Exam-solution-2018 - Altklausur

Machine learning (Technische Universität München)

Machine Learning Final Exam SOLUTION

1	2	3	4	5	6	7	8	9	10	11	12	∑
5	7	[illegible]	[illegible]	[illegible]	[illegible]	8	7	3	6	9	8	??

[illegible] 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 15-18 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 ?? pages, ?? problems. You can earn ?? points.

1 Decision Trees

Problem 1 [(1+4)=5 points] You are developing a model to classify games at which machine learning will beat the world champion within five years. The following table contains the data you have collected.

x_1 (Team or Indivi[illegible]	[illegible]r Physical)	x_3 (Skill or Chance)	y (Win or Lose)
T	[illegible]	S	W
I	[illegible]	S	W
T	[illegible]	S	W
I	[illegible]	C	W
T	[illegible]	S	L
I	M	C	L
T	P	C	L
T	P	C	L
T	P	C	L
I	P	S	W

You can look up the value of $\log_2(x)$ in this table:

x	0.10	0.2	0.25	0.33	0.50	0.66	0.75	0.8	1.0
$\log_2(x)$	-3.32	-2.32	-2.0	-1.60	-1.0	-0.60	-0.42	-0.32	0.0

a) Calculate the entropy $i_H(y)$ of the class labels y.

$$p(y = W) = p(y = L) = 1/ \qquad \textbf{-0.25pt. for each calculation mistake}$$
$$H(y) = p(y = W)\log p(y = W) + p(y = L)\log p(y = L) = 1$$

b) Build the optimal decision tree of depth 1 using entropy as the impurity measure. Which attribute is selected as the root of the decision tree?

Splitting on x_1: **1pt total, -0.25pt. for each calculation mistake**

$$p(y = W|x_1 = T) = 2/6 \qquad p(y = W|x_1 = I) = 3/4$$
$$i_H(x_1 = T) = 1/3 \cdot log(1/3) + 2/3 \cdot log(2/3) \approx 0.93$$
$$i_H(x_1 = I) = 3/4 \cdot log(3/4) + 1/4 \cdot log(1/4) = 0.815$$
$$\Delta(x1) = 1 - \frac{6}{10} \cdot 0.93 - \frac{4}{10} \cdot 0.815 \approx 0.12$$

Splitting on x_2: **1pt total, -0.25pt. for each calculation mistake**

$$p(y = W|x_2 = M) = 1/4 \qquad p(y = W|x_2 = P) = 2/6$$
$$\Delta(x2) = \Delta(x1)$$

Splitting on x_3: **1pt total, -0.25pt. for each calculation mistake**

$$p(y = W|x_3 = S) = 4/5 \qquad p(y = W|x_3 = C) = 1/5$$
$$i_H(x_3 = S) = 4/5 \cdot log(4/5) + 1/5 \cdot log(1/5) \approx \frac{3.6}{5}$$
$$\Delta(x3) = 1 - \frac{1}{2}\frac{3.6}{5} - \frac{1}{2}\frac{3.6}{5} = 1 - \frac{3.6}{5} = \frac{1.4}{5} = 0.28$$

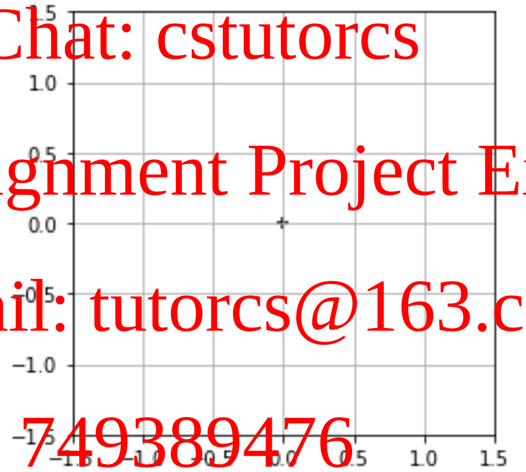
We would split on x_3 since it yields the highest information gain. **1pt. for final answer**

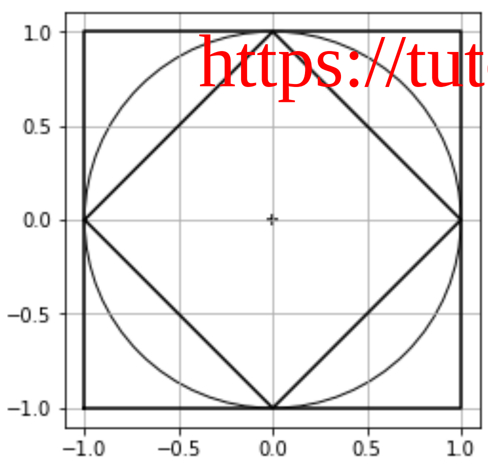
2 KNN

Problem 2 [(1.5+5.5)=7 points]

a) Let $\boldsymbol{x} \in \mathbb{R}^2$. Draw e following norms. Make sure to clearly label which circle corresponds to wh

