Machine Learning — Repeat Exam

1	2	3	4	5	6	7	8	9	10	11	$\sum$
4	5	6	4	6	5	4	7	4	2	7	54

Do not write anything above this line

Name:

Student ID: Signature:

- Only write on the sheets given to you by supervisors. If you need more paper, ask the supervisors.
- Pages 16-18 can be used as scratch paper.
- All sheets (including scratch paper) have to be returned at the end.
- **Do not unstaple the sheets!**
- Wherever answer boxes are provided, please write your answers in them.
- Please write your student ID (*Matrikelnummer*) on every sheet you hand in.
- **Only use a black or a blue pen (no pencils, red or green pens!).**
- You are allowed to use your A4 sheet of handwritten notes (two sides). **No other materials (e.g. books, cell phones, calculators) are allowed!**
- Exam duration - 120 minutes.
- This exam consists of 21 pages, 11 problems. You can earn 54 points.

Probability distributions

For your reference, we provide the following probability distribution.

- Univariate normal distribution

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Bernoulli distribution

$$\text{Bern}(x|\theta) = \theta^x(1-\theta)^{(1-x)}$$

Decision Trees

Problem 1 [(2+2)=4 points] Assume you want to build a decision tree. Your data set consists of N samples, each with k features ($k \leq N$).

a) If the features are binary, what is the maximum possible number of leaf nodes and the maximum depth of your decision tree?

> Each feature can only be used once on a path from the root to the leaf.
>
> Maximum number of leaf nodes: $\min\left(2^k, N\right)$ **1pt.**
>
> Maximum depth: k **1pt.**

b) If the features are continuous, what is the maximum possible number of leaf nodes and the maximum depth of your decision tree?

> Each feature can be used multiple times on a path from the root to the leaf.
>
> Maximum number of leaf nodes: N **1pt.**
>
> Maximum depth: N **1pt.**

Regression

Problem 2 [(1+4)=5 points] We want to perform regression on a dataset consisting of N samples $\boldsymbol{x}_i \in \mathbb{R}^D$ with corresponding targets $y_i \in \mathbb{R}$ (represented compactly as $\boldsymbol{X} \in \mathbb{R}^{N \times D}$ and $\boldsymbol{y} \in \mathbb{R}^N$).

Assume that we have fitted an L_2-regularized linear regression model and obtained the optimal weight vector $\boldsymbol{w}^* \in \mathbb{R}^D$ as

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \frac{\lambda}{2} \boldsymbol{w}^T \boldsymbol{w}$$

Note that there is no bias term.

Now, assume that we obtained a new data matrix $\boldsymbol{X}_{new}$ by scaling all samples by the same positive factor $a \in (0, \infty)$. That is, $\boldsymbol{X}_{new} = a\boldsymbol{X}$ (and respectively $\boldsymbol{x}_i^{new} = a\boldsymbol{x}_i$).

a) Find the weight vector $\boldsymbol{w}_{new}$ that will produce the same predictions on $\boldsymbol{X}_{new}$ as $\boldsymbol{w}^*$ produces on $\boldsymbol{X}$.

> Predictions of a linear regression model are generated as $\hat{y} = \boldsymbol{w}^T \boldsymbol{x}$.
>
> This means that we need to ensure that $\boldsymbol{w}^{*T} \boldsymbol{x}_i = \boldsymbol{w}_{new}^T \boldsymbol{x}_i^{new}$ or equivalently $\boldsymbol{w}^{*T} \boldsymbol{x}_i = \boldsymbol{w}_{new}^T a \boldsymbol{x}_i$. Solving for $\boldsymbol{w}_{new}$ we get $\boldsymbol{w}_{new} = \frac{\boldsymbol{w}^*}{a}$
>
> **1 pt.** for a correct answer.

b) Find the regularization factor $\lambda_{new} \in \mathbb{R}$, such that the solution $\boldsymbol{w}_{new}^*$ of the new L_2-regularized

linear regression problem

$$\boldsymbol{w}^*_{new} = \arg\min_{\boldsymbol{w}} \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{w}^T\boldsymbol{x}_i^{new} - y_i)^2 + \frac{\lambda_{new}}{2}\boldsymbol{w}^T\boldsymbol{w}$$

will produce the same predictions on $\boldsymbol{X}_{new}$ as $\boldsymbol{w}^*$ produces on $\boldsymbol{X}$.

Provide a mathematical justification for your answer.

The closed form solution for $\boldsymbol{w}^*$ on the original data $\boldsymbol{X}$ is

$$\boldsymbol{w}^* = (\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

0.5 pt.

The closed form solution for $\boldsymbol{w}^*_{new}$ on the new data $\boldsymbol{X}_{new}$ is

$$\begin{aligned}\boldsymbol{w}^*_{new} &= (\boldsymbol{X}^T_{new}\boldsymbol{X}_{new} + \lambda_{new}\boldsymbol{I})^{-1}\boldsymbol{X}^T_{new}\boldsymbol{y} \\ &= a(a^2\boldsymbol{X}^T\boldsymbol{X} + \lambda_{new}\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y}\end{aligned}$$

1 pt.

by setting $\lambda_{new} = a^2\lambda$, we get

$$\begin{aligned}&= a(a^2\boldsymbol{X}^T\boldsymbol{X} + a^2\lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ &= \frac{1}{a}(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ &= \frac{1}{a}\boldsymbol{w}^*\end{aligned}$$

Which (according to our answer in part (a) of this problem) will produce the same predictions on $\boldsymbol{X}_{new}$ as $\boldsymbol{w}^*$ does on $\boldsymbol{X}$, as desired.

