HOME ASSIGNMENT 2

Multivariate Data Analysis

SUPERVISOR
Xijia Liu

STUDENTS
Ebba Sköld (ebsk0003@student.umu.se)
Hugo Englund (hugo.englund@umu.se)
Viktor Mostberg (vimo0015@student.umu.se)

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Umeå University
Department of Mathematics and Mathematical Statistics

1 Part I: Theoretical Problems

1.1 Exercise 8.3

Given the covariance matrix

$$\mathbf{\Sigma} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix},$$

the eigenvalues can easily be extracted by the following equation

$$(\mathbf{\Sigma} - \lambda I) = 0$$

which in its full form can be written as

$$\begin{bmatrix} 2-\lambda & 0 & 0 \\ 0 & 4-\lambda & 0 \\ 0 & 0 & 4-\lambda \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Since this leaves one with three trivial equations these calculations will be skipped and the conclusion can be made that the eigenvalues related to $\mathbf{\Sigma}$ are

$$\lambda_1 = 2, \lambda_2 = 4 \text{ and } \lambda_3 = 4.$$

It should be noted that $\lambda_2 = \lambda_3$ which makes their associated eigenvectors (and principal components) non-unique.

The eigenvectors are then computed by considering the following equation for $i = 1, 2, 3$

$$(\mathbf{\Sigma} - \lambda \boldsymbol{I})\boldsymbol{v}_i = 0$$

which can be written as

$$\begin{bmatrix} 2-\lambda & 0 & 0 \\ 0 & 4-\lambda & 0 \\ 0 & 0 & 4-\lambda \end{bmatrix} \begin{bmatrix} v_i^{(1)} \\ v_i^{(2)} \\ v_i^{(3)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Inserting the derived eigenvalues one by one in the equation above we are left with the following eigenvectors

$$\boldsymbol{v}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \boldsymbol{v}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \text{ and } \boldsymbol{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

Further, given that $\mathbf{\Sigma} = \boldsymbol{X}^T\boldsymbol{X}$ the matrix $\boldsymbol{X}$ can be determined using Cholesky decomposition. This leaves us with

$$\boldsymbol{X} = \begin{bmatrix} \sqrt{2} & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

Thus, the principal components Y_1, Y_2 and Y_3 can be deduced using the following equation

$$\boldsymbol{Y} = \boldsymbol{X}^T\boldsymbol{V}$$

represented by

$$\boldsymbol{Y} = \begin{bmatrix} \sqrt{2} & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

resulting in the following principal components

$$Y_1 = \begin{bmatrix} \sqrt{2} \\ 0 \\ 0 \end{bmatrix}, Y_2 = \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix} \text{ and } Y_3 = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}.$$

1.2 Exercise 8.4

Given the covariance matrix

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma^2 & \sigma^2\rho & 0 \\ \sigma^2\rho & \sigma^2 & \sigma^2\rho \\ 0 & \sigma^2\rho & \sigma^2 \end{pmatrix},$$

we first have to determine the eigenvalues and then, the corresponding eigenvectors. In order to find the eigenvalues, we solve

$$| \mathbf{\Sigma} - \mathbb{1}\lambda |= 0 \implies (\sigma^2 - \lambda)^3 - 2(\sigma^2 - \lambda)(\sigma^2\rho)^2 = (\sigma^2 - \lambda)\left((\sigma^2 - \lambda)^2 - 2(\sigma^2\rho)^2\right) = 0$$

which trivially yields $\lambda = \sigma^2$ and

$$\begin{aligned}(\sigma^2 - \lambda)^2 - 2(\sigma^2\rho)^2 = 0 &\implies \sigma^2 - \lambda = \sqrt{2}\sigma^2\rho \\ &\implies \lambda = \sigma^2(1 \pm \sqrt{2}\rho).\end{aligned}$$

