

Exercise 2: Math Background (Solution)

1 Linear algebra

a) $\mathbf{A} \in \mathbb{R}^{M \times N}$, $\mathbf{B} \in \mathbb{R}^{M \times M}$, $\mathbf{C} \in \mathbb{R}^{1 \times N}$, $\mathbf{D} \in \mathbb{R}^{1 \times 1}$.

b) $f(\mathbf{x}) = \sum_{i=1}^N \sum_{j=1}^N x_i x_j M_{ij} = \sum_{i=1}^N x_i \sum_{j=1}^N x_j M_{ij} = \sum_{i=1}^N x_i (\mathbf{M} \cdot \mathbf{x})_i = \mathbf{x}^\top \mathbf{M} \mathbf{x}$.

c) Proof: Consider $\|\mathbf{u} - \mathbf{v}\|^2$, we have:

$$\begin{aligned} \|\mathbf{u} - \mathbf{v}\|^2 &= \langle \mathbf{u} - \mathbf{v}, \mathbf{u} - \mathbf{v} \rangle \\ &= \langle \mathbf{u}, \mathbf{u} \rangle - \langle \mathbf{u}, \mathbf{v} \rangle - \langle \mathbf{v}, \mathbf{u} \rangle + \langle \mathbf{v}, \mathbf{v} \rangle \\ &= \|\mathbf{u}\|^2 - 2\langle \mathbf{u}, \mathbf{v} \rangle + \|\mathbf{v}\|^2 \\ &= 0 \end{aligned}$$

Hence, $\mathbf{u} = \mathbf{v}$.

* $\|x\|$ refers to the L2-norm $\|x\|_2$, unless stated otherwise.

2 Linear Least Square

a) By definition of the gradient, we need to determine $\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{pmatrix}$. For $1 \leq k \leq n$, we

have

$$\frac{\partial f(\mathbf{x})}{\partial x_k} = \frac{\partial}{\partial x_k} \left(\sum_{i=1}^n b_i x_i \right) = \sum_{i=1}^n \frac{\partial}{\partial x_k} (b_i x_i) = \sum_{i=1}^n \delta_{ik} b_i = b_k.$$

The Kronecker delta is defined as follows: $\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$

Hence, we obtain $\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{pmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = \mathbf{b}$.

- b) To determine the gradient of the function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A} \mathbf{x}$, where \mathbf{A} is a symmetric matrix in \mathbb{S}_n , we can use the definition of the gradient:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right]$$

We start by computing the partial derivative of f with respect to x_i .

$$\begin{aligned} \frac{\partial f}{\partial x_i} &= \frac{\partial}{\partial x_i} (\mathbf{x}^\top \cdot (\mathbf{A} \mathbf{x})) = \frac{\partial \mathbf{x}^\top}{\partial x_i} \cdot (\mathbf{A} \mathbf{x}) + \mathbf{x}^\top \cdot \frac{\partial (\mathbf{A} \mathbf{x})}{\partial x_i} = \mathbf{e}_i^\top \cdot (\mathbf{A} \mathbf{x}) + \mathbf{x}^\top \cdot \mathbf{A} \mathbf{e}_i \\ &= \sum_j A_{ij} x_j + \sum_j A_{ij} x_j = 2 \sum_j A_{ij} x_j = 2(\mathbf{A} \mathbf{x})_i \end{aligned}$$

where \mathbf{e}_i is the standard basis vector in the i 'th direction (1 at the i 'th, and all other entries are 0's).

Thus, the gradient of f is:

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = [2(\mathbf{A} \mathbf{x})_1, 2(\mathbf{A} \mathbf{x})_2, \dots, 2(\mathbf{A} \mathbf{x})_n] = 2\mathbf{A} \mathbf{x}$$

Therefore, the gradient of the quadratic function $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A} \mathbf{x}$ is $\frac{\partial f}{\partial \mathbf{x}} = 2\mathbf{A} \mathbf{x}$.

- c) Let us first rewrite the expression:

$$\begin{aligned} f(\mathbf{x}) &= \|\mathbf{A} \mathbf{x} - \mathbf{b}\|_2^2 \\ &= (\mathbf{A} \mathbf{x} - \mathbf{b})^\top (\mathbf{A} \mathbf{x} - \mathbf{b}) \\ &= ((\mathbf{A} \mathbf{x})^\top - \mathbf{b}^\top) (\mathbf{A} \mathbf{x} - \mathbf{b}) \\ &= (\mathbf{x}^\top \mathbf{A}^\top - \mathbf{b}^\top) (\mathbf{A} \mathbf{x} - \mathbf{b}) \\ &= \mathbf{x}^\top \mathbf{A}^\top \mathbf{A} \mathbf{x} - \mathbf{x}^\top \mathbf{A}^\top \mathbf{b} - \mathbf{b}^\top \mathbf{A} \mathbf{x} + \mathbf{b}^\top \mathbf{b} \\ &= \mathbf{x}^\top \mathbf{A}^\top \mathbf{A} \mathbf{x} - 2\mathbf{x}^\top \mathbf{A}^\top \mathbf{b} + \mathbf{b}^\top \mathbf{b}. \end{aligned}$$

