

## Homework Set 3

Introduction to Artificial Intelligence with Mathematics (MAS473)

Total Points = 50pts

1. (5pts) Consider the EM algorithm of a Gaussian mixture model

$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x} | \mu_k, \Sigma_k)$$

in our lecture. Assume that  $\Sigma_k = \epsilon I$  for all  $k = 1, \dots, K$ . Letting  $\epsilon \rightarrow 0$ , prove that the limiting case is equivalent to the  $K$ -means clustering.

*Solution.* From the assumption, we can calculate in the same way as the general GMM model and we can see that the EM algorithm of the given model is

- (E-step) Using the current parameters  $\theta = \{\mu_1, \dots, \mu_K, \pi_1, \dots, \pi_K\}$ , compute

$$p(z_{ik} = 1 | \mathbf{x}_i) = \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \mu_k, \epsilon I)}{\sum_{l=1}^K \pi_l \mathcal{N}(\mathbf{x}_i | \mu_l, \epsilon I)}.$$

- (M-step) Update all parameters  $\theta$

$$\begin{aligned} \mu_k &= \sum_{i=1}^N \frac{p(z_{ik} = 1 | \mathbf{x}_i)}{\sum_{j=1}^N p(z_{jk} = 1 | \mathbf{x}_j)} \mathbf{x}_i, \\ \pi_k &= \frac{1}{N} \sum_{i=1}^N p(z_{ik} = 1 | \mathbf{x}_i). \end{aligned}$$

- Repeat E-step and M-step until convergence.

Letting  $\epsilon \rightarrow 0$ ,

$$p(z_{ik} = 1 | \mathbf{x}_i) = \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \mu_k, \epsilon I)}{\sum_{l=1}^K \pi_l \mathcal{N}(\mathbf{x}_i | \mu_l, \epsilon I)} = \frac{\pi_k \cdot \exp(-\|\mathbf{x}_i - \mu_k\|^2 / 2\epsilon)}{\sum_{l=1}^K \pi_l \cdot \exp(-\|\mathbf{x}_i - \mu_l\|^2 / 2\epsilon)}$$

converges to  $\frac{1}{|\mathcal{I}_i|} \mathbf{1}_{\{k \in \mathcal{I}_i\}}$  where  $\mathcal{I}_i = \operatorname{argmin}_j \|\mathbf{x}_i - \mu_j\|^2$ . By the further assumption :

At any time,  $\mu_1, \dots, \mu_K$  satisfy that  $\operatorname{argmin}_{j \in \{1, \dots, K\}} \|\mathbf{x}_i - \mu_j\|^2$  has only 1 element for all  $i = 1, \dots, N$

E-step is equivalent to E-step of  $K$ -means clustering algorithm if we set  $r_{ik} = \frac{1}{|\mathcal{I}_i|} \mathbf{1}_{\{k \in \mathcal{I}_i\}}$ . Then the update rule for  $\mu_1, \dots, \mu_K$  in M-step is same as M-step of  $K$ -means clustering.  $\pi_1, \dots, \pi_K$  does not affect  $p(z_{ik} = 1 | \mathbf{x}_i)$  and  $\mu_k$  as long as  $\pi_1, \dots, \pi_K > 0$ .

2. (15pts) **(Latent Class Analysis)** Consider a  $D$ -dimensional random vector  $\mathbf{x}_0 = [x_1, \dots, x_D]$  where  $x_i \sim \text{Bernoulli}(\mu_i)$  ( $i = 1, \dots, D$ ) are independent. Now we consider a mixture model of distributions of random vectors like  $\mathbf{x}_0$ . In other words, consider

$$p(\mathbf{x}|\mu, \pi) = \sum_{k=1}^K \pi_k p(\mathbf{x}|\mu_k)$$

where  $\mu = [\mu_1, \dots, \mu_K]$ ,  $\mu_k = [\mu_{k1}, \dots, \mu_{kD}] \in [0, 1]^D$  for any  $k = 1, \dots, K$ ,  $\pi = [\pi_1, \dots, \pi_K] \in \Delta^{K-1} = \{[y_1, \dots, y_K] \in \mathbb{R}^K : y_i \geq 0 \text{ for any } i = 1, \dots, K \text{ and } \sum_{i=1}^K y_i = 1\}$  and

$$p(\mathbf{x}|\mu_k) = \prod_{i=1}^D \mu_{ki}^{x_i} (1 - \mu_{ki})^{1-x_i}.$$

Assume  $\mathcal{D} = \{\mathbf{x}_i : 1 \leq i \leq N\}$  is a given dataset. Using the similar argument as Gaussian mixture models, prove that the EM algorithm for this model is

