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

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SAP SE / DHBW Mannheim

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Find all slides on GitHub (DaWe1992/Applied_ML_Fundamentals)

Lecture Overview

Agenda for this Unit

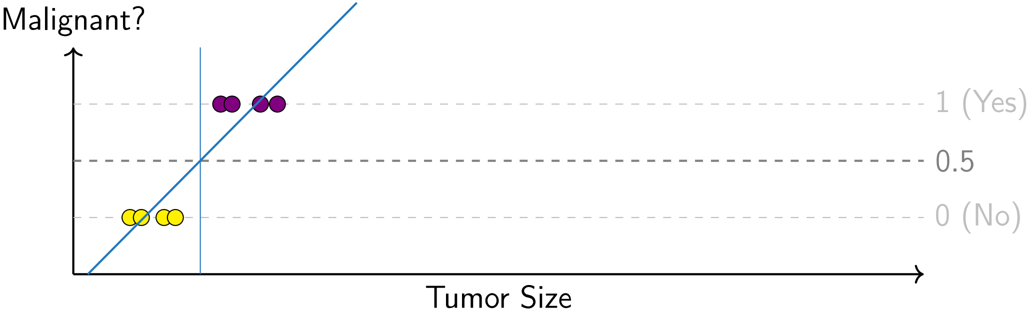
Section:

Introduction

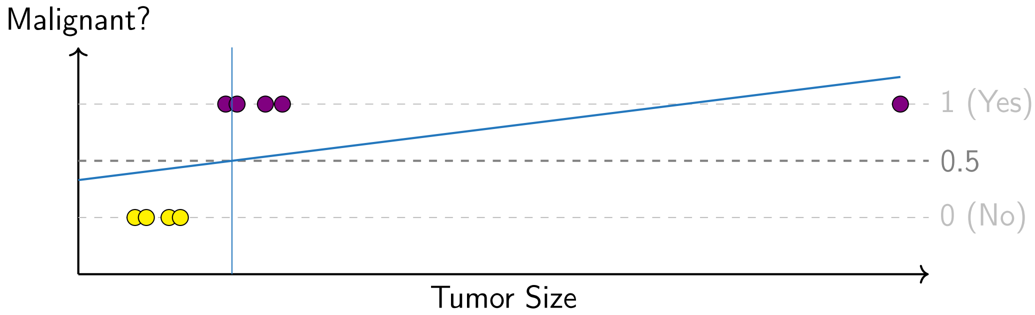
What is logistic Regression?

- 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' is encoded as **1** / $\oplus$
  - The 'negative class' as **0** / $\ominus$
- **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: $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{\theta}^\intercal \boldsymbol{x}$
- By putting a **threshold** at 0.5, we can turn linear regression into a classifier
  - If $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geqslant 0.5$, predict $y = 1$
  - If $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$, predict $y = 0$
- **Outliers affect the decision boundary**
- Furthermore, we only want $0 \leqslant h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leqslant 1$
- Linear regression can output $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \ll 0$ or $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \gg 1$
- **We need a better strategy!**

Section:

Model Architecture

Logistic Regression Model

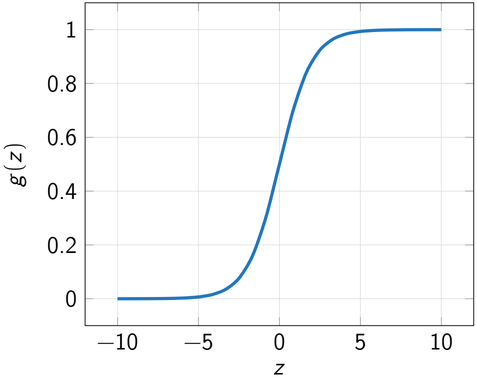
- Remember that we want: $0 \leqslant h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leqslant 1$
- **Solution:** **Logistic / Sigmoid function:**

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

- We plug $\boldsymbol{\theta}^\intercal \boldsymbol{x}$ into the sigmoid function:

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

Logistic/Sigmoid Function



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

Where does the Sigmoid come from?