Note that $\mathbf{x}^\top \mathbf{A}^\top \mathbf{b} = \mathbf{b}^\top \mathbf{A} \mathbf{x}$, because both result with a scalar. Since if $s \in \mathbb{R} \rightarrow s^\top = s \rightarrow \mathbf{x}^\top \mathbf{A}^\top \mathbf{b} = (\mathbf{x}^\top \mathbf{A}^\top \mathbf{b})^\top = \mathbf{b}^\top \mathbf{A} \mathbf{x}$.

Thus, by using part a) $\rightarrow \frac{\partial \mathbf{b}^\top \mathbf{x}}{\partial \mathbf{x}} = \mathbf{b}$ and b) $\rightarrow \frac{\partial \mathbf{x}^\top \mathbf{B} \mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{B} \mathbf{x}$ (\mathbf{B} is symmetric), we obtain:

$$\begin{aligned} \nabla_{\mathbf{x}} f(\mathbf{x}) &= \nabla_{\mathbf{x}} (\mathbf{x}^\top \mathbf{A}^\top \mathbf{A} \mathbf{x} - 2\mathbf{x}^\top \mathbf{A}^\top \mathbf{b} + \mathbf{b}^\top \mathbf{b}) = \nabla_{\mathbf{x}} \mathbf{x}^\top \mathbf{A}^\top \mathbf{A} \mathbf{x} - \nabla_{\mathbf{x}} 2\mathbf{x}^\top \mathbf{A}^\top \mathbf{b} + 0 \\ &= 2\mathbf{A}^\top \mathbf{A} \mathbf{x} - 2\mathbf{A}^\top \mathbf{b} = 2\mathbf{A}^\top (\mathbf{A} \mathbf{x} - \mathbf{b}) \end{aligned}$$

3 Calculus - derivatives

a) The derivatives are:

- $f_1'(x) = [(x^3 + x + 1)^2]' = 2(x^3 + x + 1)(x^3 + x + 1)' = 2(x^3 + x + 1)(3x^2 + 1)$
- $f_2'(x) = \left[\frac{e^{2x}-1}{e^{2x}+1}\right]' = \frac{(e^{2x}-1)'(e^{2x}+1) - (e^{2x}-1)(e^{2x}+1)'}{(e^{2x}+1)^2} = \frac{2e^{2x}(e^{2x}+1) - (e^{2x}-1)2e^{2x}}{(e^{2x}+1)^2} = \frac{4e^{2x}}{(e^{2x}+1)^2}$
- $f_3'(x) =$
 $= [(1-x)\log(1-x)]'$
 $= \log(1-x) \cdot (1-x)' + (1-x) \cdot \log'(1-x)$
 $= -\log(1-x) + (1-x) \cdot \frac{\partial \log(y)}{y} \cdot \frac{y}{x} = -\log(1-x) + (1-x) \cdot \frac{1}{1-x} \cdot (1-x)'$
 $= -\log(1-x) - 1$

b) The gradients are:

- $\nabla f_4 = \frac{\partial}{\partial \mathbf{x}} \left(\frac{1}{2}\|\mathbf{x}\|_2^2\right) = \frac{\partial}{\partial \mathbf{x}} \left(\frac{1}{2}\mathbf{x}^\top \mathbf{x}\right) = \frac{\partial}{\partial \mathbf{x}} \left(\frac{1}{2}\mathbf{x}^\top I \mathbf{x}\right) = \frac{1}{2} \cdot 2I \mathbf{x} = \mathbf{x}$
- $\nabla f_5 = \frac{\partial}{\partial \mathbf{x}} \left(\frac{1}{2}\|\mathbf{x}\|_2\right) = \frac{\partial}{\partial \mathbf{x}} \left(\frac{1}{2}\sqrt{\mathbf{x}^\top \mathbf{x}}\right) = \frac{1}{2} \cdot \frac{1}{2}(\mathbf{x}^\top \mathbf{x})^{-\frac{1}{2}} \cdot \frac{\partial(\mathbf{x}^\top \mathbf{x})}{x} = \frac{1}{2} \cdot \frac{1}{2}(\mathbf{x}^\top \mathbf{x})^{-\frac{1}{2}} \cdot 2I \mathbf{x} = \frac{1}{2} \frac{\mathbf{x}}{\|\mathbf{x}\|_2}$

c) The Jacobians are:

