Data Analytics and Machine Learning Group Department of Informatics Technical University of Munich



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# **Machine Learning**

Graded Exercise: IN2064 / Retake Date: Thursday 1st April, 2021

**Examiner:** Prof. Dr. Stephan Günnemann **Time:** 16:30 – 18:30

#### **Working instructions**

- This graded exercise consists of 34 pages with a total of 11 problems.
   Please make sure now that you received a complete copy of the graded exercise.
- The total amount of achievable credits in this graded exercise is 40.
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### Problem 1: Probabilistic Inference (Version A) (4 credits)

We have observed *N* coin flips of which *T* landed tails and *H* landed heads (T + H = N). We model each coin flip with a Bernoulli( $\theta$ ) distribution with a shared unknown probability  $\theta$  of coming up heads, i.e. p(heads  $|\theta| = \theta$ .

Furthermore, we assume that  $\theta$  follows a Beta(a, b) distribution with parameters a > 0 and b > 0. In this problem we are not interested in estimating  $\theta$ , but rather estimating the parameters a and b.



a) Is it possible to compute a maximum likelihood estimate (MLE)  $\arg \max_{a,b} p(\mathcal{D} \mid a,b)$  of a and b in this model? If yes, briefly describe a way to do it and how the variable  $\theta$  is handled.

If no, explain why it is not possible and the role of the variable  $\theta$ .



b) Is it possible to compute a maximum a posteriori (MAP) estimate  $\arg \max_{a,b} p(a,b \mid \mathcal{D})$  of a and b in this model? If yes, briefly describe how to compute the MAP estimate of a and b.

If no, describe how and why the model would need to be changed/extended to allow MAP estimation of a and b.

### Problem 1: Probabilistic Inference (Version B) (4 credits)

If yes, briefly describe how to compute the MAP estimate of a and b.

Furthermore, we assume that  $\theta$  follows a Beta(a, b) distribution with parameters a > 0 and b > 0. In this problem we are not interested in estimating  $\theta$ , but rather estimating the parameters a and b.

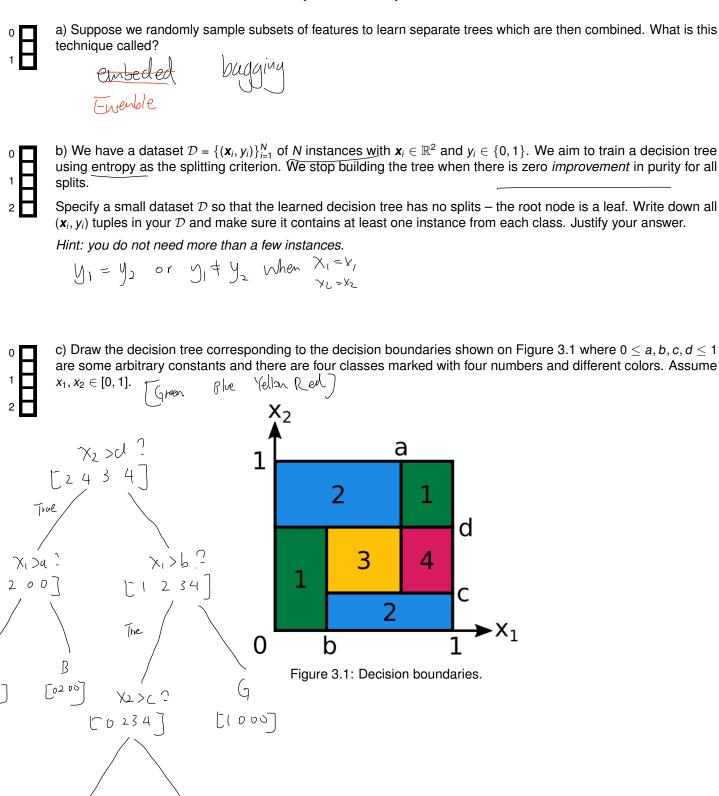
a) Is it possible to compute a maximum likelihood estimate (MLE)  $\arg\max_{a,b} p(\mathcal{D} \mid a,b)$  of a and b in this model? If yes, briefly describe a way to do it and how the variable  $\theta$  is handled. If no, explain why it is not possible and the role of the variable  $\theta$ .

b) Is it possible to compute a maximum a posteriori (MAP) estimate  $\max_{a,b} p(a,b \mid \mathcal{D})$  of a and b in this model?

If no, describe how and why the model would need to be changed/extended to allow MAP estimation of a and b.

We have observed *N* coin flips of which *T* landed tails and *H* landed heads (T + H = N). We model each coin flip with a Bernoulli( $\theta$ ) distribution with a shared unknown probability  $\theta$  of coming up heads, i.e. p(heads  $|\theta| = \theta$ .

#### Problem 2: Decision Trees (Version A) (5 credits)



#### Problem 2: Decision Trees (Version B) (5 credits)

a) Suppose we randomly sample subsets of features to learn separate trees which are then combined. What is this technique called?

b) We have a dataset  $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$  of N instances with  $\mathbf{x}_i \in \mathbb{R}^2$  and  $y_i \in \{0, 1\}$ . We aim to train a decision tree using entropy as the splitting criterion. We stop building the tree when there is zero *improvement* in purity for all splits.

Specify a small dataset  $\mathcal{D}$  so that the learned decision tree has no splits – the root node is a leaf. Write down all  $(\mathbf{x}_i, y_i)$  tuples in your  $\mathcal{D}$  and make sure it contains at least one instance from each class. Justify your answer.

Hint: you do not need more than a few instances.

c) Draw the decision tree corresponding to the decision boundaries shown on Figure 4.1 where  $0 \le a, b, c, d \le 1$  are some arbitrary constants and there are four classes marked with four numbers and different colors. Assume  $x_1, x_2 \in [0, 1]$ .

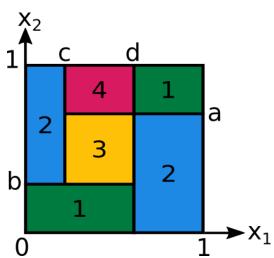
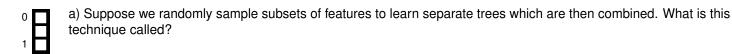
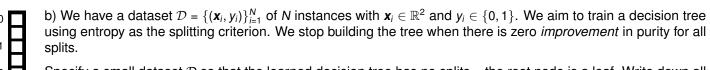


Figure 4.1: Decision boundaries.