1 pt. for setting $\boldsymbol{w}^*_{new} = \frac{1}{a}\boldsymbol{w}^*$

1 pt. for correct (and justified) value of λ_{new}

Equivalent solution

$$\begin{aligned}\boldsymbol{w}^*_{new} \overset{!}{=} \frac{\boldsymbol{w}^*}{a} &= \frac{1}{a}\arg\min_{\boldsymbol{w}} \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{w}^T\boldsymbol{x}_i - y_i)^2 + \frac{\lambda}{2}\boldsymbol{w}^T\boldsymbol{w} \\ &= \frac{1}{a}\arg\min_{\boldsymbol{w}} \frac{1}{2}\sum_{i=1}^{N}(\frac{\boldsymbol{w}^T}{a}a\boldsymbol{x}_i - y_i)^2 + \frac{a^2\lambda}{2}\frac{\boldsymbol{w}^T}{a}\frac{\boldsymbol{w}}{a} \\ &= \frac{a}{a}\arg\min_{\boldsymbol{w}_{new}=\frac{\boldsymbol{w}}{a}} \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{w}^T_{new}\boldsymbol{x}_i^{new} - y_i)^2 + \frac{a^2\lambda}{2}\boldsymbol{w}^T_{new}\boldsymbol{w}_{new} \\ &\overset{!}{=} \boldsymbol{w}^*_{new} = \arg\min_{\boldsymbol{w}_{new}} \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{w}^T_{new}\boldsymbol{x}_i^{new} - y_i)^2 + \frac{\lambda_{new}}{2}\boldsymbol{w}^T_{new}\boldsymbol{w}_{new}\end{aligned}$$

1 pt. for setting $\boldsymbol{w}^*_{new} \overset{!}{=} \frac{\boldsymbol{w}^*}{a}$ and inserting a in the right spots (while keeping the loss function independent of a)

1 pt. for correctly substituting $\boldsymbol{w}_{new}$

For this equality to hold we need to match the regularization term by setting $\lambda_{new} = a^2\lambda$.

1 pt. for matching regularization term

1 pt. for correct (and justified) value of λ_{new}

Classification

Problem 3 [(1+2+3)=6 points] We would like to perform binary classification on multivariate binary data. That is, the data points $\boldsymbol{x}_i \in \{0,1\}^D$ are binary vectors of length D, and each sample belongs to one of two classes $y_i \in \{1,2\}$.

Consider the following generative classification model. We place a categorical prior on y

$$p(y=1) = \pi_1 \qquad p(y=2) = \pi_2.$$

The class-conditional distributions are products of independent Bernoulli distributions

$$p(\boldsymbol{x} \mid y=1, \boldsymbol{\alpha}) = \prod_{j=1}^{D} \mathrm{Bern}(x_j \mid \alpha_j),$$
$$p(\boldsymbol{x} \mid y=2, \boldsymbol{\beta}) = \prod_{j=1}^{D} \mathrm{Bern}(x_j \mid \beta_j),$$

where $\boldsymbol{\alpha} \in [0,1]^D$ and $\boldsymbol{\beta} \in [0,1]^D$ are the respective parameter vectors for both classes.
That is, each component x_j is distributed as $x_j \sim \mathrm{Bern}(\alpha_j)$ if $y=1$ or $x_j \sim \mathrm{Bern}(\beta_j)$ if $y=2$.

a) Write down the expression for the posterior distribution $p(y \mid \boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\pi})$.

Using the Bayes formula

$$\begin{aligned} p(y \mid \boldsymbol{x}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\pi}) &= \frac{p(\boldsymbol{x} \mid y, \boldsymbol{\alpha}, \boldsymbol{\beta}) p(y \mid \boldsymbol{\pi})}{p(\boldsymbol{x} \mid \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\pi})} \\ &= \frac{p(\boldsymbol{x} \mid y, \boldsymbol{\alpha}, \boldsymbol{\beta}) p(y \mid \boldsymbol{\pi})}{p(\boldsymbol{x} \mid y=1, \boldsymbol{\alpha}, \boldsymbol{\beta}) p(y=1 \mid \boldsymbol{\pi}) + p(\boldsymbol{x} \mid y=2, \boldsymbol{\alpha}, \boldsymbol{\pi}) p(y=2 \mid \boldsymbol{\pi})} \end{aligned}$$

b) Assume that $D=3$, $\boldsymbol{\alpha} = [1/3, 1/3, 3/4]$, $\boldsymbol{\beta} = [2/3, 1/2, 1/2]$, $\pi_1 = 1/3$ and $\pi_2 = 2/3$.

Write down a data point $\boldsymbol{x}_1 \in \{0,1\}^3$ that will be classified as class 1 by our model. Additionally, compute the posterior probability $p(y=1 \mid \boldsymbol{x}_1, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\pi})$.

Consider $\boldsymbol{x}_1 = (0, 0, 1)^T$. The probability that $\boldsymbol{x}_1$ belongs to class 1 is

$$\begin{aligned}
p(y = 1 \mid \boldsymbol{x}_1, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\pi}) &= \frac{p(\boldsymbol{x}_1 \mid y = 1, \boldsymbol{\alpha}, \boldsymbol{\beta}) p(y = 1 \mid \boldsymbol{\pi})}{p(\boldsymbol{x}_1 \mid y = 1, \boldsymbol{\alpha}, \boldsymbol{\beta}) p(y = 1 \mid \boldsymbol{\pi}) + p(\boldsymbol{x}_1 \mid y = 2, \boldsymbol{\alpha}, \boldsymbol{\pi}) p(y = 2 \mid \boldsymbol{\pi})} \\
&= \frac{p(\boldsymbol{x}_1 \mid y = 1, \boldsymbol{\alpha}, \boldsymbol{\beta}) \pi_1}{p(\boldsymbol{x}_1 \mid y = 1, \boldsymbol{\alpha}, \boldsymbol{\beta}) \pi_1 + p(\boldsymbol{x}_1 \mid y = 2, \boldsymbol{\alpha}, \boldsymbol{\pi}) \pi_2} \\
&= \frac{(1 - \alpha_1) \cdot (1 - \alpha_2) \cdot \alpha_3 \cdot \pi_1}{(1 - \alpha_1) \cdot (1 - \alpha_2) \cdot \alpha_3 \cdot \pi_1 + (1 - \beta_1) \cdot (1 - \beta_2) \cdot \beta_3 \cdot \pi_2} \\
&= \frac{2/3 \cdot 2/3 \cdot 3/4 \cdot 1/3}{2/3 \cdot 2/3 \cdot 3/4 \cdot 1/3 + 1/3 \cdot 1/2 \cdot 1/2 \cdot 2/3} \\
&= \frac{1/9}{1/9 + 1/18} \\
&= \frac{2}{3}
\end{aligned}$$

