Problem Solutions

e-Chapter 9

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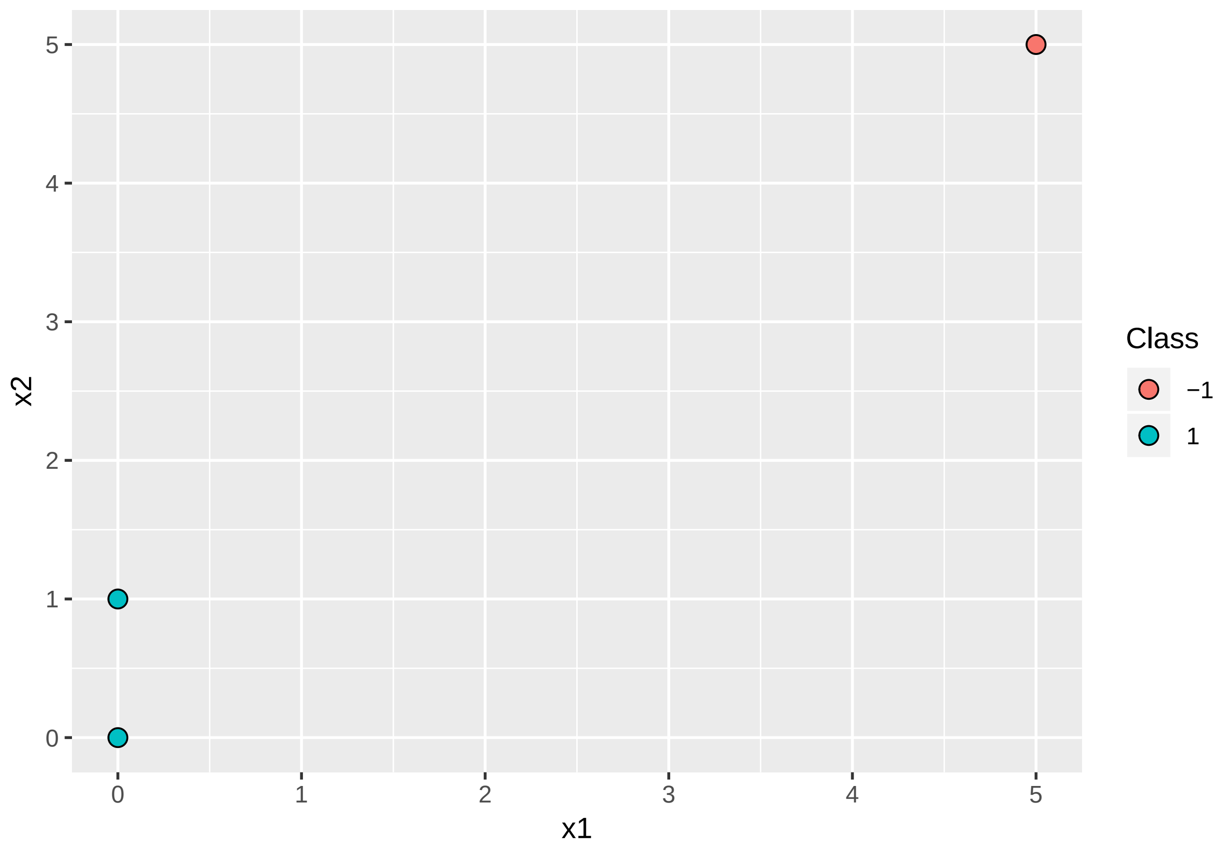
Problem 9.1

(a) We begin by implementing the nearest neighbor method on the raw data.

```
data <- data.frame(x1 = c(0, 0, 5), x2 = c(0, 1, 5))
class <- as.factor(c(1, 1, -1))

ggplot(data, aes(x = x1, y = x2, fill = class)) + geom_point(size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class"))
```

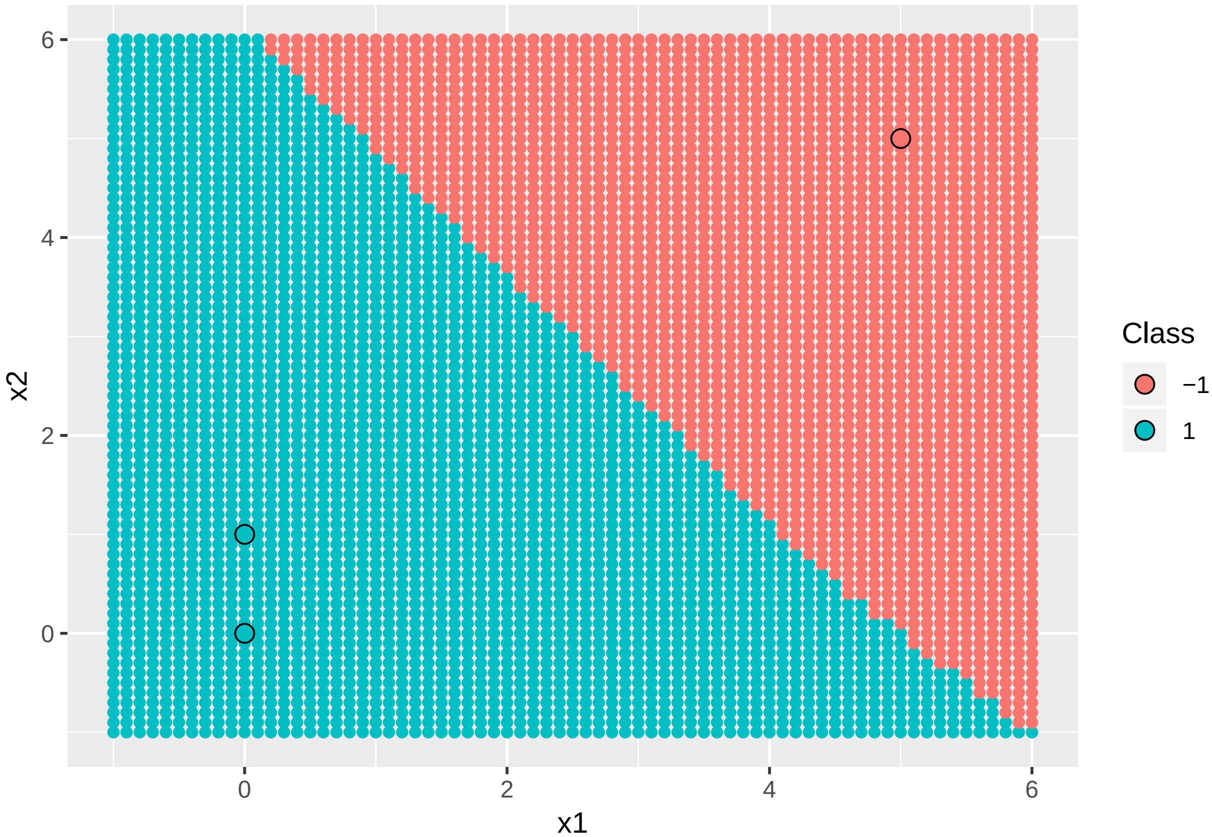



```
grid <- expand.grid(x1 = seq(min(data[, 1] - 1), max(data[, 1] + 1), by = 0.1),
                    x2 = seq(min(data[, 2] - 1), max(data[, 2] + 1), by = 0.1))

knn_mod <- knn(data, grid, class, k = 1, prob = TRUE)
```

Below, we show the decision regions of the final hypothesis.