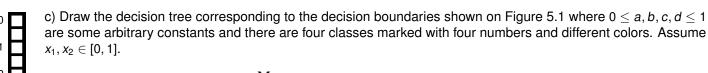
#### Problem 2: Decision Trees (Version C) (5 credits)





Specify a small dataset  $\mathcal{D}$  so that the learned decision tree has no splits – the root node is a leaf. Write down all  $(\mathbf{x}_i, \mathbf{y}_i)$  tuples in your  $\mathcal{D}$  and make sure it contains at least one instance from each class. Justify your answer.

Hint: you do not need more than a few instances.



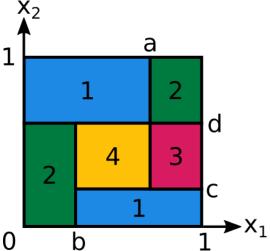


Figure 5.1: Decision boundaries.

#### Problem 2: Decision Trees (Version D) (5 credits)

a) Suppose we randomly sample subsets of features to learn separate trees which are then combined. What is this technique called?

b) We have a dataset  $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$  of N instances with  $\mathbf{x}_i \in \mathbb{R}^2$  and  $y_i \in \{0, 1\}$ . We aim to train a decision tree using entropy as the splitting criterion. We stop building the tree when there is zero *improvement* in purity for all splits.

Specify a small dataset  $\mathcal{D}$  so that the learned decision tree has no splits – the root node is a leaf. Write down all  $(\mathbf{x}_i, y_i)$  tuples in your  $\mathcal{D}$  and make sure it contains at least one instance from each class. Justify your answer.

Hint: you do not need more than a few instances.

c) Draw the decision tree corresponding to the decision boundaries shown on Figure 6.1 where  $0 \le a, b, c, d \le 1$  are some arbitrary constants and there are four classes marked with four numbers and different colors. Assume  $x_1, x_2 \in [0, 1]$ .

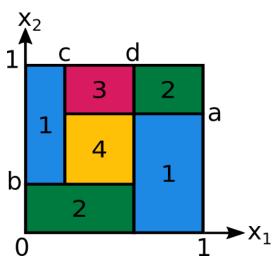


Figure 6.1: Decision boundaries.

# Problem 3: Linear Regression (Version A) (2 credits)



We have a dataset  $\{(\mathbf{x}_i, y_i) \mid \mathbf{x}_i \in \mathbb{R}^2, y_i \in \mathbb{R}\}_{i=1}^N$  and want to fit the following model with three parameters  $\mathbf{w} = \begin{pmatrix} a & b & c \end{pmatrix}^T \in \mathbb{R}^3$  to it.

$$f(\mathbf{x}, \mathbf{w}) = a \sin(\mathbf{x}_2) + \frac{1}{2}b\|\mathbf{x}\|_1 - \mathbf{x}_1^2 \mathbf{x}_2 c$$

Give a closed form expression for the optimal w minimizing the squared error between the predictions and targets

$$\sum_{i=1}^{N} \left( f(\boldsymbol{x}_i, \boldsymbol{w}) - y_i \right)^2.$$

Justify your answer.

Note: You can use results from the lecture without deriving them again.

$$f(x,w) = W^{T} \begin{pmatrix} \frac{\sin(x_{2})}{2} & = W^{T} \phi(x) \\ -x_{1}^{2} x_{2} \end{pmatrix} = W^{T} \phi(x)$$

$$= \alpha y w \ln \left[ W^{T} - y \right]^{2}$$

$$= \left( P^{T} - y \right)^{-1} P^{T} y$$

# Problem 3: Linear Regression (Version B) (2 credits)

We have a dataset  $\{(\boldsymbol{x}_i,y_i) \mid \boldsymbol{x}_i \in \mathbb{R}^2, y_i \in \mathbb{R}\}_{i=1}^N$  and want to fit the following model with three parameters  $\boldsymbol{w} = \begin{pmatrix} a & b & c \end{pmatrix}^T \in \mathbb{R}^3$  to it.

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$f(\mathbf{x}, \mathbf{w}) = a \|\mathbf{x}\|_2 - \frac{1}{2} \mathbf{x}_1^2 \mathbf{x}_2 b + c \cos(\mathbf{x}_1)$$

Give a closed form expression for the optimal  $\mathbf{w}$  minimizing the squared error between the predictions and targets

$$\sum_{i=1}^{N} \left( f\left( \boldsymbol{x}_{i}, \boldsymbol{w} \right) - y_{i} \right)^{2}.$$

Justify your answer.

Note: You can use results from the lecture without deriving them again.

# Problem 3: Linear Regression (Version C) (2 credits)



We have a dataset  $\{(\boldsymbol{x}_i,y_i) \mid \boldsymbol{x}_i \in \mathbb{R}^2, y_i \in \mathbb{R}\}_{i=1}^N$  and want to fit the following model with three parameters  $\boldsymbol{w} = \begin{pmatrix} a & b & c \end{pmatrix}^T \in \mathbb{R}^3$  to it.

$$f(\boldsymbol{x}, \boldsymbol{w}) = -\boldsymbol{x}_1 \boldsymbol{x}_2^2 a + b \tan(\boldsymbol{x}_2) + \frac{1}{2} c \|\boldsymbol{x}\|_{\infty}$$

Give a closed form expression for the optimal w minimizing the squared error between the predictions and targets

$$\sum_{i=1}^{N} \left( f(\mathbf{x}_i, \mathbf{w}) - y_i \right)^2.$$

Justify your answer.

Note: You can use results from the lecture without deriving them again.

### Problem 4: Logistic Regression (Version A) (6 credits)

Let  $\mathcal{D} = \{(\mathbf{x}_i, y_i) \mid \mathbf{x}_i \in \mathbb{R}^d, y_i \in \{0, 1\}\}$  be a classification dataset that is *not*-linearly separable. Furthermore, let  $\mathcal{D}_{\alpha} = \{(\alpha \mathbf{x}_i, y_i) \mid (\mathbf{x}_i, y_i) \in \mathcal{D}\}\$  be a scaled copy of  $\mathcal{D}$  with  $\alpha > 1$ .  $f(\mathbf{x}, \mathbf{w}) : \mathbb{R}^m \times \mathbb{R}^m \to [0, 1]$  is a logistic regression model on  $\mathbb{R}^m$  for some m with parameters  $\mathbf{w}$ .  $f(\mathbf{x}, \mathbf{w})$  outputs the predicted probabilities for class 1.

