## Statistik un Data Science für die Informatik

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## Übungsblatt 5

## Task 1

Gegeben: 
$$\mathbf{x} = \begin{pmatrix} -2 \\ -1 \\ 0 \\ 1 \\ 2 \end{pmatrix} \in \mathbb{R}^{5x1}, \, \mathbf{y} = \begin{pmatrix} 2 \\ 0 \\ 0 \\ 2 \\ 6 \end{pmatrix} \in \mathbb{R}^{5x1} \text{ and } f(x) = a + bx.$$

To be found: a and b.

Let W be a weight matrix such that  $\mathbf{w} = \begin{pmatrix} a \\ b \end{pmatrix} \in \mathbb{R}^{2x_1}$ 

The loss function (i.e. the mean squared error (MSE) function) is defined as follows:

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i) = \frac{1}{n} ||Xw - y||^2.$$

The MSE function is continuous and differentiable. It also has one minimum, the global minimum. To find the solution to this equation (namely, to find the weights vector w with the least mean squared error), we need to compute the derivative of the loss function and set it to 0:

$$\frac{dL}{dw} = \begin{pmatrix} \frac{dL}{dw_0} \\ \frac{dL}{dw_1} \end{pmatrix} = 0$$

The closed-form solution:

$$\frac{dL}{dw} = \begin{pmatrix} \frac{dL}{dw_0} \\ \frac{dL}{dw_1} \end{pmatrix} = X^T X w - X^T y = 0 \quad 1 + X^T y$$

$$\iff X^T X w = X^T y \quad |*(X^T X)^{-1}|$$

$$\iff w = (X^T X)^{-1} X^T y$$

X is a design matrix (meaning it has an additional column of 1s to the original x vector to fully vectorize the computations):  $f(x) = a + bx = ax_1 + bx_2 = a * 1 + b * x_2$ .

$$X = \begin{pmatrix} 1 & -2 \\ 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \in \mathbb{R}^{5x2}, X^T = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \end{pmatrix} \in \mathbb{R}^{2x5}$$

$$X^{T}X = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 1 & -2 \\ 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 5 & 0 \\ 0 & 10 \end{pmatrix} \in \mathbb{R}^{2x2}$$

To compute the inverse of  $X^TX$  we need to apply Cramer's rule:

$$(X^TX)^{-1} = \frac{1}{det(X^TX)} \begin{pmatrix} (-1)^{1+1} det(X^TX_{11)} & (-1)^{2+1} det(X^TX_{21)} \\ (-1)^{1+2} det(X^TX_{12)} & (-1)^{2+2} det(X^TX_{22)} \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{11}) & (-1)^{2+1} det(X^TX_{21}) \\ (-1)^{1+2} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{11}) & (-1)^{2+1} det(X^TX_{21}) \\ (-1)^{1+2} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+1} det(X^TX_{21}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{12}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+1} det(X^TX_{21}) \\ (-1)^{1+2} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+1} det(X^TX_{22}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+1} det(X^TX_{22}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{22}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{22}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{22}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{12}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{12}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{12}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{12}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{12}) \\ (-1)^{1+2} det(X^TX) & (-1)^{2+2} det(X^TX_{12}) \end{pmatrix} = \frac{1}{det(X^TX)^{-1}} \begin{pmatrix} (-1)^{1+1} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{12}) \\ (-1)^{1+2} det(X^TX_{12}) & (-1)^{2+2} det(X^TX_{12}) \end{pmatrix}$$

$$=\frac{1}{det(X^TX)}\begin{pmatrix} det(X^TX_{11}) & -det(X^TX_{21}) \\ -det(X^TX_{12}) & det(X^TX_{22}) \end{pmatrix}$$

$$(X^T X)^{-1} = \frac{1}{50} \begin{pmatrix} 10 & 0 \\ 0 & 5 \end{pmatrix} = \begin{pmatrix} 0.2 & 0 \\ 0 & 0.1 \end{pmatrix} \in \mathbb{R}^{2x2}$$

$$X^{T}y = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} 2 \\ 0 \\ 0 \\ 2 \\ 6 \end{pmatrix} = \begin{pmatrix} 10 \\ 10 \end{pmatrix} \in \mathbb{R}^{2x1}$$

$$w = (X^T X)^{-1} X^T y = \begin{pmatrix} 0.2 & 0 \\ 0 & 0.1 \end{pmatrix} \begin{pmatrix} 10 \\ 10 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \in \mathbb{R}^{2x1}$$

$$\implies$$
  $w_0 = a = 2, w_1 = b = 1$ 

$$\implies f(x) = 2 + x.$$