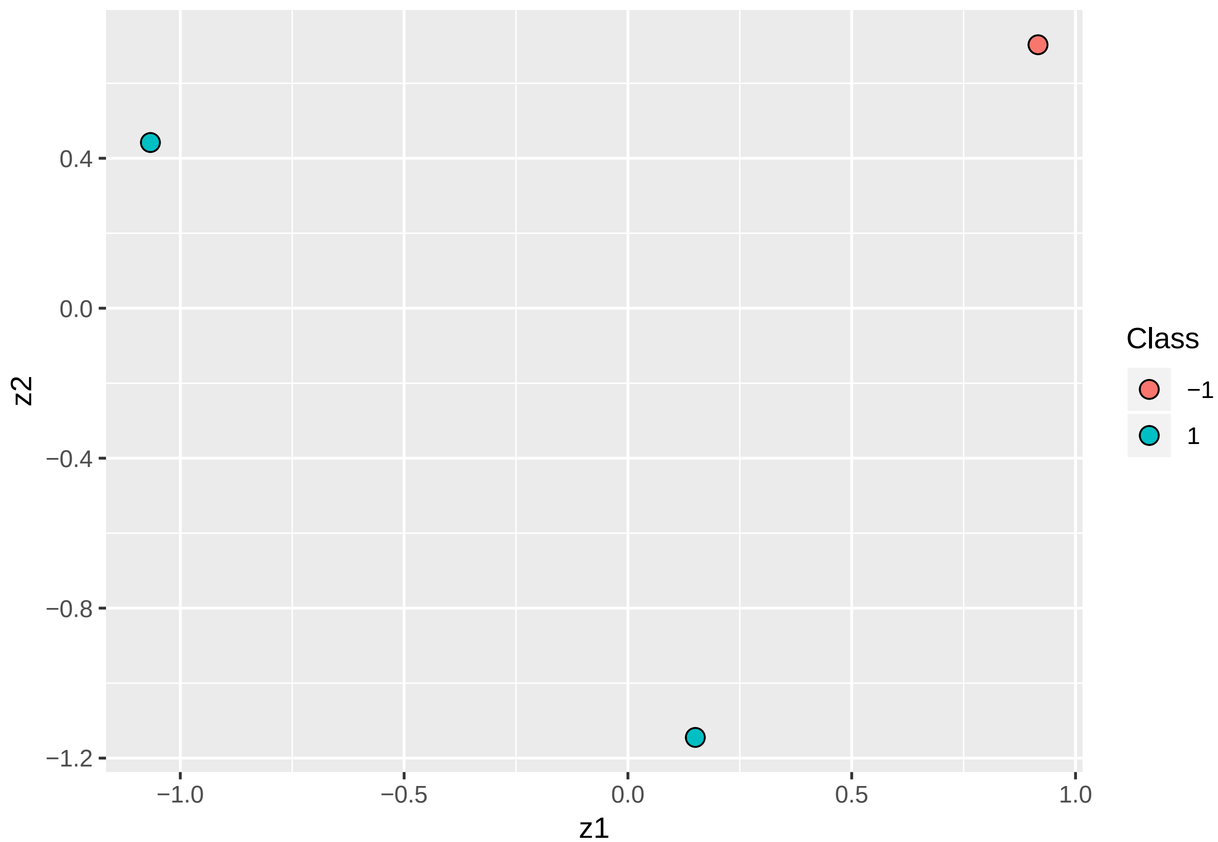
```
ggplot() + geom_point(data = grid, aes(x = x1, y = x2, col = knn_mod)) +
  geom_point(data = data, aes(x = x1, y = x2, fill = class), size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class")) +
```

```
  guides(col = guide_legend(title = "Class"))
```



(b) Here, we transform to whitened coordinates and we run the nearest neighbor rule.

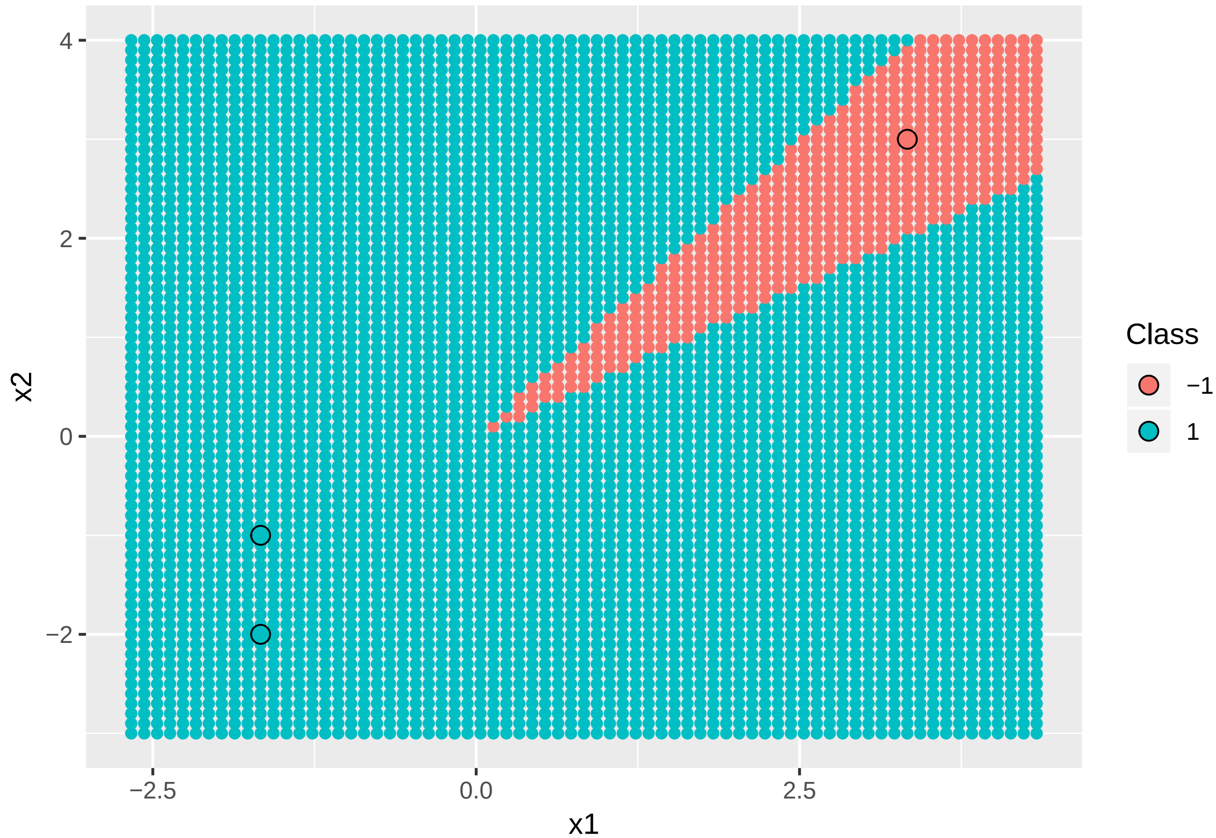
```
data_centered <- apply(data, 2, function(y) y - mean(y))
sigma <- t(data_centered) %*% as.matrix(data_centered) / 2
sigma_sqr <- sqrtm(sigma)
sigma_sqr_inv <- solve(sigma_sqr)
data_whitened <- as.matrix(data_centered) %*% sigma_sqr_inv
data_whitened <- as.data.frame(data_whitened)
colnames(data_whitened) <- c("z1", "z2")

ggplot(data_whitened, aes(x = z1, y = z2, fill = class)) + geom_point(size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class"))
```




```
grid_centered <- expand.grid(x1 = seq(min(data_centered[, 1] - 1),
                                      max(data_centered[, 1] + 1), by = 0.1),
                             x2 = seq(min(data_centered[, 2] - 1),
                                      max(data_centered[, 2] + 1), by = 0.1))
grid_whitened <- as.matrix(grid_centered) %*% sigma_sqr_inv

knn_mod_whitened <- knn(data_whitened, grid_whitened, class, k = 1, prob = TRUE)
```

