

# \*\*\* Applied Machine Learning Fundamentals \*\*\*

## Logistic Regression

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SAP SE / DHBW Mannheim

Winter term 2021/2022



Find all slides on [GitHub](https://github.com/DaWe1992/Applied_ML_Fundamentals) (DaWe1992/Applied\_ML\_Fundamentals)

# Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
<b>Unit VI</b>	<b>Classification I</b>
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	Clustering
Unit X	Dimensionality Reduction

# Agenda for this Unit

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

## 2 Model Architecture

- Sigmoid Function
- Probabilistic Interpretation
- Model Training
- Decision Boundary

## 3 Non-linear Data

- Feature Mapping
- Regularization

## 4 Multi-Class Classification

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- Multinomial Logistic Regression
- One-vs-Rest (OVR)
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## 5 Wrap-Up

- Summary
- Self-Test Questions
- Lecture Outlook
- Recommended Literature and further Reading
- Meme of the Day

Section:  
**Introduction**

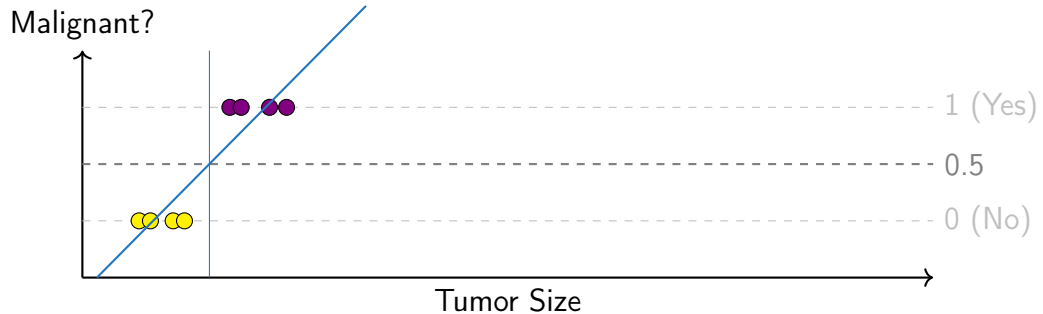


# What is logistic Regression?

- Learning algorithm for **classification** (*despite the name...*)
- In its standard form it's applicable to **binary classification problems only**, but you can use techniques like:
  - **One-vs-One (OVO)**
  - **One-vs-Rest (OVR)**
- **Class labels:**
  - The 'positive class'  $\oplus$  is encoded as **1**
  - The 'negative class'  $\ominus$  as **0**
- **Probabilistic interpretation:** The output of the algorithm is between 0 and 1 (*probability of the instance belonging to the positive class*)

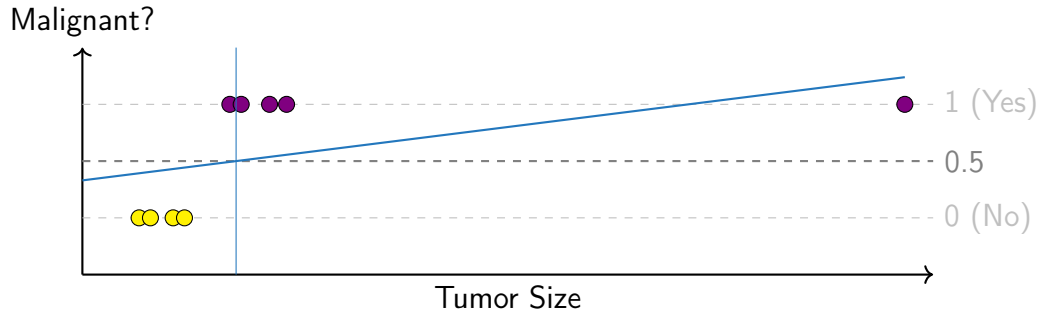


# Why you should not use linear Regression...





# Why you should not use linear Regression...



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

- Linear regression:  $h_{\theta}(\mathbf{x}) = \theta^T \mathbf{x}$
- By putting a **threshold** at 0.5, we can turn linear regression into a classifier
  - If  $h_{\theta}(\mathbf{x}) \geq 0.5$ , predict  $y = 1$
  - If  $h_{\theta}(\mathbf{x}) < 0.5$ , predict  $y = 0$
- **Problems:**
  - ① Outliers heavily affect the decision boundary
  - ② Furthermore, we only want  $0 \leq h_{\theta}(\mathbf{x}) \leq 1$ , linear regression can output values  $h_{\theta}(\mathbf{x}) \ll 0$  or  $h_{\theta}(\mathbf{x}) \gg 1$
- We need a better strategy!