c) Consider the case when $D = 2$, $\pi_1 = \pi_2 = 1/2$, and $\boldsymbol{\alpha} \in [0, 1]^2$ and $\boldsymbol{\beta} \in [0, 1]^2$ are known and fixed. Show that the resulting classification rule can be represented as a linear function of $\boldsymbol{x}$. That is, find $\boldsymbol{w} \in \mathbb{R}^2$ and $b \in \mathbb{R}$, such that

$$\{\boldsymbol{x} \in \{0, 1\}^2 : \boldsymbol{w}^T \boldsymbol{x} + b > 0\} = \{\boldsymbol{x} \in \{0, 1\}^2 : p(y = 1 \mid \boldsymbol{x}) > p(y = 2 \mid \boldsymbol{x})\}$$

$$\begin{aligned}
& p(y = 1 \mid \boldsymbol{x}) > p(y = 2 \mid \boldsymbol{x}) \\
\iff & p(\boldsymbol{x} \mid y = 1) p(y = 1) > p(\boldsymbol{x} \mid y = 2) p(y = 2) \\
\iff & p(\boldsymbol{x} \mid y = 1) > p(\boldsymbol{x} \mid y = 2) \\
\iff & \log p(\boldsymbol{x} \mid y = 1) > \log p(\boldsymbol{x} \mid y = 2) \\
\iff & \log p(x_1 \mid y = 1) + \log p(x_2 \mid y = 1) > \log p(x_1 \mid y = 2) + \log p(x_2 \mid y = 2) \\
\iff & x_1 \log \alpha_1 + (1 - x_1) \log(1 - \alpha_1) + x_2 \log \alpha_2 + (1 - x_2) \log(1 - \alpha_2) \\
& - x_1 \log \beta_1 - (1 - x_1) \log(1 - \beta_1) - x_2 \log \beta_2 - (1 - x_2) \log(1 - \beta_2) > 0 \\
\iff & (\log \alpha_1 - \log(1 - \alpha_1) - \log \beta_1 + \log(1 - \beta_1)) x_1 \\
& + (\log \alpha_2 - \log(1 - \alpha_2) - \log \beta_2 + \log(1 - \beta_2)) x_2 \\
& + (\log(1 - \alpha_1) + \log(1 - \alpha_2) - \log(1 - \beta_1) - \log(1 - \beta_2)) > 0
\end{aligned}$$

We can equivalently represent this inequality as $\boldsymbol{w}^T \boldsymbol{x} + b > 0$, where

$$\boldsymbol{w} = \begin{pmatrix} \log \alpha_1 - \log(1 - \alpha_1) - \log \beta_1 + \log(1 - \beta_1) \\ \log \alpha_2 - \log(1 - \alpha_2) - \log \beta_2 + \log(1 - \beta_2) \end{pmatrix} \in \mathbb{R}^2$$

and

$$b = (\log(1 - \alpha_1) + \log(1 - \alpha_2) - \log(1 - \beta_1) - \log(1 - \beta_2)) \in \mathbb{R}$$

Kernels

Problem 4 [(4)=4 points] Prove or disprove whether the following operations on sets $A, B \subseteq \mathcal{X}$, where $\mathcal{X}$ is a finite set, define a valid kernel.

a) $k(A, B) = |A \times B|$, where $A \times B = \{(a, b) : a \in A, b \in B\}$ denotes the cartesian product and $|S|$ denotes the cardinality of set S, i.e. the number of elements in S.

Yes, using cardinality as a feature map $|A \times B| = |A| \cdot |B|$ obviously defines a kernel.

0.5pt. for definition of a kernel or stating Mercer's theorem (only once and only if no subtask was solved).

1pt. for a correct answer.

b) $k(A, B) = |A \cap B|$

Since the set $\mathcal{X}$ is finite we can denote its members as x_i, with $i \in \{1, 2, ...|\mathcal{X}|\}$, and define the membership vector $\boldsymbol{a}$, with

$$a_i = \begin{cases} 1 & \text{if } x_i \in A, \\ 0 & \text{otherwise.} \end{cases}$$

Using this as a feature map we can write

$$|A \cap B| = \boldsymbol{a}^T \boldsymbol{b},$$

showing that $|A \cap B|$ is a kernel.

0.5pt. for definition of a kernel or stating Mercer's theorem (only once and only if no subtask was solved).

1pt. for a correct answer.

c) $k(A, B) = |A \cup B|$

Looking at the determinant of a Gram matrix defined by two objects $A, B \subseteq \mathcal{X}$ we have

$$\det \begin{pmatrix} |A| & |A \cup B| \\ |A \cup B| & |B| \end{pmatrix} = |A||B| - |A \cup B|^2,$$

which is negative if $A \neq B$. Hence, the Gram matrix is not positive semidefinite and according to Mercer's theorem $|A \cup B|$ is not a kernel.

0.5pt. for definition of a kernel or stating Mercer's theorem (only once and only if no subtask was solved).

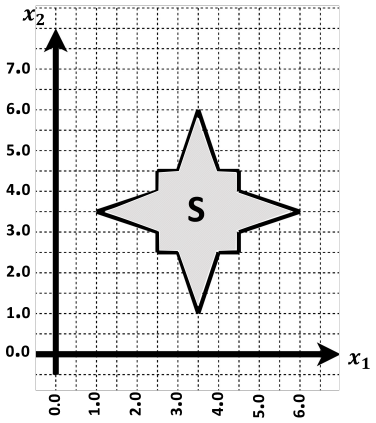
2pt. for a correct counterexample.

Optimization

Problem 5 [(1+3+2)=6 points] Let f be the following convex function on $\mathbb{R}^2$:

$$f(x_1, x_2) = e^{x_1 + x_2} - 5 \cdot \log(x_2)$$

a) Consider the following shaded region $\boldsymbol{S}$ in $\mathbb{R}^2$. Is this region convex? Why?