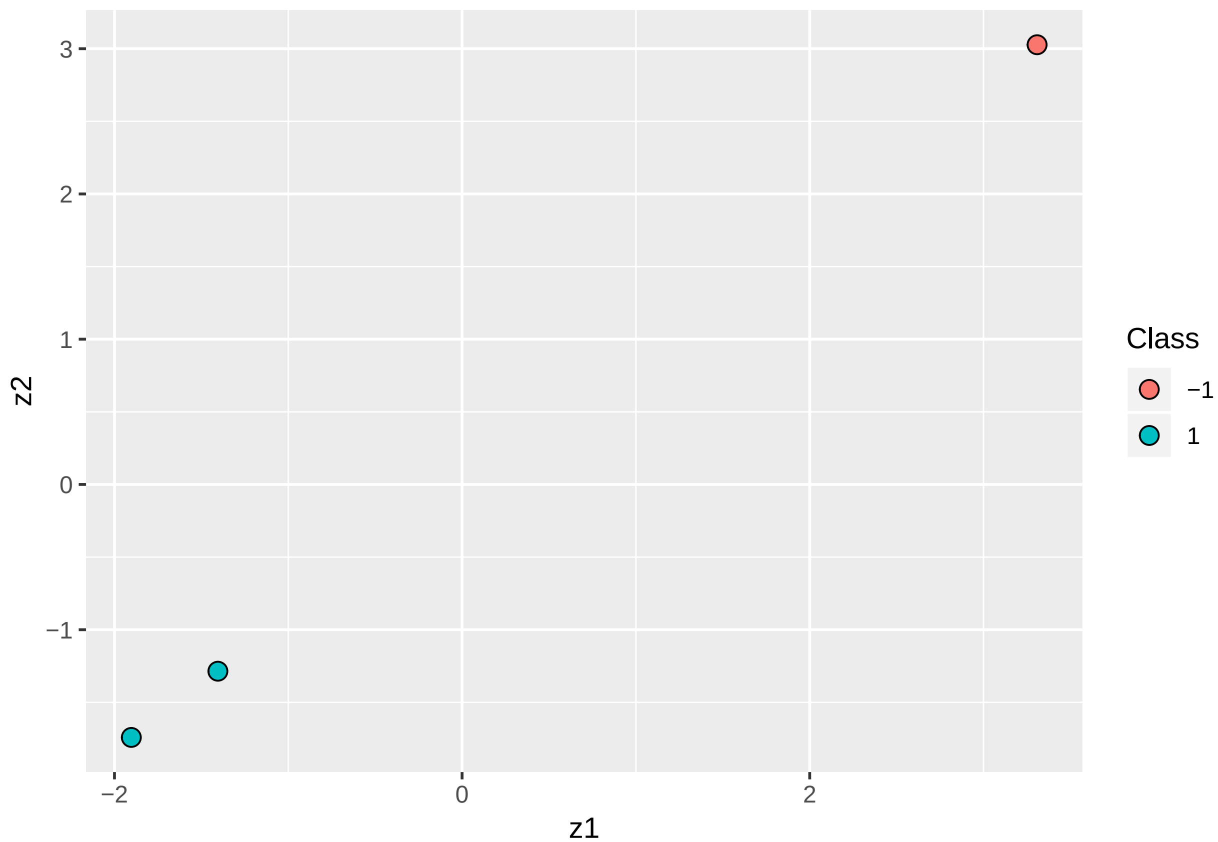
We show the decision region of the final hypothesis in the original space as well.

```
ggplot() + geom_point(data = grid_centered, aes(x = x1, y = x2, col = knn_mod_whitened)) +
  geom_point(data = as.data.frame(data_centered), aes(x = x1, y = x2, fill = class),
             size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class")) +
  guides(col = guide_legend(title = "Class"))
```



(*c*) Finally, we use principal component analysis to reduce the data to 1 dimension for our nearest neighbor classifier.

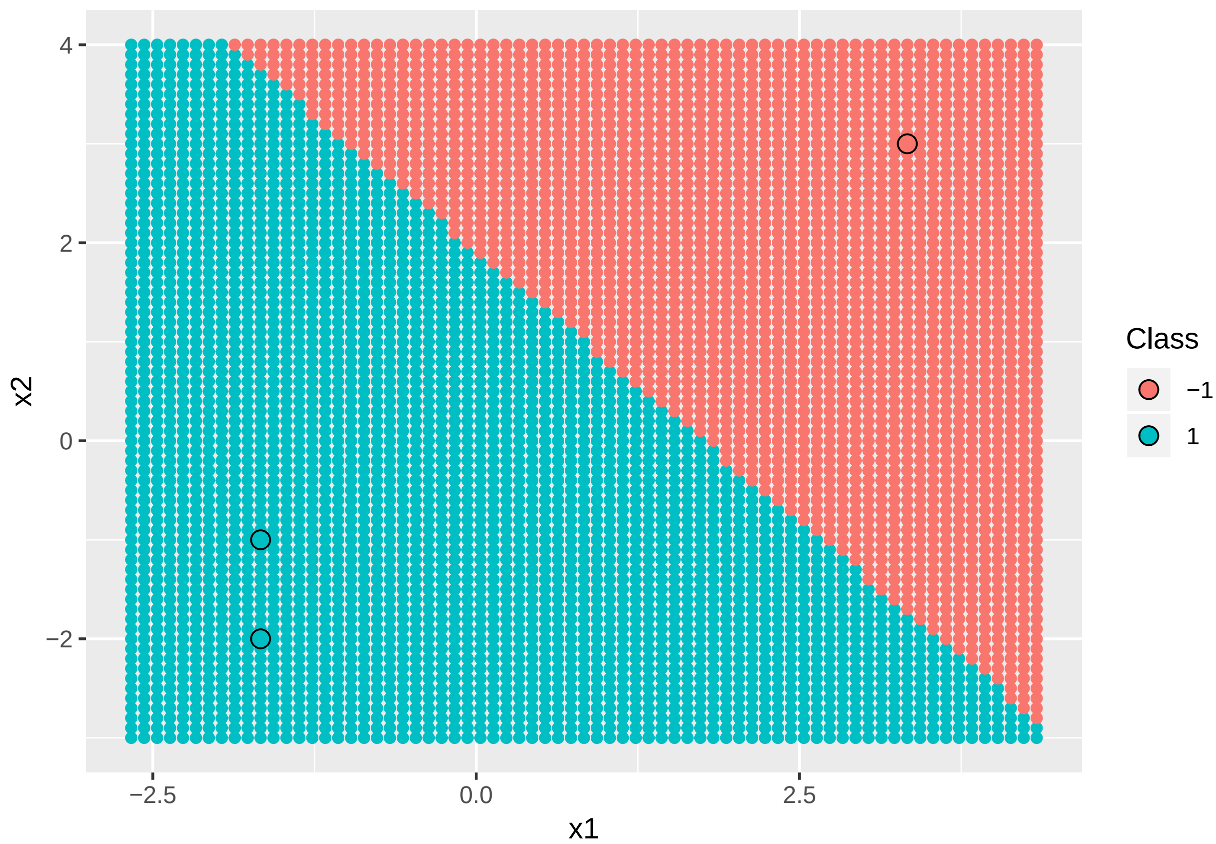
```
SVD_decomp <- svd(data_centered)
V1 <- SVD_decomp$v[, 1]
Z <- data_centered %*% V1
data_pca <- Z %*% t(V1)
data_pca <- as.data.frame(data_pca)
colnames(data_pca) <- c("z1", "z2")

ggplot(data_pca, aes(x = z1, y = z2, fill = class)) + geom_point(size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class"))
```




```
grid_pca <- (as.matrix(grid_centered) %*% V1) %*% t(V1)

knn_mod_pca <- knn(data_pca, grid_pca, class, k = 1, prob = TRUE)
```

Once again, we show the decision regions of the final hypothesis in the original space.

```
ggplot() + geom_point(data = grid_centered, aes(x = x1, y = x2, col = knn_mod_pca)) +
  geom_point(data = as.data.frame(data_centered), aes(x = x1, y = x2, fill = class),
             size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class")) +
  guides(col = guide_legend(title = "Class"))
```



Problem 9.2

(a) Here, we have $x'_n = x_n + b$. Let us compute $\overline{x'}$, $\sigma_i'^2$ and Σ'. We have

$$\overline{x'} = \frac{1}{N}\sum_{n=1}^{N} x'_n = \frac{1}{N}\sum_{n=1}^{N}(x_n + b) = \overline{x} + b;$$

moreover, we have

$$\sigma_i'^2 = \frac{1}{N}\sum_{n=1}^{N}(x'_{ni} - \overline{x'}_i)^2 = \frac{1}{N}\sum_{n=1}^{N}(x_{ni} + b_i - \overline{x'}_i - b_i)^2 = \sigma_i^2;$$

and finally

$$\Sigma' = \frac{1}{N}\sum_{n=1}^{N}(x'_n - \overline{x'})(x'_n - \overline{x'})^T = \frac{1}{N}\sum_{n=1}^{N}(x_n + b - \overline{x} - b)(x_n + b - \overline{x} - b)^T = \Sigma.$$