- Initialization
- (E-step) Using the current parameters, compute

$$p(z_{ik} = 1|\mathbf{x}_i) = \frac{\pi_k p(\mathbf{x}_i|\mu_k)}{\sum_{l=1}^K \pi_l p(\mathbf{x}_i|\mu_l)}$$

- (M-step) Update all parameters

$$\begin{aligned} \mu_k &= \frac{\sum_{i=1}^N p(z_{ik} = 1|\mathbf{x}_i) \mathbf{x}_i}{\sum_{i=1}^N p(z_{ik} = 1|\mathbf{x}_i)} \\ \pi_k &= \frac{1}{N} \sum_{i=1}^N p(z_{ik} = 1|\mathbf{x}_i) \end{aligned}$$

- Repeat E-step and M-step until convergence.

where  $\mathbf{z}_i = [\mathbf{z}_{i1}, \dots, \mathbf{z}_{iK}]$  is a one-hot vector which indicates that a group containing  $\mathbf{x}_i$ .

*Solution.* Note that

$$\begin{aligned} p(\mathbf{x}_i|\mathbf{z}_i = 1) &= \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}}, \\ p(\mathbf{x}_i|\mathbf{z}_i = 1) &= \prod_{k=1}^K \left( \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}} \right)^{z_{ik}}. \end{aligned}$$

Then

$$p(\mathbf{x}_i, \mathbf{z}_i) = p(\mathbf{x}_i|\mathbf{z}_i) p(\mathbf{z}_i) = \prod_{k=1}^K \left( \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}} \right)^{z_{ik}}.$$

Moreover,

$$p(z_{ik} = 1|\mathbf{x}_i) = \frac{p(z_{ik} = 1, \mathbf{x}_i)}{p(\mathbf{x}_i)} = \frac{p(\mathbf{x}_i|z_{ik} = 1)p(z_{ik} = 1)}{\sum_{l=1}^K p(\mathbf{x}_i|z_{il} = 1)p(z_{il} = 1)} = \frac{\pi_k p(\mathbf{x}_i|\mu_k)}{\sum_{l=1}^K \pi_l p(\mathbf{x}_i|\mu_l)}.$$

From the log likelihood function of  $\mathbf{x}$

$$J(\mu, \pi) = \sum_{i=1}^N \log p(\mathbf{x}_i | \mu, \pi) = \sum_{i=1}^N \log \left( \sum_{k=1}^K \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}} \right),$$

we have

$$\begin{aligned} \nabla_{\mu_l} J(\mu, \pi) &= \sum_{i=1}^N \frac{\pi_l \prod_{j=1}^D \mu_{lj}^{\mathbf{x}_{ij}} (1 - \mu_{lj})^{1-\mathbf{x}_{ij}}}{\sum_{k=1}^K \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}}} \cdot ((1 - \mathbf{x}_i) \odot \mu_l - (1 - \mathbf{x}_i) \odot (1 - \mu_l)) \\ &= \sum_{i=1}^N \frac{\pi_l \prod_{j=1}^D \mu_{lj}^{\mathbf{x}_{ij}} (1 - \mu_{lj})^{1-\mathbf{x}_{ij}}}{\sum_{k=1}^K \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}}} \cdot ((\mathbf{x}_i - \mu_l) \odot (\mu_l(1 - \mu_l))) \end{aligned}$$

From  $\nabla_{\mu_l} J(\mu, \pi) = 0$ , we obtain

$$(\mu_l(1 - \mu_l)) \odot \nabla_{\mu_l} J(\mu, \pi) = \sum_{i=1}^N \frac{\pi_l \prod_{j=1}^D \mu_{lj}^{\mathbf{x}_{ij}} (1 - \mu_{lj})^{1-\mathbf{x}_{ij}}}{\sum_{k=1}^K \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}}} \cdot (\mathbf{x}_i - \mu_l) = 0.$$

