Exercise 2: Math Background (Solution)

Exercise 1.1

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

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

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

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

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

Exercise 1.2

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

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

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 $\nabla_x f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$.

b) Similar to the first part, we obtain $f(x) = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij} x_i x_j$ and the partial derivative of the variable x_k with $1 \leq k \leq n$ is

$$\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k}\left(\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_ix_j\right) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial}{\partial x_k}\left(A_{ij}x_ix_j\right) \\
&= \sum_{j=1,j\neq k}^{n} \frac{\partial}{\partial x_k}\left(x_kA_{kj}x_j\right) + \sum_{i=1,i\neq k}^{n} \frac{\partial}{\partial x_k}\left(A_{ik}x_ix_k\right) + \frac{\partial}{\partial x_k}\left(A_{kk}x_k^2\right) \\
&= \sum_{j=1,j\neq k}^{n} A_{kj}x_j + \sum_{i=1,i\neq k}^{n} A_{ik}x_i + 2A_{kk}x_k \\
&= \sum_{j=1}^{n} A_{kj}x_j + \sum_{i=1}^{n} A_{ik}x_i \\
&\overset{A\in\mathbb{S}_n}{=} 2\cdot\sum_{j=1}^{n} A_{kj}x_j \\
&= 2\cdot(Ax)_k.
\end{aligned}$$

Hence, we obtain $\nabla_x f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{pmatrix} = \begin{pmatrix} 2\cdot(Ax)_1 \\ 2\cdot(Ax)_2 \\ \vdots \\ 2\cdot(Ax)_n \end{pmatrix} = 2Ax.$

c) Let us first rewrite the expression:

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

Using part (a) and (b), we obtain

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

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Exercise 1.3

a) The derivatives are:

- $f_1'(x) = \left[(x^3+x+1)^2\right]' = 2(x^3+x+1)(x^3+x+1)' = 2(x^3+x+1)(3x^2+1)$

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

b) The gradients are:

- $\nabla f_4 = (x_1, x_2)^\top = \mathbf{x}$
- $\nabla f_5 = \frac{1}{2}(x_1^2 + x_2^2)^{-\frac{1}{2}}(x_1, x_2)^\top = \frac{1}{2}\frac{\mathbf{x}}{\|\mathbf{x}\|_2}$

c) The Jacobians are:

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

d) The divergences are:

- $\mathrm{div} f_8 = 0$
- $\mathrm{div} f_9 = 2$

Exercise 1.4

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

- $\sigma(z)_i$ 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)
- $\sigma(z)_i$ 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:

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

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:

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

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

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

Exercise 1.5

a) We use the definition of the variance, namely

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

and equivalently,

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

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

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

$(*) X, Y$ 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, we observe:

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

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