Problem Solutions

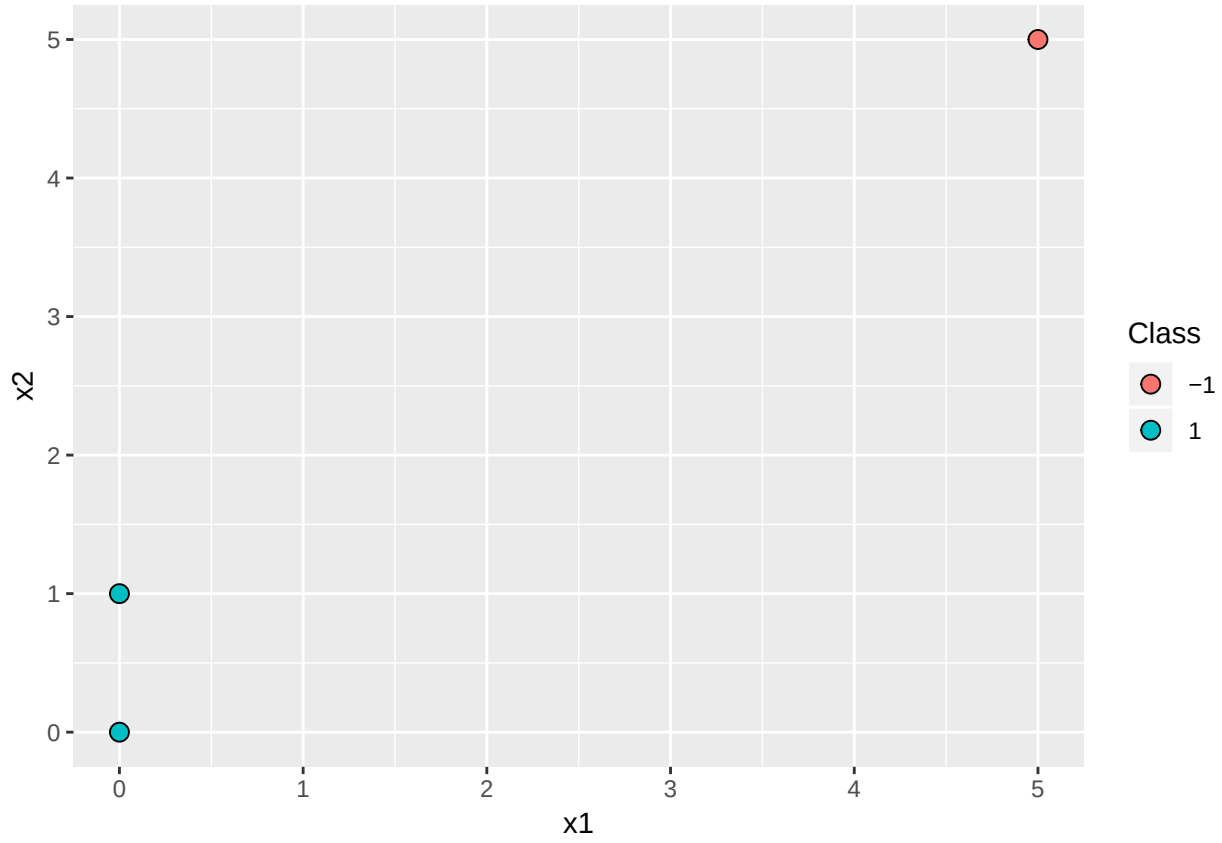
e-Chapter 9

Pierre Paquay

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"))
```

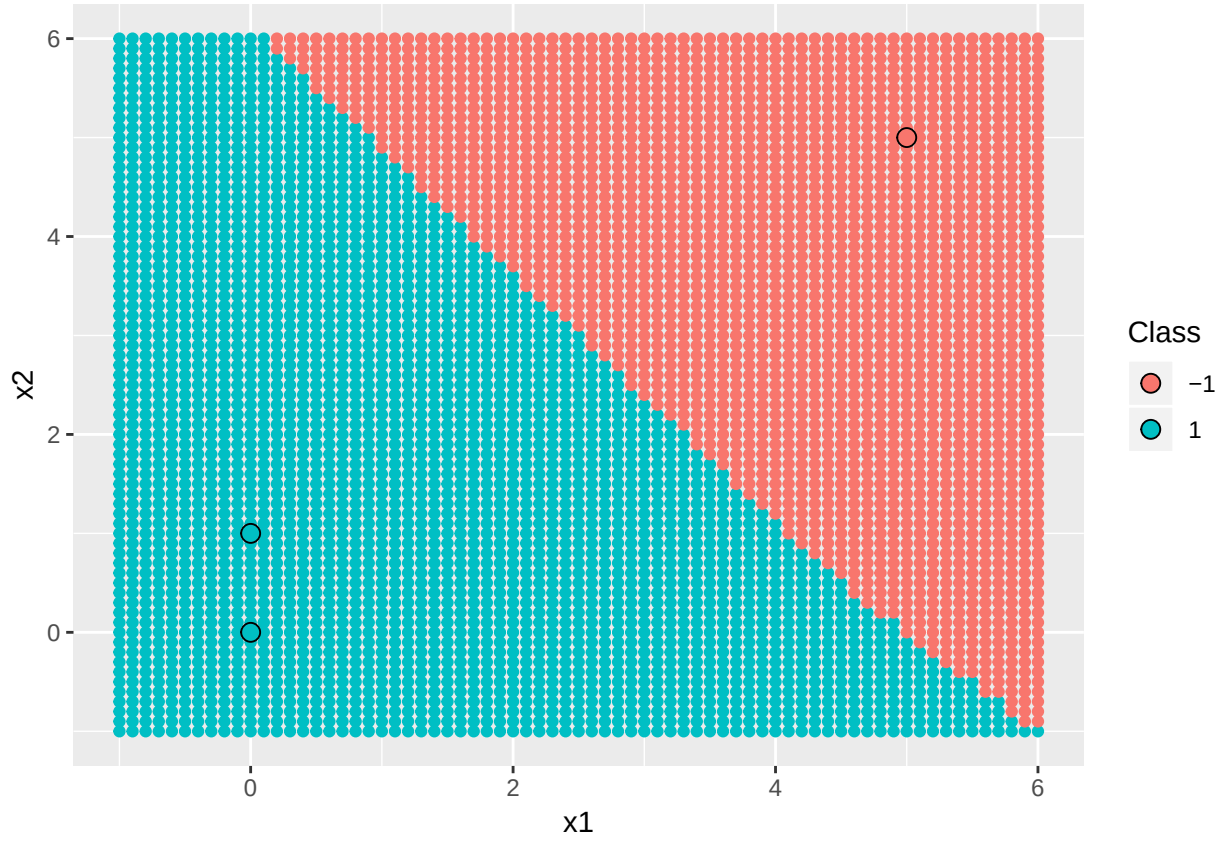



```
grid <- expand.grid(x1 = seq(min(data[, 1] - 1), max(data[, 1] + 1), by = 0.1),
                    x2 = seq(min(data[, 2] - 1), max(data[, 2] + 1), by = 0.1))

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

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

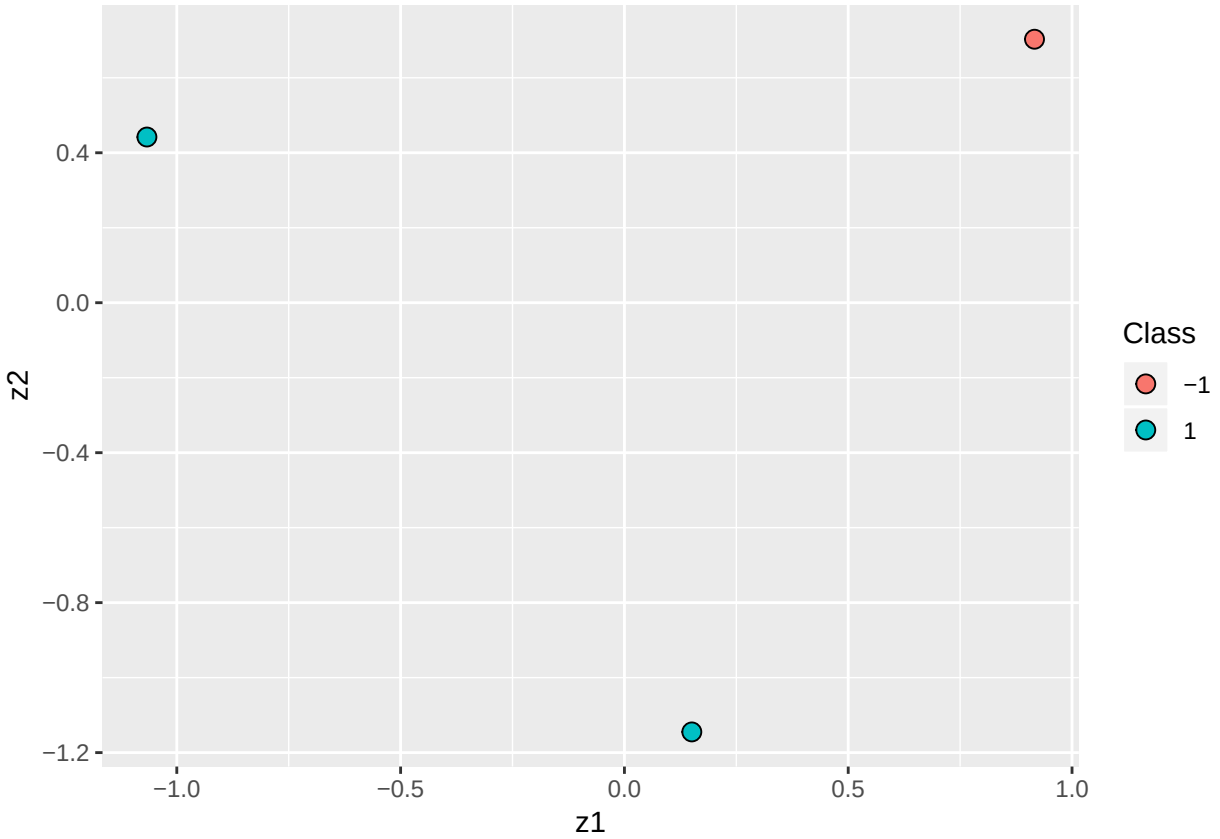
```
ggplot() + geom_point(data = grid, aes(x = x1, y = x2, col = knn_mod)) +
  geom_point(data = data, aes(x = x1, y = x2, fill = class), size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class")) +