You train two logistic regression models on  $\mathcal D$  and  $\mathcal D_{\alpha}$  without regularization and obtain the optimal parameters  $\mathbf{w}^*$  and  $\mathbf{w}^{*,\alpha}$ , respectively. Consider a test point  $\mathbf{x}_{\text{test}} \in \mathbb{R}^d$  and the predicted probabilities by the two models,  $s = f(\mathbf{x}_{test}, \mathbf{w}^*)$  and  $t = f(\mathbf{x}_{test}, \mathbf{w}^{*,\alpha})$ .

LW\*, = W

a) Is s > t possible? Is s = t possible? Is s < t possible? Justify your answers.

$$\mathcal{D}_3 = \left\{ (\boldsymbol{x}_i, 1) \mid \boldsymbol{x}_i \in \mathbb{R}^2, \boldsymbol{x}_{i, 1} > 0, \boldsymbol{x}_{i, 2} > 0 \right\} \cup \left\{ (\boldsymbol{x}_i, 0) \mid \boldsymbol{x}_i \in \mathbb{R}^2, \boldsymbol{x}_{i, 1} < 0, \boldsymbol{x}_{i, 2} < 0 \right\}$$

In the following, treat  $\infty$  as an actual value, i.e.  $\infty \begin{pmatrix} 1 \\ 1 \end{pmatrix}$  would be a vector in the same direction as  $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$  but with infinite length/norm.

b) Briefly explain why the maximum likelihood estimate of  $\mathbf{w}$  on  $\mathcal{D}_3$  obtained by training without regularization is not unique in this setting.

$$E(w) = -2 y_i \ln 6 (w T x_i) + (1 - y_i) / n (1 - 6 (w T x_i))$$
Win E(w) 
$$w \uparrow \rightarrow \infty$$



c) Give two possible maximum likelihood estimates (without regularization) of the parameters  $\mathbf{w}$  on  $\mathcal{D}_3$ ,  $\mathbf{w}^{*,a}$  and  $\mathbf{w}^{*,b}$ , and a test point  $\mathbf{x}_{\text{test}}$  such that either  $f(\mathbf{x}_{\text{test}}, \mathbf{w}^{*,a}) < \frac{1}{2} < f(\mathbf{x}_{\text{test}}, \mathbf{w}^{*,b})$  or  $f(\mathbf{x}_{\text{test}}, \mathbf{w}^{*,a}) > \frac{1}{2} > f(\mathbf{x}_{\text{test}}, \mathbf{w}^{*,b})$  holds. Justify your answer.

### Problem 4: Logistic Regression (Version B) (6 credits)

Let  $\mathcal{D} = \{(\mathbf{x}_i, y_i) \mid \mathbf{x}_i \in \mathbb{R}^d, y_i \in \{0, 1\}\}$  be a classification dataset that is *not* linearly separable. Furthermore, let  $\mathcal{D}_{\alpha} = \{(\alpha \mathbf{x}_i, y_i) \mid (\mathbf{x}_i, y_i) \in \mathcal{D}\}$  be a scaled copy of  $\mathcal{D}$  with  $\alpha > 1$ .  $f(\mathbf{x}, \mathbf{w}) : \mathbb{R}^m \times \mathbb{R}^m \to [0, 1]$  is a logistic regression model on  $\mathbb{R}^m$  for some m with parameters  $\mathbf{w}$ .  $f(\mathbf{x}, \mathbf{w})$  outputs the predicted probabilities for class 1.

You train two logistic regression models on  $\mathcal{D}$  and  $\mathcal{D}_{\alpha}$  without regularization and obtain the optimal parameters  $\mathbf{w}^*$  and  $\mathbf{w}^{*,\alpha}$ , respectively. Consider a test point  $\mathbf{x}_{\text{test}} \in \mathbb{R}^d$  and the predicted probabilities by the two models,  $\mathbf{s} = f(\mathbf{x}_{\text{test}}, \mathbf{w}^*)$  and  $t = f(\mathbf{x}_{\text{test}}, \mathbf{w}^{*,\alpha})$ .



a) Is s > t possible? Is s = t possible? Is s < t possible? Justify your answers.

Now consider another dataset  $\mathcal{D}_3$  and a logistic regression model  $f(\mathbf{x}, \mathbf{w})$  on  $\mathcal{D}_3$ .

$$\mathcal{D}_3 = \{(\mathbf{x}_i, 1) \mid \mathbf{x}_i \in \mathbb{R}^2, \mathbf{x}_{i,1} > 0, \mathbf{x}_{i,2} > 0\} \cup \{(\mathbf{x}_i, 0) \mid \mathbf{x}_i \in \mathbb{R}^2, \mathbf{x}_{i,1} < 0, \mathbf{x}_{i,2} < 0\}$$

In the following, treat  $\infty$  as an actual value, i.e.  $\infty \begin{pmatrix} 1 \\ 1 \end{pmatrix}$  would be a vector in the same direction as  $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$  but with infinite length/norm.



b) Briefly explain why the maximum likelihood estimate of  $\mathbf{w}$  on  $\mathcal{D}_3$  obtained by training without regularization is not unique in this setting.



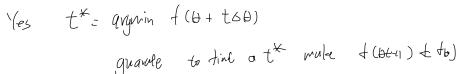
c) Give two possible maximum likelihood estimates (without regularization) of the parameters  $\boldsymbol{w}$  on  $\mathcal{D}_3$ ,  $\boldsymbol{w}^{*,a}$  and  $\boldsymbol{w}^{*,b}$ , and a test point  $\boldsymbol{x}_{\text{test}}$  such that either  $f(\boldsymbol{x}_{\text{test}}, \boldsymbol{w}^{*,a}) < \frac{1}{2} < f(\boldsymbol{x}_{\text{test}}, \boldsymbol{w}^{*,b})$  or  $f(\boldsymbol{x}_{\text{test}}, \boldsymbol{w}^{*,a}) > \frac{1}{2} > f(\boldsymbol{x}_{\text{test}}, \boldsymbol{w}^{*,b})$  holds. Justify your answer.

# Problem 5: Optimization (Version A) (3 credits)

Suppose we're minimizing some differentiable convex function  $f: \mathbb{R}^d \to \mathbb{R}$  using one of the following variants of gradient descent. Let  $\theta_t$  be the value of the parameter at iteration t, and  $\theta_{t+1}$  be the value of the parameter at the iteration t + 1 for some integer t.

