## MTH6101 - Introduction to Machine Learning

## Sample exam 2021

Read the following carefully:

This sample paper should take about two hours to solve, provided you have done prior revision and are ready for examination in the Module.

This sample paper is provided to be used for practice, at a later stage in your revision. It is not a suggestion how to study and it is not to be used as a first step in your revision.

Importantly, this sample paper is not to be used as a guide for what topics to revise/what topics to exclude. The final exam will cover anything seen in lectures, labs, practicals and note that the presence of a topic on this sample paper is not an indication of the presence of the topic in the final exam. Ditto absence of a topic in this sample exam.

To do well in the final exam, it is not compulsory nor necessary that you practice this sample paper. However if you practice with this sample exam, it should be a honest attempt, meaning to do this paper in proper exam conditions, answering everything.

1. Do exercise $4(3)$ of the booklet.

1 Compute the singular value decomposition (use R) and report the results.
(3 marks)

This exercise is about singular value decomposition of the following matrix:

$$
3:\left(\begin{array}{rrrr}
-1 & 0 & 1 & 0 \\
1 & 1 & 0 & 1 \\
-1 & 0 & -1 & -1
\end{array}\right)
$$

These are the results of the singular value decomposition of the matrix.

```
## $d
## [1] 2.2724982 1.4923587 0.7801395
##
## $u
## [,1] [,2] [,3]
## [1,] 0.2260912 -0.8460412 0.4828013
## [2,] -0.7154086 0.1921651 0.6717612
## [3,] 0.6611152 0.4972795 0.5618183
##
## $v
## [,1] [,2] [,3]
## [1,] -0.7052217 0.3624643-0.4779381
## [2,] -0.3148115 0.1287660 0.8610783
## [3,] -0.1914299 -0.9001326 -0.1012858
## [4,] -0.6057315 -0.2044511 0.1409272
```

Although not asked in this question, you should always check what you do and be able to retrieve the original matrix.

```
round(SS$u%*%%diag(SS$d)%*%t(SS$v),5)
## [,1] [,2] [,3] [,4]
## [1,] -1 0 1 0
## [2,] 1
## [3,] -1 0
M
## [,1] [,2] [,3] [,4]
## [1,] -1 0 1 0
## [2,] 1
## [3,] -1 0
```

2 Using the results you just obtained with eigenvalues $d_{1}, d_{2}, \ldots$ sorted out in decreasing order and corresponding eigenvectors $\mathbf{u}_{1}, \mathbf{u}_{2}, \ldots$ and $\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots$, compute a series of approximations of rank one using R. These are $d_{1} \mathbf{u}_{1} \mathbf{v}_{1}^{T}, d_{1} \mathbf{u}_{1} \mathbf{v}_{1}^{T}+d_{2} \mathbf{u}_{2} \mathbf{v}_{2}^{T}, \ldots$ as appropriate according to the matrix dimensions. Comment on your results.

The eigenvalues $2.2725,1.49236,0.78014$ are already sorted out. Here we give the resulting matrices only.

```
## [1] "First term only"
## [,1] [,2] [,3] [,4]
## [1,] -0.36234 -0.16175 -0.09836 -0.31122
## [2,] 1.14652 0.51181 0.31122 0.98478
## [3,] -1.05951 -0.47297 -0.28760 -0.91004
## [1] "With 2 terms"
## [,1] [,2] [,3] [,4]
## [1,] -0.81998 -0.32433 1.03815 -0.05308
## [2,] 1.25047 0.54874 0.05308 0.92614
## [3,] -0.79052 -0.37741 -0.95561 -1.06177
## [1] "With 3 terms"
## [,1] [, 2] [, 3] [,4]
## [1,] -1 0
## [2,] 1
## [3,] -1 0
```

The matrix of this problem has rank 3. The matrix with one term only is of course an approximation to it but it is quite rough. The second matrix with two terms is especially interesting as it is close to the matrix itself and thus it is a low rank approximation to the matrix. The matrix of the final computation equals the original.
2. Do exercise $8(1)$ of the booklet.