- **Centering.** We may write that

$$z'_n = x'_n - \overline{x'} = x_n + b - \overline{x} - b = z_n.$$

- **Normalization.** Here, we have that

$$z'_n = D'(x'_n - \overline{x'})$$

  where

$$D' = \mathrm{diag}(1/\sigma'_1, \cdots, 1/\sigma'_d) = \mathrm{diag}(1/\sigma_1, \cdots, 1/\sigma_d) = D.$$

  In that case, we have

$$z'_n = D(x'_n - \overline{x'}) = D(x_n + b - \overline{x} - b) = z_n.$$

- **Whitening.** We have

$$z'_n = \Sigma'^{-1/2}(x'_n - \overline{x'}) = \Sigma^{-1/2}(x_n + b - \overline{x} - b) = z_n.$$

(b) Here, we have $x'_n = \alpha x_n$ with $\alpha > 0$. Let us compute $\overline{x'}$, $\sigma_i'^2$ and Σ'. We have

$$\overline{x'} = \frac{1}{N}\sum_{n=1}^{N} x'_n = \frac{1}{N}\sum_{n=1}^{N} \alpha x_n = \alpha\overline{x};$$

moreover, we have

$$\sigma_i'^2 = \frac{1}{N}\sum_{n=1}^{N}(x'_{ni} - \overline{x'}_i)^2 = \frac{1}{N}\sum_{n=1}^{N}(\alpha x_{ni} - \alpha\overline{x'}_i)^2 = \alpha^2\sigma_i^2;$$

and finally

$$\Sigma' = \frac{1}{N}\sum_{n=1}^{N}(x'_n - \overline{x'})(x'_n - \overline{x'})^T = \frac{1}{N}\sum_{n=1}^{N}(\alpha x_n - \alpha\overline{x})(\alpha x_n - \alpha\overline{x})^T = \alpha^2\Sigma.$$

- **Centering.** We may write that

$$z'_n = x'_n - \overline{x'} = \alpha x_n - \alpha\overline{x} = \alpha z_n \neq z_n.$$

- **Normalization.** Here, we have that

$$z'_n = D'(x'_n - \overline{x'})$$

  where

$$D' = \mathrm{diag}(1/\sigma'_1, \cdots, 1/\sigma'_d) = \mathrm{diag}(1/(\alpha\sigma_1), \cdots, 1/(\alpha\sigma_d)) = \frac{1}{\alpha}D.$$

  In that case, we have

$$z'_n = \frac{1}{\alpha}D(x'_n - \overline{x'}) = \frac{1}{\alpha}D(\alpha x_n - \alpha\overline{x}) = D(x_n - \overline{x}) = z_n.$$

- **Whitening.** We have

$$z'_n = \Sigma'^{-1/2}(x'_n - \overline{x'}) = \frac{1}{\alpha}\Sigma^{-1/2}(\alpha x_n - \alpha\overline{x}) = z_n.$$

(c) Here, we have $x'_n = Ax_n$ with $A = \mathrm{diag}(a_1, \cdots, a_d)$ $(a_i \neq 0)$. Let us compute $\overline{x'}$, $\sigma_i'^2$ and Σ'. We have

$$\overline{x'} = \frac{1}{N}\sum_{n=1}^{N} x'_n = \frac{1}{N}\sum_{n=1}^{N} Ax_n = A\overline{x};$$

moreover, we have

$$\sigma_i'^2 = \frac{1}{N}\sum_{n=1}^{N}(x'_{ni} - \overline{x'}_i)^2 = \frac{1}{N}\sum_{n=1}^{N}(a_i x_{ni} - a_i\overline{x'}_i)^2 = a_i^2\sigma_i^2;$$

and finally

$$\Sigma' = \frac{1}{N}\sum_{n=1}^{N}(x'_n - \overline{x'})(x'_n - \overline{x'})^T = \frac{1}{N}\sum_{n=1}^{N}(Ax_n - A\overline{x})(Ax_n - A\overline{x})^T = A\Sigma A^T.$$

- **Centering.** We may write that

$$z'_n = x'_n - \overline{x'} = Ax_n - A\overline{x} = Az_n \neq z_n.$$

- **Normalization.** Here, we have that
$$z'_n = D'(x'_n - \overline{x'})$$
where
$$D' = \mathrm{diag}(1/\sigma'_1, \cdots, 1/\sigma'_d) = \mathrm{diag}(1/(a_1\sigma_1), \cdots, 1/(a_d\sigma_d));$$
which means that $D'A = D$. In that case, we have
$$z'_n = D'(x'_n - \overline{x'}) = D'A(x_n - \overline{x}) = D(x_n - \overline{x}) = z_n.$$

- **Whitening.** We have
$$z'_n = \Sigma'^{-1/2}(x'_n - \overline{x'}) = (A\Sigma A^T)^{-1/2}A(x_n - \overline{x}) \neq z_n.$$

(d) Here, we have $x'_n = Ax_n$ with $\det(A) \neq 0$. Let us compute $\overline{x'}$, $\sigma_i'^2$ and Σ'. We have
$$\overline{x'} = \frac{1}{N}\sum_{n=1}^{N} x'_n = \frac{1}{N}\sum_{n=1}^{N} Ax_n = A\overline{x};$$
moreover, we have
$$\sigma_i'^2 = \frac{1}{N}\sum_{n=1}^{N}(x'_{ni} - \overline{x'}_i)^2 = \frac{1}{N}\sum_{n=1}^{N}(l_i^T x_n - l_i^T \overline{x})^2 = \frac{1}{N}\sum_{n=1}^{N} l_i^T (x_n - \overline{x})(x_n - \overline{x})^T l_i = l_i^T \Sigma l_i$$
where l_i is the ith row of A; and finally
$$\Sigma' = \frac{1}{N}\sum_{n=1}^{N}(x'_n - \overline{x'})(x'_n - \overline{x'})^T = \frac{1}{N}\sum_{n=1}^{N}(Ax_n - A\overline{x})(Ax_n - A\overline{x})^T = A\Sigma A^T.$$

- **Centering.** We may write that
$$z'_n = x'_n - \overline{x'} = Ax_n - A\overline{x} = Az_n \neq z_n.$$

- **Normalization.** Here, we have that
$$z'_n = D'(x'_n - \overline{x'})$$
where
$$D' = \mathrm{diag}(1/\sigma'_1, \cdots, 1/\sigma'_d) = \mathrm{diag}(1/(l_1^T \Sigma l_1), \cdots, 1/(l_d^T \Sigma l_d)).$$
In that case, we have
$$z'_n = D'(x'_n - \overline{x'}) = D'A(x_n - \overline{x}) = D'Az_n \neq z_n.$$

- **Whitening.** We have
$$z'_n = \Sigma'^{-1/2}(x'_n - \overline{x'}) = (A\Sigma A^T)^{-1/2}A(x_n - \overline{x}) \neq z_n.$$

Problem 9.3

We may write
$$\Gamma = \mathrm{diag}(\lambda_1, \cdots, \lambda_d)$$
where $\lambda_i > 0$. With this in mind, it is easy to describe $\Gamma^{1/2}$ and $\Gamma^{-1/2}$; we have
$$\Gamma^{1/2} = \mathrm{diag}(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_d}) \text{ and } \Gamma^{-1/2} = \mathrm{diag}(1/\sqrt{\lambda_1}, \cdots, 1/\sqrt{\lambda_d}).$$

To prove the first fact, we simply need to compute $\Gamma^{1/2}\Gamma^{1/2}$, we have

$$\Gamma^{1/2}\Gamma^{1/2} = \mathrm{diag}(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_d})\mathrm{diag}(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_d}) = \mathrm{diag}(\lambda_1, \cdots, \lambda_d) = \Gamma;$$

to prove the second fact, we need to compute $\Gamma^{1/2}\Gamma^{-1/2}$ (the same reasoning can be applied to $\Gamma^{-1/2}\Gamma^{1/2}$), we have

$$\Gamma^{1/2}\Gamma^{-1/2} = \mathrm{diag}(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_d})\mathrm{diag}(1/\sqrt{\lambda_1}, \cdots, 1/\sqrt{\lambda_d}) = I.$$

Now, to prove that $\Sigma^{1/2} = U\Gamma^{1/2}U^T$, we write that

$$\Sigma^{1/2}\Sigma^{1/2} = U\Gamma^{1/2}\underbrace{U^TU}_{=I}\Gamma^{1/2}U^T = U\Gamma U^T = \Sigma.$$

Then, to prove that $\Sigma^{-1/2} = U\Gamma^{-1/2}U^T$, we write that

$$\Sigma^{-1/2}\Sigma^{1/2} = U\Gamma^{-1/2}\underbrace{U^TU}_{=I}\Gamma^{1/2}U^T = UIU^T = I.$$

Problem 9.4

We know that $A = V\psi$, consequently we get

$$V^TA = \underbrace{V^TV}_{=I}\psi = \psi$$

because V is an orthogonal matrix. Moreover, we also have that

$$\psi^T\psi = A^T\underbrace{VV^T}_{=I}A = A^TA = I$$

since A is an orthogonal matrix as well; this means that ψ is also an orthogonal matrix.