Hence, we have $\lambda_1 = \sigma^2$, $\lambda_2 = \sigma^2(1 + \sqrt{2}\rho)$ and $\lambda_3 = \sigma^2(1 - \sqrt{2}\rho)$. Then, we can find the eigenvectors, $\mathbb{v}_i$, by solving $(\mathbf{\Sigma} - \mathbb{1}\lambda_i)\mathbb{v}_i = \mathbb{0}$ for $i = 1, 2, 3$. For $\lambda_1 = \sigma^2$, we get

$$\begin{pmatrix} 0 & \sigma^2\rho & 0 \\ \sigma^2\rho & 0 & \sigma^2\rho \\ 0 & \sigma^2\rho & 0 \end{pmatrix} \mathbb{v}_1 = \mathbb{0} \implies \begin{cases} \sigma^2\rho v_1^{(2)} = 0 \\ \sigma^2\rho v_1^{(1)} + \sigma^2\rho v_1^{(3)} = 0 \\ \sigma^2\rho v_1^{(2)} = 0 \end{cases}$$

Thus, $v_1^{(2)} = 0$ and $v_1^{(1)} = -v_1^{(3)}$ which yields $\mathbb{v}_1^\intercal = (1, 0, -1)$. For $\lambda_2 = \sigma^2(1 + \sqrt{2}\rho)$, we get

$$\begin{pmatrix} -\sigma^2\sqrt{2}\rho & \sigma^2\rho & 0 \\ \sigma^2\rho & -\sigma^2\sqrt{2}\rho & \sigma^2\rho \\ 0 & \sigma^2\rho & -\sigma^2\sqrt{2}\rho \end{pmatrix} \mathbb{v}_2 = \mathbb{0} \implies \begin{cases} -\sigma^2\sqrt{2}\rho v_2^{(1)} + \sigma^2\rho v_2^{(2)} = 0 \\ \sigma^2\rho v_2^{(1)} - \sigma^2\sqrt{2}\rho v_2^{(2)} + \sigma^2\rho v_2^{(3)} = 0 \\ \sigma^2\rho v_2^{(2)} - \sigma^2\sqrt{2}\rho v_2^{(3)} = 0 \end{cases}$$

Thus, $\sqrt{2}v_2^{(1)} = v_2^{(2)}$ and $v_2^{(2)} = \sqrt{2}v_2^{(3)}$ which yields $\mathbb{v}_2^\intercal = \left(1/\sqrt{2}, 1, 1/\sqrt{2}\right)$. For $\lambda_3 = \sigma^2(1 - \sqrt{2}\rho)$, we analogously obtain

$$\begin{cases} \sigma^2\sqrt{2}\rho v_3^{(1)} + \sigma^2\rho v_3^{(2)} = 0 \\ \sigma^2\rho v_3^{(1)} + \sigma^2\sqrt{2}\rho v_3^{(2)} + \sigma^2\rho v_3^{(3)} = 0 \\ \sigma^2\rho v_3^{(2)} + \sigma^2\sqrt{2}\rho v_3^{(3)} = 0 \end{cases}$$

Thus, $\sqrt{2}v_3^{(1)} = -v_3^{(2)}$ and $v_3^{(2)} = -\sqrt{2}v_3^{(3)}$ which yields $\mathbb{v}_3^\intercal = \left(-1/\sqrt{2}, 1, -1/\sqrt{2}\right)$. Assume that we have some observation $\mathbf{X}^\intercal = (X_1, X_2, X_3)$, then, the principal components becomes

$$\begin{aligned} Y_1 &= \mathbb{v}_1\mathbf{X} = X_1 - X_3 \\ Y_2 &= \mathbb{v}_2\mathbf{X} = \frac{1}{\sqrt{2}}X_1 + X_2 + \frac{1}{\sqrt{2}}X_3 \\ Y_3 &= \mathbb{v}_3\mathbf{X} = -\frac{1}{\sqrt{2}}X_1 + X_2 - \frac{1}{\sqrt{2}}X_3 \end{aligned}$$

Since $\mathrm{Var}(Y_i) = \lambda_i$, the total variance is

$$\sum_{i=1}^{3} \lambda_i = \sigma^2 + \sigma^2(1 + \sqrt{2}\rho) + \sigma^2(1 - \sqrt{2}\rho) = 3\sigma^2,$$

and the proportion of variance explained by each principal component becomes $\lambda_i/3\sigma^2$, presented in Table 1.