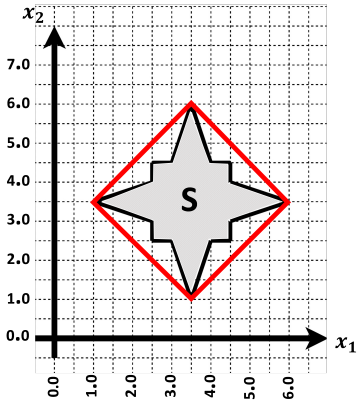


It is not. Because we can choose two points in $\boldsymbol{S}$ where the line connecting the points does not completely resides in $\boldsymbol{S}$.

1pt. for a correct answer and explanation.

b) Find the maximizer (x_1^*, x_2^*) of f over the shaded region $\boldsymbol{S}$. For your computations, you can pick values from the following table. Justify your answer.

$e^{4.5} = 90.017$	$e^{5.0} = 148.41$	$e^{5.5} = 244.69$	$e^{6.5} = 665.14$
$e^{7.0} = 1096.63$	$e^{7.5} = 1808.04$	$e^{8.0} = 2980.95$	$e^{8.5} = 4914.76$
$e^{9.0} = 8103.08$	$e^{9.5} = 13359.726$	$e^{10.0} = 22026.46$	$e^{10.5} = 36315.50$
$\log(1.0) = 0$	$\log(2.5) = 0.9162$	$\log(3.0) = 1.0986$	$\log(3.5) = 1.2527$
$\log(4.0) = 1.3862$	$\log(4.5) = 1.5040$	$\log(5.0) = 1.6094$	$\log(6.0) = 1.7917$



According to the lecture, we need to compute the value of f only on the four corners of the convex hull. Afterwards, we pick the corner at which the value of f is larger.

$$f(1, 3.5) = e^{4.5} - 5 \cdot \log(3.5) = 83.7533 \qquad f(3.5, 1.0) = e^{4.5} - 5 \cdot \log(1.0) = 90.01$$
$$f(6, 3.5) = e^{9.5} - 5 \cdot \log(3.5) = 13353.46 \qquad f(3.5, 6.0) = e^{9.5} - 5 \cdot \log(6.0) = 13350.76$$

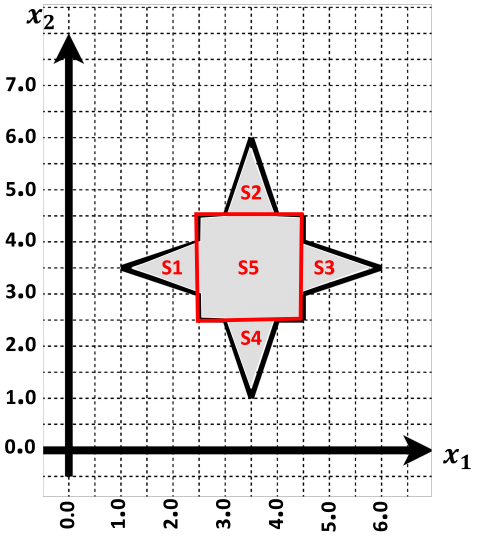
Therefore, the maximum of f occurs at point $(6, 3.5)$, and the maximum of f is 13353.46.

1pt. for writing down the correct answer.
2pt. for completely correct explanation (checking only the 4 corners of the convex-hull).
1pt. for partially correct explanation (checking all 16 corners, gradient ascent, etc.)

c) Assume that we are given an algorithm `ConvOpt`$(f, \mathcal{X})$ that takes as input a convex function f and any convex region $\mathcal{X}$, and returns the minimum of f over $\mathcal{X}$.

Using the `ConvOpt` algorithm, how would you find the global minimum of f over the shaded region $\boldsymbol{S}$?

We can partition the shaded region S to the following five convex regions. Afterwards, we run the `ConvOpt` algorithm separately for the 5 regions.



2pt. for a feasible approach.
1pt. for an approach with a few addressable issues.

SVM

Problem 6 [(5)=5 points] Given the data points

$$\boldsymbol{x}_1 = (1,1,0,1)^T \qquad \boldsymbol{x}_2 = (1,1,1,0)^T \qquad \boldsymbol{x}_3 = (0,1,1,1)^T \qquad \boldsymbol{x}_4 = (0,0,1,1)^T$$

Prove or disprove whether the following combinations of labels $\boldsymbol{y}$ and dual variables $\boldsymbol{\alpha}$ are the optimal solutions of a soft-margin SVM with $C = 1$.

a) $\boldsymbol{y} = (-1,-1,1,1)^T$, $\boldsymbol{\alpha} = (0.6, 0.6, 1, 0)^T$

b) $\boldsymbol{y} = (-1,-1,1,1)^T$, $\boldsymbol{\alpha} = \left(\frac{2}{3}, \frac{2}{3}, \frac{4}{3}, 0\right)^T$

c) $\boldsymbol{y} = (-1,1,-1,1)^T$, $\boldsymbol{\alpha} = (1,1,1,1)^T$

a) No, $\sum_i \alpha_i y_i \neq 0$. **1pt.** (**0.5pt.** for constraint)

b) No, $\alpha_3 > C$. **1pt.** (**0.5pt.** for constraint)

c) This solution is feasible, so we need to check optimality. The dual problem of the soft-margin SVM is

$$g(\boldsymbol{\alpha}) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j y_i y_j \alpha_i \alpha_j \boldsymbol{x}_i^T \boldsymbol{x}_j.$$

0.5pt., also for a correct approach for deriving it.

To check whether this is an optimal solution we first look at the gradient, which is given by

$$\left(\nabla_{\boldsymbol{\alpha}} g(\boldsymbol{\alpha})\right)_i = 1 - \sum_j y_i y_j \alpha_j \boldsymbol{x}_i^T \boldsymbol{x}_j.$$

1pt.

To calculate the gradient, we need the kernel matrix, with $K_{ij} = \boldsymbol{x}_i^T \boldsymbol{x}_j$:

$$K = \begin{pmatrix} 3 & 2 & 2 & 1 \\ 2 & 3 & 2 & 1 \\ 2 & 2 & 3 & 2 \\ 1 & 1 & 2 & 2 \end{pmatrix}.$$

0.5pt.