- L_1-norm: $||\boldsymbol{x}$
- L_2-norm: $||\boldsymbol{x}$
- L_∞-norm: $||\boldsymbol{x}||_\infty = \max_i |x_i|$





0.5pt. for each correctly drawn unit circle

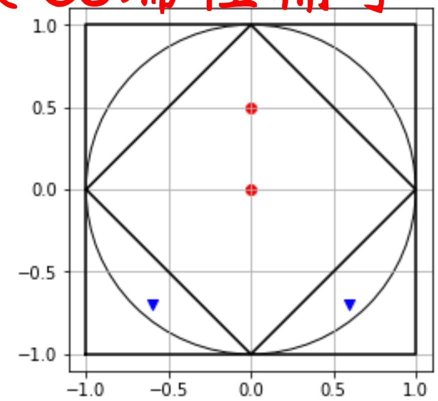
b) Construct a binary classification dataset that consists of 4 data points, that is specify $\boldsymbol{x}_i \in \mathbb{R}^2$ and $y_i \in \{0, 1\}$ (i.e. write the coordinates and labels) for each data point i, such that:

Performing leave-one-out cross validation (LOOCV) with a 1-NN (one nearest neighbor) classifier using L_1 distance yields 0% misclassification rate. Meanwhile, performing LOOCV with a 1-NN classifier using L_∞ distance on the same dataset yields misclassification rate of 50%.

Hint: Remember the shape of the unit circles.

Class red: $p_1 =$
$q_1 = (-0.6, -0.7$

Class blue:



$$L_1(p_1, q_1) = 1.3, \quad L_1(p_1, q_2) = 1.3, \quad L_1(q_1, q_2) = 1.2$$
$$L_\infty(p_1, q_1) = 0.7, \quad L_\infty(p_1, q_2) = 0.7, \quad L_\infty(q_1, q_2) = 1.4$$

0.5pt. 2 samples (red) are in L_1 unit circle
1pt. 2 samples (blue) are in L_∞ unit circle but not in L_1 unit circle
1pt. L_1-distance between red samples is smaller than L_1 distance to a blue sample
1pt. L_∞-distance between red samples is smaller than L_∞ distance to a blue sample
1pt. L_1-distance between blue samples is smaller than L_1 distance to a red sample
1pt. L_∞-distance between blue samples is greater than L_∞ distance to a blue sample

3 Probabilistic Inference

Problem 3 [(6)=6 points] A kangaroo starts from a random location $\boldsymbol{x}_0 \in \mathbb{R}^2$ in the jungle and after one jump reaches the location $\boldsymbol{x}_1 \in \mathbb{R}^2$.

The prior over the start[illegible]andard bivariate normal distribution

$$[illegible]\ \mathcal{N}\left(\boldsymbol{x}_0 \,\middle|\, \begin{bmatrix}0\\0\end{bmatrix}, \boldsymbol{I}_{2\times2}\right),$$

where $\boldsymbol{I}_{2\times2}$ denotes the [illegible]ix.

The conditional distribu[illegible]rmal distribution with mean $\boldsymbol{x}_0$ and identity covariance

$$p(\boldsymbol{x}_1|\boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_1|\boldsymbol{x}_0, \boldsymbol{I}_{2\times2})$$

Assume that we observe $\boldsymbol{x}_1$, the position of the kangaroo after the jump.

Write down the closed-form expression for $p(\boldsymbol{x}_0|\boldsymbol{x}_1)$. Make sure that you obtain a valid probability distribution (i.e. it integrates to one). Show your work.

Important: You are not allowed to simply use facts about conditionals of multivariate normal distribution (e.g. from Bishop's book). Derive the result starting from the Bayes formula.

$$p(\boldsymbol{x}_0|\boldsymbol{x}_1) \propto p(\boldsymbol{x}_1|\boldsymbol{x}_0)p(\boldsymbol{x}_0)$$ Bayes formula **1 pt**

$$\propto \mathcal{N}\left(\boldsymbol{x}_0 \,\middle|\, \begin{bmatrix}0\\0\end{bmatrix}, \boldsymbol{I}_{2\times2}\right) \times \mathcal{N}(\boldsymbol{x}_1|\boldsymbol{x}_0, \boldsymbol{I}_{2\times2})$$

$$\propto \exp\left(-\frac{1}{2}\boldsymbol{x}_0^T\boldsymbol{x}_0\right)\exp\left(-\frac{1}{2}(\boldsymbol{x}_0^T - \boldsymbol{x}_1)^T(\boldsymbol{x}_0 - \boldsymbol{x}_1)\right)$$ Writing the densities **1 pt**

Simplify & absorb all the terms constant in $\boldsymbol{x}_0$ into $\propto$

$$\propto \exp\left(-\frac{1}{2}\left(2\boldsymbol{x}_0^T\boldsymbol{x}_0 - 2\boldsymbol{x}_1^T\boldsymbol{x}_0\right)\right)$$ Simplifying **1 pt**

We see that there is a quadratic term $2\boldsymbol{x}_0^T\boldsymbol{x}_0$ and a linear term $-2\boldsymbol{x}_1^T\boldsymbol{x}_0$ in the exponent. Therefore we conclude that this is a normal distribution.