Table 1: *The proportion of variance explained for each principal component Y_i, $i = 1, 2, 3$.*

Principal Component	**Proportion**
Y_1	$\frac{1}{3}$
Y_2	$\frac{1}{3}\left(1 + \sqrt{2}\rho\right)$
Y_3	$\frac{1}{3}\left(1 - \sqrt{2}\rho\right)$

2 Part II: Programming Problems

2.1 The Method of PCA

Given a sample covariance matrix $\mathbf{S} = \mathbf{X}^T\mathbf{X}$, with $\mathbf{X}$ having dimension $n \times p$, eigen decomposition is performed such that

$$\mathbf{S} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$$

where $\mathbf{Q} = (\mathbf{q}_1, \mathbf{q}_2, ..., \mathbf{q}_n)$ is the matrix of eigenvectors.

Further, for the ith case the jth principal component can be obtained by

$$y_{ij} = \mathbf{x}_i^\top \mathbf{q}_j$$

where $i = 1, 2, ..., n$ and $j = 1, 2, ..., p$.

2.2 Task 1

Set random seed for reproducibility.

```
set.seed(1337)
```

```
# convert vector to matrix
vec2mat = function(vec, dim) {
    return(matrix(unlist(vec), ncol=dim, byrow=T)[,dim:1])
}
```

Firstly, we fetch the data and extract the observations related to our favorite number 2.

```
# read data
dat = read.table('HA_2_zip.train')
dat_two <- dat[which(dat[,1] == 2), 2:257]
```

Then, we plotted the first 24 observations of our number.

```
# plot first 24 digits
par(mfrow = c(3, 4))
no = 1
for (n in 1:2) {
    for (i in 1:12) {
        img_i = vec2mat(dat_two[no, 256:1], dim=16)
        image(
            t(img_i), xaxt='n', yaxt='n',
            xlab='', ylab='', main=paste("Image", no)
        )
        no = no + 1
    }
}
```