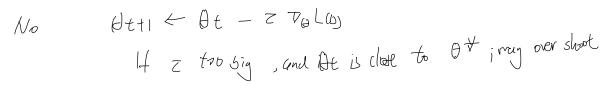
a) Suppose we are using gradient descent with line search.

Is the inequality  $f(\theta_{t+1}) \le f(\theta_t)$  guaranteed to always hold? Justify your answer.



b) Suppose we are using gradient descent with fixed step size.

Is the inequality  $f(\theta_{t+1}) \le f(\theta_t)$  guaranteed to always hold? Justify your answer.



c) Suppose we are using gradient descent with adaptive learning rate (Adam - Adaptive moment estimation). Is the inequality  $f(\theta_{t+1}) \leq f(\theta_t)$  guaranteed to always hold? Justify your answer.

No beauting time to those optimize does know the next value  $f(0+1) \leq f(0+1)$  by spainting Z

# Problem 5: Optimization (Version B) (3 credits)

Suppose we're minimizing some differentiable convex function  $f: \mathbb{R}^d \to \mathbb{R}$  using one of the following variants of gradient descent. Let  $\theta_t$  be the value of the parameter at iteration t, and  $\theta_{t+1}$  be the value of the parameter at the iteration t+1 for some integer t.

a) Suppose we are using gradient descent with fixed step size.

Is the inequality  $f(\theta_{t+1}) \leq f(\theta_t)$  guaranteed to always hold? Justify your answer.

0	b) Suppose we are using gradient descent with adaptive learning rate (Adam - Adaptive moment estimation)
	Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.

c) Suppose we are using gradient descent with line search.

Is the inequality  $f(\theta_{t+1}) \leq f(\theta_t)$  guaranteed to always hold? Justify your answer.

# Problem 5: Optimization (Version C) (3 credits)

Suppose we're minimizing some differentiable convex function  $f: \mathbb{R}^d \to \mathbb{R}$  using one of the following variants of gradient descent. Let  $\theta_t$  be the value of the parameter at iteration t, and  $\theta_{t+1}$  be the value of the parameter at the iteration t+1 for some integer t.

a) Suppose we are using gradient descent with line search.	0
Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.	Н¹
b) Suppose we are using gradient descent with adaptive learning rate (Adam - Adaptive moment estimation). Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.	0 1
c) Suppose we are using gradient descent with fixed step size. Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.	0

# Problem 5: Optimization (Version D) (3 credits)

Suppose we're minimizing some differentiable convex function  $f: \mathbb{R}^d \to \mathbb{R}$  using one of the following variants of gradient descent. Let  $\theta_t$  be the value of the parameter at iteration t, and  $\theta_{t+1}$  be the value of the parameter at the iteration t+1 for some integer t.

0	a) Suppose we are using gradient descent with adaptive learning rate (Adam - Adaptive moment estimation).
0   1   1	Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.
0	b) Suppose we are using gradient descent with fixed step size. Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.
0   1	c) Suppose we are using gradient descent with line search. Is the inequality $f(\theta_{t+1}) \leq f(\theta_t)$ guaranteed to always hold? Justify your answer.

# 1 1+ exp(xíy) · exp(x7y) · y

#### Problem 6: Deep Learning (Version A) (3 credits)

Suppose  $\mathbf{x} \in \mathbb{R}^N$  and  $\mathbf{y} \in \mathbb{R}^N$  are two vectors. We define the function  $f: \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$  as

$$f(\mathbf{x}, \mathbf{y}) = \log (1 + \exp(\mathbf{x}^T \mathbf{y})).$$

The code below implements the computation of f(x, y) as well as its gradients w.r.t. x and y using backpropagation (similarly to how we did in Exercise sheet 7). However, some code fragments are missing. Your task is to complete the missing code fragments.

```
import numpy as np
class F:
  def forward(self, x, y):
     self.cache = (x, y)
     out = np. (og (I+ np. exp(npdot(x.Tv))
     # MISSING CODE FRAGMENT #1
     return out
  def backward(self, d_out):
     # x, y are np.arrays of shape (N,)
     # MISSING CODE FRAGMENT #2
                                           \times npexp (x.1 Qy) \times y
     return d_x, d_y
# Example usage
f = F()
x = np.array([1., 2., 3])
y = np.array([-2., 3., -1.])
z = f.forward(x, y)
dz = 1.0
d_x, d_y = f.backward(d_z)
```

a) Complete the MISSING CODE FRAGMENT #1

b) Complete the MISSING CODE FRAGMENT #2

1 2

#### Problem 6: Deep Learning (Version B) (3 credits)

Suppose  $\mathbf{x} \in \mathbb{R}^N$  and  $\mathbf{y} \in \mathbb{R}^N$  are two vectors. We define the function  $f: \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$  as

$$f(\mathbf{x}, \mathbf{y}) = \log (\exp(\mathbf{x}^T \mathbf{y}) - 1)$$
.

The code below implements the computation of f(x, y) as well as its gradients w.r.t. x and y using backpropagation (similarly to how we did in Exercise sheet 7). However, some code fragments are missing. Your task is to complete the missing code fragments.

```
import numpy as np
class F:
  def forward(self, x, y):
     self.cache = (x, y)
     # MISSING CODE FRAGMENT #1
     return out
  def backward(self, d_out):
     \# x, y are np.arrays of shape (N,)
     x, y = self.cache
     # MISSING CODE FRAGMENT #2
     return d_x, d_y
# Example usage
f = F()
x = np.array([1., 2., 3])
y = np.array([-2., 3., -1.])
z = f.forward(x, y)
dz = 1.0
d_x, d_y = f.backward(d_z)
```

a) Complete the MISSING CODE FRAGMENT #1



b) Complete the MISSING CODE FRAGMENT #2

#### Problem 6: Deep Learning (Version C) (3 credits)

Suppose  $\mathbf{x} \in \mathbb{R}^N$  and  $\mathbf{y} \in \mathbb{R}^N$  are two vectors. We define the function  $f: \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$  as