Section:  
**Model Architecture**





# Logistic Regression Model

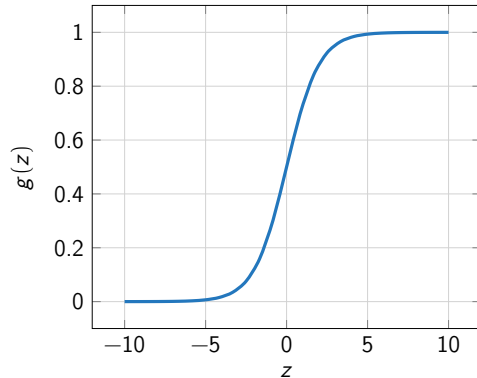
- Remember that we want:  $0 \leq h_{\theta}(\mathbf{x}) \leq 1$
- **Solution:** **Logistic / Sigmoid function:**

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

- We plug  $\theta^T \mathbf{x}$  into the sigmoid function:

$$h_{\theta}(\mathbf{x}) = g(\theta^T \mathbf{x}) = \frac{1}{1 + e^{-(\theta^T \mathbf{x})}} \quad (2)$$

# Logistic/Sigmoid Function



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



## Where does the Sigmoid come from?

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{\sum_j p(\mathbf{x}, \mathcal{C}_j)} = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)}$$

$$= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

$$= \frac{1}{1 + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)/(p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1))}$$

$$= \frac{1}{1 + \exp\{-z\}} = g(z)$$

→ **logistic sigmoid**

$$z = \log \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

→ **log odds**

# Interpretation of Hypothesis Output

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

$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ tumorSize \end{bmatrix} \quad (3)$$

- If  $h_{\theta}(\mathbf{x}) = 0.7$ , we have to tell the patient that there is a **70 % chance** of the tumor being malignant  $\Rightarrow p(y = 1|\mathbf{x}, \theta)$
- **Binary case:**  $p(y = 0|\mathbf{x}, \theta) = 1 - p(y = 1|\mathbf{x}, \theta)$

# Training Setup

- We have a labeled training set ( $\Rightarrow$  **supervised learning**):

$$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \dots, (\mathbf{x}^{(n)}, y^{(n)})\} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^n \quad (4)$$

- Each  $\mathbf{x}$  is a vector of features:

$$\mathbf{x} = \begin{bmatrix} x_0 \\ \vdots \\ x_m \end{bmatrix} \in \mathbb{R}^{m+1} \quad \text{and} \quad x_0 = 1 \quad \text{and} \quad y \in \{0, 1\} \quad (5)$$

- How to choose the parameters  $\theta$ ?

# Logistic Regression Cost Function

- Gradient descent is performed in order to find the parameters  $\theta$
- To this end, a cost function is needed:

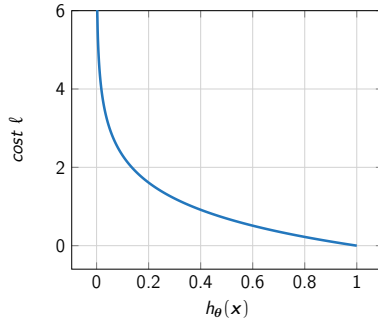
$$\mathcal{J}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(h_{\theta}(\mathbf{x}^{(i)}), y^{(i)}) \quad (6)$$

- The cost function  $\ell(h_{\theta}(\mathbf{x}), y)$  is defined as follows:  
(square loss would be **non-convex**...)

