negative class $\ominus$, if

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5 \iff \boldsymbol{\theta}^\intercal \boldsymbol{x} < 0$$

Decision Boundary (Ctd.)



Example: Decision Boundary

- Let us consider a simple example
- Suppose our model function takes the form:

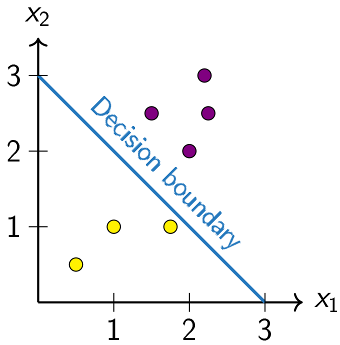
$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

- Assume we obtain the following model parameters using gradient descent:

$$\theta_0 = -3, \qquad \theta_1 = 1, \qquad \theta_2 = 1$$

- Predict $y = 1$, if $-3 + x_1 + x_2 \geqslant 0$

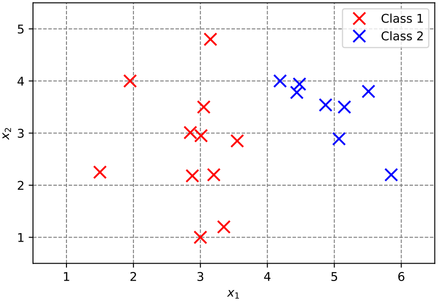
Example: Decision Boundary (Ctd.)

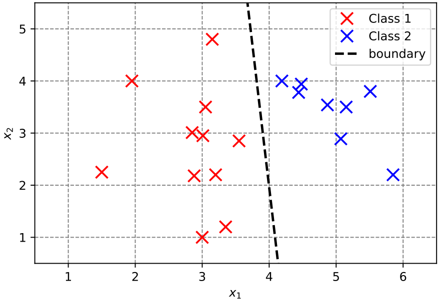


- Predict $y = 1$, if $-3 + x_1 + x_2 \geqslant 0$
- The decision boundary satisfies $-3 + x_1 + x_2 = 0$
- If $x_2 = 0$, then $x_1 = 3$ and vice versa

Logistic regression is not a maximum-margin classifier, but the cost function can be adjusted to get that $\Longrightarrow$ Hinge loss

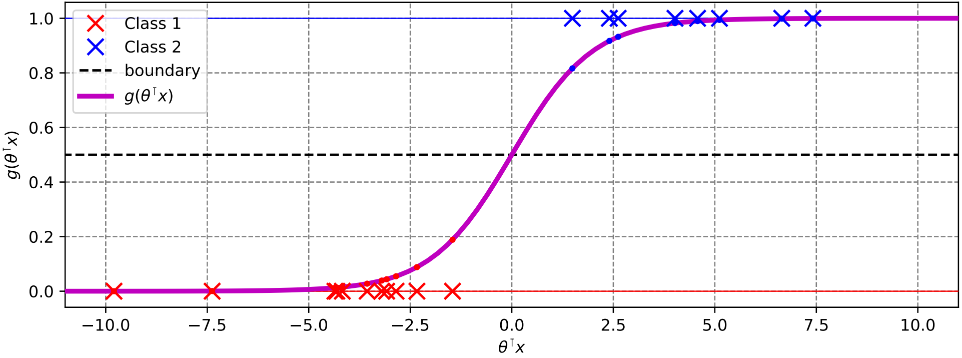
Another Example: Decision Boundary





Where is the sigmoid function?

Another Example: Logistic Function



Section:

Non-linear Data

- Feature Mapping
- Regularization

Non-Linear Decision Boundaries

Feature mapping can be used to obtain non-linear decision boundaries/surfaces (same procedure already introduced for linear regression)

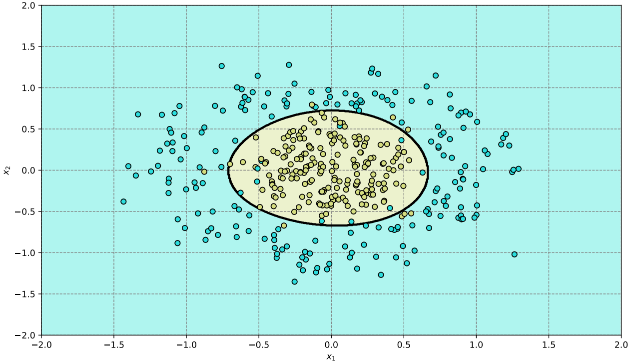
Example:

- Let a circular two-dimensional dataset be given (features x_1 and x_2)
- We choose the following model function:

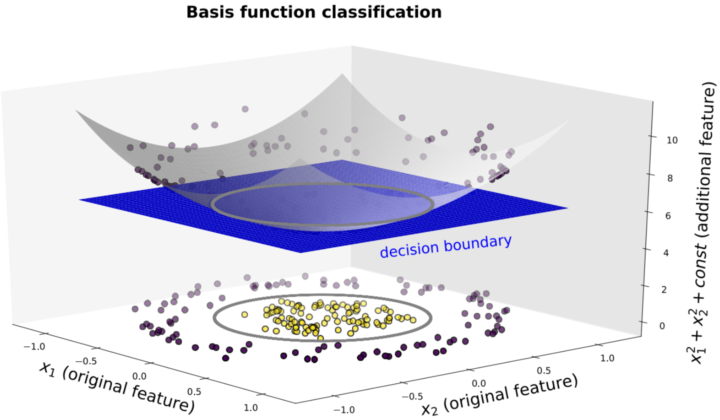
$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2\right)$$

- The algorithm could choose the parameters $\boldsymbol{\theta}^\star := \left(-1, 0, 0, 1, 1\right)^\intercal$
- So we would get: $x_1^2 + x_2^2 = 1$ **(equation of a unit circle)**

Example: Non-Linear Decision Boundary



It is still linear!