Image 1

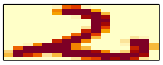


Image 2

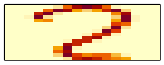


Image 3

Image 4

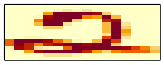


Image 5

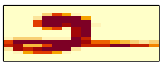


Image 6

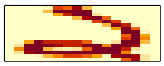


Image 7

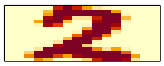


Image 8

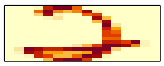


Image 9

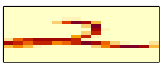


Image 10

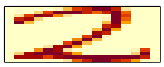


Image 11

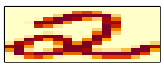
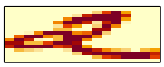
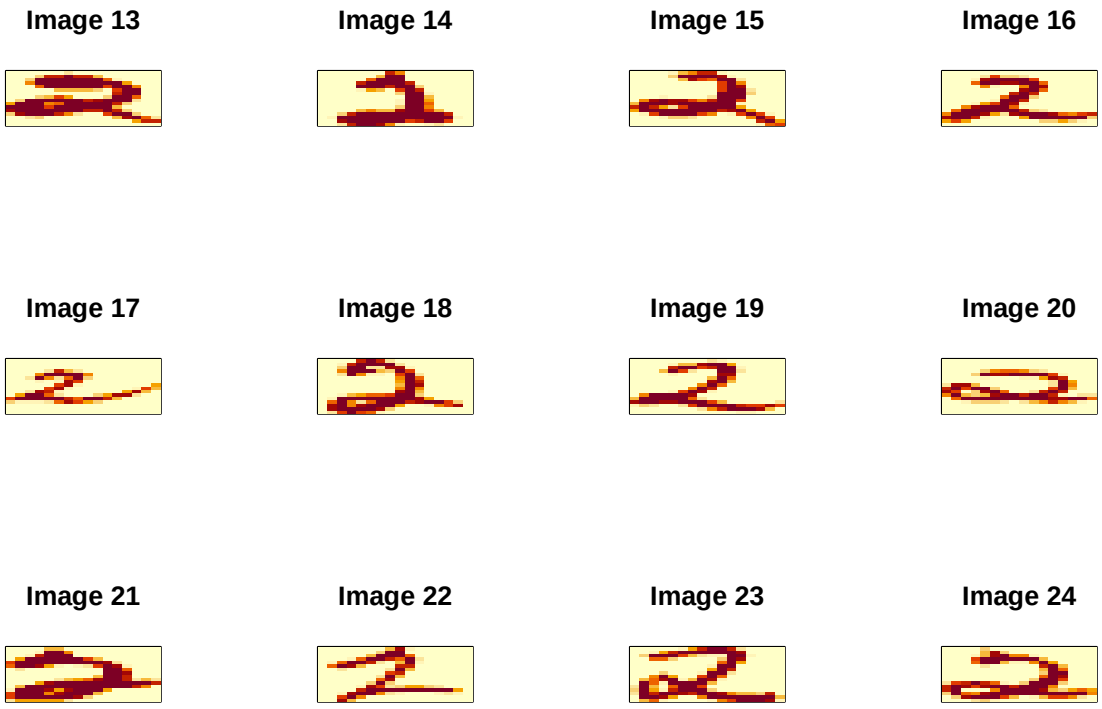


Image 12





2.3 Task 2

Consequently, we computed the principal components and plotted the four first and last, respectively, as 16x16 pixel images.

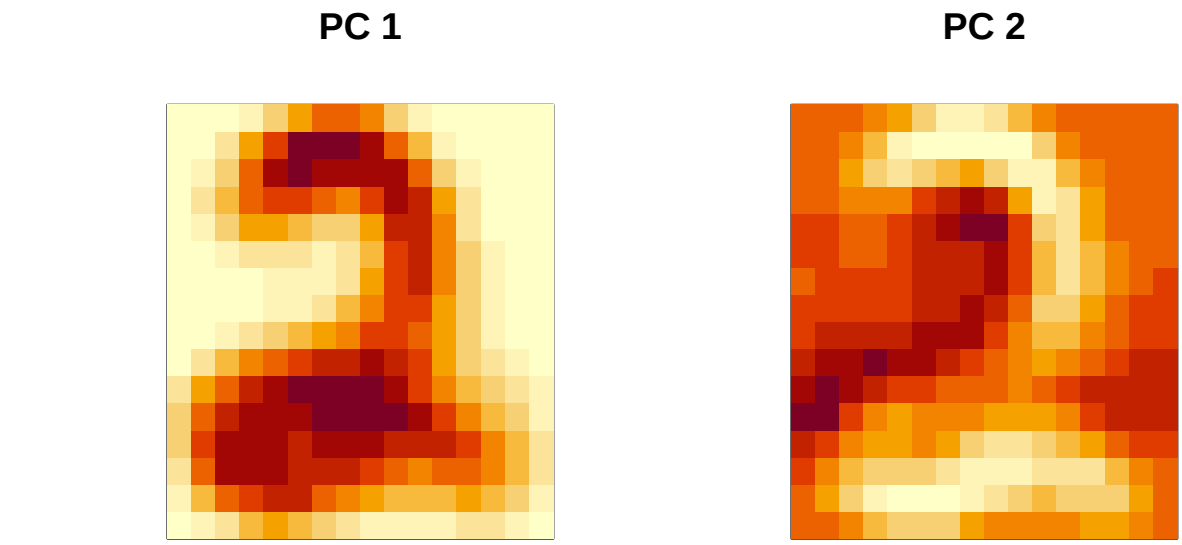
```
# convert data with digit 2 to matrix
dat_two_mat = matrix(
    unlist(dat_two),
    nrow=dim(dat_two)[1],
    ncol=dim(dat_two)[2]
)

# compute PC's and eigenvectors
S_two = t(dat_two_mat) %*% dat_two_mat
eigen_el = eigen(S_two)
Q_two = eigen_el$vectors
eigen_val = eigen_el$values
pc_two = dat_two_mat %*% Q_two
```