```

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



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

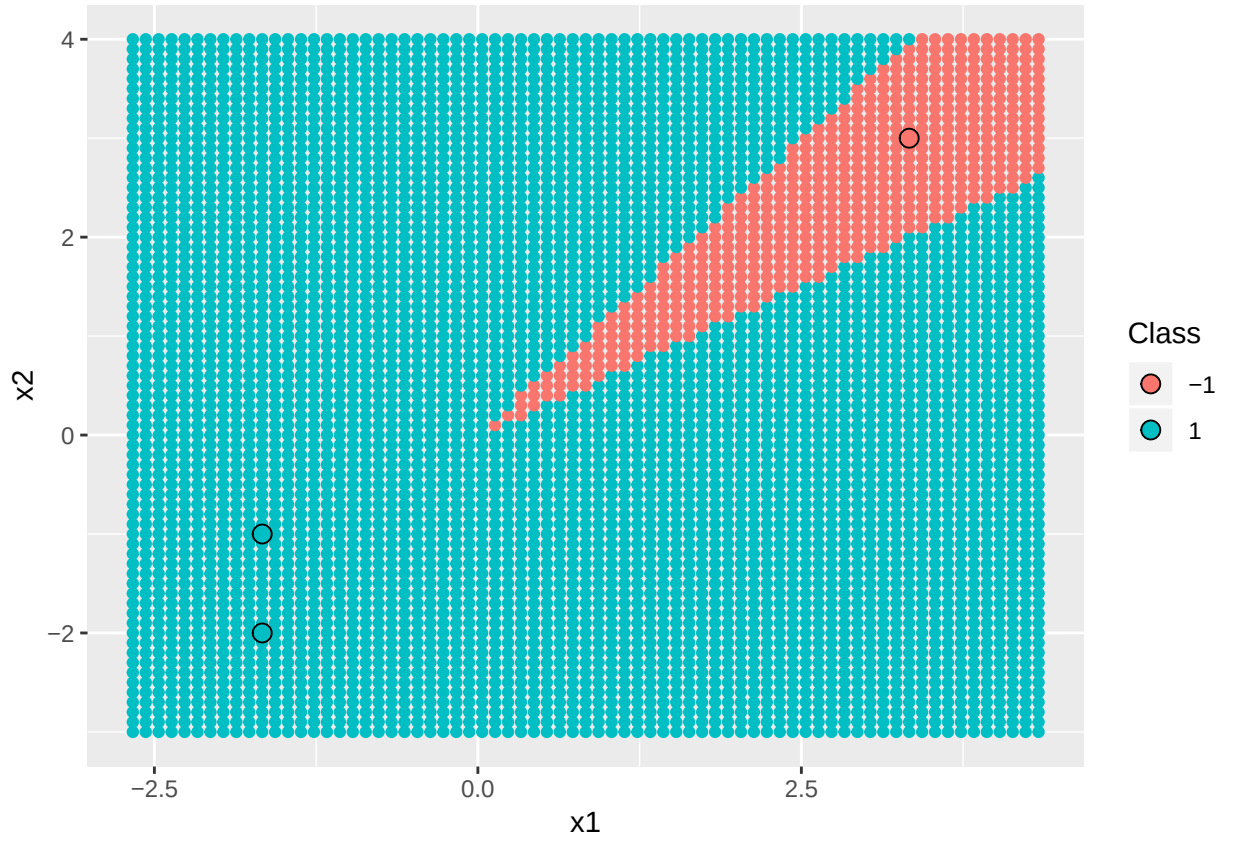
```
data_centered <- apply(data, 2, function(y) y - mean(y))
sigma <- t(data_centered) %*% as.matrix(data_centered) / 2
sigma_sqr <- sqrtm(sigma)
sigma_sqr_inv <- solve(sigma_sqr)
data_whitened <- as.matrix(data_centered) %*% sigma_sqr_inv
data_whitened <- as.data.frame(data_whitened)
colnames(data_whitened)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

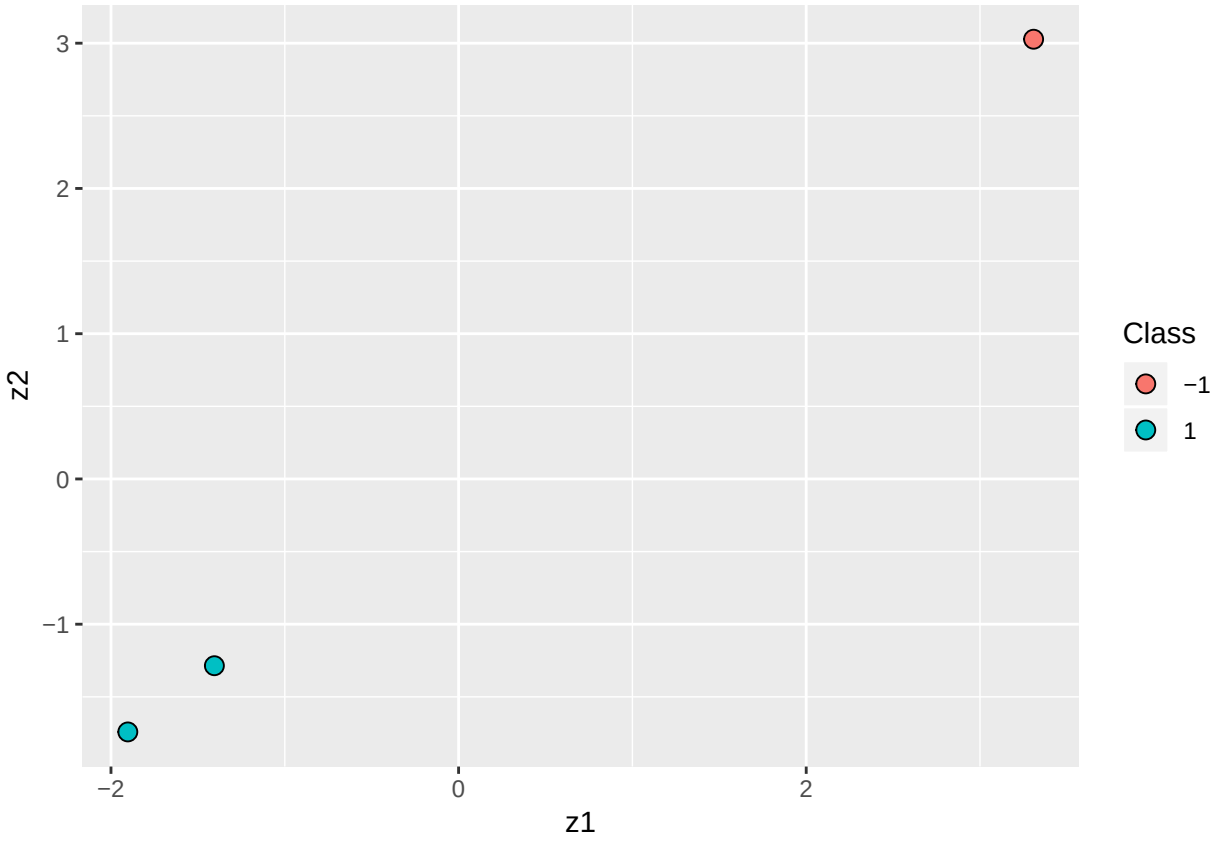
We show the decision region of the final hypothesis in the original space as well.