$$\propto \mathcal{N}(\boldsymbol{x}_0 \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$$ Showing that posterior is $\mathcal{N}$ **1 pt**

$$\propto \exp\left(-\frac{1}{2}(\boldsymbol{x}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x}_0 - 2\boldsymbol{x}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu})\right)$$

We need to complete the square and determine its parameters $\boldsymbol{\Sigma}$ and $\boldsymbol{\mu}$.

$$\boldsymbol{x}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x}_0 \overset{!}{=} 2\boldsymbol{x}_0^T\boldsymbol{x}_0 \iff \boldsymbol{\Sigma} = \frac{1}{2}\boldsymbol{I}$$ Computing $\boldsymbol{\Sigma}$ **1 pt**

$$2\boldsymbol{x}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} \overset{!}{=} 2\boldsymbol{x}_0^T\boldsymbol{x}_1 \iff \boldsymbol{\mu} = \frac{1}{2}\boldsymbol{x}_1$$ Computing $\boldsymbol{\mu}$ **1 pt**

Therefore the posterior distribution is

$$p(\boldsymbol{x}_0 \mid \boldsymbol{x}_1) = \mathcal{N}\left(\boldsymbol{x}_0 \mid \frac{1}{2}\boldsymbol{x}_1, \frac{1}{2}\boldsymbol{I}\right)$$

4 Regression

Problem 4 [(7)=7 points] Consider the following one-dimensional regression problem:

$$\ldots_i, \tau) = \mathcal{N}(y_i \mid wx_i, \tau^2)$$
$$\ldots \mid \sigma) = \mathcal{N}(w \mid 0, \sigma^2)$$

where $x_i, y_i \in \mathbb{R}$, and τ [illegible] ariance parameters. You fit the parameter w using, e.g., the MLE or the MAP a[illegible] $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_N)\}$ of N i.i.d. instances.

Your task is to qualitati[illegible] appens to the quantities in each column as the parameters in each row vary. Speci[illegible] f the table below you have to write one and only one of the following three options: *(i) increases*, *(ii) decreases* or *(iii) no change.*

For example in the top left cell you have to specify whether the quantity $\mathrm{Var}(p(w|\sigma))$ increases, decreases or does not change as we increase the value of the parameter σ.

	$\mathrm{Var}(p(w\|\sigma))$	$\|w_{MLE} - w_{MAP}\|$	$\|\mathbb{E}_{p(w\|\mathcal{D})}[w] - w_{MAP}\|$
σ increases	increases	decreases	no change
σ decreases	decreases	increases	no change
N increases	no change	decreases	no change

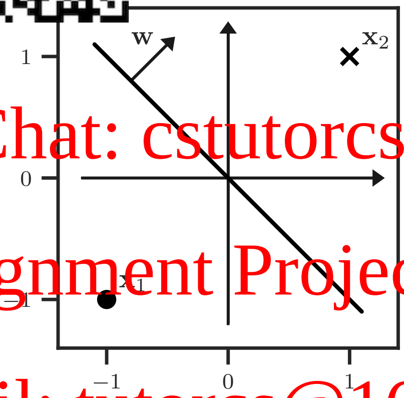
In the table above

- $\mathrm{Var}(p(w|\sigma))$ denotes the variance of the distribution $p(w|\sigma)$
- w_{MLE} and w_{MAP} denote the maximum likelihood estimate and the MAP estimate of the parameter w respectively.
- $\mathbb{E}_{p(w|\mathcal{D})}[w]$ is the expectation of the posterior distribution over w.
- $|\cdot|$ denotes the absolute value.

column 1: 0.5pt. for the first two cells and 1pt. point for the last cell
column 2: 1pt. for each cell
column 3: 2pt. if all cells are correct otherwise 0

Classification

Problem 5 [(5)=5 points] Consider the classification problem in the figure below. There are two points, $\mathbf{x}_1 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$ with [illegible] $= \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ with class $y_2 = 1$. Further you are given a logistic regression model with [illegible] $\begin{bmatrix} \log 2 \\ \log 2 \end{bmatrix}$. Here, log denotes natural logarithms, i.e. base e. Assume that there is n[illegible]



Prove or disprove that the weight vector $\boldsymbol{w}$ is the MAP estimate for a logistic regression model with a Gaussian prior on $\boldsymbol{w}$ with precision $\lambda = 1$.

$$\mathbf{w}_{MAP} = \arg\max_{\mathbf{w}} p(\mathbf{w}|\mathcal{D}) \qquad \textbf{0.5pt}$$

$$= \arg\max_{\mathbf{w}} \log p(\mathbf{w}|\mathcal{D}) \qquad \textbf{0.5pt}$$

$$\Leftrightarrow \nabla_{\mathbf{w}} \log p(\mathbf{w}|\mathcal{D}) \stackrel{!}{=} 0 \qquad \textbf{1pt}$$

The students also get the points if they directly start with log likelihood + regularization.

