Univ.-Prof. Dr. rer. nat. Rudolf Mathar

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## Written Examination <br> Fundamentals of Big Data Analytics

Tuesday, March 21, 2017, 01:00 p.m.

Name: $\qquad$ Matr.-No.: $\qquad$
Field of study: $\qquad$

## Please pay attention to the following:

1) The exam consists of 4 problems. Please check the completeness of your copy. Only written solutions on these sheets will be considered. Removing the staples is not allowed.
2) The exam is passed with at least $\mathbf{5 0}$ points.
3) You are free in choosing the order of working on the problems. Your solution shall clearly show the approach and intermediate arguments.
4) Admitted materials: The sheets handed out with the exam and a non-programmable calculator.
5) The results will be published on Friday evening, the 24.03.17, on the homepage of the institute.

The corrected exams can be inspected on Monday, 27.03.17, 14:00h. at the seminar room 333 of the Chair for Theoretical Information Technology, Kopernikusstr. 16.

Problem 1. (25 points)
Analysis of Multivariate Densities and Maximum Likelihood Estimation:
Let $f_{\mathbf{Z}}(x, y)$ be the joint density of the random vector $\mathbf{Z}=(X, Y)^{\mathrm{T}}$. It is given by

$$
f_{\mathbf{Z}}(x, y)=\left\{\begin{array}{ll}
c, & 0 \leq y \leq a \\
0, & \text { otherwise }
\end{array} \text { and } y \leq x \leq y+a\right.
$$

for a proper number $c$ with the parameter $a>0$.
a) Sketch the support (topview) of the density $f_{\mathbf{Z}}(x, y)$ for $a=1$ and mark important points. (2P)

b) What is the value of $c$ as a function of $a$ such that $f_{\mathbf{Z}}(x, y)$ is a proper density function. (2P)
c) Calculate the missing value $\mu_{X}=\mathrm{E}(X)$ of the mean vector

$$
\mathrm{E}(\mathbf{Z})=\binom{\mu_{X}}{\frac{1}{2}}
$$

for $a=1$. (3P)
d) Compute the missing values of the covariance matrix

$$
\boldsymbol{\Sigma}_{\mathbf{Z}}=\left(\begin{array}{cc}
\frac{1}{6} & \sigma_{1,2} \\
\sigma_{2,1} & \sigma_{2,2}
\end{array}\right)
$$

of the density $f_{\mathbf{Z}}$ for $a=1$ by calculating the variance $\sigma_{2,2}$ of $Y$ and the co-variances $\sigma_{1,2}$ and $\sigma_{2,1} \cdot(3+2+1 \mathrm{P})$
e) Determine the marginal densities for $X$ and $Y$ for $a=1$. $(2+2 \mathrm{P})$
f) Are $X$ and $Y$ independent random variables? Please justify the reason behind your answer. (1P)
g) Calculate the mean vector $\mathrm{E}(\mathbf{Z})$ and the covariance matrix $\operatorname{Cov}(\mathbf{Z})$ for the general case $a>0 .(1+1 \mathrm{P})$
h) Assuming $n$ IID random vectors $\mathbf{Z}_{1}, \mathbf{Z}_{2}, \ldots, \mathbf{Z}_{n}$ with densities $f_{\mathbf{Z}_{i}}\left(x_{i}, y_{i}\right)=f_{\mathbf{Z}}\left(x_{i}, y_{i}\right)$, calculate the likelihood function $L\left(a, \mathbf{Z}_{1}, \mathbf{Z}_{2}, \ldots, \mathbf{Z}_{n}\right)$. (1P)
i) Show that the $\log$-likelihood function $\ell\left(a, \mathbf{Z}_{1}, \mathbf{Z}_{2}, \ldots, \mathbf{Z}_{n}\right)=\log \left(L\left(a, \mathbf{Z}_{1}, \mathbf{Z}_{2}, \ldots, \mathbf{Z}_{n}\right)\right)$ is strictly monotonic in $a$. (2P)
j) Why is the quantity $\hat{a}=\max _{1 \leq i \leq n}\left\{y_{i}, x_{i}-y_{i}\right\}$ the maximum likelihood estimator for the parameter $a$ ? (2P)

Problem 2. (25 points)
Principal Component Analysis:
Part I
Assume four independent two-dimensional samples:

$$
\mathbf{x}_{1}=\sqrt{3}\binom{4}{4}, \quad \mathbf{x}_{2}=\sqrt{3}\binom{4}{-4}, \quad \mathbf{x}_{3}=\sqrt{3}\binom{0}{8}, \quad \mathbf{x}_{4}=\sqrt{3}\binom{0}{-4} .
$$