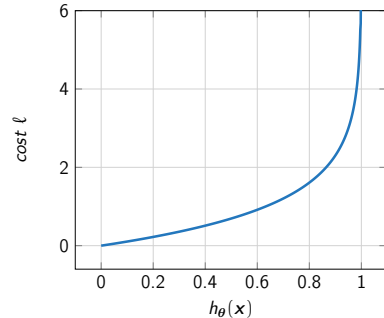
$$\ell(h_{\theta}(\mathbf{x}), y) = \begin{cases} -\log(h_{\theta}(\mathbf{x})) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(\mathbf{x})) & \text{if } y = 0 \end{cases} \quad (7)$$

# Logistic Regression Cost Function (Ctd.)

$y = 1$ :



$y = 0$ :





# Logistic Regression Cost Function (Ctd.)

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

$$\ell(h_{\theta}(\mathbf{x}), y) = -y \log(h_{\theta}(\mathbf{x})) - (1 - y) \log(1 - h_{\theta}(\mathbf{x})) \quad (8)$$

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

$$\mathcal{J}(\theta) = \frac{1}{n} \sum_{i=1}^n [-y^{(i)} \log(h_{\theta}(\mathbf{x}^{(i)})) - (1 - y^{(i)}) \log(1 - h_{\theta}(\mathbf{x}^{(i)}))] \quad (9)$$



# Derivation of Cross Entropy

- The likelihood function can be written in the form:

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^n h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})^{y^{(i)}} \cdot (1 - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}))^{1-y^{(i)}} \quad (10)$$

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

$$\mathcal{J}(\boldsymbol{\theta}) = -\log \mathcal{L}(\boldsymbol{\theta}) \quad (11)$$



# Derivative of the Sigmoid Function

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

$$\frac{d}{dz}g(z) = \frac{0 \cdot (1 + e^{-z}) - (-e^{-z})}{(1 + e^{-z})^2}$$

$$= \frac{e^{-z}}{(1 + e^{-z})^2} = \frac{(1 - 1) + e^{-z}}{(1 + e^{-z})^2} = \frac{1 + e^{-z}}{(1 + e^{-z})^2} - \frac{1}{(1 + e^{-z})^2}$$

$$= \frac{1}{1 + e^{-z}} \left[ 1 - \frac{1}{1 + e^{-z}} \right]$$

$$= \boxed{g(z)(1 - g(z))}$$



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

$$\frac{\partial}{\partial \theta_j} \mathcal{J}(\boldsymbol{\theta}) = -\frac{\partial}{\partial \theta_j} y \log(g(\boldsymbol{\theta}^\top \mathbf{x})) - \frac{\partial}{\partial \theta_j} (1 - y) \log(1 - g(\boldsymbol{\theta}^\top \mathbf{x}))$$
 (derivative of sum terms)

$$= \left[ -\frac{y}{g(\boldsymbol{\theta}^\top \mathbf{x})} + \frac{1 - y}{1 - g(\boldsymbol{\theta}^\top \mathbf{x})} \right] \frac{\partial}{\partial \theta_j} g(\boldsymbol{\theta}^\top \mathbf{x})$$
 (derivative of log function)

$$= \left[ -\frac{y}{g(\boldsymbol{\theta}^\top \mathbf{x})} + \frac{1 - y}{1 - g(\boldsymbol{\theta}^\top \mathbf{x})} \right] g(\boldsymbol{\theta}^\top \mathbf{x})(1 - g(\boldsymbol{\theta}^\top \mathbf{x})) \frac{\partial}{\partial \theta_j} \boldsymbol{\theta}^\top \mathbf{x}$$
 (chain rule)

$$= \left[ \frac{g(\boldsymbol{\theta}^\top \mathbf{x}) - y}{g(\boldsymbol{\theta}^\top \mathbf{x})(1 - g(\boldsymbol{\theta}^\top \mathbf{x}))} \right] g(\boldsymbol{\theta}^\top \mathbf{x})(1 - g(\boldsymbol{\theta}^\top \mathbf{x})) x_j$$
 (algebraic manipulation)

$$= (g(\boldsymbol{\theta}^\top \mathbf{x}) - y) x_j = \boxed{(h_{\boldsymbol{\theta}}(\mathbf{x}) - y) x_j}$$
 (cancelling terms)

# Gradient Descent

- The goal is to minimize  $\mathcal{J}(\boldsymbol{\theta})$ :  $\boldsymbol{\theta}^* = \arg \min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$
- Repeat until convergence {  
 $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(t)})$  // simultaneously update all  $\theta_j$   
}
- The gradient  $\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$  is given by:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n \left( h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)} \right) \mathbf{x}^{(i)} \quad (12)$$

Algorithm looks identical to linear regression, but  $h_{\boldsymbol{\theta}}(\mathbf{x})$  is different!