```
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.

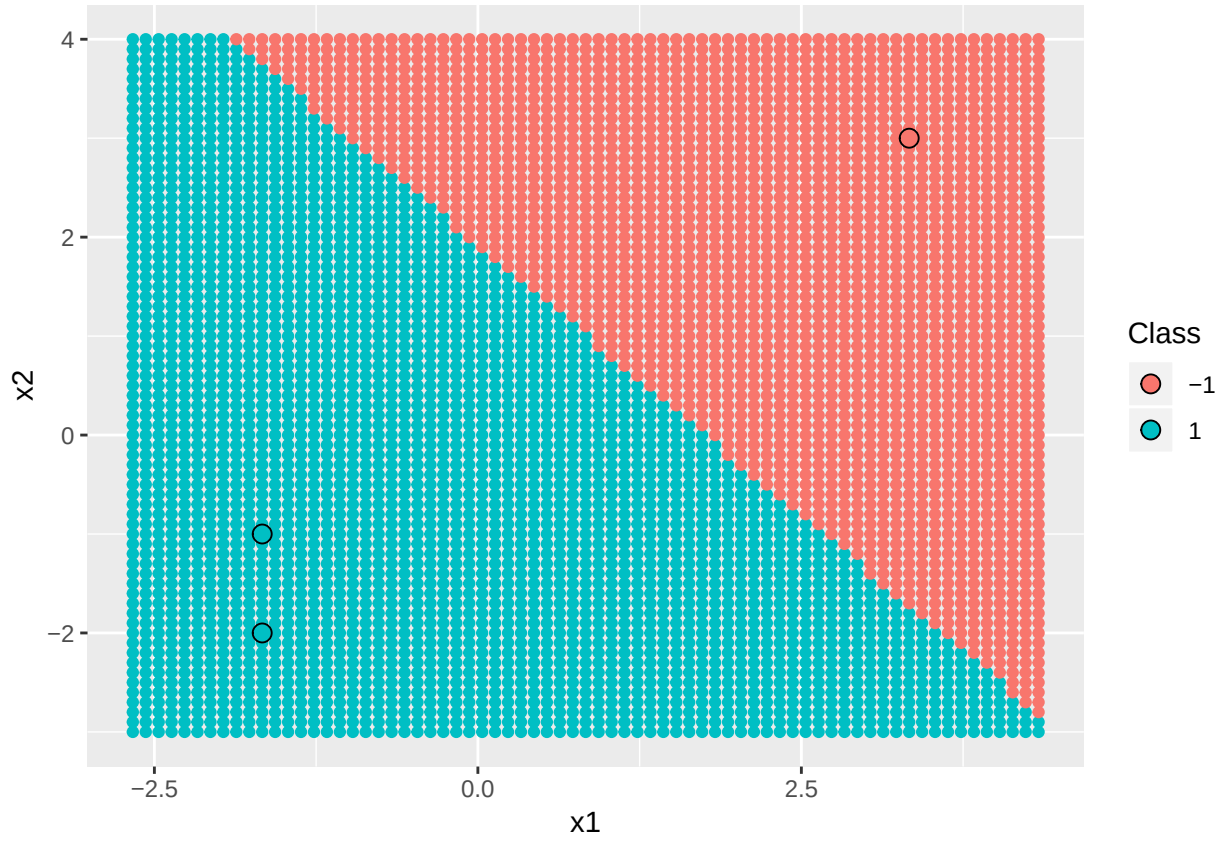
```
SVD_decomp <- svd(data_centered)
V1 <- SVD_decomp$v[, 1]
Z <- data_centered %*% V1
data_pca <- Z %*% t(V1)
data_pca <- as.data.frame(data_pca)
colnames(data_pca) <- c("z1", "z2")

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 $\overline{x'}$, σ'^2_i 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

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

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 $\overline{x'}$, σ'^2_i 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

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