Using this we can directly calculate

$$\begin{aligned} \partial_{\alpha_1} g(\boldsymbol{\alpha}) &= 1 - (3 - 2 + 2 - 1) = -1 \\ \partial_{\alpha_2} g(\boldsymbol{\alpha}) &= 1 - (-2 + 3 - 2 + 1) = 1 \\ \partial_{\alpha_3} g(\boldsymbol{\alpha}) &= 1 - (2 - 2 + 3 - 2) = 0 \\ \partial_{\alpha_4} g(\boldsymbol{\alpha}) &= 1 - (-1 + 1 - 2 + 2) = 1 \end{aligned}$$

0.5pt.

Now let us consider the constraints. Since all $\alpha_i = 1 = C$ we cannot increase any α_i. However, we also can't decrease α_1 without decreasing either α_2 or α_4 due to the constraint $\sum_i \alpha_i y_i = 0$. The absolute values of these three derivatives are equally high, which means that decreasing these values would not increase $g(\boldsymbol{\alpha})$. Hence, we cannot increase $g(\boldsymbol{\alpha})$ any further and this is indeed an optimal solution. **0.5pt.**

Deep Learning

Problem 7 [(2+2)=4 points] You are trying to solve a regression task and you want to choose between two approaches:

1. A simple linear regression model.
2. A feed forward neural network $f_{\boldsymbol{W}}(\boldsymbol{x})$ with L hidden layers, where each hidden layer $l \in \{1, ..., L\}$ has a weight matrix $\boldsymbol{W}_l \in \mathbb{R}^{D \times D}$ and a ReLU activation function. The output layer has a weight matrix $\boldsymbol{W}_{L+1} \in \mathbb{R}^{D \times 1}$ and no activation function.

In both models, there are no bias terms.

Your dataset $\mathcal{D}$ contains data points with nonnegative features $\boldsymbol{x}_i$ and the target y_i is continuous:

$$\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N, \qquad \boldsymbol{x}_i \in \mathbb{R}^D_{\geq 0}, \qquad y_i \in \mathbb{R}$$

Let $\boldsymbol{w}^*_{LS} \in \mathbb{R}^D$ be the optimal weights for the linear regression model corresponding to a global minimum of the following least squares optimization problem:

$$\boldsymbol{w}^*_{LS} = \arg\min_{\boldsymbol{w} \in \mathbb{R}^D} \mathcal{L}_{LS}(\boldsymbol{w}) = \arg\min_{\boldsymbol{w} \in \mathbb{R}^D} \frac{1}{2} \sum_{i=1}^N (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2$$

Let $\boldsymbol{W}^*_{NN} = \{\boldsymbol{W}^*_1, \ldots, \boldsymbol{W}^*_{L+1}\}$ be the optimal weights for the neural network corresponding to a global minimum of the following optimization problem:

$$\boldsymbol{W}^*_{NN} = \arg\min_{\boldsymbol{W}} \mathcal{L}_{NN}(\boldsymbol{W}) = \arg\min_{\boldsymbol{W}} \frac{1}{2} \sum_{i=1}^N (f_{\boldsymbol{W}}(\boldsymbol{x}_i) - y_i)^2$$

a) Assume that the optimal $\boldsymbol{W}^*_{NN}$ you obtain are non-negative.
What will be the relation $(<, \leq, =, \geq, >)$ between the neural network loss $\mathcal{L}_{NN}(\boldsymbol{W}^*_{NN})$ and the linear regression loss $\mathcal{L}_{LS}(\boldsymbol{w}^*_{LS})$? Provide a mathematical argument to justify your answer.

Note that for any non-negative $\boldsymbol{x}$ and any non-negative $\boldsymbol{W}$ it holds $\text{ReLU}(\boldsymbol{xW}) = \boldsymbol{xW}$.

1pt: Therefore, since our data points have non-negative features $\boldsymbol{x}_i$ and the optimal weights $\boldsymbol{W}^*_{NN}$ are non-negative, every ReLU layer is equivalent to a linear layer when plugging in the optimal weights. This means we can write

$$\begin{aligned} f_{\boldsymbol{W}^*_{\boldsymbol{NN}}}(\boldsymbol{x}_i) &= ReLU(ReLU(ReLU(\boldsymbol{x}_i^T \boldsymbol{W}^*_1)\boldsymbol{W}^*_2) \cdots \boldsymbol{W}^*_L)\boldsymbol{W}^*_{L+1} \\ &= \boldsymbol{x}_i^T \boldsymbol{W}^*_1 \boldsymbol{W}^*_2 \cdots \boldsymbol{W}^*_{L+1} \\ &= \boldsymbol{x}_i^T \boldsymbol{w}^*_{NN} \end{aligned}$$

where we defined $\boldsymbol{w}^*_{NN} = \boldsymbol{W}^*_1 \boldsymbol{W}^*_2 \cdots \boldsymbol{W}^*_{L+1}$. From this we can see that the neural network with optimal weights behaves like a linear regression with a different set of weights $\boldsymbol{w}^*_{NN}$.

-0.5pt: if mentioned only non-negative weights or features but not both

-0.5pt: if the answer under (a) is actually the correct answer for (b) and vice versa

1pt: Note also that linear regression is a special case of the above neural network, i.e. for any weights $\boldsymbol{w}_{LS}$ you can find weights $\boldsymbol{W}_{NN}$ that produce the same output.

Given the above facts and since we the optimal weights correspond to a global minima we can conclude that $\mathcal{L}_{NN}(\boldsymbol{W}^*_{NN}) = \mathcal{L}_{LS}(\boldsymbol{w}^*_{LS})$ and the optimal weights found by solving the least squares optimization problem will be $\boldsymbol{w}^*_{LS} = \boldsymbol{w}^*_{NN}$.

b) In contrast to (a), now assume that the optimal weights $\boldsymbol{w}^*_{LS}$ you obtain are non-negative. What will be the relation $(<, \leq, =, \geq, >)$ between the linear regression loss $\mathcal{L}_{LS}(\boldsymbol{w}^*_{LS})$ and the neural network loss $\mathcal{L}_{NN}(\boldsymbol{W}^*_{NN})$? Provide a mathematical argument to justify your answer.