It then follows that

$$\mu_l = \frac{\sum_{i=1}^N p(z_{ik} = 1 | \mathbf{x}_i) \mathbf{x}_i}{\sum_{i=1}^N p(z_{ik} = 1 | \mathbf{x}_i)}.$$

To maximizing the log likelihood function with a constraint  $\sum_{k=1}^K \pi_k = 1$  w.r.t.  $\{\pi_k : k = 1, \dots, K\}$ , we introduce a Lagrange multiplier  $\lambda$  :

$$\mathcal{L}(\mu, \pi) = J(\mu, \pi) + \lambda \cdot \left( \sum_{k=1}^K \pi_k - 1 \right).$$

From  $\frac{\partial}{\partial \pi} \mathcal{L}(\mu, \pi) = 0$ , i.e.

$$\sum_{i=1}^N \frac{\prod_{j=1}^D \mu_{lj}^{\mathbf{x}_{ij}} (1 - \mu_{lj})^{1-\mathbf{x}_{ij}}}{\sum_{k=1}^K \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}}} + \lambda = 0, \quad 1 \leq k \leq K,$$

we get

$$\frac{1}{\pi_k} \sum_{i=1}^N \frac{\pi_k \prod_{j=1}^D \mu_{lj}^{\mathbf{x}_{ij}} (1 - \mu_{lj})^{1-\mathbf{x}_{ij}}}{\sum_{k=1}^K \pi_k \prod_{j=1}^D \mu_{kj}^{\mathbf{x}_{ij}} (1 - \mu_{kj})^{1-\mathbf{x}_{ij}}} + \lambda = 0, \quad 1 \leq k \leq K.$$

Thus,

$$\pi_k = -\frac{1}{\lambda} \sum_{i=1}^N p(z_{ik} = 1 | \mathbf{x}_i).$$

From the constraint,

$$\sum_{k=1}^K \pi_k = -\sum_{k=1}^K \frac{1}{\lambda} \sum_{i=1}^N p(z_{ik} = 1 | \mathbf{x}_i) = -\sum_{i=1}^N \sum_{k=1}^K \frac{1}{\lambda} p(z_{ik} = 1 | \mathbf{x}_i) = -N.$$

Therefore, we get

$$\pi_k = \frac{1}{N} \sum_{i=1}^N p(z_{ik} = 1 | \mathbf{x}_i).$$

3. (10pts) Prove that

$$\mathcal{N}(\mathbf{x}|\mathbf{a}, A)\mathcal{N}(\mathbf{x}|\mathbf{b}, B) = Z^{-1}\mathcal{N}(\mathbf{x}|\mathbf{c}, C)$$

where

$$\mathbf{c} = C(A^{-1}\mathbf{a} + B^{-1}\mathbf{b}), C = (A^{-1} + B^{-1})^{-1}, \text{ and } Z^{-1} = (2\pi)^{-D/2}|A+B|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{a} - \mathbf{b})^\top (A + B)^{-1}(\mathbf{a} - \mathbf{b})\right).$$

Also, prove that

$$(Z + U W V^\top)^{-1} = Z^{-1} - Z^{-1}U(W^{-1} + V^\top Z^{-1}U)^{-1}V^\top Z^{-1}$$

where  $Z \in \mathbb{R}^{n \times n}$ ,  $W \in \mathbb{R}^{m \times m}$ ,  $U, V \in \mathbb{R}^{n \times m}$  with assumptions that the relevant inverses all exist.