1 Build explicitly $\mathbf{B}=\mathbf{A}^{T} \mathbf{A}$ and then $\mathbf{A z}$ and $\mathbf{z}^{T} \mathbf{B z} . \quad$ (4 marks)
This question uses $\mathbf{A}=\left(\begin{array}{ll}-1 & 1\end{array}\right)$ and $\mathbf{z}=\left(z_{1}, z_{2}\right)^{T}$.
This computation is straightforward with the given matrix $\mathbf{A}$. We have $\mathbf{B}=\left(\begin{array}{rr}1 & -1 \\ -1 & 1\end{array}\right)$;
$\mathbf{A} \mathbf{z}=-z_{1}+z_{2}$ and
$\mathbf{z}^{T} \mathbf{B z}=z_{1}^{2}-2 z_{1} z_{2}+z_{2}^{2}$.

2 Compute the derivatives $\frac{\partial}{\partial \mathbf{z}}(\mathbf{A z})$ and $\frac{\partial}{\partial \mathbf{z}}\left(\mathbf{z}^{T} \mathbf{B} \mathbf{z}\right)$.
(6 marks)
These derivatives are
$\frac{\partial}{\partial \mathbf{z}}(\mathbf{A} \mathbf{z})=\frac{\partial}{\partial \mathbf{z}}\left(-z_{1}+z_{2}\right)=\left(\begin{array}{ll}-1 & 1\end{array}\right)=\mathbf{A}$ and
$\frac{\partial}{\partial \mathbf{z}}\left(\mathbf{z}^{T} \mathbf{B} \mathbf{z}\right)=\frac{\partial}{\partial \mathbf{z}}\left(z_{1}^{2}-2 z_{1} z_{2}+z_{2}^{2}\right)=\binom{2 z_{1}-2 z_{2}}{-2 z_{1}+2 z_{2}}=2 \mathbf{B} \mathbf{z}$.

3 Verify that your results coincide with the result given in lectures.
(2 marks)

As indicated above, at the end of each derivative.
3. Do exercise 12 of the booklet. Analyze the centered (not scaled) data, considering only variables (Sepal.Length, Sepal.Width, Petal.Length).

1 Report the output of prcomp using summary, then comment on it and interpret the first principal component.
(10 marks)

This analysis is performed with a single instruction.

```
PC<-prcomp(x=iris[,1:3], center = TRUE,scale=!TRUE)
summary(PC)
## Importance of components:
## PC1 PC2 PC3
## Standard deviation 1.9212 0.49130 0.24383
## Proportion of Variance 0.9246 0.06047 0.01489
## Cumulative Proportion 0.9246 0.98511 1.00000
```

The first component is enough to recover $92.464 \%$ of the total variability in the data.
The first principal component has coefficients (0.39, -0.091, 0.916) for variables (Sepal.Length, Sepal.Width, Petal.Length). Given the very low weight of the coefficient for Sepal.Width, this first PC is a weighted average of variable Sepal.Length, Petal.Length, with variable Petal.Length having the biggest weight.

2 Report the eigenvalues of the singular value decomposition of these data.
(3 marks)

These are 23.4516, 5.9971, 2.9763.
Although the R code is strictly not required, the eigenvalues are the result of

```
svd(x=scale(x=iris[,1:3], center=TRUE, scale=!TRUE))$d
## [1] 23.451585 5.997100 2.976341
```

3 Explain the relation between the singular eigenvalues of step 2 and the entries labelled Standard deviation of the summary in step 1 . Verify numerically your assertion.
(6 marks)

The $i$-th entry under Standard deviation is the square root of the eigenvalue $\lambda_{i}$ of the Karhunen-Loeve decomposition of the variance covariance matrix of the data. The relation between $\lambda_{i}$ and the singular eigenvalue $d_{i}$ is a result seen in the Module lectures: $\sqrt{\lambda_{i}}=d_{i} / \sqrt{n-1}$.
For the numerical verification, recall that for these data $n=150$ and see that
$23.4516 / \sqrt{150-1}=23.4516 / 12.2066=1.9212287$;
$5.9971 / \sqrt{150-1}=5.9971 / 12.2066=0.4913016$ and
$2.9763 / \sqrt{150-1}=2.9763 / 12.2066=0.2438313$, which are the values reported above.
4. This question is concerned with the transept data gilgais from the R package MASS. You will perform a lasso fit to these data before answering the questions below. For this analysis, the response variable will be the superficial pH pHOO , and explanatory variables are e 00 , e30, e80, c00, c30, c80. You will use all the data available for these variables, and use scale to make sure that the data is centered and scaled. Finally, when invoking the lars function set both parameters intercept and normalize to FALSE.