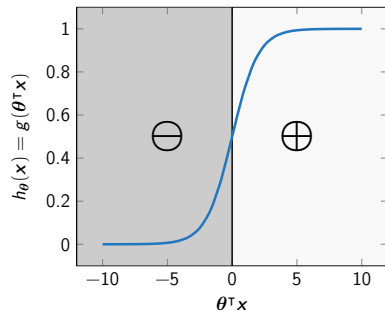
# Decision Boundary

- We have to set a threshold
- Setting the threshold to 0.5 means:
  - Predict the positive class, if

$$h_{\theta}(\mathbf{x}) \geq 0.5 \Leftrightarrow \theta^T \mathbf{x} \geq 0$$

- Predict the negative class, if

$$h_{\theta}(\mathbf{x}) < 0.5 \Leftrightarrow \theta^T \mathbf{x} < 0$$



## Decision Boundary (Ctd.)

- Suppose we have the following hypothesis:

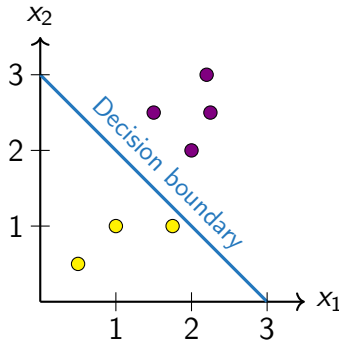
$$h_{\theta}(\mathbf{x}) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

- Using gradient descent we obtained the following coefficients:

$$\theta_0 = -3 \quad \theta_1 = 1 \quad \theta_2 = 1$$

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

## Decision Boundary (Ctd.)

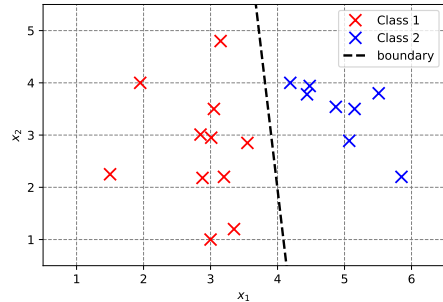
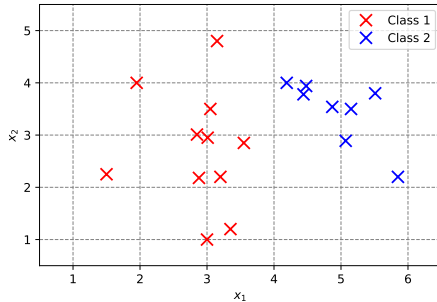


- Predict  $y = 1$ , if  $-3 + x_1 + x_2 \geq 0$
- The decision boundary satisfies  $-3 + x_1 + x_2 = 0$
- If  $x_2 = 0$ , then  $x_1 = 3$  and vice versa

Logistic regression is not a maximum-margin classifier (although the cost function can be adjusted to get that  $\Rightarrow$  Hinge loss)

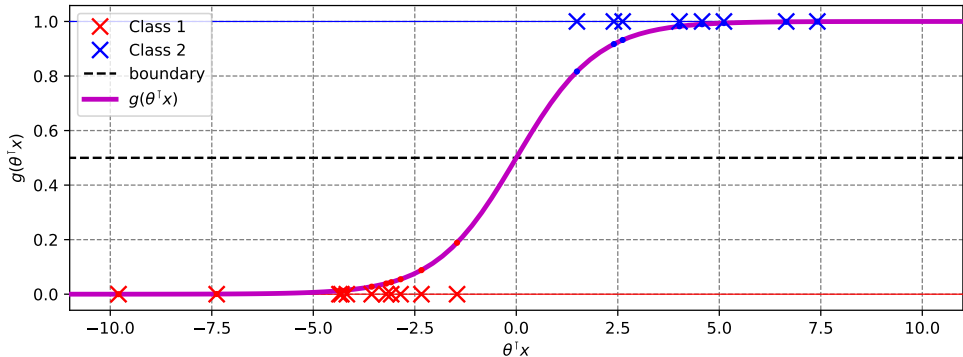


## Example: Decision Boundary



Where is the sigmoid function?