Problem 9.5

(a) if A is a diagonal matrix ($N = d$), it suffices to define U, Γ and V as follows

$$U = V = I_N \text{ and } \Gamma = A.$$

In this case, we have

$$A = U\Gamma V^T.$$

(c) If A is a matrix with pairwise orthogonal columns, we may write that

$$A^TA = \mathrm{diag}(a_1, \cdots, a_d)$$

where $a_i > 0$. Now if we define D as follows

$$D = \mathrm{diag}(1/\sqrt{a_1}, \cdots, 1/\sqrt{a_d}),$$

it is easy to see that $U = AD$ is actually a matrix with orthonormal columns since

$$U^TU = D^TA^TAD = I_d.$$

In this case, we have

$$A = U\Gamma V^T$$

with $\Gamma = \mathrm{diag}(\sqrt{a_1}, \cdots, \sqrt{a_d})$ and $V = I_d$.

(d) If A has SVD $U\Gamma V^T$ and $Q^TQ = I$, we may write that

$$QA = (QU)\Gamma V^T$$

with QU a matrix with orthonormal columns since

$$(QU)^T(QU) = U^T \underbrace{Q^TQ}_{=I} U = I_d.$$

(e) If A has blocks A_i along the diagonal such that A_i has SVD $U_i\Gamma_i V_i^T$, we simply have to define U, Γ, and V as follows

$$U = \begin{pmatrix} U_1 & & \\ & \ddots & \\ & & U_m \end{pmatrix}, \ \Gamma = \begin{pmatrix} \Gamma_1 & & \\ & \ddots & \\ & & \Gamma_m \end{pmatrix} \text{ and } V = \begin{pmatrix} V_1 & & \\ & \ddots & \\ & & V_m \end{pmatrix}.$$

In that case, we immediately get that

$$A = U\Gamma V^T$$

with

$$U^TU = \begin{pmatrix} U_1^T & & \\ & \ddots & \\ & & U_m^T \end{pmatrix} \begin{pmatrix} U_1 & & \\ & \ddots & \\ & & U_m \end{pmatrix} = I,$$

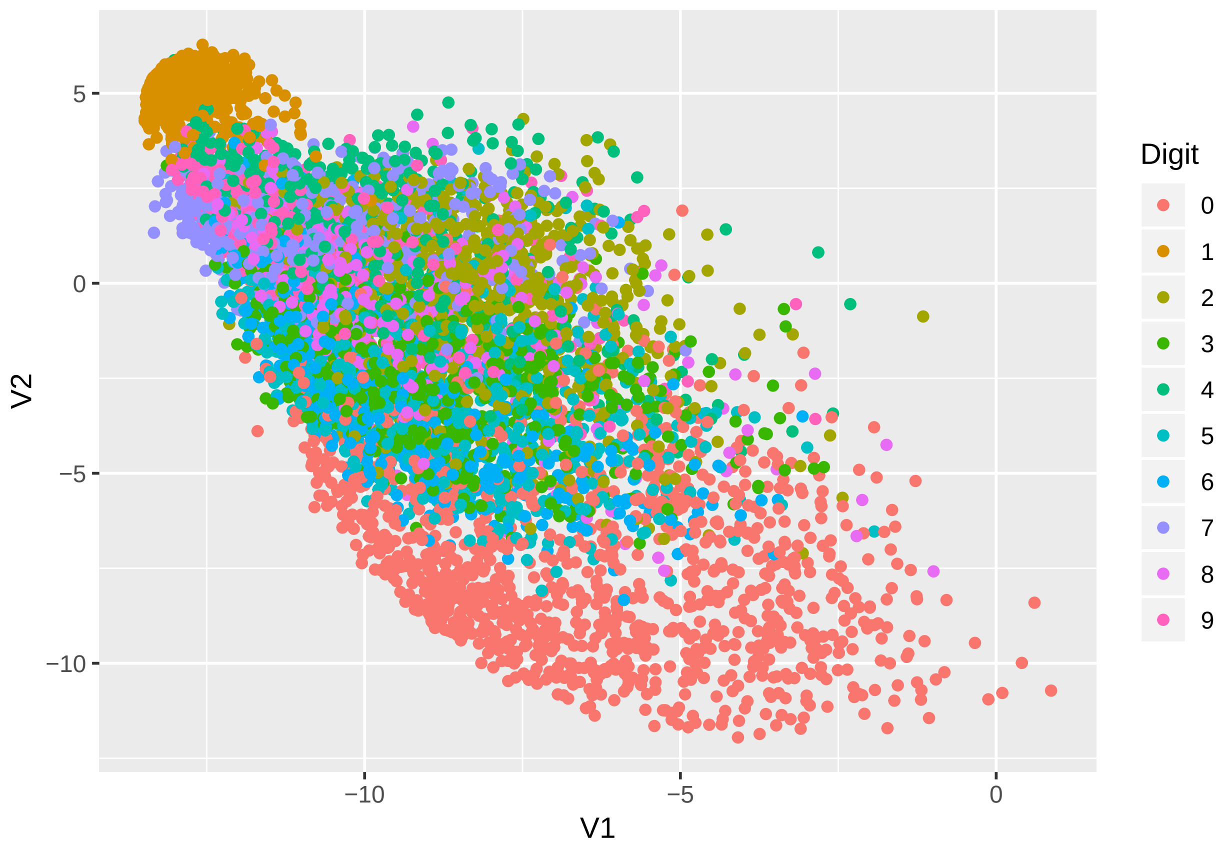
$$V^TV = \begin{pmatrix} V_1^T & & \\ & \ddots & \\ & & V_m^T \end{pmatrix} \begin{pmatrix} V_1 & & \\ & \ddots & \\ & & V_m \end{pmatrix} = VV^T = I,$$

and Γ diagonal.

Problem 9.6

Here, we suppose that the digits data were not centered and we perform PCA to obtain a 2-dimensional feature vector.

```
digits <- read.delim("zip.train", header = FALSE, sep = " ")
digits$V258 <- NULL
colnames(digits) <- c("digit", 1:256)

X <- as.matrix(digits[, -1])
y <- digits[, 1]
SVD_decomp <- svd(X)
V2 <- SVD_decomp$v[, 1:2]
Z <- X %*% V2
digits_pca <- Z %*% t(V2)
digits_pca_proj <- digits_pca %*% V2
digits_pca_proj <- as.data.frame(digits_pca_proj)

ggplot(digits_pca_proj, aes(x = V1, y = V2, col = as.factor(y))) + geom_point() +
  guides(col = guide_legend(title = "Digit"))
```



The transformed data is not whitened since its covariance matrix is not the identity matrix.

```
cov(digits_pca_proj)
```

```
##            V1        V2
## V1  6.842064 -8.121955
## V2 -8.121955 17.058353
```

Problem 9.7

As we have that

$$z_n = \sqrt{N}\Gamma_k^{-1}V_k^T x_n,$$

we may let Z be

$$Z = \sqrt{N}X(\Gamma_k^{-1}V_k^T)^T = \sqrt{N}XV_k\Gamma_k^{-1}.$$

Moreover, since X is centered, it is easy to see that Z is centered as well because

$$\overline{z} = \frac{1}{N}Z^T 1 = \frac{\sqrt{N}}{N}\Gamma_k^{-1}V_k^T \underbrace{X^T 1}_{=0} = 0.$$