*Solution.* First, we prove the second formula and then prove the first formula using the second one. The second formula is obtained by a directly calculation

$$\begin{aligned} & (Z^{-1} - Z^{-1}U(W^{-1} + V^\top Z^{-1}U)^{-1}V^\top Z^{-1})(Z + U W V^\top) \\ &= I + Z^{-1}U W V^\top - Z^{-1}U(W^{-1} + V^\top Z^{-1}U)^{-1}V^\top Z^{-1}(Z + U W V^\top) \\ &= I + Z^{-1}U W V^\top - Z^{-1}U(W^{-1} + V^\top Z^{-1}U)^{-1}(V^\top + V^\top Z^{-1}U W V^\top) \\ &= I + Z^{-1}U W V^\top - Z^{-1}U(W^{-1} + V^\top Z^{-1}U)^{-1}(W^{-1}W V^\top + V^\top Z^{-1}U W V^\top) \\ &= I + Z^{-1}U W V^\top - Z^{-1}U(W^{-1} + V^\top Z^{-1}U)^{-1}(W^{-1} + V^\top Z^{-1}U)W V^\top \\ &= I + Z^{-1}U W V^\top - Z^{-1}U W V^\top = I. \end{aligned}$$

Next,

$$\begin{aligned} & \mathcal{N}(\mathbf{x}|\mathbf{a}, A)\mathcal{N}(\mathbf{x}|\mathbf{b}, B) \\ &= \frac{1}{(2\pi)^D} \cdot \frac{1}{|A|^{1/2}} \cdot \frac{1}{|B|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{a})^\top A^{-1}(\mathbf{x} - \mathbf{a}) - \frac{1}{2}(\mathbf{x} - \mathbf{b})^\top B^{-1}(\mathbf{x} - \mathbf{b})\right) \\ &= \frac{1}{(2\pi)^D} \cdot \frac{1}{|A|^{1/2}} \cdot \frac{1}{|B|^{1/2}} \exp\left(-\frac{1}{2}\mathbf{x}^\top (A^{-1} + B^{-1})\mathbf{x} + (A^{-1}\mathbf{a} + B^{-1}\mathbf{b})^\top \mathbf{x} - \frac{1}{2}\mathbf{a}^\top A^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top B^{-1}\mathbf{b}\right) \\ &= \frac{1}{(2\pi)^D} \cdot \frac{1}{|A|^{1/2}} \cdot \frac{1}{|B|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - (A^{-1} + B^{-1})^{-1}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b}))^\top (A^{-1} + B^{-1}) \cdot \right. \\ & \quad \left. (\mathbf{x} - (A^{-1} + B^{-1})^{-1}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})) - \frac{1}{2}\mathbf{a}^\top A^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top B^{-1}\mathbf{b} + \frac{1}{2}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})^\top (A^{-1} + B^{-1})^{-1}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})\right) \\ &= \frac{1}{(2\pi)^D} \cdot \frac{1}{|A|^{1/2}} \cdot \frac{1}{|B|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{c})^\top C^{-1}(\mathbf{x} - \mathbf{c}) - \frac{1}{2}\mathbf{a}^\top A^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top B^{-1}\mathbf{b} \right. \\ & \quad \left. + \frac{1}{2}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})^\top (A^{-1} + B^{-1})^{-1}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})\right) \\ &= \mathcal{N}(\mathbf{x}|\mathbf{c}, C) \cdot \frac{1}{(2\pi)^{D/2}} \cdot \frac{|C|^{1/2}}{|A|^{1/2}|B|^{1/2}} \exp\left(\frac{1}{2}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})^\top (A^{-1} + B^{-1})^{-1}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b}) - \frac{1}{2}\mathbf{a}^\top A^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top B^{-1}\mathbf{b}\right). \end{aligned}$$

By the second formula,

$$(A^{-1} + B^{-1})^{-1} = A - A(A + B)^{-1}A = B - B(A + B)^{-1}B.$$

Thus

$$\begin{aligned}
& \frac{1}{2}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b})^\top (A^{-1} + B^{-1})^{-1}(A^{-1}\mathbf{a} + B^{-1}\mathbf{b}) - \frac{1}{2}\mathbf{a}^\top A^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top B^{-1}\mathbf{b} \\
&= \frac{1}{2}\mathbf{a}^\top A^{-1}(A - A(A+B)^{-1}A)A^{-1}\mathbf{a} + \frac{1}{2}\mathbf{b}^\top B^{-1}(B - B(A+B)^{-1}B)B^{-1}\mathbf{b} \\
&\quad + \mathbf{a}^\top A^{-1}(A^{-1} + B^{-1})^{-1}B^{-1}\mathbf{b} - \frac{1}{2}\mathbf{a}^\top A^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top B^{-1}\mathbf{b} \\
&= -\frac{1}{2}\mathbf{a}^\top (A+B)^{-1}\mathbf{a} - \frac{1}{2}\mathbf{b}^\top (A+B)^{-1}\mathbf{b} + \mathbf{a}^\top (A+B)^{-1}\mathbf{b} \\
&= -\frac{1}{2}(\mathbf{a} - \mathbf{b})^\top (A+B)^{-1}(\mathbf{a} - \mathbf{b}).
\end{aligned}$$