$$p(\mathcal{C}_1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{x})} = \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{\sum_j p(\boldsymbol{x}, \mathcal{C}_j)} = \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{\sum_j p(\boldsymbol{x}|\mathcal{C}_j)p(\mathcal{C}_j)} \tag{3}$$

$$= \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\boldsymbol{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \tag{4}$$

$$= \frac{1}{1 + p(\boldsymbol{x}|\mathcal{C}_2)p(\mathcal{C}_2)/(p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1))} \tag{5}$$

$$= \frac{1}{1 + \exp\{-z\}} = g(z) \qquad \longrightarrow \textbf{logistic sigmoid} \tag{6}$$

$$z = \log \frac{p(\boldsymbol{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \qquad \longrightarrow \textbf{log odds} \tag{7}$$

Interpretation of Hypothesis Output

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

$$\boldsymbol{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ tumorSize \end{bmatrix} \tag{8}$$

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

$$\mathcal{D} = \left\{(\boldsymbol{x}^{(1)}, y^{(1)}), (\boldsymbol{x}^{(2)}, y^{(2)}), \dots, (\boldsymbol{x}^{(n)}, y^{(n)})\right\} = \left\{(\boldsymbol{x}^{(i)}, y^{(i)})\right\}_{i=1}^{n} \tag{9}$$

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

$$\boldsymbol{x} = \begin{bmatrix} x_0 \\ \vdots \\ x_m \end{bmatrix} \in \mathbb{R}^{m+1} \quad \text{and} \quad x_0 = 1 \quad \text{and} \quad y \in \{0, 1\} \tag{10}$$

- How to choose the parameters θ?

Logistic Regression Cost Function

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

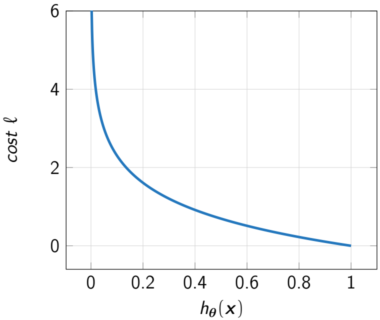
$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)}) \tag{11}$$

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

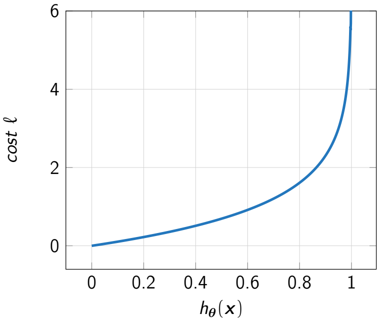
$$\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 1 \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 0 \end{cases} \tag{12}$$

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:

$$\ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = -y \log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) - (1 - y) \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \tag{13}$$

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

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \left[-y^{(i)} \log(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) - (1 - y^{(i)}) \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) \right] \tag{14}$$

Derivation of Cross Entropy

- The likelihood function can be written in the form:

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{n} h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})^{y^{(i)}} \cdot (1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}))^{1-y^{(i)}} \tag{15}$$

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

$$\mathcal{J}(\boldsymbol{\theta}) = -\log \mathcal{L}(\boldsymbol{\theta}) \tag{16}$$

Gradient Descent

- The goal is to minimize $\mathcal{J}(\boldsymbol{\theta})$: $\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$
- `Repeat until convergence {`

  $$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(t)}) \qquad \textit{// simultaneously update all } \theta_j$$

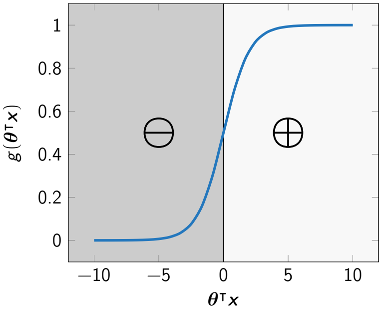
  `}`
- The gradient $\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$ is given by:

$$\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)} \right) \boldsymbol{x}^{(i)} \tag{17}$$

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

Decision Boundary

- **For classification we have to set a threshold**
- Suppose we predict $y = 1$, if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geqslant 0.5$
    - This means $g(z) \geqslant 0.5$
    - This is equivalent to $z \geqslant 0$ and $\boldsymbol{\theta}^{\intercal}\boldsymbol{x} \geqslant 0$
- Suppose we predict $y = 0$, if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5 \Rightarrow \boldsymbol{\theta}^{\intercal}\boldsymbol{x} < 0$



Decision Boundary (Ctd.)