# Example: Logistic Function



Section:  
**Non-linear Data**



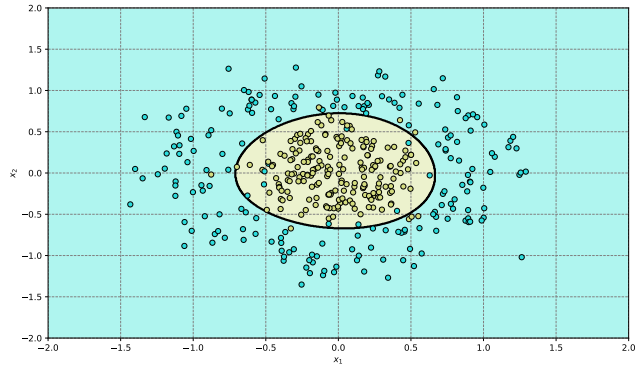
# Non-Linear Decision Boundaries

- **Feature mapping** can be used to obtain non-linear decision boundaries
- **Example:**
  - Imagine a circular data set
  - Using the features...

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

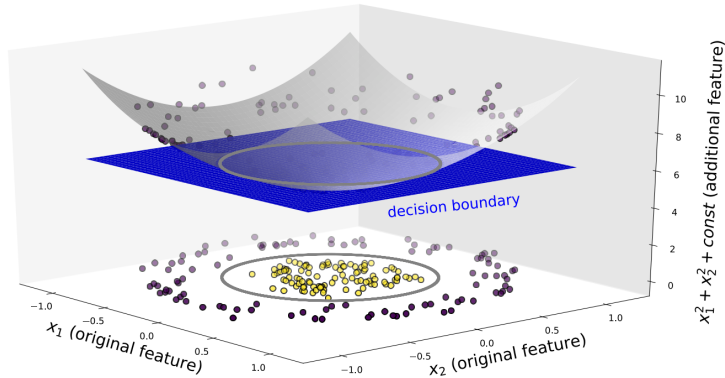
- ...the algorithm could e. g. choose:  $\theta = [-1, 0, 0, 1, 1]^T$
- So we would get:  $x_1^2 + x_2^2 = 1 \Rightarrow$  **equation of a unit circle**

# Example: Non-Linear Decision Boundary



# It is still linear!

**Basis function classification**



# Logistic Regression with Regularization

- We should apply regularization for non-linear decision boundaries:

$$\frac{1}{n} \sum_{i=1}^n \left[ -y^{(i)} \log(h_{\theta}(\mathbf{x}^{(i)})) - (1 - y^{(i)}) \log(1 - h_{\theta}(\mathbf{x}^{(i)})) \right] + \frac{\lambda}{2m} \sum_{j=1}^m \theta_j^2 \quad (13)$$

- The last term prevents the parameters  $\theta_j$  from becoming too large
- $\lambda \geq 0$  controls the degree of regularization
- This leads to smoother decision boundaries

Section:  
**Multi-Class Classification**





# 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  
(→ **Multinomial Logistic Regression** / **Softmax Regression**)
  - ② Transform the problem into several binary problems.  
Two common techniques are:
    - **One-vs-Rest (OvR)** → One-against-All
    - **One-vs-One (OvO)** → Pairwise classification
- Let's examine these approaches a bit closer



# Multinomial Logistic Regression Introduction

- The logistic regression model has to be changed in order to deal with multiple classes
- The sigmoid function is replaced by the **Softmax** function:

$$\mathbf{g} : \mathbb{R}^K \rightarrow \mathbb{R}^K \quad \mathbf{z} \mapsto \mathbf{g}(\mathbf{z}) \quad g_k(\mathbf{z}) = \frac{e^{z_k}}{\sum_{n=1}^K e^{z_n}} \quad (14)$$

- $\kappa$  is the number of possible outcomes / classes
- The softmax function returns a **probability distribution over the possible outcomes**, i. e.  $\sum_{k=1}^K g_k(\mathbf{z}) = 1$