Also,

$$\frac{|C|^{1/2}}{|A|^{1/2}|B|^{1/2}} = \frac{|A^{-1} + B^{-1}|^{-1/2}}{|A|^{1/2}|B|^{1/2}} = \frac{1}{|A(A^{-1} + B^{-1})B|^{1/2}} = \frac{1}{|A+B|^{1/2}}.$$

We are done.

4. (10pts) **(Probabilistic PCA)** Let  $\mathcal{D} = \{\mathbf{x}_i \in \mathbb{R}^D : 1 \leq i \leq N\}$ ,  $\bar{\mathbf{x}} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i$  and

$$S = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top.$$

Introduce a latent random variable  $\mathbf{z}$ . Suppose

$$\mathbf{z} \sim \mathcal{N}(\mathbf{z}|0, I)$$

and

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|W\mathbf{z} + \mu, \sigma^2 I)$$

where  $W \in \mathbb{R}^{D \times M}$  and  $\mu \in \mathbb{R}^D$ .

(a) Find  $p(\mathbf{x})$  and  $p(\mathbf{z}|\mathbf{x})$ .

(b) Prove that the maximum likelihood estimator of  $\mu$  is

$$\mu_{ML} = \bar{\mathbf{x}}.$$

(c) Prove that the maximum likelihood estimator of  $W$  satisfies

$$S(WW^\top + \sigma^2 I)^{-1}W = W.$$

In fact, we can obtain the closed form of  $W_{ML}$  and  $\sigma_{ML}^2$ . If you are interested in this result, read “Probabilistic principal component analysis” written by M. E. Tipping and C. M. Bishop (1999).

*Solution.*

(a) First,

$$\begin{aligned} p(\mathbf{x}) &= \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} \\ &\propto \int \exp\left(-\frac{1}{2\sigma^2}(\mathbf{x} - W\mathbf{z} - \mu)^\top(\mathbf{x} - W\mathbf{z} - \mu) - \frac{1}{2}\mathbf{z}^\top\mathbf{z}\right) d\mathbf{z} \\ &= \int \exp\left(-\frac{1}{2}\mathbf{z}^\top\left(\frac{1}{\sigma^2}W^\top W + I\right)\mathbf{z} - \frac{1}{\sigma^2}(\mu - \mathbf{x})^\top W\mathbf{z} - \frac{1}{2\sigma^2}(\mu - \mathbf{x})^\top(\mu - \mathbf{x})\right) d\mathbf{z} \\ &= \int \exp\left(-\frac{1}{2}\left(\mathbf{z} + \frac{1}{\sigma^2}\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top(\mu - \mathbf{x})\right)^\top\left(\frac{1}{\sigma^2}W^\top W + I\right)\left(\mathbf{z} + \frac{1}{\sigma^2}\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top(\mu - \mathbf{x})\right) + \right. \\ &\quad \left. \frac{1}{2\sigma^4}(\mathbf{x} - \mu)^\top W\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top(\mathbf{x} - \mu) - \frac{1}{2\sigma^2}(\mathbf{x} - \mu)^\top(\mathbf{x} - \mu)\right) d\mathbf{z}. \end{aligned}$$