We suggest to keep the symbolic value $\sqrt{3}$ within your calculations without any conversion to a low-precision number!
a) Calculate the sample mean $\overline{\mathbf{x}}_{4} \cdot(2 \mathrm{P})$
b) Calculate the sample covariance matrix $\mathbf{S}_{4}$. (4P)
c) Determine the Gerschgorin's circles of the normalized matrix $\frac{1}{4} \mathbf{S}_{4}$ and sketch them on the complex domain. $(4+2 \mathrm{P})$

d) Is the matrix $\mathbf{S}_{4}$ positive definite, negative definite, or indefinite? Give a reason for your statement. (1P)

## Part II

e) Now we independently take $n$ samples in total such that the corresponding sample covariance matrix $\mathbf{S}_{n}$ is given by

$$
\mathbf{S}_{n}=\left(\begin{array}{cc}
14 & -14 \\
-14 & 110
\end{array}\right)
$$

Calculate the spectral decomposition $\mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{\mathrm{T}}$ of $\mathbf{S}_{n}$ by determining the matrices $\mathbf{V}$ and几. $(3+5 \mathrm{P})$
f) Determine the best projection matrix $\mathbf{Q}$ to transform the two-dimensional samples to a one-dimensional data and calculate the projection of $\mathbf{x}_{1} .(2+1 \mathrm{P})$
g) Determine the residuum $\frac{1}{n-1} \max _{\mathbf{Q}} \sum_{i=1}^{n}\left\|\mathbf{Q} \mathbf{x}_{i}-\mathbf{Q} \overline{\mathbf{x}}_{n}\right\|^{2}$ for the above choice of $\mathbf{Q}$.

Problem 3. (25 points)

## Discriminant Analysis:

A training dataset consists of three-dimensional vectors belonging to three classes denoted by the labels $y_{i} \in\{1,2,3\}$. This dataset is given below.

| Data | Label | Data | Label | Data | Label |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{x}_{1}=\left(\begin{array}{l}1 \\ 1 \\ 1\end{array}\right)$ | $y_{1}=1$ | $\mathbf{x}_{4}=\left(\begin{array}{c}1 \\ -1 \\ -1\end{array}\right)$ | $y_{4}=2$ | $\mathbf{x}_{7}=\left(\begin{array}{c}-1 \\ 1 \\ 1\end{array}\right)$ | $y_{7}=3$ |
| $\mathbf{x}_{2}=\left(\begin{array}{c}1 \\ 2 \\ 0\end{array}\right)$ | $y_{2}=1$ | $\mathbf{x}_{5}=\left(\begin{array}{c}0 \\ -2 \\ -1\end{array}\right)$ | $y_{5}=2$ | $\mathbf{x}_{8}=\left(\begin{array}{c}-1 \\ 0 \\ 2\end{array}\right)$ | $y_{8}=3$ |
| $\mathbf{x}_{3}=\left(\begin{array}{c}1 \\ 1 \\ -1\end{array}\right)$ | $y_{3}=1$ | $\mathbf{x}_{6}=\left(\begin{array}{c}-1 \\ -1 \\ -1\end{array}\right)$ | $y_{6}=2$ | $\mathbf{x}_{9}=\left(\begin{array}{c}-1 \\ -1 \\ 1\end{array}\right)$ | $y_{9}=3$ |

Consider only those vectors $\mathbf{x}_{i}$ in the dataset with labels $y_{i}=1$ and $y_{i}=2$.
a) Find the matrix $\mathbf{W}$, that is the matrix corresponding to the sum of squares within groups. (5P)
b) Find Fisher's linear discriminant rule for classification of vectors with labels $y_{i}=1$ and $y_{i}=2$. Explain each step. (3P)
Hint: For a matrix $\mathbf{A}=\left(\begin{array}{c}\alpha_{1} \mathbf{x}^{\mathrm{T}} \\ \alpha_{2} \mathbf{x}^{\mathrm{T}} \\ \alpha_{3} \mathbf{x}^{\mathrm{T}}\end{array}\right) \in \mathbb{R}^{3 \times 3}$ and any $\mathbf{x}=\left(\begin{array}{l}x_{1} \\ x_{2} \\ x_{3}\end{array}\right) \in \mathbb{R}^{3}$, the eigenvalues and its dominant eigenvector are given by $(0,0, \operatorname{tr}(\mathbf{A}))$ and $\left(\begin{array}{l}\alpha_{1} \\ \alpha_{2} \\ \alpha_{3}\end{array}\right)$, respectively.