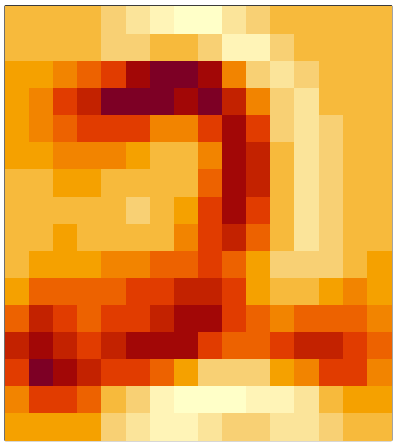
```
# first 4 PC's
par(mfrow=c(1, 2), oma=c(0, 0, 2, 0))

for (i in 1:4) {
    if (i == 3) {
        par(mfrow=c(1, 2))
```

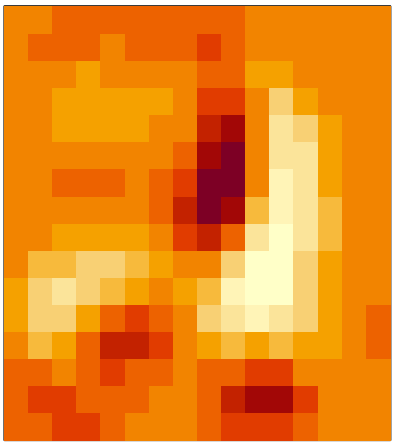
```
    }
    pc = Q_two[, i]
    img = vec2mat(pc[256:1], dim=16)
    image(t(img), xaxt='n', yaxt='n', xlab='', ylab='', main=paste("PC", i))
    if (i == 2) {
        title("First four PC's", outer=T)
    }
}
```