Since  $\frac{1}{\sigma^2}W^\top W + I$  is positive definite and is independent of  $\mathbf{x}$ ,

$$\exp\left(-\frac{1}{2}\left(\mathbf{z} + \frac{1}{\sigma^2}\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top(\mu - \mathbf{x})\right)^\top\left(\frac{1}{\sigma^2}W^\top W + I\right)\left(\mathbf{z} + \frac{1}{\sigma^2}\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top(\mu - \mathbf{x})\right)\right)$$

is an unnormalized normal pdf with respect to  $\mathbf{z}$  and the integration is also independent of  $\mathbf{x}$  (Note that the integration is invariant to a translation). Thus,

$$\begin{aligned} p(\mathbf{x}) &\propto \exp\left(\frac{1}{2\sigma^4}(\mathbf{x} - \mu)^\top W\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top(\mathbf{x} - \mu) - \frac{1}{2\sigma^2}(\mathbf{x} - \mu)^\top(\mathbf{x} - \mu)\right) \\ &= \exp\left(\frac{1}{2\sigma^2}(\mathbf{x} - \mu)^\top\left(I - \frac{1}{\sigma^2}W\left(\frac{1}{\sigma^2}W^\top W + I\right)^{-1}W^\top\right)(\mathbf{x} - \mu)\right). \end{aligned}$$

Therefore

$$p(\mathbf{x}) = \mathcal{N} \left( \mathbf{x} \mid \mu, \sigma^2 \left( I - \frac{1}{\sigma^2} W \left( \frac{1}{\sigma^2} W^\top W + I \right)^{-1} W^\top \right)^{-1} \right).$$

Note that

$$\sigma^2 \left( I - \frac{1}{\sigma^2} W \left( \frac{1}{\sigma^2} W^\top W + I \right)^{-1} W^\top \right)^{-1} = \sigma^2 \left( I + \frac{1}{\sigma^2} W W^\top \right) = \sigma^2 I + W W^\top$$

by the second formula in Problem 3. Next,

$$\begin{aligned} p(\mathbf{z}|\mathbf{x}) &\propto p(\mathbf{x}|\mathbf{z})p(\mathbf{z}) \\ &\propto \exp \left( -\frac{1}{2\sigma^2} (\mathbf{x} - W\mathbf{z} - \mu)^\top (\mathbf{x} - W\mathbf{z} - \mu) - \frac{1}{2} \mathbf{z}^\top \mathbf{z} \right) \\ &\propto \exp \left( -\frac{1}{2} \left( \mathbf{z} + \frac{1}{\sigma^2} \left( \frac{1}{\sigma^2} W^\top W + I \right)^{-1} W^\top (\mu - \mathbf{x}) \right)^\top \left( \frac{1}{\sigma^2} W^\top W + I \right) \left( \mathbf{z} + \frac{1}{\sigma^2} \left( \frac{1}{\sigma^2} W^\top W + I \right)^{-1} W^\top (\mu - \mathbf{x}) \right) \right). \end{aligned}$$

The detail calculation is already done above. Therefore,

$$p(\mathbf{z}|\mathbf{x}) = \mathcal{N} \left( \mathbf{z} \mid \frac{1}{\sigma^2} \left( \frac{1}{\sigma^2} W^\top W + I \right)^{-1} W^\top (\mathbf{x} - \mu), \left( \frac{1}{\sigma^2} W^\top W + I \right)^{-1} \right).$$

(b) From (a),  $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mu, \sigma^2 I + W W^\top)$ . To maximize

$$\mathcal{L}(\mu, W) = \sum_{i=1}^N \log p(\mathbf{x}_i) = -\frac{ND}{2} \log(2\pi) - \frac{N}{2} \log |\sigma^2 I + W W^\top| - \frac{1}{2} \sum_{i=1}^N (\mathbf{x}_i - \mu)^\top (\sigma^2 I + W W^\top)^{-1} (\mathbf{x}_i - \mu),$$

differentiate w.r.t.  $\mu$  :

$$\frac{\partial}{\partial \mu} \mathcal{L}(\mu, W) = -(\sigma^2 I + W W^\top)^{-1} \sum_{i=1}^N (\mathbf{x}_i - \mu).$$

Since  $\sigma^2 I + W W^\top$  is positive definite,

$$\mu_{ML} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i = \bar{\mathbf{x}}.$$