$$f(\mathbf{x}, \mathbf{y}) = \log (1 + \exp(\mathbf{x}^T \mathbf{y})).$$

The code below implements the computation of f(x, y) as well as its gradients w.r.t. x and y using backpropagation (similarly to how we did in Exercise sheet 7). However, some code fragments are missing. Your task is to complete the missing code fragments.

```
import numpy as np
class F:
  def forward(self, x, y):
     self.cache = (x, y)
     # MISSING CODE FRAGMENT #1
     return out
  def backward(self, d_out):
     # x, y are np.arrays of shape (N,)
     x, y = self.cache
     # MISSING CODE FRAGMENT #2
     return d_x, d_y
# Example usage
f = F()
x = np.array([1., 2., 3])
y = np.array([-2., 3., -1.])
z = f.forward(x, y)
dz = 1.0
d_x, d_y = f.backward(d_z)
```

a) Complete the MISSING CODE FRAGMENT #1

b) Complete the MISSING CODE FRAGMENT #2

0 1 2

#### Problem 6: Deep Learning (Version D) (3 credits)

Suppose  $\mathbf{x} \in \mathbb{R}^N$  and  $\mathbf{y} \in \mathbb{R}^N$  are two vectors. We define the function  $f: \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$  as

$$f(\mathbf{x}, \mathbf{y}) = \log (\exp(\mathbf{x}^T \mathbf{y}) - 1)$$
.

The code below implements the computation of f(x, y) as well as its gradients w.r.t. x and y using backpropagation (similarly to how we did in Exercise sheet 7). However, some code fragments are missing. Your task is to complete the missing code fragments.

```
import numpy as np
class F:
  def forward(self, x, y):
     self.cache = (x, y)
     # MISSING CODE FRAGMENT #1
     return out
  def backward(self, d_out):
     \# x, y are np.arrays of shape (N,)
     x, y = self.cache
     # MISSING CODE FRAGMENT #2
     return d_x, d_y
# Example usage
f = F()
x = np.array([1., 2., 3])
y = np.array([-2., 3., -1.])
z = f.forward(x, y)
dz = 1.0
d_x, d_y = f.backward(d_z)
```



a) Complete the MISSING CODE FRAGMENT #1



b) Complete the MISSING CODE FRAGMENT #2

## Problem 7: Kernels (Version A) (3 credits)

Let  $\Sigma \in \mathbb{R}^{D \times D}$  be a given invertible, positive semi-definite matrix and  $c \in \mathbb{R}$  be a given constant. Consider the kernel:

$$k: \mathbb{R}^D imes \mathbb{R}^D o \mathbb{R}, \quad k(\pmb{x}_1, \pmb{x}_2) = c^2 \exp\left(-rac{1}{2}(\pmb{x}_1 - \pmb{x}_2)\pmb{\Sigma}^{-1}(\pmb{x}_1 - \pmb{x}_2)
ight).$$

Prove or disprove that 
$$k$$
 is a valid kernel.

$$=c^{1}\exp\left(-\frac{1}{2}\left(x_{1}^{T}\overline{2}^{-1}-y_{2}^{T}\overline{2}^{-1}\right)\left(x_{1}-x_{2}\right)\right)$$

Hint: If  $k_1(\boldsymbol{x}_1, \boldsymbol{x}_2)$  then  $\exp(k_1(\boldsymbol{x}_1, \boldsymbol{x}_2))$  is also a kernel.

$$= c \exp(-\frac{1}{2} (x_1^{7} + x_2^{7}))$$

$$= c^{2} \exp(-\frac{1}{2} (x_1^{7} + x_2^{7} + x_2^{$$

$$= c^{2} \exp(-\frac{1}{5} x_{1}^{7} z^{-1} x_{1}) \exp(-\frac{1}{5} x_{2}^{7} z^{-1} x_{2}) \exp(x_{1}^{7} z^{-1} x_{2})$$

$$= (2 \exp(-\frac{1}{5} x_{1}^{7} z^{-1} x_{2}) \exp(x_{1}^{7} z^{-1} x_{2})$$

$$= (2 \exp(-\frac{1}{5} x_{1}^{7} z^{-1} x_{2}) \exp(x_{1}^{7} z^{-1} x_{2})$$

$$= (2 \exp(-\frac{1}{5} x_{1}^{7} z^{-1} x_{2}) \exp(x_{1}^{7} z^{-1} x_{2})$$

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$$= (2 \exp(-\frac{1}{5} x_{1}^{7} z^{-1} x_{2}) \exp(x_{1}^{7} z^{-1} x_{2})$$

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# Problem 7: Kernels (Version B) (3 credits)

Let  $\Sigma \in \mathbb{R}^{D \times D}$  be a given invertible, positive semi-definite matrix and  $a \in \mathbb{R}$  be a given constant. Consider the kernel:

$$k: \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}, \quad k(\boldsymbol{x}_1, \boldsymbol{x}_2) = a^2 \exp\left(-\frac{1}{2}(\boldsymbol{x}_1 - \boldsymbol{x}_2)\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}_1 - \boldsymbol{x}_2)\right).$$



Prove or disprove that k is a valid kernel.

Hint: If  $k_1(\mathbf{x}_1, \mathbf{x}_2)$  then  $\exp(k_1(\mathbf{x}_1, \mathbf{x}_2))$  is also a kernel.

# Problem 8: Probabilistic inference & SVD (Version A) (4 credits)

Consider a generative model where  $\mathbf{X} \in \mathbb{R}^{N \times D}$  is the observed variable and  $\mathbf{a} \in \mathbb{R}^{N}$ ,  $\mathbf{b} \in \mathbb{R}^{D}$  are the model parameters. We assume the following generative process:

$$p(\boldsymbol{X}|\boldsymbol{a},\boldsymbol{b}) = \prod_{i=1}^{N} \prod_{j=1}^{D} p(X_{ij}|\boldsymbol{a},\boldsymbol{b}) = \prod_{i=1}^{N} \prod_{j=1}^{D} \mathcal{N}(X_{ij}|a_i \cdot b_j, 1).$$

Here  $\mathcal{N}(x|\mu,\sigma)$  denotes the density of the normal distribution

$$\mathcal{N}(\mathbf{x}|\mu,\sigma) \propto \exp\left(-rac{(\mathbf{x}-\mu)^2}{2\sigma^2}
ight).$$

a) Suppose you observed X. Derive a maximum likelihood estimate (MLE)  $a^*$ ,  $b^*$  of the parameters a, b.