PC 3



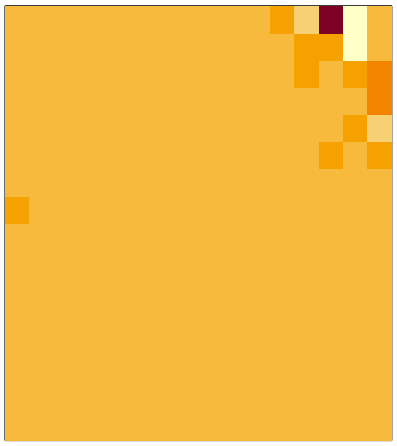
PC 4



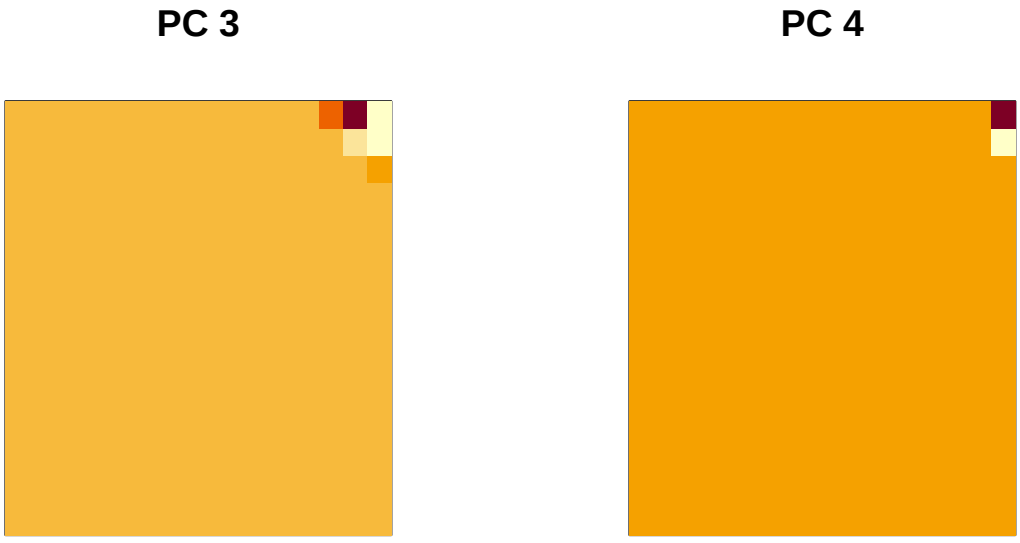
```
# last 4 PC's
par(mfrow=c(1, 2), oma=c(0, 0, 2, 0))
for (i in 1:4) {
    if (i == 3) {
        par(mfrow=c(1, 2))
    }
    pc = Q_two[, (dim(dat_two_mat)[2] - 4) + i]
    img = vec2mat(pc[256:1], dim=16)
    image(t(img), xaxt='n', yaxt='n', xlab='', ylab='', main=paste("PC", i))
    if (i == 2) {
        title("Last four PC's", outer=T)
    }
}
```

