W3WI DS304.1 Applied Machine Learning Fundamentals

Exercise Sheet #3 - Linear Regression

Question 1 (Matrix operations)

Let $X \in \mathbb{R}^{n \times (m+1)}$, $y \in \mathbb{R}^n$, and $\theta \in \mathbb{R}^{m+1}$ be given. What is the result of the following operations (matrix, vector, or scalar), and what is the dimension?

$$ullet X^\intercal X$$
 $ullet X^\intercal y$ $ullet y^\intercal y$ $ullet \|X heta - y\|^2$

Question 2×2022 (Normal equation)

Let the training dataset

$$\mathcal{D}_{train} = \{(1, 2), (2, 1), (3, 3)\}$$

be given. Each training example is a tuple of the form (x, y), where $x \in \mathbb{R}$ is the only feature, and $y \in \mathbb{R}$ the corresponding label. Please work through the following questions:

1. Compute the optimal model parameters θ^* using the **normal equation**

$$oldsymbol{ heta}^\star = ig(oldsymbol{X}^\intercal oldsymbol{X}ig)^{-1} oldsymbol{X}^\intercal oldsymbol{y}.$$

Do not apply any regularization. Hint: Let $\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathbb{R}^{2 \times 2}$ be an invertible matrix. Its inverse is given by $\mathbf{A}^{-1} = \frac{1}{ad-bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$.

2. Figure 1 below plots the training dataset $\mathcal{D}_{\text{train}}$. Add the regression function of your model to the plot.

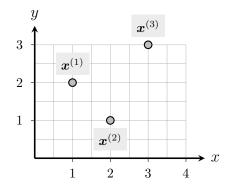


Figure 1: Plot of the training data set $\mathcal{D}_{\text{train}}$.

Question 3 2022 (Least squares error)

A colleague of yours provides you with a dedicated test dataset \mathcal{D}_{test} so that you can thoroughly validate the model you have trained in question 2:

$$\mathcal{D}_{test} = \{(0.5, 3), (1, 1.5), (2.5, 1), (3, 1.5)\}.$$

Each tuple has the same form as in question 2. Please answer the following questions:

- 1. Calculate the least squares error of your model from question 2 on the training dataset $\mathcal{D}_{\text{train}}$. Hint: Use $\boldsymbol{\theta}^* = \begin{pmatrix} 1 \\ 0.5 \end{pmatrix}$ in your calculations.
- 2. Compute the least squares error on $\mathcal{D}_{\text{test}}$! Hint: Use $\boldsymbol{\theta}^{\star} = \begin{pmatrix} 1 \\ 0.5 \end{pmatrix}$ in your calculations.
- 3. Figure 2 visualizes both datasets, \mathcal{D}_{train} and \mathcal{D}_{test} . How do you rate the model performance given figure 2 as well as the least squares errors you have computed on both datasets? What can you do to improve the model?

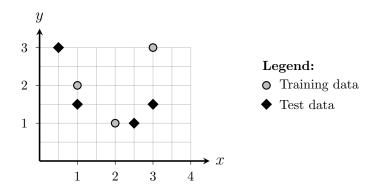


Figure 2: Plot of the complete dataset comprising train and test data.

Question 4 2022 (Regularization)

- ☐ Regularization mitigates the danger of underfitting.
- ☐ Regularization mitigates the danger of overfitting.
- \square The regularization parameter λ should be chosen as large as possible.
- \square The formula for ridge regression is given by $\boldsymbol{\theta}^{\star} = \left(\boldsymbol{X}^{\intercal} \boldsymbol{X} + \lambda \boldsymbol{I} \right)^{-1} \boldsymbol{X}^{\intercal} \boldsymbol{y}$.
- ☐ It is not possible to use regularization and basis functions simultaneously.

Question 5 2020, modified (Basis functions)

Name some examples of basis functions. Also do some research online: What other types exist? What is the purpose of basis functions? Can any function serve as a basis function?

Question 6 (Polynomial basis functions)

You are given the following dataset consisting of the two features x_1 and x_2 :

Row	x_1	x_2	y
1	3	2	5
2	1	1	4
3	4	3	2
4	1	2	3
5	6	1	1

Please compute the transformations $\varphi(x^{(i)})$ of the data points $x^{(i)}$ using the following polynomial basis functions:

$$oldsymbol{arphi}: \mathbb{R}^2
ightarrow \mathbb{R}^6, \qquad oldsymbol{arphi}(oldsymbol{x}) = egin{pmatrix} arphi_0(oldsymbol{x}) \ arphi_1(oldsymbol{x}) \ arphi_2(oldsymbol{x}) \ arphi_3(oldsymbol{x}) \ arphi_4(oldsymbol{x}) \ arphi_5(oldsymbol{x}) \end{pmatrix} = egin{pmatrix} 1 \ x_1 \ x_1 x_2^2 \ x_1^2 x_2^2 \ x_1^2 x_2 \ x_2^3 \ x_2^5 \ \end{pmatrix} \in \mathbb{R}^6.$$

Question 7 (Normal equation, polynomial basis functions, and regularization)

The following training dataset is presented to you (see figure 3):

$$\mathcal{D}_{train} = \{(1, 1/2), (2, 1), (3, 1/2), (4, 2)\}.$$

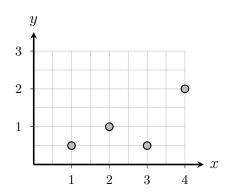


Figure 3: Plot of the training dataset $\mathcal{D}_{\text{train}}$.

Your task is to train a linear regression model on \mathcal{D}_{train} . Due to the fact that the data is slightly non linear, you decide to use **polynomial basis functions** to transform the features

in a non-linear fashion. You choose the feature functions

$$\varphi(x) = \begin{pmatrix} 1 \\ x \\ x^3 \end{pmatrix},$$

so that the model function will be of the form

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^3.$$

In order to prevent overfitting you decide to regularize the model using the regularization parameter $\lambda = 1/2$.

Please answer the following questions:

- 1. Compute the optimal model parameters θ^* . (It is a valuable exercise to compute it by hand, but you may also use software.)
- 2. What is the prediction for the unknown data point $x_q = 1/2$?