1 Which is the variable whose coefficient first shrinks to zero in the lasso path? Give the value of $\lambda$ at which this occurs. (4 marks)

The variable is c 80 , and this occurs at $\lambda=2.2487$.
Note that what is shown below was not asked specifically here, but this is the fit, table of coefficients and values of $\lambda$ generated.

```
library(MASS)
data(gilgais)
lars(x=scale(x=gilgais[,-c(1:3)],center = TRUE,scale=TRUE),
            y = scale(x=gilgais[,1],center=TRUE,scale=TRUE),
    type = "lasso", intercept = FALSE, normalize = FALSE)->A
round(A$beta,4)
## e00 e30 e80 c00 c30 c80
## 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.000
## 1 0.0000 0.0000 0.0924 0.0000}00.0000 0.000
## 2 0.0000 0.0966 0.1891 0.0000 0.0000 0.000
## 3 0.0000 0.1638 0.2001 -0.0740 0.0000 0.000
## 4 0.6883 0.1995 0.1899 -0.7839 0.0000 0.000
## 5 1.1289 0.4835 0.1919 -1.2521 -0.2699 0.000
## 6 1.2794 0.5780 0.1823 -1.4077 -0.3884 0.038
## attr(,"scaled:scale")
## [1] 1 1 1 1 1 1
round(A$lambda,4)
## [1] 116.5936 82.9464 25.8163 18.1039 8.9388 2.2487
```

2 Which is the variable whose coefficient is the last to shrink to zero in the lasso path? Give the corresponding $\lambda$.
(4 marks)

The variable is e80, and this occurs at $\lambda=116.5936$.

3 Compute and report the shrinkage $s=s(\lambda)=\|\hat{\beta}(\lambda)\|_{1} / \max _{\lambda}\|\hat{\beta}(\lambda)\|_{1}$ attained at the breakpoints in the lasso path.
(8 marks)

The computation of $s$ is simply computing the Manhattan norm at each point in the path, and then normalizing it with respect to the norm of the ordinary least squares estimate.
The computation of the norm can be done in a variety of ways. The first is the simplest, used in lectures.

```
## used in lectures
apply(X = abs(A$beta), MARGIN = 1, FUN = sum) ->SS
round(SS,4)
## rrrrrrrr
## 0.0000 0.0924 0.2857 0.4379 1.8615 3.3264 3.8736
## equivalent computation
for(i in 1:nrow(A$beta))
    print(dist(rbind(A$beta[i,],0),method="manh") [1])
## [1] 0
## [1] 0.09243733
## [1] 0.2856825
## [1] 0.4378502
## [1] 1.86154
## [1] 3.32638
## [1] 3.873632
## normalization
s<-SS/max(SS) # shrinkage s
```

The values of shrinkage $s$ are $0,0.0239,0.0738,0.113,0.4806$, 0.8587 , 1.

4 Construct and report a table with the following 8 columns: a column for breakpoints lambda, then 6 columns for coefficients of variables (e00, e30, e80, c00, c30, c80). The last column will have shrinkage $s$, to be given as values in $[0,1]$. ( 6 marks)

The table is constructed with cbind and columns renamed.

```
## LP for lasso path
LP<-cbind(c(A$lambda,0),A$beta,s)
colnames(LP)[c(1,8)]<-c("lambda", "s")
round(LP,4)
\begin{tabular}{lrrrrrrrr} 
\#\# & lambda & \(e 00\) & \(e 30\) & \(e 80\) & \(c 00\) & \(c 30\) & \(c 80\) & s \\
\#\# 0 & 116.5936 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.000 & 0.0000 \\
\#\# 1 & 82.9464 & 0.0000 & 0.0000 & 0.0924 & 0.0000 & 0.0000 & 0.000 & 0.0239 \\
\#\# 2 & 25.8163 & 0.0000 & 0.0966 & 0.1891 & 0.0000 & 0.0000 & 0.000 & 0.0738 \\
\#\# 3 & 18.1039 & 0.0000 & 0.1638 & 0.2001 & -0.0740 & 0.0000 & 0.000 & 0.1130 \\
\#\# 4 & 8.9388 & 0.6883 & 0.1995 & 0.1899 & -0.7839 & 0.0000 & 0.000 & 0.4806 \\
\#\# 5 & 2.2487 & 1.1289 & 0.4835 & 0.1919 & -1.2521 & -0.2699 & 0.000 & 0.8587 \\
\#\# 6 & 0.0000 & 1.2794 & 0.5780 & 0.1823 & -1.4077 & -0.3884 & 0.038 & 1.0000
\end{tabular}
```