Loss function:

$$\mathcal{L}(\mathbf{w}) = -\left(\sum_{i=1}^{2} y_i \log \sigma(\mathbf{w}^\top \mathbf{x}_i) + (1 - y_i) \log(1 - \sigma(\mathbf{w}^\top \mathbf{x}_i))\right) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \quad \textbf{1 pt for correct loss fn}$$

First we derive the gradient of the negative log likelihood.

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = -\left(\sum_{i=1}^{n} \mathbf{x}_i \left[y_i - \sigma\left(\mathbf{w}^\top \mathbf{x}_i\right)\right]\right) + \lambda \mathbf{w}. \qquad \textbf{1 pt for correct derivative}$$

Plugging in our numbers we get

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = -\mathbf{x}_1 \left[0 - \sigma\left(\mathbf{w}^\top \mathbf{x}_1\right)\right] - \mathbf{x}_2 \left[1 - \sigma\left(\mathbf{w}^\top \mathbf{x}_2\right)\right] + \lambda \mathbf{w}$$

$$= -\begin{bmatrix} 1/5 \\ 1/5 \end{bmatrix} - \begin{bmatrix} 1/5 \\ 1/5 \end{bmatrix} + \begin{bmatrix} \log 2 \\ \log 2 \end{bmatrix} = \begin{bmatrix} -2/5 + \log 2 \\ -2/5 + \log 2 \end{bmatrix}$$

Since the gradient w.r.t. the weights is not zero the solution is not optimal. That is, $\mathbf{w}$ is not the MAP estimate of the logistic regression model.

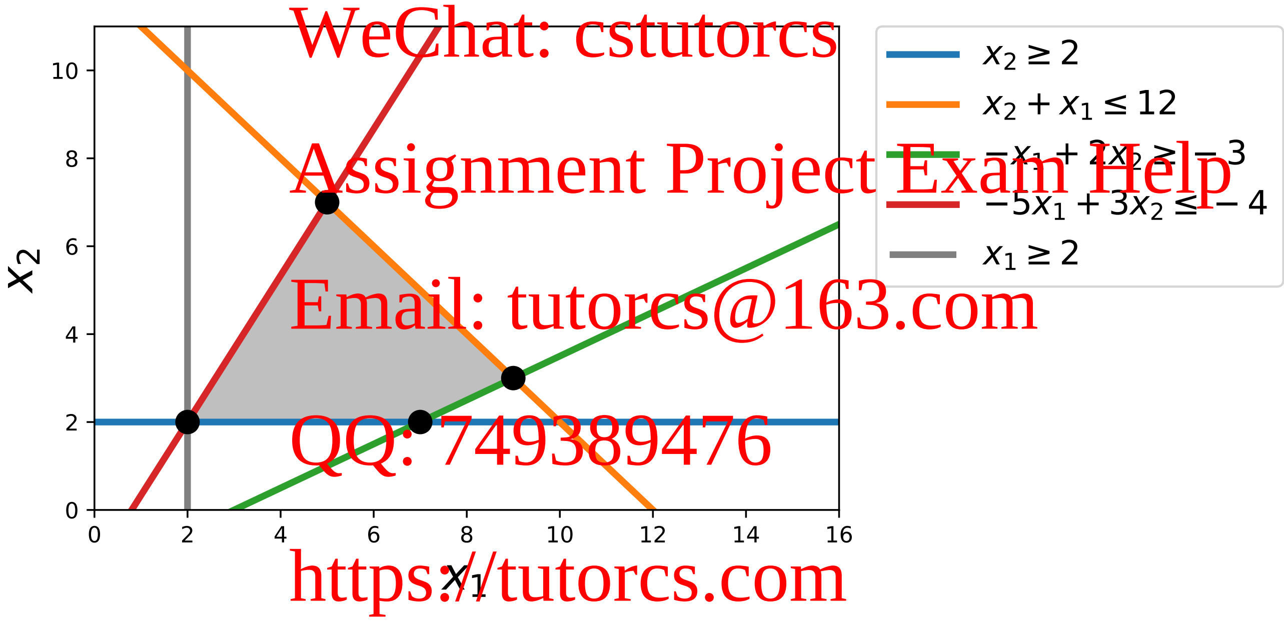
1 pt for correct result [illegible] here are some arithmetic mistakes but they still arrive at the gradient $\neq 0$ a[illegible] they can also get the point. No points for just stating the conclusion withou[illegible]

5 Constrained Optimization

Problem 6 [(3+3)=6 points] Consider the following optimization problem

$$\min_{x_1,x_2} 2x_1 - 3x_2$$
$$x_1 \geq 2$$
$$x_2 \geq 2$$
$$x_1 + x_2 \leq 12$$
$$-x_1 + 2x_2 \geq -3$$
$$-5x_1 + 3x_2 \leq -4$$

a) Draw the set of feasible points



3pt. if all correct.
-0.5pt. for every incorrect line.
-1pt. if feasible set not marked.

b) Solve the optimization problem, i.e. find the minimizer (x_1^*, x_2^*).