Suppose that the vectors $\mathbf{x}_{i}$ with label $y_{i}$ are randomly drawn from a multivariate normal distribution with the covariance matrix $\boldsymbol{\Sigma}_{i}$ and the expected value $\boldsymbol{\mu}_{i}$ for $i=1,2,3$.
c) Find the maximum likelihood estimation of the expected values. (4P)
d) If $\boldsymbol{\Sigma}_{1}=\boldsymbol{\Sigma}_{2}=\boldsymbol{\Sigma}_{3}=\boldsymbol{\Sigma}$, find the maximum likelihood estimation of the covariance matrix $\hat{\boldsymbol{\Sigma}}$ by using the whole dataset (5P).

Consider only those vectors $\mathbf{x}_{i}$ in the dataset with labels $y_{i}=2$ and $y_{i}=3$.
e) Find the maximum likelihood estimation of the covariance matrix, $\hat{\boldsymbol{\Sigma}}$. (3P)
f) Find the Gaussian maximum likelihood discriminant rule for classification of vectors with labels $y_{i}=2$ and $y_{i}=3$. Explain each step. (5P)

## Support Vector Machines:

a) Suppose that a training dataset is composed of vectors $\mathbf{x}_{i} \in \mathbb{R}^{3}$ belonging to two classes. The class membership is indicated by the labels $y_{i} \in\{-1,+1\}$. Suppose that the dataset is separable. A Support vector machine is used to find the maximum-margin hyperplane $\mathbf{a}^{\mathrm{T}} \mathbf{x}+b=0$. The primal optimization problem gives the optimal $\mathbf{a}^{\star}$ as $\left(\begin{array}{lll}1 & 3 & 0\end{array}\right)^{\mathrm{T}}$. Two support vectors with different labels are given as :

$$
\mathbf{x}_{1}^{\mathrm{T}}=\left(\begin{array}{lll}
1 & -1 & 1
\end{array}\right), \quad \mathbf{x}_{2}^{\mathrm{T}}=\left(\begin{array}{lll}
-1 & -1 & -1
\end{array}\right)
$$

Find the optimal value $b^{\star}$. (3P)

Consider another training dataset that is non-separable. The following dual problem is solved for a support vector machine

$$
\begin{aligned}
\max _{\boldsymbol{\lambda}} & \sum_{i=1}^{6} \lambda_{i}-\frac{1}{2} \sum_{i, j} y_{i} y_{j} \lambda_{i} \lambda_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j} \\
\text { s.t. } & 0 \leq \lambda_{i} \leq 5 \quad \text { and } \quad \sum_{i=1}^{6} \lambda_{i} y_{i}=0 .
\end{aligned}
$$

The dataset with the outputs of the optimization problem are given in the following table.

| Data | Label | Solution | Data | Label | Solution |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{x}_{1}=\binom{1}{1}$ | $y_{1}=-1$ | $\lambda_{1}^{\star}=0$ | $\mathbf{x}_{4}=\binom{0.5}{-0.5}$ | $y_{4}=1$ | $\lambda_{4}^{\star}=4.73$ |
| $\mathbf{x}_{2}=\binom{2}{0}$ | $y_{2}=-1$ | $\lambda_{2}^{\star}=0.67$ | $\mathbf{x}_{5}=\binom{-2}{1}$ | $y_{5}=1$ | $\lambda_{5}^{\star}=0.94$ |
| $\mathbf{x}_{3}=\binom{0}{0}$ | $y_{3}=-1$ | $\lambda_{3}^{\star}=5$ | $\mathbf{x}_{6}=\binom{0}{-1}$ | $y_{6}=1$ | $\lambda_{1}^{\star}=0$ |

b) Determine the support vectors. (4P)
c) Find the maximum-margin hyperplane by finding $\mathbf{a}^{\star}$ and $b^{\star}$. (6P)
d) Suppose that a kernel is given by $K(\mathbf{x}, \mathbf{y})=\left(2 \mathbf{x}^{T} \mathbf{y}+1\right)^{2}$ for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{p}$. Determine the feature mapping function $\phi(\mathbf{x})$, i.e., the function $\phi: \mathbb{R}^{p} \rightarrow \mathbb{R}^{d}$ where $K(\mathbf{x}, \mathbf{y})=$ $\boldsymbol{\phi}(\mathbf{x})^{T} \boldsymbol{\phi}(\mathbf{y})$. Determine the dimension of the feature space. (6P)

Consider a training dataset that is separable and consists of vectors $\mathbf{x}_{i} \in \mathbb{R}^{p}$ with labels $y_{i} \in\{-1,+1\}$.
e) Write down the optimization problem for the kernel-based support vector machine using the kernel $K(\mathbf{x}, \mathbf{y})=\exp \left(-\gamma\|\mathbf{x}-\mathbf{y}\|^{2}\right)$. (3P)
f) Write down the kernel-based support vector machine classifier for this dataset. (3P)

Additional sheet
Problem:

Additional sheet
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