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 $\overline{x'}$, σ'^2_i 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

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

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
$$D' = \text{diag}(1/\sigma'_1, \cdots, 1/\sigma'_d) = \text{diag}(1/(a_1\sigma_1), \cdots, 1/(a_d\sigma_d));$$
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 $\overline{x'}$, σ'^2_i 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
$$\sigma'^2_i = \frac{1}{N}\sum_{n=1}^{N}(x'_{ni} - \overline{x'}_i)^2 = \frac{1}{N}\sum_{n=1}^{N}(l_i^T x_n - l_i^T\overline{x})^2 = \frac{1}{N}\sum_{n=1}^{N} l_i^T(x_n - \overline{x})(x_n - \overline{x})^T l_i = l_i^T\Sigma l_i$$
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
$$D' = \text{diag}(1/\sigma'_1, \cdots, 1/\sigma'_d) = \text{diag}(1/(l_1^T\Sigma l_1), \cdots, 1/(l_d^T\Sigma l_d)).$$
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
$$\Gamma = \text{diag}(\lambda_1, \cdots, \lambda_d)$$
where $\lambda_i > 0$. With this in mind, it is easy to describe $\Gamma^{1/2}$ and $\Gamma^{-1/2}$; we have
$$\Gamma^{1/2} = \text{diag}(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_d}) \text{ and } \Gamma^{-1/2} = \text{diag}(1/\sqrt{\lambda_1}, \cdots, 1/\sqrt{\lambda_d}).$$

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