The domain (feasible set) is a convex set. Minimizing a concave function is equivalent to maximizing a convex function. We know from the lecture that in this case the optimum lies on one of the vertices of the domain. That is, we only need to check the points $(2, 2)$, $(7, 2)$, $(5, 7)$ and $(9, 3)$. By checking these 4 points we conclude that $(x_1^*, x_2^*) = (5, 7)$ is the solution.

1.5pt. for the correct minimizer
1.5pt. for the explanation

6 SVM

Problem 7 [(7+1)=8 points]

a) Consider training a hard-margin SVM using a linear kernel $k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{x}_i^T \boldsymbol{x}_j$ on a linearly separable training set $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), \dots (\boldsymbol{x}_N, y_N)\}$. Let s denote the number of support vectors we would obtain if we would train on the entire dataset. Furthermore, let ε denote the leave-one-out cross validation (LOOCV) misclassification rate.

Does the following [illegible]stify your answer.

$$\varepsilon \leq \frac{s}{N}$$

Intuitively, the [illegible]e following claim (which we prove below): if $\boldsymbol{x}_i$ is not a support vector when training on the entire training set, then the optimal $\boldsymbol{w}^*$ and b^* do not change when leaving $\boldsymbol{x}_i$ out of the training set.

Since the original data are linearly separable and since we are using a hard-margin classifier, the hypothesis given by the original $\boldsymbol{w}^*$ and b^* will not make an error on $\boldsymbol{x}_i$, and hence, no error will be made in the i-th step of the LOOCV. Equivalently, the only *possible* errors in the LOOCV procedure are made on $\boldsymbol{x}_i$'s which are support vectors when training on the entire training set, and hence $\varepsilon \leq \frac{s}{N}$.

(The following details are not required for full points).

Formally, let $(\boldsymbol{w}^*_{\mathcal{D}}, b^*_{\mathcal{D}})$ and $\boldsymbol{\alpha}^*_{\mathcal{D}}$ denote the optimal primal and dual solutions for the SVM when training on the entire $\mathcal{D}$. Also let $\mathcal{D}_i = \mathcal{D} \setminus \{(\boldsymbol{x}_i, y_i)\}$ be the set of training examples when omitting the i-th example, and let $(\boldsymbol{w}^*_{\mathcal{D}_i}, b^*_{\mathcal{D}_i})$ and $\boldsymbol{\alpha}^*_{\mathcal{D}_i}$ be the optimal primal and dual variables of the optimization problem when training on $\mathcal{D}_i$.

$\boldsymbol{\alpha}_{\mathcal{D}_i}$ consists of only $n-1$ variables, namely $\boldsymbol{\alpha}_{\mathcal{D}_i,1}, \dots, \boldsymbol{\alpha}_{\mathcal{D}_i,i-1}, \boldsymbol{\alpha}_{\mathcal{D}_i,i+1}, \dots, \boldsymbol{\alpha}_{\mathcal{D}_i,N}$. Now consider setting the dual variables as follows $\boldsymbol{\alpha}_{\mathcal{D}_i,j} = \boldsymbol{\alpha}^*_{\mathcal{D},j}$ for $j \neq i$. Note that, if $\boldsymbol{x}_i$ is not a support vector when training on $\mathcal{D}$ then $\boldsymbol{\alpha}^*_{\mathcal{D},i} = 0$. We can verify that $(\boldsymbol{w}^*_{\mathcal{D}}, b^*_{\mathcal{D}})$ and $\boldsymbol{\alpha}_{\mathcal{D}_i}$ satisfy the KKT conditions for the SVM optimization problem when training on $\mathcal{D}_i$ (e.g. the condition regarding the derivatives of the Lagrangian with respect to the primal variables is guaranteed to hold by our construction). From this, and the fact that $\boldsymbol{w}^*_{\mathcal{D}}$, $b^*_{\mathcal{D}}$ are unique since the objective function is strictly convex we can conclude that $\boldsymbol{w}^*$, b^* do not change when omitting $\{(\boldsymbol{x}_i, y_i)\}$ as desired.

3pt. for stating that w^* and b^* do not change when leaving out a non-support vector
3pt. for stating that only possible errors are made by leaving out support vectors
1pt. for combining the above two statements to get the inequality

b) Consider a setting similar to the previous problem, except that we now we use SVM with an arbitrary valid kernel k. Assume that the data is linearly separable in the feature space corresponding to the kernel. Does $\varepsilon \leq \frac{s}{N}$ hold in this case? Justify your answer.

Yes. The above argument only uses the facts that the optimum of a convex optimization problem is not affected by leaving out non-active constraints, and that the training data can be perfectly classified by the obtained hypothesis based on training on the full dataset. The choice of kernel has no influence. **1pt**

7 Kernels

Problem 8 [(7)=7 points] Let $\mathcal{M}$ denote the set of all real-valued matrices of arbitrary size.

Prove or disprove that the function $k : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ is a valid kernel:

$$k(X, Y) = \min\{\text{rank}(X), \text{rank}(Y)\}$$

Consider the feature [illegible] $\underbrace{\ldots, 1}_{\text{ones}}, \underbrace{0, 0, 0, 0, 0, 0, 0, 0, 0 \ldots}_{\text{zeros everywhere else}})$.