Logistic Regression with Regularization

- Again, we should apply **regularization** when using the feature mapping approach to avoid running into ☠ **overfitting** ☠
- Add a **regularizer** to the cost function:

$$\widetilde{\mathcal{J}}(\boldsymbol{\theta}) := \mathcal{J}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|^2 \tag{16}$$

- The regularizer prevents the parameters θ_j from becoming too large
- $\lambda \geqslant 0$ controls the degree of regularization
- This leads to smoother decision boundaries

Section:

Multi-Class Classification

- Techniques Overview
- One-vs-Rest (OvR)
- One-vs-One (OvO)

Multi-Class Classification

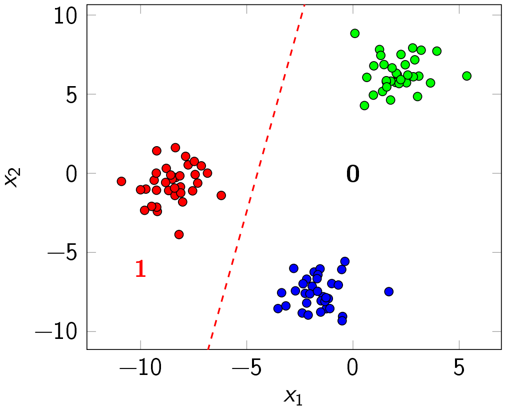
- In its basic form logistic regression can handle two classes only
- **What if there are more than two classes?**
- Two approaches:
  1. Change the algorithm so that it can deal with more classes ($\longrightarrow$ **Multinomial Logistic Regression** / **Softmax Regression**)
  2. Transform the problem into several binary problems
     Two common techniques are:
     - **One-vs-Rest (OvR)** $\longrightarrow$ One-against-All
     - **One-vs-One (OvO)** $\longrightarrow$ Pairwise classification
- Let's have a closer look into the second approach!

Transforming the Problem into several binary Problems

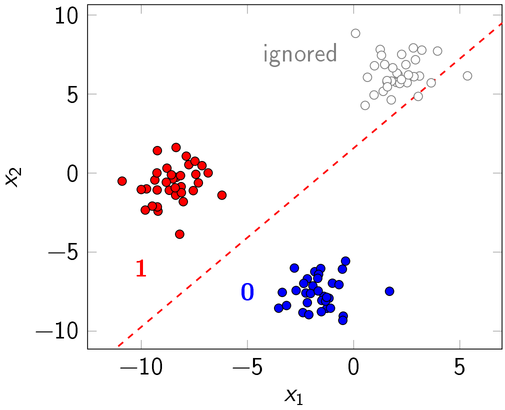
- Instead of adjusting the algorithm, we can also **transform the multi-class problem into several binary problems**
- Two common techniques are:
  - **One-vs-Rest (OvR)** $\longrightarrow$ One-against-All
  - **One-vs-One (OvO)** $\longrightarrow$ Pairwise classification
- **General idea:**
  - Several classifiers are trained individually
  - During prediction the classifiers **vote for the correct class**
- Such techniques can be used **for all binary classifiers**

Multi-Class Classification: One-vs-Rest (OvR)

- **Train one classifier per class** (expert for that class)
- We get K classifiers
- The k-th classifier learns to distinguish the k-th class from all the others
- Set the labels of examples from class k to $\mathbf{1}$, all the others to $\mathbf{0}$



Multi-Class Classification: One-vs-One (OvO)



- **Train one classifier for each pair of classes**
- We get $\binom{K}{2}$ classifiers
- Ignore all other examples that do not belong to either of the two classes
- **Voting**: Count how often each class wins; The class with the highest score is predicted

Section:
Wrap-Up

Summary
Self-Test Questions
Lecture Outlook

Summary

- Logistic regression is used for classification (!!!)
- It is used for **binary classification problems** (generalizations exist)
- **Output:** Probability of instance belonging to positive class
- Apply a **threshold** ρ to get the classification
- The algorithm minimizes the **cross entropy cost function**
- There is **no closed-form solution** (unlike for linear regression)
- **Basis functions** can be used for non-linear data
- **Multi-class classification:** One-vs-Rest, One-vs-One

Important

Self-Test Questions

1. Why should you not use linear regression for classification?
2. How is the logistic function defined?
3. Why do we use cross entropy instead of the squared error?
4. Does logistic regression find the best-separating (i. e. maximum margin) hyper-plane?
5. What techniques do you know for multi-class classification problems?

What's next...?

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Regression
Unit V	**Classification I**
Unit VI	Evaluation
Unit VII	Classification II
Unit VIII	Clustering
Unit IX	Dimensionality Reduction

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Logistic Regression
Term: Winter term 2023/2024

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Do you have any questions?