(c) Differentiate w.r.t.  $W$ :

$$\begin{aligned} \frac{\partial}{\partial W} \mathcal{L}(\mu, W) &= \frac{\partial}{\partial W} \left( -\frac{N}{2} \log |\sigma^2 I + W W^\top| - \frac{1}{2} \sum_{i=1}^N \text{tr} \left( (\sigma^2 I + W W^\top)^{-1} (\mathbf{x}_i - \mu) (\mathbf{x}_i - \mu)^\top \right) \right) \\ &= \frac{\partial}{\partial W} \left( -\frac{N}{2} \log |\sigma^2 I + W W^\top| - \frac{N}{2} \sum_{i=1}^N \text{tr} \left( (\sigma^2 I + W W^\top)^{-1} S \right) \right). \end{aligned}$$

Let  $C = \sigma^2 I + W W^\top$ . From Problem 5(c) in Homework 1,

$$\frac{\partial}{\partial C} \log |C| = C^{-1}.$$

Also,

$$\frac{\partial}{\partial C} \text{tr} (C^{-1} S) = -C^{-1} S C^{-1}.$$

To prove this, we first observe that

$$CC^{-1} = I \Rightarrow \frac{\partial C}{\partial x} C^{-1} + C \frac{\partial C^{-1}}{\partial x} = 0 \Rightarrow \frac{\partial C^{-1}}{\partial x} = -C^{-1} \frac{\partial C}{\partial x} C^{-1}.$$

From Problem 5(a) in Homework 1,

$$\frac{\partial}{\partial C^{-1}} \text{tr}(C^{-1}S) = S.$$

By the chain rule,

$$\frac{\partial}{\partial C_{ij}} \text{tr}(C^{-1}S) = \left( -C^{-1} \frac{\partial C}{\partial C_{ij}} C^{-1} \right) : S$$

where  $A : B = \text{tr}(A^\top B) = \sum_{i,j} A_{ij} B_{ij}$ . Then

$$\frac{\partial}{\partial C_{ij}} \text{tr}(C^{-1}S) = -\text{tr} \left( C^{-1} S C^{-1} \frac{\partial C}{\partial C_{ij}} \right) = -(C^{-1} S C^{-1})_{ij}$$

and so

$$\frac{\partial}{\partial C} \text{tr}(C^{-1}S) = -C^{-1} S C^{-1}.$$

Now, back to the problem. By the matrix differentiation formula,

$$\frac{\partial}{\partial C} \left( -\frac{N}{2} \log |C| - \frac{N}{2} \sum_{i=1}^N \text{tr}(C^{-1}S) \right) = -\frac{N}{2} (C^{-1} - C^{-1} S C^{-1}) =: P.$$

Also,

$$\frac{\partial}{\partial W_{ij}} C = \sum_{k=1}^D e_{ki} W_{kj} + \sum_{k=1}^D e_{ik} W_{kj}$$

where  $e_{mn}$  is a  $D \times D$  matrix such that  $(m, n)$ -entry is one and other entries are zeros. By the chain rule,

$$\frac{\partial}{\partial W_{ij}} \left( -\frac{N}{2} \log |C| - \frac{N}{2} \sum_{i=1}^N \text{tr}(C^{-1}S) \right) = P : \left( \sum_{k=1}^D e_{ki} W_{kj} + \sum_{k=1}^D e_{ik} W_{kj} \right)$$

where  $A : B = \text{tr}(A^\top B) = \sum_{i,j} A_{ij} B_{ij}$ . Then

$$P : \left( \sum_{k=1}^D e_{ki} W_{kj} + \sum_{k=1}^D e_{ik} W_{kj} \right) = \sum_{k=1}^D P_{ki} W_{kj} + \sum_{k=1}^D P_{ik} W_{kj} = (P^\top W)_{ij} + (PW)_{ij}.$$

Thus,

$$\frac{\partial}{\partial W} \left( -\frac{N}{2} \log |C| - \frac{N}{2} \sum_{i=1}^N \text{tr}(C^{-1}S) \right) = P^\top W + PW = 2PW = -N(C^{-1}W - C^{-1}SC^{-1}W)$$

since  $P$  is symmetric. Therefore,

$$W_{ML} = SC^{-1}W_{ML} = S(WW^\top + \sigma^2 I)^{-1}W_{ML}.$$