Then $\phi(X)^T \phi(Y) = \sum$ [illegible] $\min\{\text{rank}(X), \text{rank}(Y)\} = k(X, Y)$ is the inner product. Hence, $k(X, Y)$ is a v[illegible]

1pt. for definition of [illegible] **cer's theorem (0.5pt. for only using Mercer's theorem / stating it partially)**
6pt. for the proof

8 Deep Learning

Problem 9 [(1+1+1)=3 points] You are given a dataset containing images $x_i \in [0, 1]^D$ (all the pixel values are normalized between 0 and 1) and respective class labels $y_i \in \{1, ..., C\}$. You implement a fully connected neural network with two hidden layers, *tanh* activations and L_2 regularization on all weights excluding biases.

a) Consider two strategies for initializing the weights of your neural network.

1) Sample the weights from Uniform$(-10, 10)$
2) Sample the weights from Uniform$(-1, 1)$

Which choice (1 or 2) is more reasonable, given that we are training the network with backpropagation? Justify your answer.

We choose 2) to prevent saturation and vanishing gradients (because of *tanh*). Just mentioning activation function without vanishing gradients is not enough.
Answering that L_2 norm will dominate the loss is not necessarily correct. If you sample 100 weights from 1) and 2), L_2 norm will be around 5×10^{-4} and 5×10^{-3} respectively. However, $tanh'(1) = 0.42$ and $tanh'(10) = 0.0$ leading to the vanishing gradient problem.
Answers containing exploding gradients are also not correct because max of $tanh'$ is 1.

1pt only if the correct option is selected **with** a valid explanation.

b) When training neural networks, why do we usually stop training when the loss on the validation set starts to increase?

Overfitting. (**1pt**)

c) After training has finished, your model has high training loss and high validation loss. What should you do? Justify your answer.

Since both training and validation loss are high we are underfitting. Solution:
Increase the network capacity/complexity by choosing bigger/wider network (more neurons/parameters/layers) or reduce regularization (in our case L_2).
Incorrect answers:

Student ID:

It is not obvious why data augmentation would help since we have normalized images. Overfitting to a small subset of the training set is a good initial approach but not mentioning network capacity or a way to increase it (further steps) is incomplete answer.
Learning rate c ending on the shape of our loss function it may not matter. On the ing rate can have slower convergence but given enough iterations we wi um (assume using b) as a training procedure).
Change of activ d not matter since we only have 2 layers so gradient problems can be r intialization (see a)).

1pt if the answer contains increasing complexity **or** lower regularization.
0.5pt if the answer is suggesting "different architecture" or reseting and trying again while acknowledging that the network did not learn anything
Points are not deducted for writing some items from a list of incorrect answers unless they are fundamentally wrong (e.g. saying the model is overfitting).

9 Dimensionality Reduction

Problem 10 [(6)=6 points] Let the matrix $\boldsymbol{X} \in \mathbb{R}^{N \times D}$ represent N data points of dimension $D = 10$ (samples stored as rows). We applied PCA to $\boldsymbol{X}$. By using the $K = 5$ top principal components, we transformed/projected $\boldsymbol{X}$ into $\tilde{\boldsymbol{X}} \in \mathbb{R}^{N \times K}$. We computed that $\tilde{\boldsymbol{X}}$ preserves 70% of the variance of the original data $\boldsymbol{X}$.

Suppose now we apply PCA on the following matrices:

a) $\boldsymbol{Y}_1 = \boldsymbol{X}\boldsymbol{S}$ where $\boldsymbol{S} = \lambda \boldsymbol{I}$, with $\lambda \in \mathbb{R}$ and $\boldsymbol{I} \in \mathbb{R}^{D \times D}$ is the identity matrix

b) $\boldsymbol{Y}_2 = \boldsymbol{X}\boldsymbol{R}$ where $\boldsymbol{R} \in \mathbb{R}^{D \times D}$ and $\boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{I}$

c) $\boldsymbol{Y}_3 = \boldsymbol{X}\boldsymbol{P}$ where $\boldsymbol{P} = \text{diag}(+5, -5, \dots, +5, -5)$ is a $D \times D$ diagonal matrix

d) $\boldsymbol{Y}_4 = \boldsymbol{X}\boldsymbol{Q}$ where $\boldsymbol{Q} = \text{diag}(1, 2, 3, \dots, D-1, D)$ is a $D \times D$ diagonal matrix

e) $\boldsymbol{Y}_5 = \boldsymbol{X} + \mathbf{1}_N \boldsymbol{\mu}^T$ where $\boldsymbol{\mu} \in \mathbb{R}^D$ and $\mathbf{1}_N$ is an N-dimensional column vector of all ones

f) $\boldsymbol{Y}_6 = \boldsymbol{X}\boldsymbol{A}$ where $\boldsymbol{A} \in \mathbb{R}^{D \times D}$ and $\text{rank}(\boldsymbol{A}) = 5$

and obtain the projected data $\tilde{\boldsymbol{Y}}_1, \dots \tilde{\boldsymbol{Y}}_6 \in \mathbb{R}^{N \times K}$ using the principal components corresponding to the top $K = 5$ largest eigenvalues of the respective $\boldsymbol{Y}_i$.