- $J_{f_6} = \begin{bmatrix} \frac{\partial f_1}{\partial r} & \frac{\partial f_1}{\partial \varphi} \\ \frac{\partial f_2}{\partial r} & \frac{\partial f_2}{\partial \varphi} \end{bmatrix} = \begin{bmatrix} \cos(\varphi) & -r \sin(\varphi) \\ \sin(\varphi) & r \cos(\varphi) \end{bmatrix}$
- $J_{f_7} = \begin{bmatrix} \frac{\partial f_1}{\partial t} \\ \frac{\partial f_2}{\partial t} \end{bmatrix} = \begin{bmatrix} -r \sin t \\ r \cos t \end{bmatrix}$

d) The divergences are:

- $\operatorname{div} f_8 = \frac{\partial(-y)}{\partial x} + \frac{\partial x}{\partial y} = 0$
- $\operatorname{div} f_9 = \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} = 2$

4 Sigmoid derivative

a)

$$\frac{d}{dx}\sigma(x) = \frac{d}{dx}\frac{1}{1+e^{-x}} = \frac{d}{dx}(1+e^{-x})^{-\frac{1}{2}} = \frac{-(1+e^{-x})^{-2}(-e^{-x})}{(1+e^{-x})^2} = \frac{e^{-x}}{(1+e^{-x})^2}$$

b)

$$\begin{aligned} & \frac{e^{-x}}{(1+e^{-x})^2} \\ &= \frac{e^{-x} + 1 - 1}{(1+e^{-x})^2} \\ &= \frac{1+e^x}{(1+e^x)^2} - \frac{1}{(1+e^{-x})^2} \\ &= \frac{1}{1+e^{-x}} - \frac{1}{(1+e^{-x})^2} \\ &= \frac{1}{1+e^{-x}} \left(1 - \frac{1}{1+e^{-x}}\right) \\ &= \sigma(x)(1 - \sigma(x)) \end{aligned}$$

5 Softmax derivative

5.1 1st approach - two cases

When deriving $\sigma(z)$ with respect to z , there are $n \times n$ partial derivatives but we notice that they reduce to only two distinct kinds:

- $\hat{y}_i = \sigma(z)_i$ w.r.t z_i . For example, deriving $\frac{e^{z_1}}{\sum_{k=1}^n e^{z_k}}$ w.r.t z_1 . (z_1 appears both in the nominator and in the denominator)
- $\hat{y}_i = \sigma(z)_i$ w.r.t $z_j, i \neq j$. For example, deriving $\frac{e^{z_1}}{\sum_{k=1}^n e^{z_k}}$ w.r.t z_2 (z_2 appears only in the denominator).

We first derive the first kind:

$$\begin{aligned} \frac{\partial \hat{y}_1}{\partial z_1} &= \partial \left(\frac{e^{z_1}}{\sum_{k=1}^n e^{z_k}} \right) / \partial z_1 = \frac{e^{z_1} \cdot \sum_{k=1}^n e^{z_k} - e^{z_1} \cdot e^{z_1}}{\left(\sum_{k=1}^n e^{z_k}\right) \left(\sum_{k=1}^n e^{z_k}\right)} = \frac{e^{z_1} (\sum_{k=1}^n e^{z_k} - e^{z_1})}{\left(\sum_{k=1}^n e^{z_k}\right) \left(\sum_{k=1}^n e^{z_k}\right)} = \\ &= \frac{e^{z_1}}{\left(\sum_{k=1}^n e^{z_k}\right)} \cdot \frac{\sum_{k=1}^n e^{z_k} - e^{z_1}}{\left(\sum_{k=1}^n e^{z_k}\right)} = \hat{y}_1 \cdot \left(1 - \frac{e^{z_1}}{\sum_{k=1}^n e^{z_k}}\right) = \hat{y}_1 \cdot (1 - \hat{y}_1). \end{aligned}$$

In the last and second to last equality, we used a trick, or the observation, that we can express these terms in means of \hat{y} . In a similar fashion, we derive the second kind:

$$\frac{\partial \hat{y}_1}{\partial z_2} = \partial \left(\frac{e^{z_1}}{\sum_{k=1}^n e^{z_k}} \right) / \partial z_2 = \frac{0 \cdot \sum_{k=1}^n e^{z_k} - e^{z_2} \cdot e^{z_1}}{\left(\sum_{k=1}^n e^{z_k}\right) \left(\sum_{k=1}^n e^{z_k}\right)} = -\frac{e^{z_2}}{\left(\sum_{k=1}^n e^{z_k}\right)} \cdot \frac{e^{z_1}}{\left(\sum_{k=1}^n e^{z_k}\right)} = -\hat{y}_1 \hat{y}_2.$$

In conclusion, the partial derivatives of the softmax layer $\hat{y} = \sigma(z)$ with respect to its input z are given by:

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i \cdot (1 - \hat{y}_i) & i = j \\ -\hat{y}_i \hat{y}_j & i \neq j \end{cases}$$

5.2 2nd approach - solve all in one!