Hint: SVD can be helpful here. No need to take derivatives.

b) Suppose all singular values of the observed matrix X are distinct. Is the MLE of the parameters a, b unique in this case? Justify your answer.

$$\frac{1}{c}a$$
 cb

#### Problem 8: Probabilistic inference & SVD (Version B) (4 credits)

Consider a generative model where  $\mathbf{X} \in \mathbb{R}^{N \times D}$  is the observed variable and  $\mathbf{a} \in \mathbb{R}^{N}$ ,  $\mathbf{b} \in \mathbb{R}^{D}$  are the model parameters. We assume the following generative process:

$$p(\mathbf{X}|\mathbf{a},\mathbf{b}) = \prod_{i=1}^{N} \prod_{j=1}^{D} p(X_{ij}|\mathbf{a},\mathbf{b}) = \prod_{i=1}^{N} \prod_{j=1}^{D} \mathcal{N}(X_{ij}|a_i \cdot b_j, 1).$$

Here  $\mathcal{N}(\mathbf{x}|\mu,\sigma)$  denotes the density of the normal distribution

$$\mathcal{N}(x|\mu,\sigma) \propto \exp\left(-rac{(x-\mu)^2}{2\sigma^2}
ight).$$

a) Suppose you observed X. Derive a maximum likelihood estimate (MLE)  $a^*$ ,  $b^*$  of the parameters a, b. Hint: SVD can be helpful here. No need to take derivatives.



b) Suppose all singular values of the observed matrix **X** are distinct. Is the MLE of the parameters **a**, **b** unique in this case? Justify your answer.

# Problem 9: Dimensionality Reduction (Version A) (2 credits)

Figure 24.1 shows a scatter plot of your two-dimensional data (N = 13 instances). You want to apply a non-linear dimensionality reduction technique based on neighbor graphs (e.g. T-SNE or UMAP). As a first step you compute the  $N \times N$ , weighted adjacency matrix representing the neighbor graph. Assume that the weights are computed with

$$p_{j|i} = \frac{\exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{j}\|^{2} / 2\sigma^{2}\right)}{\sum_{k \neq i} \exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{k}\|^{2} / 2\sigma^{2}\right)}$$

where  $\mathbf{x}_i \in \mathbb{R}^2$  and you set  $p_{i|i} = 0$ . Finally, you obtain the similarity between instances i and j with  $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2}$ .

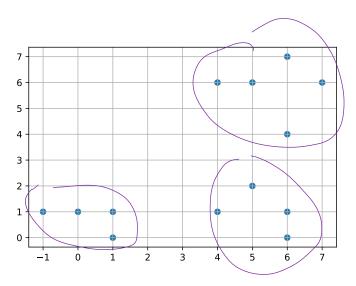
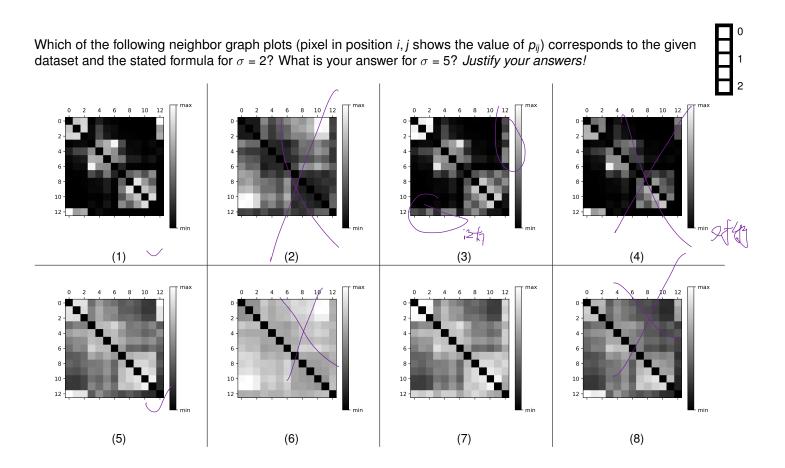


Figure 24.1: Scatter plot of the data



# Problem 9: Dimensionality Reduction (Version B) (2 credits)

Figure 25.1 shows a scatter plot of your two-dimensional data (N = 13 instances). You want to apply a non-linear dimensionality reduction technique based on neighbor graphs (e.g. T-SNE or UMAP). As a first step you compute the  $N \times N$ , weighted adjacency matrix representing the neighbor graph. Assume that the weights are computed with

$$p_{j|i} = \frac{\exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{j}\|^{2} / 2\sigma^{2}\right)}{\sum_{k \neq i} \exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{k}\|^{2} / 2\sigma^{2}\right)}$$

where  $\mathbf{x}_i \in \mathbb{R}^2$  and you set  $p_{i|i} = 0$ . Finally, you obtain the similarity between instances i and j with  $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2}$ .

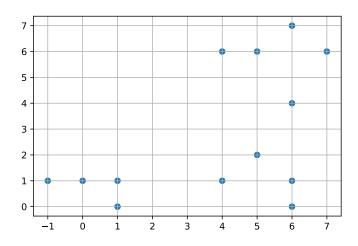
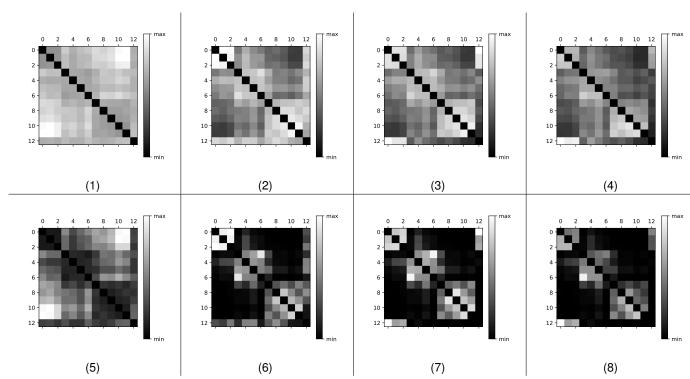


Figure 25.1: Scatter plot of the data



Which of the following neighbor graph plots (pixel in position i, j shows the value of  $p_{ij}$ ) corresponds to the given dataset and the stated formula for  $\sigma$  = 2? What is your answer for  $\sigma$  = 5? *Justify your answers!* 



### Problem 9: Dimensionality Reduction (Version C) (2 credits)

Figure 26.1 shows a scatter plot of your two-dimensional data (N = 13 instances). You want to apply a non-linear dimensionality reduction technique based on neighbor graphs (e.g. T-SNE or UMAP). As a first step you compute the  $N \times N$ , weighted adjacency matrix representing the neighbor graph. Assume that the weights are computed with

$$p_{j|i} = \frac{\exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{j}\|^{2} / 2\sigma^{2}\right)}{\sum_{k \neq i} \exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{k}\|^{2} / 2\sigma^{2}\right)}$$

where  $\mathbf{x}_i \in \mathbb{R}^2$  and you set  $p_{i|i} = 0$ . Finally, you obtain the similarity between instances i and j with  $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2}$ .