## Multinomial Logistic Regression Introduction (Ctd.)

- $z = \left( \theta_1^T x \quad \theta_2^T x \quad \dots \quad \theta_k^T x \right)^T$  is the vector of logits
- This means we learn a separate set of parameters  $\theta_k$  for each possible class
- All parameter vectors  $\theta_k$  are stacked into a single matrix  $\Theta$ :

$$\Theta = \begin{pmatrix} | & | & \dots & | \\ \theta_1 & \theta_2 & \dots & \theta_k \\ | & | & \dots & | \end{pmatrix} \quad (15)$$



# Derivative of the Cross-Entropy Function

$$\mathcal{J}(\Theta) = - \sum_{k=1}^K y_k \log(g_k(\mathbf{z})) \quad \text{with } \mathbf{z} = \begin{pmatrix} \theta_1^T \mathbf{x} \\ \theta_2^T \mathbf{x} \\ \vdots \\ \theta_K^T \mathbf{x} \end{pmatrix}$$

$$\frac{\partial}{\partial \theta_{ij}} \mathcal{J}(\Theta) = - \sum_{k=1}^K y_k \frac{\partial \log(g_k(\mathbf{z}))}{\partial g_k(\mathbf{z})} \cdot \frac{\partial g_k(\mathbf{z})}{\partial z_i} \cdot \frac{\partial z_i}{\partial \theta_{ij}} \quad \longrightarrow \text{chain rule}$$

$$= - \sum_{k=1}^K y_k \frac{1}{g_k(\mathbf{z})} \cdot \frac{\partial g_k(\mathbf{z})}{\partial z_i} \cdot \frac{\partial z_i}{\partial \theta_{ij}} \quad \longrightarrow \frac{d}{dx} \log(x) = \frac{1}{x}$$



# Derivative of the Softmax Function

$$g_k(\mathbf{z}) = \frac{e^{z_k}}{\sum_{n=1}^K e^{z_n}} \quad \frac{\partial}{\partial z_i} g_k(\mathbf{z}) = \begin{cases} g_i(\mathbf{z})(1 - g_i(\mathbf{z})) & \text{if } i = k \\ -g_k(\mathbf{z})g_i(\mathbf{z}) & \text{if } i \neq k \end{cases}$$

Case ①:  $i = k$

$$\begin{aligned} \frac{\partial}{\partial z_i} g_k(\mathbf{z}) &= \frac{e^{z_k} \sum_{n=1}^K e^{z_n} - e^{z_k} e^{z_i}}{(\sum_{n=1}^K e^{z_n})^2} \\ &= \frac{e^{z_k}}{\sum_{n=1}^K e^{z_n}} \left[ 1 - \frac{e^{z_i}}{\sum_{n=1}^K e^{z_n}} \right] \\ &= g_k(\mathbf{z})(1 - g_i(\mathbf{z})) \\ &= g_k(\mathbf{z})(1 - g_k(\mathbf{z})) \end{aligned}$$

Case ②:  $i \neq k$ :

$$\begin{aligned} \frac{\partial}{\partial z_i} g_k(\mathbf{z}) &= \frac{0 \cdot \sum_{n=1}^K e^{z_n} - e^{z_k} e^{z_i}}{(\sum_{n=1}^K e^{z_n})^2} \\ &= -\frac{e^{z_k}}{\sum_{n=1}^K e^{z_n}} \frac{e^{z_i}}{\sum_{n=1}^K e^{z_n}} \\ &= -g_k(\mathbf{z})g_i(\mathbf{z}) \end{aligned}$$



## Derivative of the Cross-Entropy Function (Ctd.)

$$\frac{\partial}{\partial \theta_{ij}} \mathcal{J}(\Theta) = - \sum_{k=1}^K \frac{y_k}{g_k(\mathbf{z})} \cdot \frac{\partial g_k(\mathbf{z})}{\partial z_i} \cdot \frac{\partial z_i}{\partial \theta_{ij}} \quad \longrightarrow \text{see slide 33}$$