To prove that the transformed data is actually whitened, we have to compute $Z^T Z$, if we use the SVD of $X = U\Gamma V^T$, we get

$$\begin{aligned}
\frac{1}{N} Z^T Z &= \frac{1}{N}(\sqrt{N} X V_k \Gamma_k^{-1})^T (\sqrt{N} X V_k \Gamma_k^{-1}) \\
&= \Gamma_k^{-1} V_k^T X^T X V_k \Gamma_k^{-1} \\
&= \Gamma_k^{-1} V_k^T V \Gamma \underbrace{U^T U}_{=I_d} \Gamma V^T V_k \Gamma_k^{-1} \\
&= \Gamma_k^{-1} V_k^T V \underbrace{\Gamma^2}_{=\mathrm{diag}(\gamma_1^2, \cdots, \gamma_d^2)} V^T V_k \Gamma_k^{-1}.
\end{aligned}$$

We also have that

$$V_k^T V = \begin{pmatrix} v_1^T \\ \vdots \\ v_k^T \end{pmatrix} (v_1, \cdots, v_k \mid v_{k+1}, \cdots, v_d) = (I_k \mid 0)$$

and

$$V^T V_k = \begin{pmatrix} I_k \\ 0 \end{pmatrix}.$$

This means that

$$\Gamma_k^{-1}(I_k \mid 0) = (\Gamma_k^{-1} \mid 0),$$

and in the same way

$$\begin{pmatrix} I_k \\ 0 \end{pmatrix} \Gamma_k^{-1} = \begin{pmatrix} \Gamma_k^{-1} \\ 0 \end{pmatrix}.$$

Consequently, we get that

$$\begin{aligned}
\frac{1}{N} Z^T Z &= (\Gamma_k^{-1} \mid 0) \Gamma^2 \begin{pmatrix} \Gamma_k^{-1} \\ 0 \end{pmatrix} \\
&= (\Gamma_k^{-1} \mid 0) \left(\begin{array}{c|c} \Gamma_k^2 & 0 \\ \hline 0 & * \end{array}\right) \begin{pmatrix} \Gamma_k^{-1} \\ 0 \end{pmatrix} \\
&= I_k,
\end{aligned}$$

which means that Z is whitened.

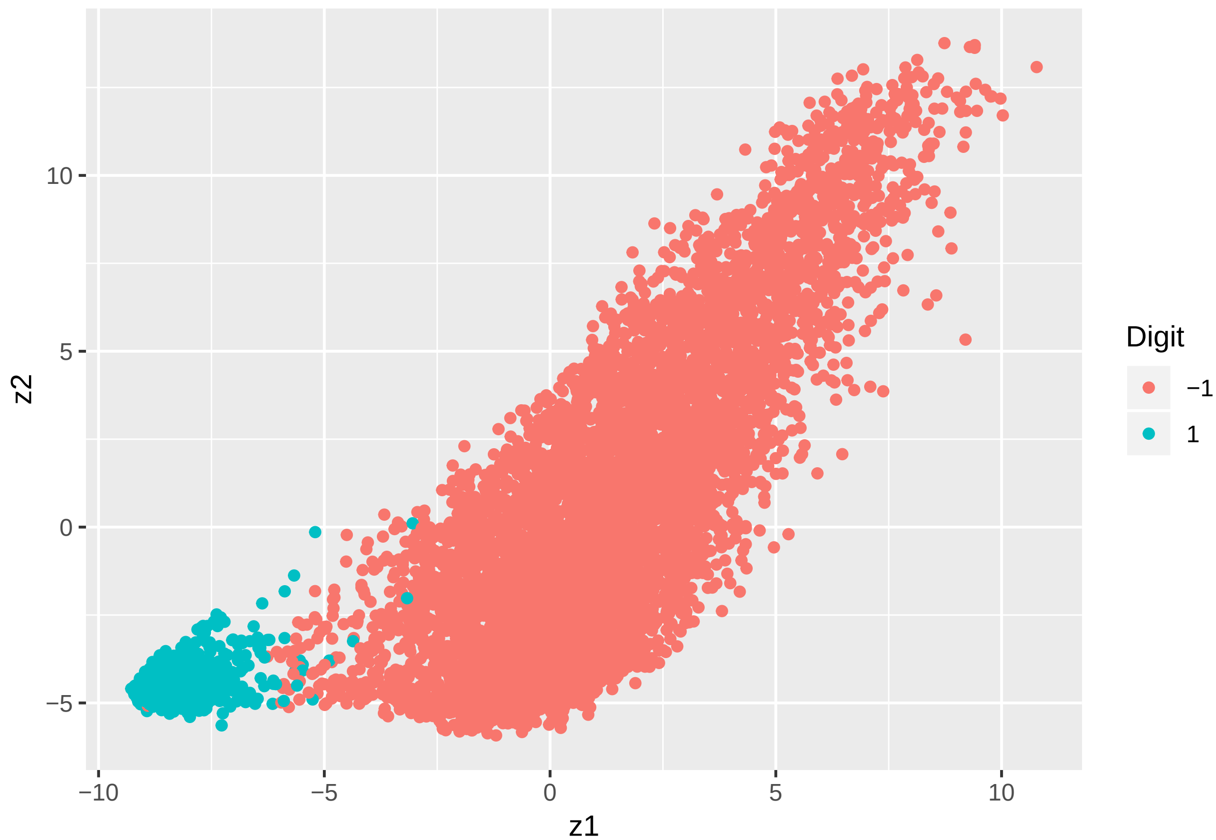
Problem 9.8

We begin by constructing a two dimensional feature as described in the book and we apply the algorithm to the digits data giving us the features z_1 and z_2.

```
digits <- read.delim("zip.train", header = FALSE, sep = " ")
digits$V258 <- NULL
colnames(digits) <- c("digit", 1:256)

X <- as.matrix(digits[, -1])
y <- digits[, 1]
X_centered <- apply(X, 2, function(x) x - mean(x))
X_centered_1 <- X_centered[y == 1, ]
X_centered_not1 <- X_centered[y != 1, ]

SVD_decomp_1 <- svd(X_centered_1)
v1 <- SVD_decomp_1$v[, 1]

SVD_decomp_not1 <- svd(X_centered_not1)
v2 <- SVD_decomp_not1$v[, 1]
```

(a) We give below a scatter plot of our resulting two features.

```
z1 <- X_centered %*% v1
z2 <- X_centered %*% v2
y_1 <- ifelse(y == 1, +1, -1)
z <- data.frame(z1, z2, y_1)

ggplot(z, aes(x = z1, y = z2, col = as.factor(y_1))) + geom_point() +
  guides(col = guide_legend(title = "Digit"))
```



(b) No, the directions of v_1 and v_2 are not necessarily orthogonal.

```
v1 %*% v2 == 0
```

```
##       [,1]
## [1,] FALSE
```

(c) Since $\hat{V} = [v_1, v_2]$ has full rank, we know that

$$\hat{V}^+ = (\hat{V}^T \hat{V})^{-1} \hat{V}^T.$$

In this case, we have

$$\hat{X} = X \hat{V} (\hat{V}^T \hat{V})^{-1} \hat{V}^T.$$

(d) This method of constructing features is supervised since we need the target values to apply it.

Problem 9.9

(a) Since $\hat{X}$ is a matrix whose rows are projected onto k basis vectors, it is pretty obvious that $\text{rank}(\hat{X}) = k$.

(b) We may write that

$$||\Gamma - U^T\hat{X}V||_F^2 = ||U^TXV - U^T\hat{X}V||_F^2 = ||U^T(X-\hat{X})V||_F^2.$$

Moreover, we may also write (see exercise 9.9) that

$$\begin{aligned}
||U^T(X-\hat{X})V||_F^2 &= ||U(U^T(X-\hat{X})V)V^T||_F^2 \\
&= ||UU^T(X-\hat{X})\underbrace{VV^T}_{=I}||_F^2 \\
&= \mathrm{trace}[(UU^T(X-\hat{X}))^T(UU^T(X-\hat{X}))] \\
&= \mathrm{trace}[(X-\hat{X})^TU\underbrace{U^TU}_{=I}U^T(X-\hat{X})] \\
&= ||U^T(X-\hat{X})||_F^2 \\
&\leq \underbrace{||U^T||_F^2}_{=\mathrm{trace}(U^TU)=d} \quad ||X-\hat{X}||_F^2 \\
&\leq d||X-\hat{X}||_F^2
\end{aligned}$$

where we used the fact that $||AB||_F^2 \leq ||A||_F^2||B||_F^2$.