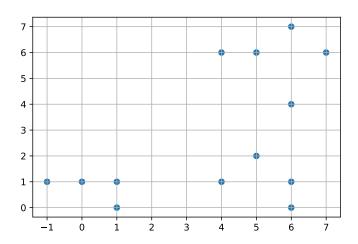
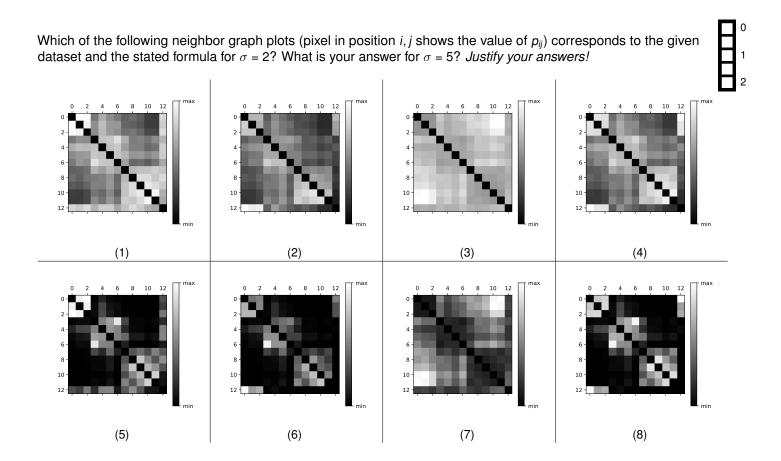


Figure 26.1: Scatter plot of the data



# Problem 9: Dimensionality Reduction (Version D) (2 credits)

Figure 27.1 shows a scatter plot of your two-dimensional data (N = 13 instances). You want to apply a non-linear dimensionality reduction technique based on neighbor graphs (e.g. T-SNE or UMAP). As a first step you compute the  $N \times N$ , weighted adjacency matrix representing the neighbor graph. Assume that the weights are computed with

$$p_{j|i} = \frac{\exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{j}\|^{2} / 2\sigma^{2}\right)}{\sum_{k \neq i} \exp\left(-\|\mathbf{x}_{i} - \mathbf{x}_{k}\|^{2} / 2\sigma^{2}\right)}$$

where  $\mathbf{x}_i \in \mathbb{R}^2$  and you set  $p_{i|i} = 0$ . Finally, you obtain the similarity between instances i and j with  $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2}$ .

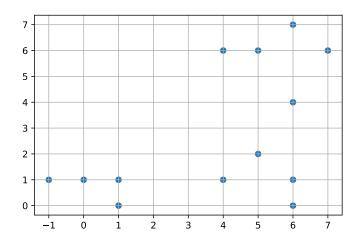
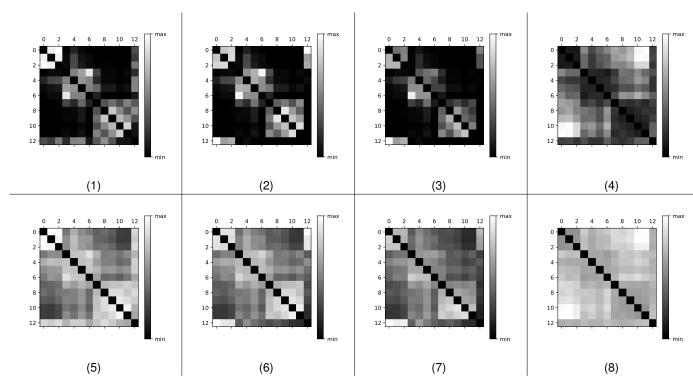


Figure 27.1: Scatter plot of the data



Which of the following neighbor graph plots (pixel in position i, j shows the value of  $p_{ij}$ ) corresponds to the given dataset and the stated formula for  $\sigma$  = 2? What is your answer for  $\sigma$  = 5? *Justify your answers!* 



### Problem 10: Clustering (Version A) (4 credits)

a) Consider the K-means algorithm with two clusters and fixed centroids  $\mu_1$ ,  $\mu_2$ . Prove that the decision boundary is a hyperplane.

Hint: Consider the equation that defines the decision boundary.

b) Now consider the Gaussian mixture model (GMM) with two clusters. In this case the assigned cluster label for instance  $x_i$  is given by  $arg max \gamma(\mathbf{z}_{ik}).$ 

(1)

where  $\gamma(z_{ik})$  are the responsibilities. Is the decision boundary in a GMM with two clusters and fixed parameters  $\pi_k$ ,

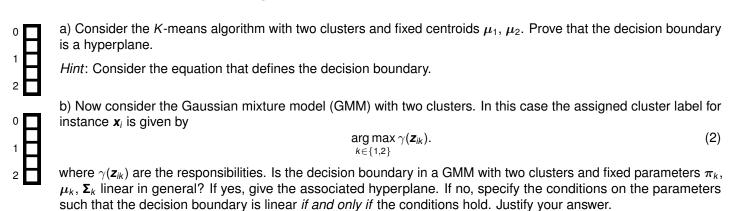
 $\mu_k$ ,  $\Sigma_k$  linear in general? If yes, give the associated hyperplane. If no, specify the conditions on the parameters such that the decision boundary is linear if and only if the conditions hold. Justify your answer.

a) For X; is on the bauday  $2|||\chi_1 - \mu_1||_2^2 = 2|||\chi_1 - \mu_2||$  $\chi^{2} - 2 \chi_{1} \mu_{1} + \mu_{1}^{2} = \chi^{2} - 2 \chi_{1} \mu_{2} + \mu_{2}^{2}$  $M_1^2 - M_2^2 = 2 \times (M_1 - M_2)$ N1 + M2 2 X1 = MI+N2  $X_{1Z} \xrightarrow{\mathcal{N}_{1}+\mathcal{N}_{2}} \Rightarrow \text{linear bandry.}$ 

 $(X_1 - \mu_1)^{\bar{1}} (X_1 - \mu_1) = (X_1 - \mu_2)^{\bar{1}} (X_1 - \mu_2)$ XTX, -2 x / M, + M/M, = X/X, -2x / /2 + /2 //2  $h_1^T h_1 - h_2^T h_2 = 2 \times_1^T (h_1 - h_2)$ 2 X T ( MI - MZ) - MI MI + MZ NZ =0 XTW +b= 0 => Myoum W= 2 (N1 - N2) b= No Tr2 - No N1

bounday & (Zi1)= & (Zi2)  $\chi^7 = \chi^7 = \chi^7 = \chi^7 = \chi^7$ 

#### Problem 10: Clustering (Version B) (4 credits)



# Problem 11: Fairness (Version A) (4 credits)

You are given data as shown on Table 30.1 where  $X \in \mathbb{R}$  denotes the non-sensitive feature,  $A \in \{a, b\}$  denotes the sensitive feature, and  $Y \in \{0, 1\}$  denotes the ground-truth label.