1pt: As stated in (a) linear regression is a special case of the above neural network, i.e. for any weights $\boldsymbol{w}_{LS}$ you can find weights $\boldsymbol{W}_{NN}$ that produce the same output. That is, everything that can be learned with a linear regression can be learned equally well with a neural network.

1pt: However, the reverse direction doesn't hold, since in principle neural networks can learn more complicated functions compared to linear regression. Moreover, the given fact that $\boldsymbol{w}^*_{LS}$ are non-negative does not tell us anything about the optimal weights of the neural network $\boldsymbol{W}^*_{NN}$.

Therefore it holds $\mathcal{L}_{NN}(\boldsymbol{W}^*_{NN}) \leq \mathcal{L}_{LS}(\boldsymbol{w}^*_{LS})$ since the neural network can potentially find a better fit for the data (e.g. by taking advantage of non-linearity).

-0.25pt: for stating $<$ instead of $\leq$

Dimensionality Reduction

Problem 8 [(3+2+2)=7 points] You are given $N = 4$ data points: $\{\boldsymbol{x}_i\}_{i=1}^4, \boldsymbol{x}_i \in \mathbb{R}^3$, represented with the matrix $\boldsymbol{X} \in \mathbb{R}^{4\times 3}$.

$$\boldsymbol{X} = \begin{bmatrix} 4 & 3 & 2 \\ 2 & 1 & -2 \\ 4 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix}$$

Hint: In this task the results of all (final and intermediate) computations happen to be integers.

a) Perform principal component analysis (PCA) of the data $\boldsymbol{X}$, i.e. find the principal components and their associated variances in the transformed coordinate system. Show your work.

First we center the data. The mean is $\bar{\boldsymbol{x}} = [2, 1, 1]$, thus we have

$$\boldsymbol{X}_c = \boldsymbol{X} - \bar{\boldsymbol{x}} = \begin{bmatrix} 2 & 2 & 1 \\ 0 & 0 & -3 \\ 2 & -2 & 1 \\ -4 & 0 & 1 \end{bmatrix}$$

Then we compute the covariance matrix.

$$\boldsymbol{\Sigma}_{X_c} = \frac{1}{N}\boldsymbol{X}_c^T\boldsymbol{X}_c = \begin{bmatrix} 6 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

Since $\boldsymbol{\Sigma}_{X_c}$ it is already in a diagonal form we can conclude that $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}_{X_c}$ and $\boldsymbol{\Gamma} = \boldsymbol{I_3}$, and that it holds $\boldsymbol{\Sigma}_{X_c} = \boldsymbol{\Gamma}\boldsymbol{\Lambda}\boldsymbol{\Gamma}^T$. The principal components are the canonical basis vectors.

1 pt. for centring the data correctly or computing the correct mean

1 pt. for computing correctly the covariance matrix.

1 pt. for giving the correct transformed coordinate system.

-0.5 pt if no centring.

b) Project the data to two dimensions, i.e. write down the transformed data matrix $\boldsymbol{Y} \in \mathbb{R}^{4\times 2}$ using the top-2 principal components you computed in (a). What fraction of variance of $\boldsymbol{X}$ is preserved by $\boldsymbol{Y}$?

The projection matrix is:

$$\boldsymbol{\Gamma}_{trunc} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}$$

since we pick the first and the third principal vector corresponding to the two largest eigenvalues. Thus, we have

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\Gamma}_{trunc} = \begin{bmatrix} 2 & 1 \\ 0 & -3 \\ 2 & 1 \\ -4 & 1 \end{bmatrix}$$

We preserve $\frac{6+3}{6+2+3} = \frac{9}{11}$ of the variance.

0.5 pt. for correct computation for projection of $\boldsymbol{X}$ or $\boldsymbol{X_c}$ based on the results obtained in question a)

0.5 pt. for correct computation for the fraction of variance based on the results obtained in question a)

0.5 pt. for correct result for projection of $\boldsymbol{X}$ or $\boldsymbol{X_c}$

0.5 pt. for correct result for the fraction of variance

c) Let $\boldsymbol{x}_5 \in \mathbb{R}^3$ be a new data point. Specify the vector $\boldsymbol{x}_5$ such that performing PCA on the data including the new data point $\{\boldsymbol{x}_i\}_{i=1}^5$ leads to exactly the same principal components as in (a).

Let $\boldsymbol{x}_5 = \bar{\boldsymbol{x}}$, i.e. the new data point equals the mean before including $\boldsymbol{x}_5$ to the dataset. Therefore, the new mean including $\boldsymbol{x}_5$ is equal to the old mean. We have:

$$\boldsymbol{X}_c = \boldsymbol{X} - \bar{\boldsymbol{x}} = \begin{bmatrix} 2 & 2 & 1 \\ 0 & 0 & -3 \\ 2 & -2 & 1 \\ -4 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

which leads to the same $\boldsymbol{\Sigma}_{X_c}$ as in (a) up to a difference in the multiplicative constant, in (a) we had $\frac{1}{4}\boldsymbol{X}_c^T\boldsymbol{X}_c$ and here we have $\frac{1}{5}\boldsymbol{X}_c^T\boldsymbol{X}_c$. While the this difference leads to different eigenvalues, the eigenvectors and thus the principal components stay the same.

2 pt. for saying $\boldsymbol{x}_5 = \bar{\boldsymbol{x}}$

1pt. for only reasoning on the shifted data

Clustering

Problem 9 [(4)=4 points] Let $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$ be the centroids computed by the K-means algorithm. Prove that the set $\mathcal{X}_j$ of all points in $\mathbb{R}^D$ assigned during inference to the cluster j is a convex set.

$$\mathcal{X}_j := \{\boldsymbol{x} \in \mathbb{R}^D : \boldsymbol{x} \text{ would be assigned to centroid } \boldsymbol{\mu}_j \text{ by } K\text{-means}\}$$

Hint: start by thinking about the case with $K = 2$.