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

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

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

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

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

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

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

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 $\Gamma = \text{diag}(\sqrt{a_1}, \cdots, \sqrt{a_d})$ 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

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

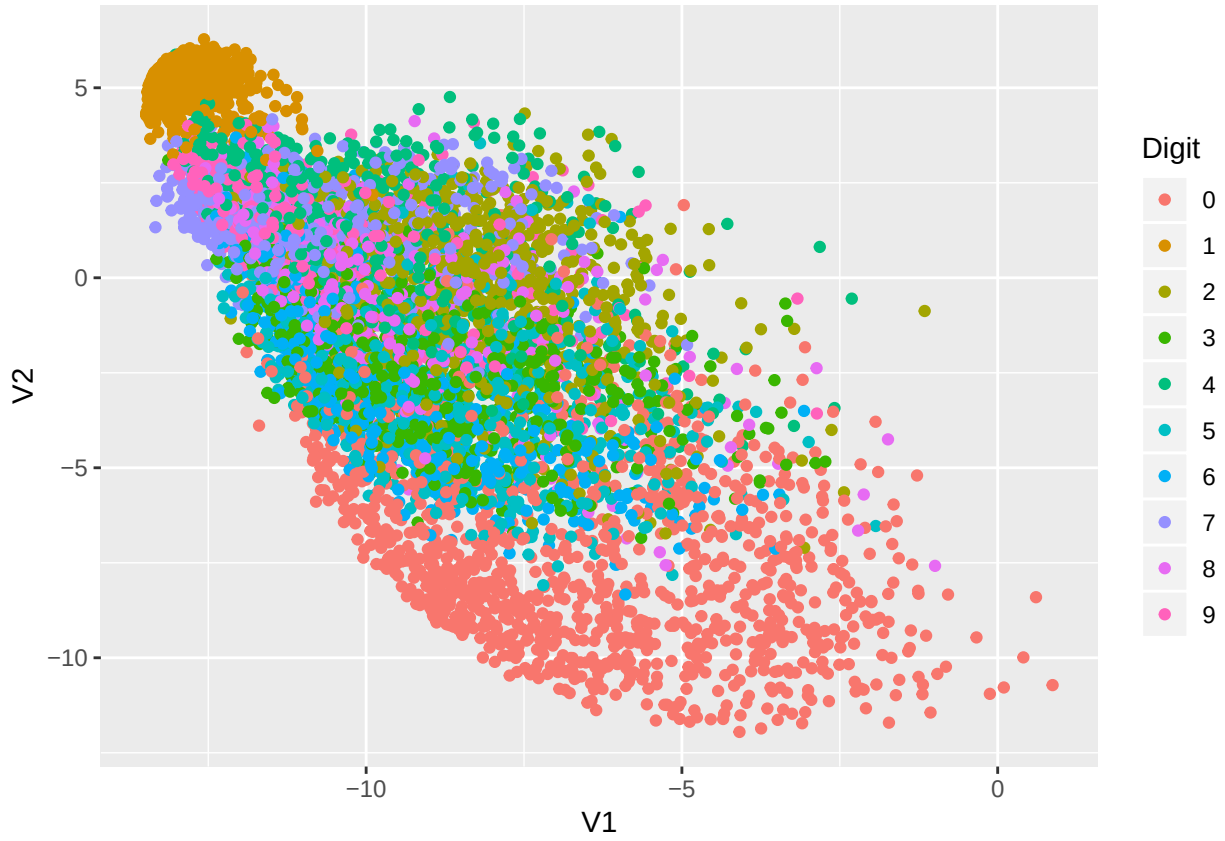
$$V^TV = \begin{pmatrix} V_1^T & & \\ & \ddots & \\ & & V_m^T \end{pmatrix} \begin{pmatrix} V_1 & & \\ & \ddots & \\ & & V_m \end{pmatrix} = VV^T = I,$$

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^TZ, if we use the SVD of $X = U\Gamma V^T$, we get

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

We also have that

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

and

$$V^TV_k = \begin{pmatrix} I_k \\ \hline 0 \end{pmatrix}.$$

This means that

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

and in the same way

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

Consequently, we get that

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

which means that Z is whitened.