Table 30.1: Fairness Data (each column is one data point)

ID	1	2	3	4	5	6	7
X	0.5	-1.0	-0.5	2.0	0.5	1.5	0.1
Α	а	b	b	а	b	а	b
Y	1	1	0	0	0	0	1

a) Let the prediction $R = r(X)$ be some arbitrary function $r$ that only depends on $X$ . The sensitive att	ribute A is
ignored. Can we conclude that the Sufficiency fairness criterion is satisfied for the data shown on T	able 30.1?
Justify your answer.	



b) Let the prediction  $R \in \{0, 1\}$  be

$$R = \begin{cases} 0 & \text{if } 2 \cdot X > 2 \text{ and } A = a \\ 0 & \text{if } 4 \cdot X > 1 \text{ and } A = b \\ 1 & \text{otherwise} \end{cases}$$



Which ones of the following three fairness criteria *Independence, Separation, and Equality of Opportunity* are satisfied for the data shown on Table 30.1? Justify your answer.

c) Modify the *least* number of instances such that none of the above criteria are satisfied. You can only modify the non-sensitive features *X*. Write down the ID(s) of the modified instance(s) and their modified *X* value. Justify your answer!

#### Problem 11: Fairness (Version B) (4 credits)

You are given data as shown on Table 31.1 where  $X \in \mathbb{R}$  denotes the non-sensitive feature,  $A \in \{a, b\}$  denotes the sensitive feature, and  $Y \in \{0, 1\}$  denotes the ground-truth label.

Table 31.1: Fairness Data (each column is one data point)

ID	1	2	3	4	5	6	7
X	0.5	-1.0	-0.5	2.0	0.5	1.5	0.1
Α	b	а	а	b	а	b	а
Y	1	1	0	0	0	0	1

0	
1	

a) Let the prediction R = r(X) be some arbitrary function r that only depends on X. The sensitive attribute A is ignored. Can we conclude that the *Sufficiency* fairness criterion is satisfied for the data shown on Table 31.1? Justify your answer.



b) Let the prediction  $R \in \{0, 1\}$  be

$$R = \begin{cases} 0 & \text{if } 2 \cdot X > 0.5 \text{ and } A = a \\ 0 & \text{if } 3 \cdot X > 3.0 \text{ and } A = b \\ 1 & \text{otherwise} \end{cases}$$

Which ones of the following three fairness criteria *Independence, Separation, and Equality of Opportunity* are satisfied for the data shown on Table 31.1? Justify your answer.



c) Modify the *least* number of instances such that none of the above criteria are satisfied. You can only modify the non-sensitive features *X*. Write down the ID(s) of the modified instance(s) and their modified *X* value. Justify your answer!

# Problem 11: Fairness (Version C) (4 credits)

You are given data as shown on Table 32.1 where  $X \in \mathbb{R}$  denotes the non-sensitive feature,  $A \in \{a, b\}$  denotes the sensitive feature, and  $Y \in \{0, 1\}$  denotes the ground-truth label.

Table 32.1: Fairness Data (each column is one data point)

ID	1	2	3	4	5	6	7
X	0.5	-1.0	-0.5	2.0	0.5	1.5	0.1
Α	а	b	b	а	b	а	b
Y	1	1	0	0	0	0	1

a) Let the prediction $R = r(X)$ be some arbitrary function $r$	that only depends on $X$ .	The sensitive attribute A is
ignored. Can we conclude that the Sufficiency fairness cr	riterion is satisfied for the	data shown on Table 32.1?
Justify your answer.		

0

b) Let the prediction  $R \in \{0, 1\}$  be

$$R = \begin{cases} 0 & \text{if } 2 \cdot X > 2 \text{ and } A = a \\ 0 & \text{if } 4 \cdot X > 1 \text{ and } A = b \\ 1 & \text{otherwise} \end{cases}$$

0 1 2

Which ones of the following three fairness criteria *Independence, Separation, and Equality of Opportunity* are satisfied for the data shown on Table 32.1? Justify your answer.

c) Modify the *least* number of instances such that none of the above criteria are satisfied. You can only modify the non-sensitive features X. Write down the ID(s) of the modified instance(s) and their modified X value. Justify your answer!

0

#### Problem 11: Fairness (Version D) (4 credits)

You are given data as shown on Table 33.1 where  $X \in \mathbb{R}$  denotes the non-sensitive feature,  $A \in \{a, b\}$  denotes the sensitive feature, and  $Y \in \{0, 1\}$  denotes the ground-truth label.

Table 33.1: Fairness Data (each column is one data point)

ID	1	2	3	4	5	6	7
X	0.5	-1.0	-0.5	2.0	0.5	1.5	0.1
Α	b	а	а	b	а	b	а
Y	1	1	0	0	0	0	1

0	
1	

a) Let the prediction R = r(X) be some arbitrary function r that only depends on X. The sensitive attribute A is ignored. Can we conclude that the *Sufficiency* fairness criterion is satisfied for the data shown on Table 33.1? Justify your answer.



b) Let the prediction  $R \in \{0, 1\}$  be

$$R = \begin{cases} 0 & \text{if } 2 \cdot X > 0.5 \text{ and } A = a \\ 0 & \text{if } 3 \cdot X > 3.0 \text{ and } A = b \\ 1 & \text{otherwise} \end{cases}$$

Which ones of the following three fairness criteria *Independence, Separation, and Equality of Opportunity* are satisfied for the data shown on Table 33.1? Justify your answer.



c) Modify the *least* number of instances such that none of the above criteria are satisfied. You can only modify the non-sensitive features *X*. Write down the ID(s) of the modified instance(s) and their modified *X* value. Justify your answer!