Bonus (applicable for arbitrary solutions):

1pt: in case of only two clusters $\mathcal{X}_j$ is a **half-space (0.5pts)** since the decision boundary is a hyperplane and therefore **convex (0.5pts** if followed from a valid statement, otherwise **0pts)**

1.5pts for the formal definition of $\mathcal{X}_j$ as an intersection of $K-1$ sets

$$\begin{aligned}\mathcal{X}_j &= \bigcap_{k \neq j} \{\boldsymbol{x} \in \mathbb{R}^D \mid \|\boldsymbol{x} - \boldsymbol{\mu}_j\|^2 < \|\boldsymbol{x} - \boldsymbol{\mu}_k\|^2\} \\ &= \bigcap_{k \neq j} \{\boldsymbol{x} \in \mathbb{R}^D \mid (\boldsymbol{\mu}_k - \boldsymbol{\mu}_j)^T (\boldsymbol{x} - (\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2) < 0\}\end{aligned}$$

0.5pts for the definition of convexity (if applied during further argumentation, otherwise **0pts**)

0.5pts for a graphical representation of the general setting for K-means (if used for further argumentation, otherwise **0pts**)

Solution 1:

In general for K clusters $\mathcal{X}_j$ is an **intersection of $K-1$ half-spaces (3pts)**:

- this point has to be clarified to get 3pts, otherwise only **1.5pts for stating this fact**,
- any complete and understandable **justification counts for 1.5pts**, for example
- consider the case $K = 2$ where $\mathcal{X}_j$ is a half-space and generalize it for larger K or
- rewrite the definition of $\mathcal{X}_j$ as above in form of an intersection of $K-1$ half-spaces.

Then $\mathcal{X}_j$ is convex since arbitrary **intersections of convex sets** are convex (**1pts** for any correct justification of convexity here).

Solution 2 (directly apply the definition of convexity):

Given $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathcal{X}_j$ and $\lambda \in (0, 1)$ we show that $\boldsymbol{x}_\lambda = \lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2 \in \mathcal{X}_j$ (**0.5pts** for the definition of convexity).

We **rewrite the definition of $\mathcal{X}_j$ (1.5pts)** as

$$\mathcal{X}_j = \{\boldsymbol{x} \in \mathbb{R}^D \mid \|\boldsymbol{x} - \boldsymbol{\mu}_j\|^2 < \|\boldsymbol{x} - \boldsymbol{\mu}_k\|^2 \text{ for all } k \neq j\}$$

2pts for the proof of "$\boldsymbol{x}_\lambda \in \mathcal{X}_j$" itself if completely correct (**1pt** if contains minor mistakes). For example: note, that for each $k \neq j$ the following conditions are equivalent (since $\|a\|^2 - \|b\|^2 = (a-b)^T(a+b)$)

$$\|\boldsymbol{x} - \boldsymbol{\mu}_j\|^2 < \|\boldsymbol{x} - \boldsymbol{\mu}_k\|^2 \;\Leftrightarrow\; (\boldsymbol{\mu}_k - \boldsymbol{\mu}_j)^T (\boldsymbol{x} - (\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2) < 0$$

and are satisfied for $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$. Then we can conclude for $\boldsymbol{x}_\lambda$ that

$$\begin{aligned}(\boldsymbol{\mu}_k - \boldsymbol{\mu}_j)^T(\boldsymbol{x}_\lambda - (\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2) &= (\boldsymbol{\mu}_k - \boldsymbol{\mu}_j)^T(\lambda\boldsymbol{x}_1 - \lambda(\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2 + (1-\lambda)\boldsymbol{x}_2 - (1-\lambda)(\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2) \\ &= \lambda \underbrace{(\boldsymbol{\mu}_k - \boldsymbol{\mu}_j)^T(\boldsymbol{x}_1 - (\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2)}_{<0} + (1-\lambda) \underbrace{(\boldsymbol{\mu}_k - \boldsymbol{\mu}_j)^T(\boldsymbol{x}_2 - (\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)/2)}_{<0} \\ &< 0\end{aligned}$$

Problem 10 [(2)=2 points] Given three 1-dimensional Gaussian distributions $\mathcal{N}(\mu_i, \sigma_i^2)$ with parameters

$$\mu_1 = 1, \quad \mu_2 = -1, \quad \mu_3 = 0,$$
$$\sigma_1 = 1, \quad \sigma_2 = 0.5, \quad \sigma_3 = 2.5$$

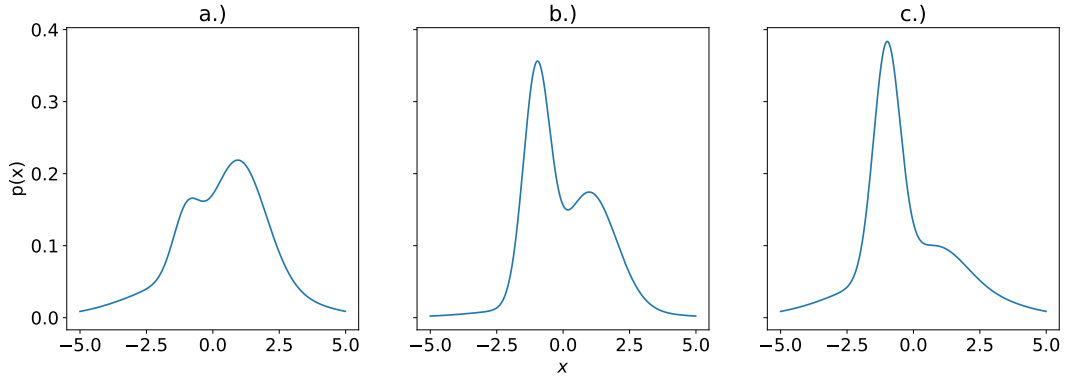
and three different vectors of mixing coefficients π defining categorical cluster priors.

Match the value of π in each row of the following table with one of the probability density functions

$$p(x) = \sum_{i=1}^{3} \pi_i \mathcal{N}(x \mid \mu_i, \Sigma_i)$$

of the resulting GMM showed below. Fill in the last column of the table, no argumentation required.