A nice trick to solve both cases in one. First, we derive:

$$\frac{\partial \log(s_i)}{\partial z_j} = \frac{1}{s_i} \frac{\partial s_i}{\partial z_j}$$

Therefore:

$$\begin{aligned} \frac{\partial s_i}{\partial z_j} &= s_i \cdot \frac{1}{s_i} \frac{\partial s_i}{\partial z_j} = s_i \cdot \frac{\partial \log(s_i)}{\partial z_j} = s_i \frac{\partial}{\partial z_j} \log\left(\frac{e^{z_i}}{\sum_{k=1}^C e^{z_k}}\right) = s_i \frac{\partial}{\partial z_j} [z_i - \log\left(\sum_{k=1}^C e^{z_k}\right)] \\ &= s_i (\delta_{ij} - \frac{1}{\sum_{k=1}^C e^{z_k}} e^{z_j}) = s_i (\delta_{ij} - s_j) \end{aligned}$$

With

$$\begin{cases} \delta_{ij} = 1 & i = j \\ \delta_{ij} = 0 & i \neq j \end{cases}$$

6 Probability

a) We use the definition of the variance, namely

$$\text{Var}(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2 \quad (1)$$

and equivalently,

$$\mathbb{E}[X^2] = \text{Var}(X) + \mathbb{E}[X]^2. \quad (2)$$

Since $X, Y \sim \mathcal{N}(0, \sigma^2)$, we are given that $\mathbb{E}[X] = \mathbb{E}[Y] = 0$. With these observations, we obtain

$$\begin{aligned} \text{Var}(XY) &\stackrel{(1)}{=} \mathbb{E}[X^2Y^2] - \mathbb{E}[XY]^2 \\ &\stackrel{(*)}{=} \mathbb{E}[X^2]\mathbb{E}[Y^2] - \mathbb{E}[X]^2\mathbb{E}[Y]^2 \\ &\stackrel{(2)}{=} (\text{Var}(X) + \mathbb{E}[X]^2)(\text{Var}(Y) + \mathbb{E}[Y]^2) - \mathbb{E}[X]^2\mathbb{E}[Y]^2 \\ &= \text{Var}(X)\text{Var}(Y) + \underbrace{\text{Var}(X)\mathbb{E}[Y]^2}_{=0} + \underbrace{\text{Var}(Y)\mathbb{E}[X]^2}_{=0} \\ &= \text{Var}(X)\text{Var}(Y) \end{aligned}$$

(*) X, Y are independent.

b) We use the properties of the expectation and the variance of a random variable. For the mean of Z , we observe:

$$\begin{aligned} \mathbb{E}[Z] &= \mathbb{E}\left[\frac{X - \mu}{\sigma}\right] \\ &= \frac{1}{\sigma} \cdot \mathbb{E}[X - \mu] \\ &= \frac{1}{\sigma} \cdot (\mathbb{E}[X] - \mathbb{E}[\mu]) \\ &= \frac{1}{\sigma} \cdot (\mu - \mu) \\ &= 0 \end{aligned}$$

For the variance, remember that:

$$\begin{aligned} \text{Var}\left[\frac{X - \mu}{\sigma}\right] &= \mathbb{E}\left[\left(\frac{X - \mu}{\sigma} - \mathbb{E}\left[\frac{X - \mu}{\sigma}\right]\right)^2\right] \\ &= \mathbb{E}\left[\left(\frac{X - \mu}{\sigma} - \frac{\mathbb{E}[X] - \mu}{\sigma}\right)^2\right] \\ &= \mathbb{E}\left[\left(\frac{X - \mathbb{E}[X]}{\sigma}\right)^2\right] \\ &= \frac{1}{\sigma^2} \mathbb{E}[(X - \mathbb{E}[X])^2] \\ &= \frac{1}{\sigma^2} \cdot \text{Var}[X]. \end{aligned}$$

Therefore, we observe that:

$$\begin{aligned}\text{Var}[Z] &= \text{Var}\left[\frac{X - \mu}{\sigma}\right] \\ &= \frac{1}{\sigma^2} \text{Var}[X] \\ &= \frac{1}{\sigma^2} \sigma^2 \\ &= 1.\end{aligned}$$

In summary, we conclude that $Z \sim \mathcal{N}(0, 1)$.