

Technical University Munich Informatics



Introduction to Deep Learning (IN 2346)

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Exercise 2: Math Background

We use the following notations in this exercise:

- Scalars are denoted with lowercase letters. E.g. x, ϕ
- Vectors are denoted with bold lowercase letters. E.g. x, ϕ
- Matrices are denoted with bold uppercase letters. E.g. X, Σ

1 Linear algebra

Tasks:

a) Let

$$f(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^{\top} \boldsymbol{A} \boldsymbol{y} + \boldsymbol{x}^{\top} \boldsymbol{B} \boldsymbol{x} - \boldsymbol{C} \boldsymbol{y} + \boldsymbol{D}$$

with $\boldsymbol{x} \in \mathbb{R}^M, \boldsymbol{y} \in \mathbb{R}^N$, function $f : \mathbb{R}^M \times \mathbb{R}^N \to \mathbb{R}$.

Compute the dimensions of the matrices A, B, C, D for the function so that the mathematical expression is valid.

- b) Let $\boldsymbol{x} \in \mathbb{R}^N$, $\boldsymbol{M} \in \mathbb{R}^{N \times N}$. Express the function $f(\boldsymbol{x}) = \sum_{i=1}^N \sum_{j=1}^N x_i x_j M_{ij}$ using only matrix-vector multiplications.
- c) Suppose $u, v \in V$, where V is a vector space. ||u|| = ||v|| = 1 and $\langle u, v \rangle = 1$. Prove that u = v.

Note: In this task we define the norm as $\|v\| := \sqrt{\langle v, v \rangle}$, where $\langle u, v \rangle$ is the inner product between two vectors.

2 Linear Least Square

In this exercise, we want to determine the gradients for a few simple functions, which will be helpful for the upcoming lectures.

Note: Remember the definition of a *gradient*: The gradient of a scalar-valued function $f: \mathbb{R}^n \to \mathbb{R}$, denoted by ∇f , is a vector-valued function that gives, geometrically, the rate and direction of the steepest ascent of f at each point in \mathbb{R}^n . The components of the gradient are the partial derivatives of f with respect to each coordinate axis, and are written as:

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

where x_1, x_2, \ldots, x_n are the coordinates of a point in \mathbb{R}^n .

- a) For $\boldsymbol{x} \in \mathbb{R}^n$, let $f : \mathbb{R}^n \to \mathbb{R}$ with $f(\boldsymbol{x}) = \boldsymbol{b}^\top \boldsymbol{x}$ for some known vector $\boldsymbol{b} \in \mathbb{R}^n$. Determine the gradient of the function f.

 Hint: Use that $f(\boldsymbol{x}) = \boldsymbol{b}^\top \boldsymbol{x} = \sum_{i=1}^n b_i x_i$.
- b) Now consider the quadratic function $f: \mathbb{R}^n \to \mathbb{R}$ with $f(x) = x^\top Ax$ for a symmetric matrix $A \in \mathbb{S}_n$. Determine the gradient of the function f. Hint: A symmetric matrix $A \in \mathbb{S}_n$ satisfies that $A_{ij} = A_{ji}$ for all $1 \le i, j \le n$.
- c) Now let us go a step further and let us determine the derivative of the following function $f: \mathbb{R}^n \to \mathbb{R}$ with

$$f(x) = ||Ax - b||_2^2 = (Ax - b)^{\top} (Ax - b)$$

where $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\mathbf{b} \in \mathbb{R}^m$.

3 Calculus - derivatives

- a) Compute the derivatives for the following functions: $f_i : \mathbb{R} \to \mathbb{R}, i \in \{1, 2, 3\}$
 - $f_1: f_1(x) = (x^3 + x + 1)^2$
 - $f_2: f_2(x) = \frac{e^{2x}-1}{e^{2x}+1}$
 - $f_3: f_3(x) = (1-x)\log(1-x)$ (Note: In this course, $\log(x) = \log_e(x) = \ln(x)$)
- b) For a function $f: \mathbb{R}^n \to \mathbb{R}$, the gradient is defined as $\nabla f = (\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n})$. Calculate the gradients of the following functions: $f_i: \mathbb{R}^2 \to \mathbb{R}, i \in \{4,5\}$
 - $f_4: f_4(\boldsymbol{x}) = \frac{1}{2}||\boldsymbol{x}||_2^2$
 - $f_5: f_5(\boldsymbol{x}) = \frac{1}{2}||\boldsymbol{x}||_2$
- c) For a function $f: \mathbb{R}^n \to \mathbb{R}^m$, the *Jacobian* is defined as

$$\mathbb{J} = \begin{bmatrix}
\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\
\frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n}
\end{bmatrix}$$