5 There is interest in retrieving the lasso estimate $\hat{\beta}^{L}(\lambda)$ that has shrinkage of $50 \%$, i.e. for which $s=0.5$. Using coef.lars or otherwise, retrieve this estimate and check that its Manhattan norm satisfies the shrinkage requirement.
Hint: Read carefully how to use coef.lars and pick a suitable value of $s$. Importantly, note that the value of $s$ can be 0.5 but this is not the only way to do this.

There are several ways to do this. The simplest is the function coef.lars with s=0.5 and mode="fraction".

```
coef.lars(object=A,s=0.5,mode="fraction")->b
round(b,4) ## the coefficient
## e00 e30 e80 c00 c30 c80
## 0.7109 0.2141 0.1900 -0.8080 -0.0139 0.0000
sum(abs(b))/max(SS) ## check the norm
## [1] 0.5
```

Another is to interpolate to determine at which fractional row the required norm would be attained. This fractional row is either approx ( $\mathrm{x}=\mathrm{s}[5: 6], \mathrm{y}=5: 6$, xout=0.5) \$y that is 5.0514; or approximately $5+2 / 38=5.0526316$, by noting that the distance between 0.8587 and 0.4806 is roughly split into 38 parts as $0.8587-0.4806=0.3782$.

```
coef.lars(object=A,s=approx(x=s [5:6],y=5:6, xout=0.5)$y) ->b
round(b,4) ## exact
## e00 e30 e80 c00 c30 c80
## 0.7109 0.2141 0.1900 -0.8080 -0.0139 0.0000
sum(abs(b))/max(SS) ## check the norm
## [1] 0.5
coef.lars(object=A,s=5+2/38)->b
round(b,4) ## approximation
## e00 e30 e80 c00 c30 c80
## 0.7115 0.2144 0.1900 -0.8085 -0.0142 0.0000
sum(abs(b))/max(SS) ## check the norm
## [1] 0.5004701
```

A third possibility is to interpolate directly the coefficients without using coef.lars. This is using either the exact proportion of the path approx $(x=s[5: 6], y=5: 6, x o u t=0.5) \$ y-5$ or the approximate $2 / 38$ so that

```
p<-1-(approx(x=s[5:6],y=5:6, xout=0.5)$y-5)
A$beta[5,]*p+A$beta[6,]*(1-p) ->b
round(b,4) ## exact
## e00 e30 e80 c00 c30 c80
## 0.7109 0.2141 0.1900 -0.8080 -0.0139 0.0000
sum(abs(b))/max(SS) ## check the norm
## [1] 0.5
p<-1-2/38
A$beta[5,]*p+A$beta[6,]*(1-p) ->b
round(b,4) ## approximate
## e00 e30 e80 c00 c30 c80
## 0.7115 0.2144 0.1900 -0.8085 -0.0142 0.0000
sum(abs(b))/max(SS) ## check the norm
## [1] 0.5004701
```

5. A logistic classifier is to be evaluated. To this end, the classifier was trained to produce the trained model termed M1. Using the trained model, 12 fresh observations were used to produce the following table of logistic predicted probabilities and true new observations Ytrue.