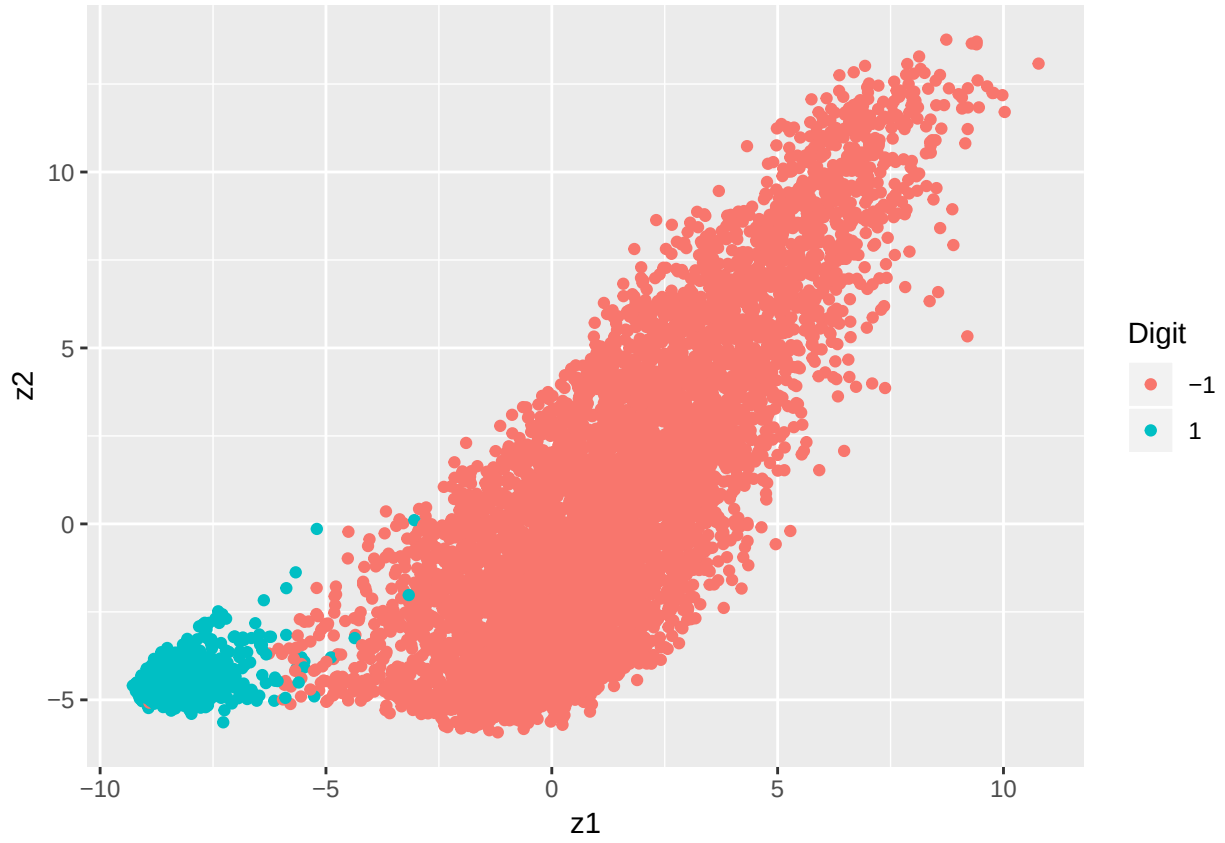
Problem 9.8

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.