- Suppose we have the following hypothesis:

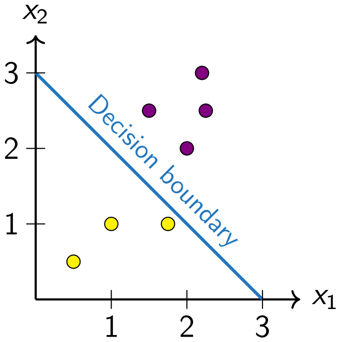
$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

- Using gradient descent we obtained the following coefficients:

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

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

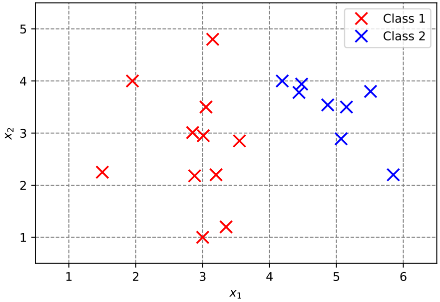
Decision Boundary (Ctd.)

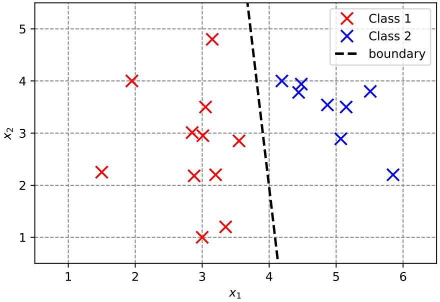


- Predict $y = 1$, if $-3 + x_1 + x_2 \geqslant 0$
- The decision boundary satisfies $-3 + x_1 + x_2 = 0$
- If $x_2 = 0$, then $x_1 = 3$ and vice versa

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

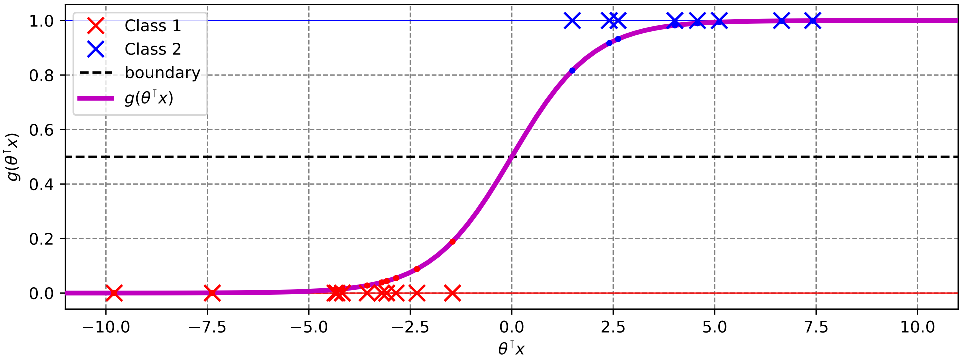
Example: Decision Boundary





Where is the sigmoid function?

Example: Logistic Function



Section:

Non-linear Data

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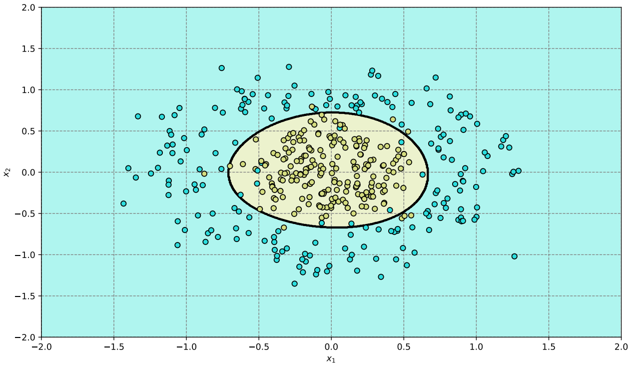
Non-Linear Decision Boundaries