(c) Since the rank of a matrix product is less than each factor, we have that

$$\mathrm{rank}(\hat{\Gamma}) = \mathrm{rank}(U^T\hat{X}V) \leq \mathrm{rank}(\hat{X}) = k.$$

(d) It is easy to see that

$$\begin{aligned}
||\Gamma - \hat{\Gamma}||_F^2 &= \sum_{i,j=1}^{d}(\gamma_{ij}-\hat{\gamma}_{ij})^2 \\
&= \sum_{i=1}^{d}(\gamma_{ii}-\hat{\gamma}_{ii})^2 + \sum_{i\neq j}(\gamma_{ij}-\hat{\gamma}_{ij})^2 \\
&\geq \sum_{i=1}^{d}(\gamma_{ii}-\hat{\gamma}_{ii})^2.
\end{aligned}$$

So, the optimal choice for $\hat{\Gamma}$ must have all off-diagonal elements equal to zero.

(e) Since we know that $\mathrm{rank}(\hat{\Gamma}) \leq k$, we may conclude that the optimal $\hat{\Gamma}$ can have at most k non-zero diagonal elements.

(f) We may write for our optimal $\hat{\Gamma}$ that

$$\begin{aligned}
||\Gamma - \hat{\Gamma}||_F^2 &= \sum_{i=1}^{d}(\gamma_{ii}-\hat{\gamma}_{ii})^2 \\
&= \sum_{i=1}^{k}(\gamma_{ii}-\hat{\gamma}_{ii})^2 + \underbrace{\sum_{i=k+1}^{d}(\gamma_{ii}-\hat{\gamma}_{ii})^2}_{\sum_{i=k+1}^{d}\gamma_{ii}^2} \\
&\geq \sum_{i=k+1}^{d}\gamma_{ii}^2.
\end{aligned}$$

Consequently, the minimum reconstruction error is equal to $\sum_{i=k+1}^{d}\gamma_{ii}^2$.

(g) If $\hat{X} = XV_kV_k^T$, we choose our optimal $\hat{\Gamma}$ such that

$$\begin{aligned}
\hat{\Gamma} &= U^T\hat{X}V \\
&= U^TXV_kV_k^TV \\
&= \underbrace{U^TU}_{=I}\Gamma V^TV_kV_k^TV \\
&= \Gamma(V^TV_k)(V_k^TV)
\end{aligned}$$

where

$$V_k^TV = (I_k \mid 0) \text{ and } V^TV_k = \left(\frac{I_k}{0}\right).$$

This means that

$$\hat{\Gamma} = \Gamma\left(\begin{array}{c|c} I_k & 0 \\ \hline 0 & 0 \end{array}\right) = \left(\begin{array}{ccc|c} \gamma_1 & & & 0 \\ & \ddots & & \vdots \\ & & \gamma_k & 0 \\ \hline 0 & \cdots & 0 & 0 \end{array}\right).$$

Thus, we finally have

$$\Gamma - \hat{\Gamma} = \left(\begin{array}{c|ccc} 0 & 0 & \cdots & 0 \\ \hline 0 & -\gamma_{k+1} & & \\ \vdots & & \ddots & \\ 0 & & & -\gamma_d \end{array}\right),$$

and consequently

$$||\Gamma - \hat{\Gamma}||_F^2 = \sum_{i=k+1}^{d} \gamma_i^2.$$

So, for this choice of $\hat{\Gamma}$, we actually check eac of the conditions obtained in points (d), (e), and (f) to characterize the optimal choice of $\hat{\Gamma}$; so $\hat{X} = XV_kV_k^T$ is the optimal choice for the reconstructed vector. In this case, we know from point (a) that

$$||X - \hat{X}||_F^2 \geq ||\Gamma - \hat{\Gamma}||_F^2,$$

so for our optimal choice of $\hat{X}$, the minimum reconstruction error is $\sum_{i=k+1}^{d} \gamma_i^2$.

Problem 9.10

(a) The main difference between Algorithm 1 and Algorithm 2 is that Algorithm 1 first performs SVD and then splits the data, and Algorithm 2 first splits the data and then performs SVD.

(b) Here, we generate N random normally distributed d-dimensional inputs $x_1, \cdots, x_N$ with their respective targets $y_n = w_f^Tx_n + \epsilon_n$ where w_f is normally distributed and ϵ_n is independant Gaussian noise with variance 0.5.

```
set.seed(10)
d <- 5
N <- 40
k <- 3

target <- function(w, x) {

  return(sum(w * as.matrix(x)) + rnorm(1, sd = sqrt(0.5)))
}
```

```
data_gen <- function(d, N) {
  wf <- rnorm(d)
  X <- data.frame(x1 = rnorm(N), x2 = rnorm(N), x3 = rnorm(N),
                  x4 = rnorm(N), x5 = rnorm(N))
  y <- apply(X, 1, target, w = wf)

  return(list(X = X, y = y, wf = wf))
}
```

Now, we use Algorithms 1 and 2 to compute estimates of E_{out}.

```
E_cross_1 <- function(X, y) {
  SVD <- svd(X)
  Vk <- SVD$v[, 1:k]
  Z <- as.matrix(X) %*% Vk
  en <- numeric(N)
  for (n in 1:N) {
    Zn <- Z[-n, ]
    yn <- y[-n]
    wn_minus <- solve(t(Zn) %*% Zn) %*% t(Zn) %*% yn
    en[n] <- (sum(Z[n, ] * wn_minus) - y[n])^2
  }
  E1 <- mean(en)

  return(E1)
}

E_cross_2 <- function(X, y) {
  en <- numeric(N)
  for (n in 1:N) {
    Xn <- X[-n, ]
    yn <- y[-n]
    SVD_minus <- svd(Xn)
    Vk_minus <- SVD_minus$v[, 1:k]
    Zn <- as.matrix(Xn) %*% Vk_minus
    wn_minus <- solve(t(Zn) %*% Zn) %*% t(Zn) %*% yn
    wn_minus2 <- Vk_minus %*% wn_minus
    en[n] <- (sum(X[n, ] * wn_minus2) - y[n] )^2
  }
  E2 <- mean(en)

  return(E2)
}
```

We compute E_{out} below.

```
E_out <- function(X, y, wf) {
  SVD <- svd(X)
  Vk <- SVD$v[, 1:k]
  Z <- as.matrix(X) %*% Vk
  w <- solve(t(Z) %*% Z) %*% t(Z) %*% y
  w2 <- Vk %*% w

  Ntest <- 1000
  X_test <- data.frame(x1 = rnorm(Ntest), x2 = rnorm(Ntest), x3 = rnorm(Ntest),
```

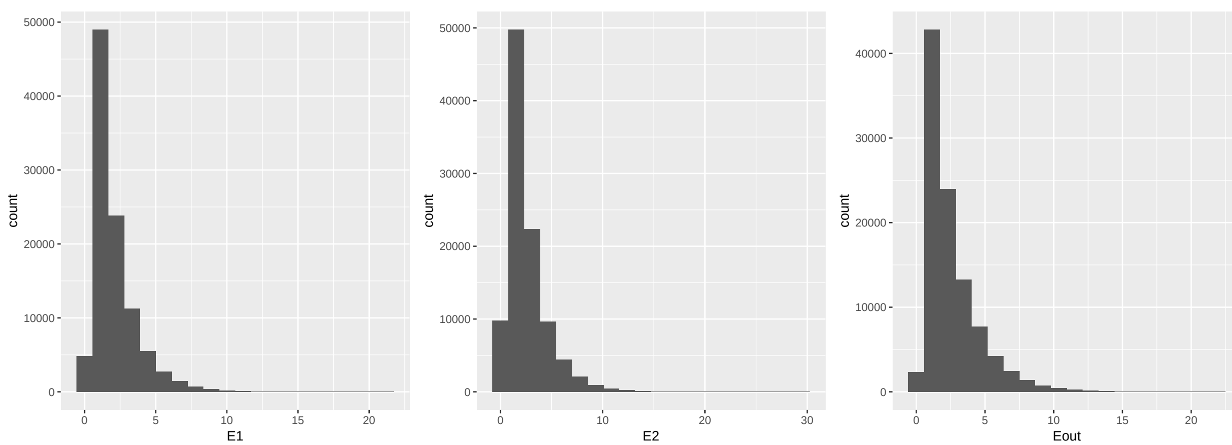
```r
                          x4 = rnorm(Ntest), x5 = rnorm(Ntest))
  y_test <- apply(X_test, 1, target, w = wf)

  E_out <- mean((as.matrix(X_test) %*% w2 - y_test)^2)

  return(E_out)
}
```