Last four PC's

PC 1



PC 2



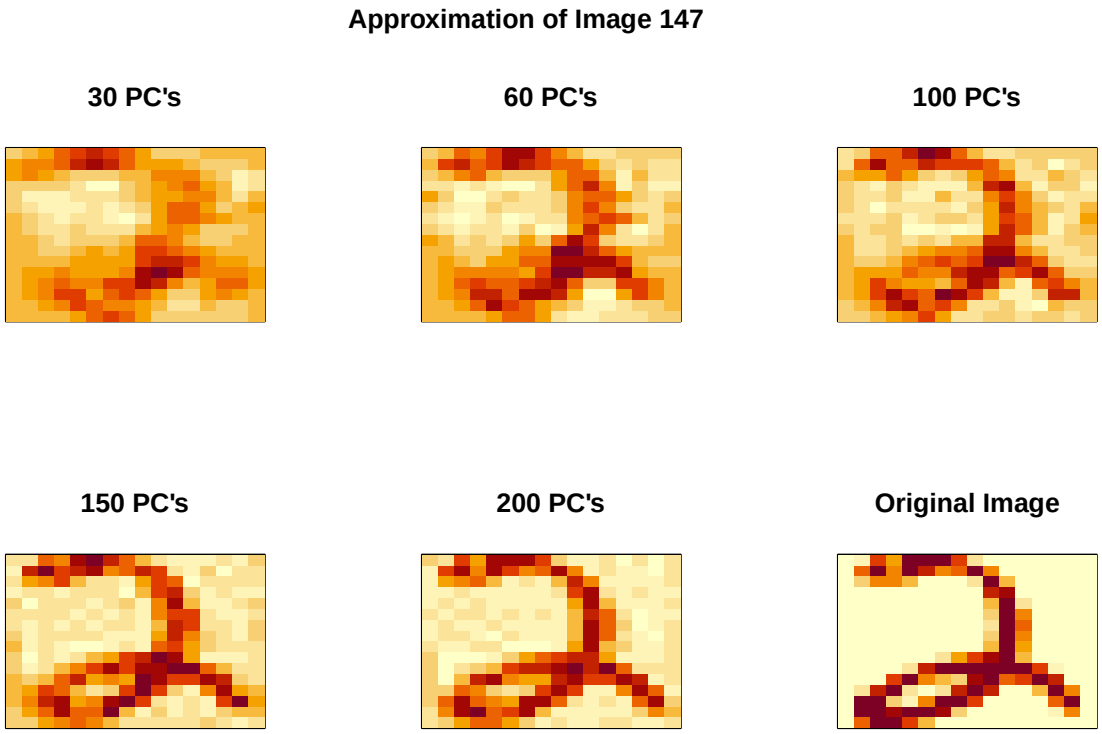
2.4 Task 3

By the principal components previously computed, a randomly selected image was selected and then reconstructed by different number of principal components. Alongside the image reconstruction, the mean-squared error (MSE) was calculated.

```
set.seed(1337)
par(mfrow=c(2, 3), oma=c(0, 0, 2, 0))
n = c(30, 60, 100, 150, 200)
rnd_idx = sample(1:dim(dat_two_mat)[1], 1)
real_vec = dat_two_mat[rnd_idx, 256:1]
real_img = vec2mat(real_vec, dim=16)
mse = vector()
j = 1
for (i in n) {
    q = Q_two[, 1:i]
    pc = real_vec %*% q
    est_vec = pc %*% t(q)
    img = vec2mat(est_vec, dim=16)
    image(t(img), xaxt='n', yaxt='n', xlab='', ylab='', main=paste(i, "PC's"))

    mse[j] = round(sum((real_vec - est_vec)^2) / length(real_vec), 4)
    j = j + 1
}
```

```
image(t(real_img), xaxt='n', yaxt='n', xlab='', ylab='', main="Original Image")
title(paste("Approximation of Image", rnd_idx), outer=T)
```




```
mse_df = data.frame(
    n_PC = c(n),
    MSE = c(mse)
)
print(mse_df)
```

```
##   n_PC    MSE
## 1   30 0.3100
## 2   60 0.2295
## 3  100 0.1536
## 4  150 0.0889
## 5  200 0.0501
```

2.5 Task 4

Related to the image reconstruction, the number of principal components needed to explain 85% of the variance was determined and also visualized by a bar plot. It was concluded that we need 21 principal components to explain 85% of the variance.

```
tot_var = sum(eigen_val)
var_exp = cumsum(eigen_val / tot_var)
```

```
barplot(
    var_exp[1:25] * 100,
    names.arg=1:25,
    xlab="Principal Component",
    ylab="Variance Epxlained (%)",
    ylim=c(0, 100),
    col=3
)
abline(h=85, col=2)
legend(x=24, y=100, legend="85%-limit", col=2, lty=1, cex=.75)
```