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

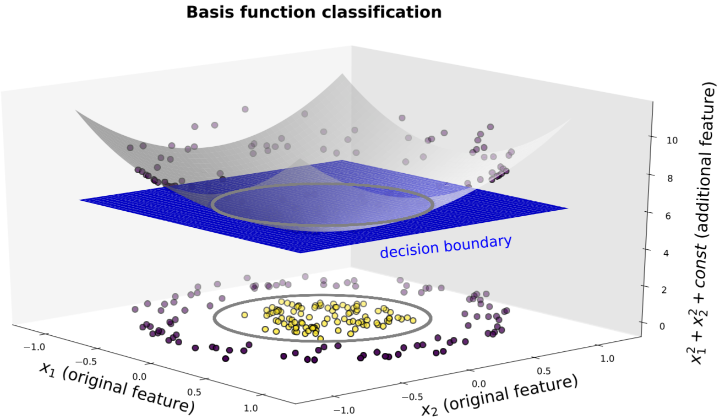
$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

  - ...the algorithm could e. g. choose: $\boldsymbol{\theta} = \begin{bmatrix} -1, 0, 0, 1, 1 \end{bmatrix}^{\intercal}$
  - 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!



Logistic Regression Cost Function (Ctd.)

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

$$\frac{1}{n}\sum_{i=1}^{n}\left[-y^{(i)}\log(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) - (1-y^{(i)})\log(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2 \tag{18}$$

- The last term 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

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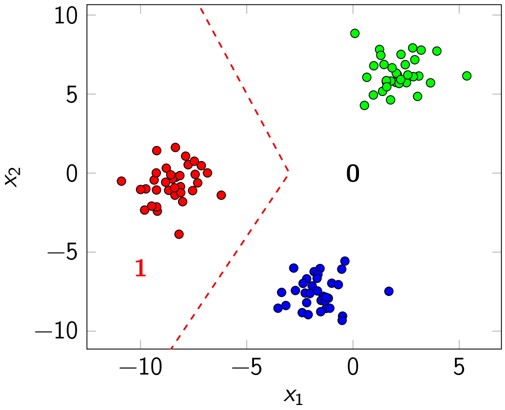
Multi-Class Classification

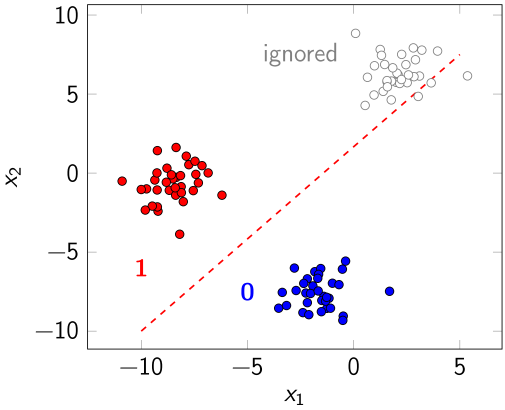
- Logistic regression can handle two classes only, namely **0** and **1**
- **What if there are more than two classes?**
- Two common techniques:
  - One-vs-Rest (OVR) $\Rightarrow$ One-against-All
  - One-vs-One (OVO) $\Rightarrow$ Pairwise classification
- Several classifiers are trained
- During prediction 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 $|\mathcal{C}|$ 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 $\mathbf{1}$, all the others to $\mathbf{0}$



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



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

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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

Important

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...?

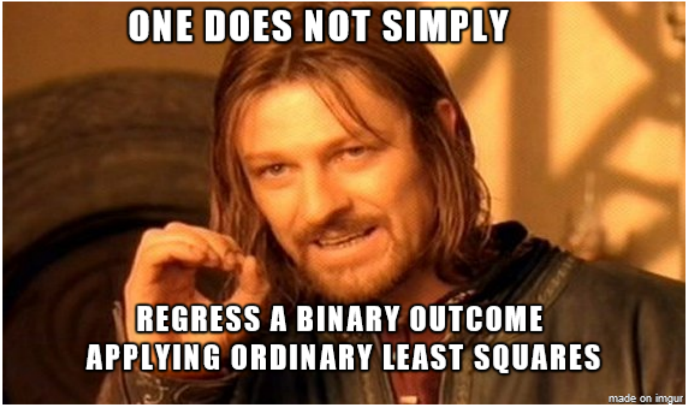
Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	**Classification I**
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	Clustering
Unit X	Dimensionality Reduction

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!

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Do you have any questions?