| \#\# | Predicted Prob | Ytrue |
| :--- | ---: | ---: |
| \#\# 6 | 0.7901 | 1 |
| \#\# 9 | 0.5903 | 0 |
| \#\# 13 | 0.3554 | 0 |
| \#\# 2 | 0.9312 | 1 |
| \#\# 17 | 0.1001 | 0 |
| \#\# 4 | 0.7901 | 1 |
| \#\# 1 | 0.9625 | 1 |
| \#\# 21 | 0.0408 | 0 |
| \#\# 10 | 0.5113 | 1 |
| \#\# 15 | 0.1743 | 1 |


| \#\# | 18 | 0.1001 |
| :--- | :--- | :--- |
| \#\# | 12 | 0.3554 |

1 Using the new data and the canonical threshold 0.5 , compute and report the confusion matrix.
(12 marks)

The probabilities are first thresholded into $0 / 1$ values $1,1,0,1$, $0,1,1,0,1,0,0,0$. These predictions "Yhat" are then compared with fresh observations.

| \#\# |  | Prob | Yhat |
| :--- | ---: | ---: | ---: |
| \#\# True | 0.7901 | 1 | 1 |
| \#\# FP | 0.5903 | 1 | 0 |
| \#\# TN | 0.3554 | 0 | 0 |
| \#\# TP | 0.9312 | 1 | 1 |
| \#\# TN | 0.1001 | 0 | 0 |
| \#\# TP | 0.7901 | 1 | 1 |
| \#\# TP | 0.9625 | 1 | 1 |
| \#\# TN | 0.0408 | 0 | 0 |
| \#\# TP | 0.5113 | 1 | 1 |
| \#\# FN | 0.1743 | 0 | 1 |
| \#\# TN | 0.1001 | 0 | 0 |
| \#\# TN | 0.3554 | 0 | 0 |

We summarize these data into the confusion matrix.

```
## 0 1
## 0 5 1
## 1 1 5
```

2 Compute and report the performance measures TPR and FPR. Briefly comment on these.

The quantities required are $\mathrm{TPR}=5 / 6=0.8333$ and $\mathrm{FPR}=1 / 6=0.1667$.

The classifier is quite a good one, with high TPR value and relatively low FPR. It is far from being random classifier with a distance to the ideal classifier of 0.2357 .

The following plot is the ROC curve for model M1. A table of Sensitivities and Specificities is also given.


| \#\# | Specificities | Sensitivities |
| :--- | ---: | ---: |
| \#\# | 0.0000 | 1.0000 |
| \#\# | 0.1667 | 1.0000 |
| \#\# | 0.5000 | 1.0000 |
| \#\# | 0.5000 | 0.8333 |
| \#\# | 0.8333 | 0.8333 |
| \#\# | 0.8333 | 0.6667 |
| \#\# | 1.0000 | 0.6667 |
| \#\# | 1.0000 | 0.3333 |


| \#\# | 1.0000 | 0.1667 |
| :--- | :--- | :--- |
| \#\# | 1.0000 | 0.0000 |

3 Use the given information to compute AUC for M1 and briefly interpret it.
( 7 marks)

The AUC is computed as a sum of areas of rectangles. Perhaps the simplest approach starts from the right, using vertical rectangles. The rectangles have areas $1 \times 0.5=0.5 ; 0.8333 \times(0.8333-0.5)=$ 0.2778 and $(1-0.8333) \times 0.6667=0.1111$ and adding these figures we achieve
$\mathrm{AUC}=0.5+0.2778+0.1111=0.8889$.
This is a good classifier, reasonably close to the ideal.
A different computation uses horizontal rectangles, starting from the bottom with areas $0.6667 \times 1=0.6667$; $(0.8333-0.6667) \times$ $0.8333=0.1389$ and $(1-0.8333) \times 0.5=0.0833$ and adding to achieve $\mathrm{AUC}=0.6667+0.1389+0.0833=0.8889$.

4 Briefly explain why does the given table of Sensitivities and Specificities contains both entries $(0,1)$ and $(1,0)$ in its extremes. What do these entries mean?
(6 marks)

The entry $(0,1)$ corresponds to a liberal classifier with all fresh observations classified as positives.
The entry $(1,0)$ is for a conservative classifier when all the observations are classified as negatives.
Both extremes can be achieved with M1 by simply using different thresholds; the former with low threshold and the latter with high threshold.

MTH6101 - INTRODUCTION TO MACHINE LEARNING - 2021/22
$A>$ Courses $>$ Science and Engineering $>$ MTH6101- Introduction to Machine Learring $-2021 / 22>$ General $>$ Semester $B$ Final Assessment 2021/22 $>$ Preview