What fraction of variance of each $\boldsymbol{Y}_i$ will be preserved by each respective $\tilde{\boldsymbol{Y}}_i$? Justify your answer.

The answer "cannot tell without additional information" is also valid if you provide a justification.

1pt. for each correct answer with justification. 0pt. without justification.

a) 70%. All eigenvalues are scaled by the same amount λ^2, so the fraction doesn't change.

b) 70%. $\boldsymbol{R}$ is a rotation/reflection/permutation matrix. The direction of the eigenvectors of the covariance matrix is changed, but the eigenvalues stay the same.

c) 70%. This is just combination of (a) and (b). All data points are scaled by 5 (i.e. eigenvalues of $\boldsymbol{X}^T\boldsymbol{X}$ are all scaled by 25), and some dimensions are reflected around origin, but the fraction of variance explained by the first K components stays the same.

d) We cannot tell without additional information: since each column (i.e. each dimension) is scaled by a different amount.

e) 70%. All data p [illegible]. But since we center the data as the first step of PCA, shifting has no [illegible]

f) 100%. Since ra [illegible] ≤ 5 as well. This means that the data lies in a ≤ 5 dimensional sub [illegible] 5 principal components capture all the variance.

10 Gaussian Mixture Models

Problem 11 [(2+5+2)=9 points] Consider two random variables $\boldsymbol{x} \in \mathbb{R}^D$ and $\boldsymbol{y} \in \mathbb{R}^D$ distributed according to two different Gaussian mixture models

$$\sum_{k=1}^{K_X} \pi_k^X \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k^X, \boldsymbol{\Sigma}_k^X),$$

$$\sum_{l=1}^{K_Y} \pi_l^Y \mathcal{N}(\boldsymbol{y}|\boldsymbol{\mu}_l^Y, \boldsymbol{\Sigma}_l^Y),$$

The first mixture $p(\boldsymbol{x}|\boldsymbol{\theta}^X)$ consists of K_X components with parameters $\boldsymbol{\theta}_k^X = (\pi_k^X, \boldsymbol{\mu}_k^X, \boldsymbol{\Sigma}_k^X)$ for $k \in \{1, \ldots, K_X\}$. Similarly, $p(\boldsymbol{y}|\boldsymbol{\theta}^Y)$ consists of K_Y components with parameters $\boldsymbol{\theta}_l^Y = (\pi_l^Y, \boldsymbol{\mu}_l^Y, \boldsymbol{\Sigma}_l^Y)$ for $l \in \{1, \ldots, K_Y\}$.

We generate a new random variable $\boldsymbol{z} \in \mathbb{R}^D$ as $\boldsymbol{z} = \boldsymbol{x} + \boldsymbol{y}$.

a) Describe the generative process (process of drawing the samples) for $\boldsymbol{z}$.

0.5pt. for mentioning that we have to **draw** one sample from $\boldsymbol{x}$ and one sample from $\boldsymbol{y}$.

0.5pt. for mentioning that $\boldsymbol{x}$ and $\boldsymbol{y}$ are GMMs and we can draw samples from them as discussed in the lecture (or describing the generative process step by step).

1pt. for stating that you have to **sum** two samples up to a get a sample from $\boldsymbol{z}$.

Example:

- Draw k from the categorical distribution on $\{1, \ldots, K_X\}$ with probabilities from $\boldsymbol{\pi}^X$.
- Draw $\tilde{\boldsymbol{x}}$ from the normal distribution $N(\boldsymbol{\mu}_k^X, \boldsymbol{\Sigma}_k^X)$
- Draw l from the categorical distribution on $\{1, \ldots, K_Y\}$ with probabilities from $\boldsymbol{\pi}^Y$.
- Draw $\tilde{\boldsymbol{y}}$ from the normal distribution $N(\boldsymbol{\mu}_l^Y, \boldsymbol{\Sigma}_l^Y)$
- Return $\tilde{\boldsymbol{z}} := \tilde{\boldsymbol{x}} + \tilde{\boldsymbol{y}}$ as a sample from $\boldsymbol{z}$.

b) Explain in a few sentences why $p(\boldsymbol{z}|\boldsymbol{\theta}^{\boldsymbol{X}}, \boldsymbol{\theta}^{\boldsymbol{Y}})$ is again a mixture of Gaussians.

Let $\boldsymbol{x}$ be drawn from the component k of $p(\boldsymbol{x} \mid \boldsymbol{\theta}^X)$ and $\boldsymbol{y}$ be drawn from the component l of $p(\boldsymbol{y} \mid \boldsymbol{\theta}^Y)$. Then $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}_k^X, \boldsymbol{\Sigma}_k^X)$ and $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}_l^Y, \boldsymbol{\Sigma}_l^Y)$. Since $\boldsymbol{z}$ is a sum of two normally distributed random variables, it also follows normal distribution $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{\mu}_k^X + \boldsymbol{\mu}_l^Y, \boldsymbol{\Sigma}_k^X + \boldsymbol{\Sigma}_l^Y)$. There are $K_X \cdot K_Y$ such possible (k, l) combinations, each having probability $\pi_k^X \pi_l^Y$ respectively.