	π_1	π_2	π_3	PDF (a, b or c)
case 1	0.111...	0.444...	0.444...	
case 2	0.444...	0.111...	0.444...	
case 3	0.444...	0.444...	0.111...	



case 1 is c.)

case 2 is a.)

case 3 is b.)

1 pt. if at least one case is correct.

2 pts. if all cases are correctly matched.

Variational Inference

Problem 11 [(3+1+1+2)=7 points] Consider the following latent variable probabilistic model

$$p(z) = \mathcal{N}(z \mid 0, 1)$$
$$p(x \mid z) = \mathcal{N}(x \mid z, 1)$$

We want to approximate the posterior distribution $p(z \mid x)$ using the following variational family

$$\mathcal{Q} = \{\mathcal{N}(z \mid \mu, 1) \text{ for } \mu \in \mathbb{R}\}$$

that includes all normal distributions with unit variance.

Questions (a), (b), (c) and (d) are all concerning this setup.

Hint: Variance of $p(z \mid x)$ is equal to 0.5.

a) Write down the closed-form expression for ELBO $\mathcal{L}(q)$ and simplify it. You can ignore all the terms constant in μ.

$$\begin{aligned}
\mathcal{L}(q) &= \mathbb{E}_q\left[\log p(x, z) - \log q(z \mid \mu)\right] && \textbf{0.5pt.} \text{ for definition of ELBO} \\
&= \mathbb{E}_q\left[\log p(x \mid z) + \log p(z) - \log q(z \mid \mu)\right] && \textbf{0.5pt.} \text{ for expanding } \log p(x, z) \\
&= \mathbb{E}_q\left[-\frac{1}{2}(x - z)^2 - \frac{1}{2}z^2 + \frac{1}{2}(z - \mu)^2\right] + \text{const.} && \textbf{1pt.} \text{ for plugging in densities} \\
&= \mathbb{E}_q\left[zx - \frac{1}{2}z^2 - z\mu + \frac{1}{2}\mu^2\right] + \text{const.} \\
&= \mathbb{E}_q\left[z\right]x - \frac{1}{2}\mathbb{E}_q\left[z^2\right] - \mathbb{E}_q\left[z\right]\mu + \frac{1}{2}\mu^2 + \text{const.} && \textbf{0.5pt.} \text{ for linearity of expectation} \\
&= \mu x - \frac{1}{2}(\mu^2 + 1^2) - \mu^2 + \frac{1}{2}\mu^2 + \text{const.} \\
&= \mu x - \frac{1}{2}(\mu^2 + 1^2) - \mu^2 + \frac{1}{2}\mu^2 + \text{const.} \\
&= \mu x - \mu^2 + \text{const.} && \textbf{0.5pt.} \text{ for simplifying}
\end{aligned}$$

b) Find the optimal variational distribution $q^* \in \mathcal{Q}$ that maximizes the ELBO

$$q^* = \arg\max_{q \in \mathcal{Q}} \mathcal{L}(q)$$

i.e. find the mean μ^* of the optimal variational distribution q^*.

We already know the ELBO: just compute the derivative w.r.t. μ and set it to zero to obtain the optimal μ^*.

$$\mathcal{L}(\mu) = \mu x - \mu^2 + \text{const.}$$
$$\frac{\partial}{\partial \mu}\mathcal{L}(\mu) = x - 2\mu \stackrel{!}{=} 0$$
$$\iff \mu^* = \frac{x}{2}$$

1 pt. for setting the gradient of ELBO to zero and solving for μ.

c) Assume that the optimal q^* (i.e., the optimal μ^*) from question (b) is given. Which of the following statements is true?

(1) $\mathbb{KL}(q(z \mid \mu^*) \parallel p(z \mid x)) < 0$

(2) $\mathbb{KL}(q(z \mid \mu^*) \parallel p(z \mid x)) = 0$

(3) $\mathbb{KL}(q(z \mid \mu^*) \parallel p(z \mid x)) > 0$

Justify your answer.

KL-divergence is non-negative, so (1) is impossible. KL-divergence is equal to zero if and only if two distribution are equal. We know that variance of $p(z \mid x)$ is 0.5 (see hint), and the variance of $q(z \mid \mu)$ for any μ is equal to 1 (by definition). Hence, $q(z \mid \mu^*) \neq p(z \mid x)$ and therefore KL-divergence is greater than zero (option (3)).

1 pt. for the correct answer with justification.

d) For each of the conditions (1), (2), (3) from question (c) above, provide a parametric variational family $\mathcal{Q}_i$, such that the optimal q_i^* from each family would fulfill the respective condition, or explain why it's impossible.

That is, provide $\mathcal{Q}_1$, such that for $q_1^* = \arg\max_{q \in \mathcal{Q}_1} \mathcal{L}(q)$ we have $\mathbb{KL}(q_1^*(z) \parallel p(z \mid x)) < 0$, for $q_2^* = \arg\max_{q \in \mathcal{Q}_2} \mathcal{L}(q)$ we have $\mathbb{KL}(q_2^*(z) \parallel p(z \mid x)) = 0$, and for $q_3^* = \arg\max_{q \in \mathcal{Q}_3} \mathcal{L}(q)$ we have $\mathbb{KL}(q_3^*(z) \parallel p(z \mid x)) > 0$.

(1) Is impossible since KL is always nonnegative. **0.5 pt.**

(2) The likelihood $p(x \mid z)$ and the prior $p(z)$ are both normal distributions, hence the posterior $p(z \mid x)$ is also a normal distribution. Therefore, the posterior is contained in the set of all normal distributions $\mathcal{Q}_2 = \{\mathcal{N}(\mu, \sigma^2) \text{ for } \mu \in \mathbb{R}, \sigma^2 \in \mathbb{R}_{>0}\}$. **1 pt.**

(3) $\mathcal{Q}_3 = \{\mathcal{N}(\mu, 1) \text{ for } \mu \in \mathbb{R}\}$ works (see answer to (c)). **0.5 pt.**