Calculate the Jacobian matrix of the following functions: $f_i : \mathbb{R}^n \to \mathbb{R}^m$, $i \in \{6,7\}$

- $f_6: \mathbb{R} \times \mathbb{R} \to \mathbb{R}^2, f_6(r,\varphi) = (r\cos\varphi, r\sin\varphi)^{\top}$
- $f_7: \mathbb{R} \to \mathbb{R}^2, f_7(t) = (r\cos t, r\sin t)^{\top}$
- d) For a function $f: \mathbb{R}^n \to \mathbb{R}^n$ the divergence is defined as $\operatorname{div} f = \sum_{i=1}^N \frac{\partial f_i}{\partial x_i}$. Calculate the divergence for the following functions: $f_i: \mathbb{R}^n \to \mathbb{R}^n$, $i \in \{8, 9\}$
 - $f_8: \mathbb{R}^2 \to \mathbb{R}^2, f_8(x, y) = (-y, x)^\top$
 - $f_9: \mathbb{R}^2 \to \mathbb{R}^2, f_9(x, y) = (x, y)^\top$

4 Sigmoid derivative

In this question we will derive the derivative of the sigmoid function:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

As seen in lecture 02, the sigmoid function is a popular activation function used in machine learning, which maps any input value to a value between 0 and 1. In logistic regression, the sigmoid function is used to map the output of the regression algorithm to a probability between 0 and 1, which can be interpreted as the probability of an input belonging to a particular class. This probability is then used to make a binary decision about whether the input belongs to the class or not.

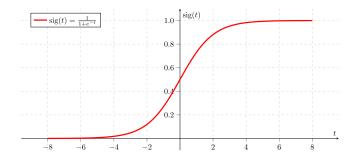


Figure 1: The sigmoid function

- a) Find the derivative of the sigmoid function: $\frac{\partial \sigma(x)}{\partial x}$
- b) Show that the derivative expression that you've found in the previous task could be represented with the sigmoid function iteslf, i.e.:

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1 - \sigma(x))$$

Hint: $e^{-x} = e^{-x} + 1 - 1$

5 Softmax derivative

In this exercise, we want to take a look at the softmax function, which is a common activation function in neural networks in order to normalize the output of a network to a probability distribution over predicted output classes. We will discuss the softmax function later in this lecture in more detail.

The softmax function $\sigma: \mathbb{R}^n \to \mathbb{R}^n$ is defined by

$$\sigma(z)_i = \frac{e^{z_i}}{\sum_{j=1}^n e^{z_j}}$$

for $1 \le i \le n$ and $z = \begin{pmatrix} z_1 & z_2 & \dots & z_n \end{pmatrix} \top$. In the expanded form, we write:

$$\hat{y} = \sigma(z_1, z_2, \dots z_n) = \left[\frac{e^{z_1}}{\sum_{k=1}^n e^{z_k}}, \frac{e^{z_2}}{\sum_{k=1}^n e^{z_k}}, \dots, \frac{e^{z_n}}{\sum_{k=1}^n e^{z_k}} \right].$$

Determine the derivative of the softmax function.

Hint: Deriving $\sigma(z)$ with respect to z will lead to $n \times n$ partial derivatives, i.e. $\frac{\partial \sigma(z)_i}{\partial z_j}$ for $1 \le i, j \le n$. It is important to consider the two cases (1) i = j and (2) $i \ne j$

6 Probability

a) Variance.

We say that two random variables X, Y are independent if and only if the joint cumulative distribution function $F_{X,Y}(x,y)$ satisfies

$$F_{X,Y}(x,y) = F_X(x)F_Y(y).$$

In the case of independence, the following property holds for these variables: Let f, g be two real-valued functions defined on the codomains of X, Y, respectively. Then

$$\mathbb{E}[g(X)h(Y)] = \mathbb{E}[g(X)] \cdot \mathbb{E}[h(Y)].$$

Assume that X, Y are two random variables that are independent and identical distributed (i.i.d.) with $X, Y \sim \mathcal{N}(0, \sigma^2)$. Prove that

$$Var(XY) = Var(X)Var(Y)$$

Remember this property, as it will play an important role at a later point of the lecture, when we take a look at the initialization of the weights of a neural network (Xavier initialization).

b) Normal distribution.

Remark: The family of random variables that are normally distributed is closed under linear transformation, that means if X is normally distributed, then for every $a, b \in \mathbb{R}$ the random variable aX + b is normally distributed.

For this exercise, assume that the random variable X is normally distributed with mean μ and variance σ^2 , i.e. $X \sim \mathcal{N}(\mu, \sigma^2)$. Let $Z = \frac{X - \mu}{\sigma}$. From the remark, we know that Z is again normally distributed. Determine the mean and the variance of the random variable Z.