That is, $p(\boldsymbol{z} \mid \boldsymbol{\theta}^X, \boldsymbol{\theta}^Y)$ is a mixture of $K_X K_Y$ gaussians.

c) Write down the probability density function $p(\boldsymbol{z}|\boldsymbol{\theta}^X, \boldsymbol{\theta}^Y)$ of $\boldsymbol{z}$.
It's enough to just state the answer (no need to show the derivation).

There are three components of the right answer: double sum over normal components of $\boldsymbol{x}$ and $\boldsymbol{y}$, mixing probabilities $\pi_k^X \pi_l^Y$ and Gaussian components $\mathcal{N}(\boldsymbol{z}|\boldsymbol{\mu}_k^X + \mu_l^Y, \boldsymbol{\Sigma}_k^X + \boldsymbol{\Sigma}_l^Y)$.

2pt. if all three parts are correct.

1pt. if at least one part is correct (even the summation).

0pt. if nothing is matchable with the correct answer.

$$\sum_{l=1}^{K_Y} \pi_k^X \pi_l^Y \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_k^X + \boldsymbol{\mu}_l^Y, \boldsymbol{\Sigma}_k^X + \boldsymbol{\Sigma}_l^Y).$$

11 Variational Inference

The exponential distribution with a scale parameter $\alpha > 0$ is defined as

$$\text{Expo}(\theta \mid \alpha) = \begin{cases} \frac{1}{\alpha}\exp(-\frac{1}{\alpha}\theta) & \text{if } \theta \geq 0 \\ 0 & \text{else} \end{cases}, \qquad \mathbb{E}[x] = \alpha, \qquad \mathbb{E}[x^2] = 2\alpha^2$$

Problem 12 [(4+2+2)=8 points] Consider the following probabilistic model.

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

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

$$q(z \mid \beta) = \text{Expo}(z \mid \beta)$$

a) Write down a closed-form for ELBO $\mathcal{L}(\beta)$ and simplify it as far as you can. You can ignore the terms that are constant in β.

Plugging in the definition of ELBO

$$\begin{aligned}
\mathcal{L}(\beta) &= \mathbb{E}_q[\log p(x,z) - \log q(z \mid \beta)] && \textbf{0.5pt.} \text{ for writing ELBO} \\
&= \mathbb{E}_q[\log p(x \mid z) + \log p(z) - \log q(z \mid \beta)] && \textbf{1pt.} \text{ for expanding } \log p(x,z) \\
&= \mathbb{E}_q\left[-\frac{1}{2}(x-z)^2 - z + \frac{1}{\beta}z\right] + \text{const.} && \textbf{1.5pt.} \text{ for computing logs} \\
&= \mathbb{E}_q\left[xz - \frac{1}{2}z^2 - z - \log\frac{1}{\beta} + \frac{1}{\beta}z\right] + \text{const.} && \uparrow (\textbf{0.5} \text{ for each distribution}) \\
&= x\mathbb{E}_q[z] - \frac{1}{2}\mathbb{E}_q[z^2] - \mathbb{E}_q[z] + \log\beta + \frac{1}{\beta}\mathbb{E}_q[z] + \text{const.} && \textbf{1pt.} \text{ for linearity of } \mathbb{E} \\
&= x\beta - \beta^2 - \beta + \log\beta + 1 + \text{const.} \\
&= -\beta^2 + (1-x)\beta + \log\beta + \text{const.}
\end{aligned}$$

b) Is the ELBO convex in β? Justify your answer.

2pt. for the correct answer with justification.

$-\beta^2$, $(1-x)\beta$ and $\log\beta$ are all concave functions of β, so their sum is also concave. Hence $\mathcal{L}(\beta)$ is not convex.

c) Outline the main steps for solving the optimization problem

$$\min_{\beta} \; \mathbb{KL}(q(z \mid \beta) \,\|\, p(z \mid x))$$

You don't need to [illegible] computations, just clearly describe each step.

Does this optimiz[illegible] closed-form solution? Why or why not?

1pt. Minimizing [illegible]

$$[illegible] \; \mathbb{KL}(q(z \mid \beta) \,\|\, p(z \mid x))$$

is equivalent to maximizing the ELBO

$$\max_{\beta} \mathbb{E}_q \left[\log p(x, z) - \log q(z \mid \beta)\right]$$

1pt. We already showed that ELBO is concave in β for this model, so we simply need to compute the gradient w.r.t. β and set it to zero

$$\nabla_\beta \mathcal{L}(\beta) = -2\beta + (1 - x) + \frac{1}{\beta} \stackrel{!}{=} 0$$

$$-2\beta^2 + (1 - x)\beta + 1 \stackrel{!}{=} 0$$

Solve the quadratic equation and choose the positive root.