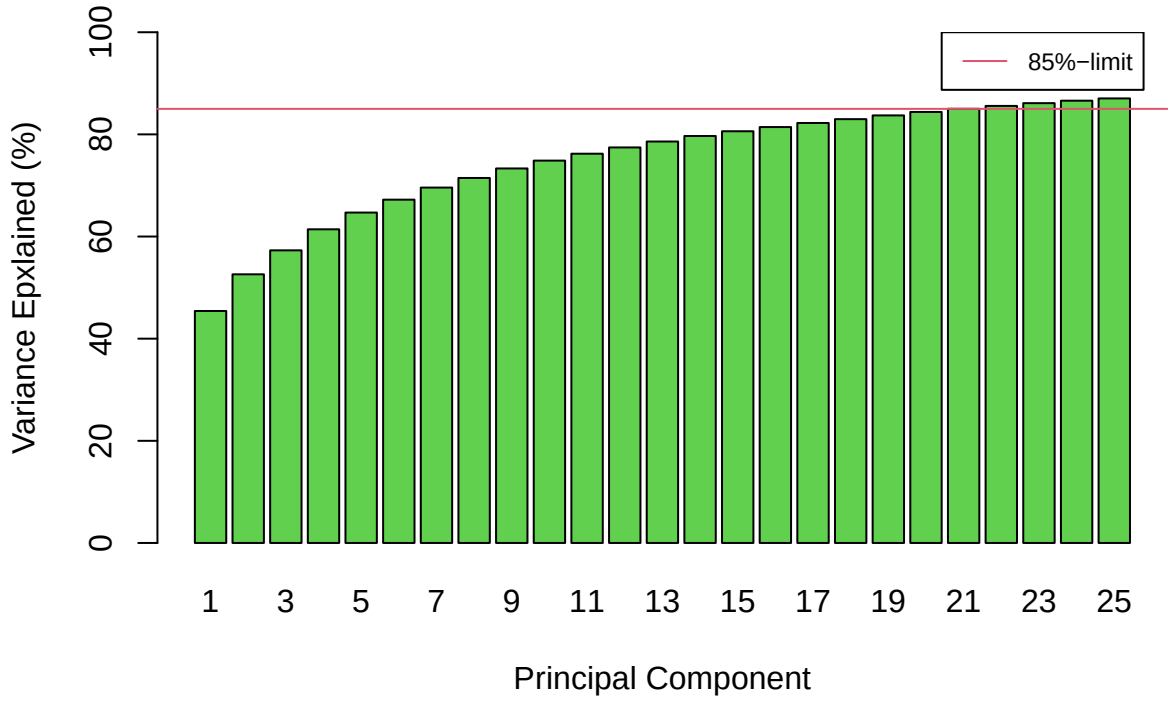


Figure 1: *The cumulative proportion of variance explained for the first 25 principal components.*

```
paste("PC's needed to explain 85% of the variance:", sum(var_exp <= 0.85) + 1)
```

```
## [1] "PC's needed to explain 85% of the variance: 21"
```

2.6 Task 5

2.6.1 Subtask 5.1

A new working data set was created by combining all observations of the digits 5 and 6.

```
dat_5 = dat[which(dat[,1] == 5), 1:257]
dat_6 = dat[which(dat[,1] == 6), 1:257]
c_dat = rbind(dat_5, dat_6)
```

2.6.2 Subtask 5.2

The data set was then divided into training set (80%) and testing set (20%) by random sampling.

```
set.seed(1337)

# randomly split data into train and test, 80%/20%
n = dim(c_dat)[1]
idx = sample(1:n, floor(0.8 * n))
train_dat = c_dat[idx, ]
test_dat = c_dat[-idx, ]

train = train_dat[, 2:257]
train_label = train_dat[, 1]

test = test_dat[, 2:257]
test_label = test_dat[, 1]
```

2.6.3 Subtask 5.3

A PCA, as presented in Section 1.2, was then performed on the training and testing set, respectively.

```
# compute eigen vectors
X_train = matrix(unlist(train), nrow=dim(train)[1], ncol=256)
X_test = matrix(unlist(test), nrow=dim(test)[1], ncol=256)

# compute PC's for train and test data
S_train= t(X_train) %*% X_train
Q_train = eigen(S_train)$vectors
pc_train = X_train %*% Q_train
pc_test = X_test %*% Q_train
```

2.6.4 Subtask 5.4

Consequently, a LDA classifier, as presented in Home Assignment 1, was fitted to the training data using only the first two principal components.

```
# format training data
train_data = as.data.frame(cbind(pc_train, train_label))

# fit LDA model
```

```
mdl = lda(
    train_label ~ V1 + V2,
    data=train_data
)
```

2.6.5 Subtask 5.5

Lastly, the LDA classifier was applied to the test set, and the confusion matrix along with the test accuracy were calculated. We obtain a test accuracy of approximately 84%, and the model tend to incorrectly classify slightly more 5's than 6's.

```
# predict test set
test_pred = predict(mdl, as.data.frame(pc_test))$class

# compute confusion matrix and test accuracy
test_res = confusionMatrix(
    data=factor(test_pred),
    reference=factor(test_label)
)
test_res$table
```

```
##            Reference
## Prediction   5   6
##          5  98  22
##          6  17 107
```

```
test_res$overall[1]
```

```
##  Accuracy
## 0.8401639
```

2.7 Conclusions

To summarize, considering the digit 2, we found that 21 principal components are needed to explain 85% of the variance. Further, the MSE was, trivially, decreasing as the number of components increased in the image reconstruction. Lastly, the LDA classifier resulted in a test accuracy of approximately 84% using only the first two components, which can be considered as a very good result. We would, however, not be even close to achieve these results with only two of the original variables, since these would not nearly explain as much as two "loaded" principal components.