Finally, we repeat this process 10^5 times and we report the averages $\overline{E}_1$, $\overline{E}_2$, and $\overline{E}_{out}$.

```r
iter <- 100000
E1 <- numeric(iter)
E2 <- numeric(iter)
Eout <- numeric(iter)
for (i in 1:iter) {
  data <- data_gen(d, N)
  X <- data$X
  y <- data$y
  wf <- data$wf

  E1[i] <- E_cross_1(X, y)
  E2[i] <- E_cross_2(X, y)
  Eout[i] <- E_out(X, y, wf)
}
E1_avg <- mean(E1)
E2_avg <- mean(E2)
Eout_avg <- mean(Eout)
```

We plot below the histograms of E_1, E_2 and E_{out}.

```r
results <- data.frame(E1 = E1, E2 = E2, Eout = Eout)
plot1 <- ggplot(results, aes(x = E1)) + geom_histogram(bins = 20)
plot2 <- ggplot(results, aes(x = E2)) + geom_histogram(bins = 20)
plot3 <- ggplot(results, aes(x = Eout)) + geom_histogram(bins = 20)
grid.arrange(plot1, plot2, plot3, nrow = 1)
```



We get $\overline{E}_1 = 2.0445914$, $\overline{E}_2 = 2.5364857$, and $\overline{E}_{out} = 2.5386052$.

(c) As we may see, the average $\overline{E}_1$ is clearly not as close to $\overline{E}_{out}$ as $\overline{E}_2$ is. This was to be expected since in cross-validation we have to compute every element of our hypothesis after the data split is done, not before.

(d) As stated in point (c), the correct estimate of E_{out} is E_2.

Problem 9.12

(a) We have

$$\begin{aligned}
E_{out}^{\pi}(h) &= \frac{1}{4}\mathbb{E}_{x,\pi}[(h(x) - f_{\pi}(x))^2] \\
&= \frac{1}{4}\mathbb{E}_{\pi}[\mathbb{E}_{x|\pi}[(h(x) - f_{\pi}(x))^2|\pi]] \\
&= \frac{1}{4}\mathbb{E}_{\pi}\left[\sum_{n=1}^{N}(h(x_n) - f_{\pi}(x_n))^2 \underbrace{\mathbb{P}(x = x_n|\pi)}_{=1/N}\right] \\
&= \frac{1}{4N}\sum_{n=1}^{N}\mathbb{E}_{\pi}[(h(x_n) - f_{\pi}(x_n))^2].
\end{aligned}$$

(b) We know from point (a) that

$$E_{out}^{\pi}(h) = \frac{1}{4N}\sum_{n=1}^{N}\mathbb{E}_{\pi}[(h(x_n) - f_{\pi}(x_n))^2];$$

so, we may write that

$$\begin{aligned}
E_{out}^{\pi}(h) &= \frac{1}{4N}\sum_{n=1}^{N}\mathbb{E}_{\pi}[(h(x_n) - \overline{y} + \overline{y} - f_{\pi}(x_n))^2] \\
&= \frac{1}{4N}\sum_{n=1}^{N}(\underbrace{\mathbb{E}_{\pi}[(h(x_n) - \overline{y})^2]}_{(1)} + \underbrace{\mathbb{E}_{\pi}[(\overline{y} - f_{\pi}(x_n))^2]}_{(2)} + 2\underbrace{\mathbb{E}_{\pi}[(h(x_n) - \overline{y})(\overline{y} - f_{\pi}(x_n))]}_{(3)}).
\end{aligned}$$

Let us treat each term separately, we immediately get

$$(1) = \mathbb{E}_{\pi}[(h(x_n) - \overline{y})^2] = (h(x_n) - \overline{y})^2.$$

We also get

$$(2) = \mathbb{E}_{\pi}[(\overline{y} - f_{\pi}(x_n))^2] = \mathbb{E}_{\pi}[(\overline{y} - y_{\pi_n})^2] = \sum_{i=1}^{N}(\overline{y} - y_i)^2 \underbrace{\mathbb{P}[\pi_n = i]}_{=1/N} = \frac{1}{N}\sum_{i=1}^{N}(\overline{y} - y_i)^2.$$

And finally, we get

$$\begin{aligned}
(3) &= \mathbb{E}_{\pi}[(h(x_n) - \overline{y})(\overline{y} - f_{\pi}(x_n))] = (h(x_n) - \overline{y})\mathbb{E}_{\pi}[(\overline{y} - y_{\pi_n})] \\
&= (h(x_n) - \overline{y})\sum_{i=1}^{N}(\overline{y} - y_i)\underbrace{\mathbb{P}[\pi_n = i]}_{=1/N} \\
&= \frac{1}{N}(h(x_n) - \overline{y})\underbrace{\sum_{i=1}^{N}(\overline{y} - y_i)}_{=0} = 0.
\end{aligned}$$

In conclusion, we get that

$$
\begin{aligned}
E^{\pi}_{out}(h) &= \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-\overline{y})^2 + \frac{1}{4N^2}\sum_{n=1}^{N}\sum_{i=1}^{N}(\overline{y}-y_i)^2 \\
&= \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-\overline{y})^2 + \underbrace{\frac{1}{4N}\sum_{i=1}^{N}(\overline{y}-y_i)^2}_{=\frac{1}{4}s_y^2} \\
&= \frac{s_y^2}{4} + \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-\overline{y})^2.
\end{aligned}
$$

(c) Similarly to E^{π}_{out}, we find that

$$
\begin{aligned}
E^{\pi}_{in}(h) &= \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-y_{\pi_n})^2 = \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-\overline{y}+\overline{y}-y_{\pi_n})^2 \\
&= \frac{1}{4N}\sum_{n=1}^{N}[(h(x_n)-\overline{y})^2 + (\overline{y}-y_{\pi_n})^2 + 2(h(x_n)-\overline{y})(\overline{y}-y_{\pi_n})] \\
&= \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-\overline{y})^2 + \frac{1}{4N}\sum_{n=1}^{N}(\overline{y}-y_{\pi_n})^2 + \frac{1}{2N}\sum_{n=1}^{N}(h(x_n)-\overline{y})(\overline{y}-y_{\pi_n}) \\
&= \frac{s_y^2}{4} + \frac{1}{4N}\sum_{n=1}^{N}(h(x_n)-\overline{y})^2 + \frac{1}{2N}\sum_{n=1}^{N}(h(x_n)-\overline{y})(\overline{y}-y_{\pi_n}).
\end{aligned}
$$

(d) We are now able to compute the permutation optimism penalty, we have

$$
\begin{aligned}
E^{\pi}_{out}(g_\pi) - E^{\pi}_{in}(g_\pi) &= -\frac{1}{2N}\sum_{n=1}^{N}(g_\pi(x_n)-\overline{y})(\overline{y}-y_{\pi_n}) \\
&= -\frac{1}{2N}\sum_{n=1}^{N}g_\pi(x_n)(\overline{y}-y_{\pi_n}) + \frac{1}{2N}\overline{y}\underbrace{\sum_{n=1}^{N}(\overline{y}-y_{\pi_n})}_{=0} \\
&= \frac{1}{2N}\sum_{n=1}^{N}(y_{\pi_n}-\overline{y})g_\pi(x_n).
\end{aligned}
$$

(e) It is easy to see that the permutation optimism penalty is proportional to the covariance between y_{π_n} and $g_\pi(x_n)$.