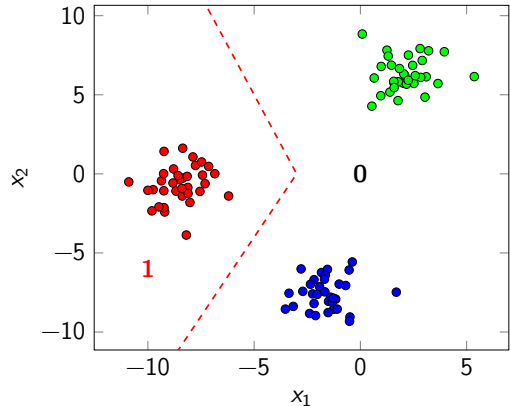
$$= \left[ -\frac{y_k}{g_k(\mathbf{z})} g_k(\mathbf{z})(1 - g_k(\mathbf{z})) + \sum_{\substack{k=1 \\ k \neq i}}^K \frac{y_k}{g_k(\mathbf{z})} g_k(\mathbf{z}) g_i(\mathbf{z}) \right] \frac{\partial z_i}{\partial \theta_{ij}} \quad \longrightarrow \text{separate cases}$$

$$= \left[ -y_k + y_k g_k(\mathbf{z}) + \sum_{\substack{k=1 \\ k \neq i}}^K y_k g_i(\mathbf{z}) \right] \frac{\partial z_i}{\partial \theta_{ij}} = \left[ -y_k + \sum_{k=1}^K y_k g_i(\mathbf{z}) \right] \frac{\partial z_i}{\partial \theta_{ij}} \quad \longrightarrow \text{cancel terms}$$

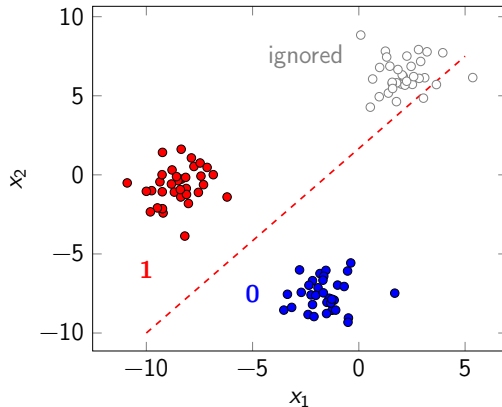
$$= (-y_k + g_k(\mathbf{z})) x_j = \boxed{(g_k(\mathbf{z}) - y_k) x_j}$$

# Multi-Class Classification: One-vs-Rest (OVR)

- **Train one classifier per class** (expert for that class)
- We get  $|\mathcal{C}|$  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 **1**, all the others to **0**



# Multi-Class Classification: One-vs-One (OVO)



- Train one classifier for each pair of classes
- We get  $\binom{|C|}{2}$  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

- **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** 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



# Self-Test Questions

- ① Why should you not use linear regression for classification?
- ② State the formula for the logistic function.
- ③ Why do we use cross entropy instead of the squared error?
- ④ Does logistic regression find the best-separating hyper-plane?
- ⑤ What techniques do you know for multi-class classification problems?

# What's next...?

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# Recommended Literature and further Reading I



## [1] Pattern Recognition and Machine Learning

*Christopher Bishop. Springer. 2006.*

→ [Link](#), cf. chapter 4.3.2

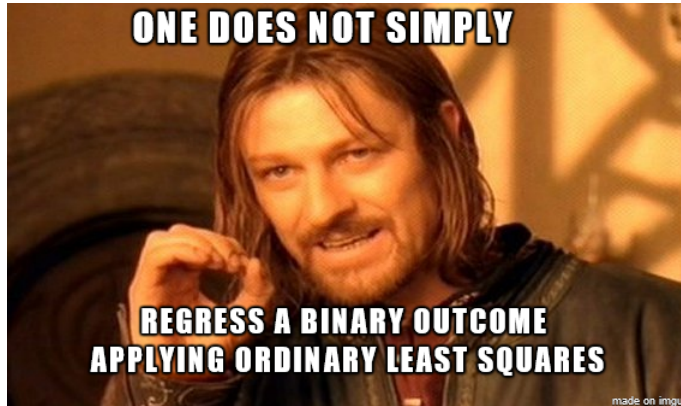


## [2] Machine Learning: A Probabilistic Perspective

*Kevin Murphy. MIT Press. 2012.*

→ [Link](#), cf. chapter 8

## Meme of the Day



Thank you very much for the attention!

**Topic:** \*\*\* Applied Machine Learning Fundamentals \*\*\* Logistic Regression

**Term:** Winter term 2021/2022

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Do you have any questions?