

# Problem Solutions

e-Chapter 9

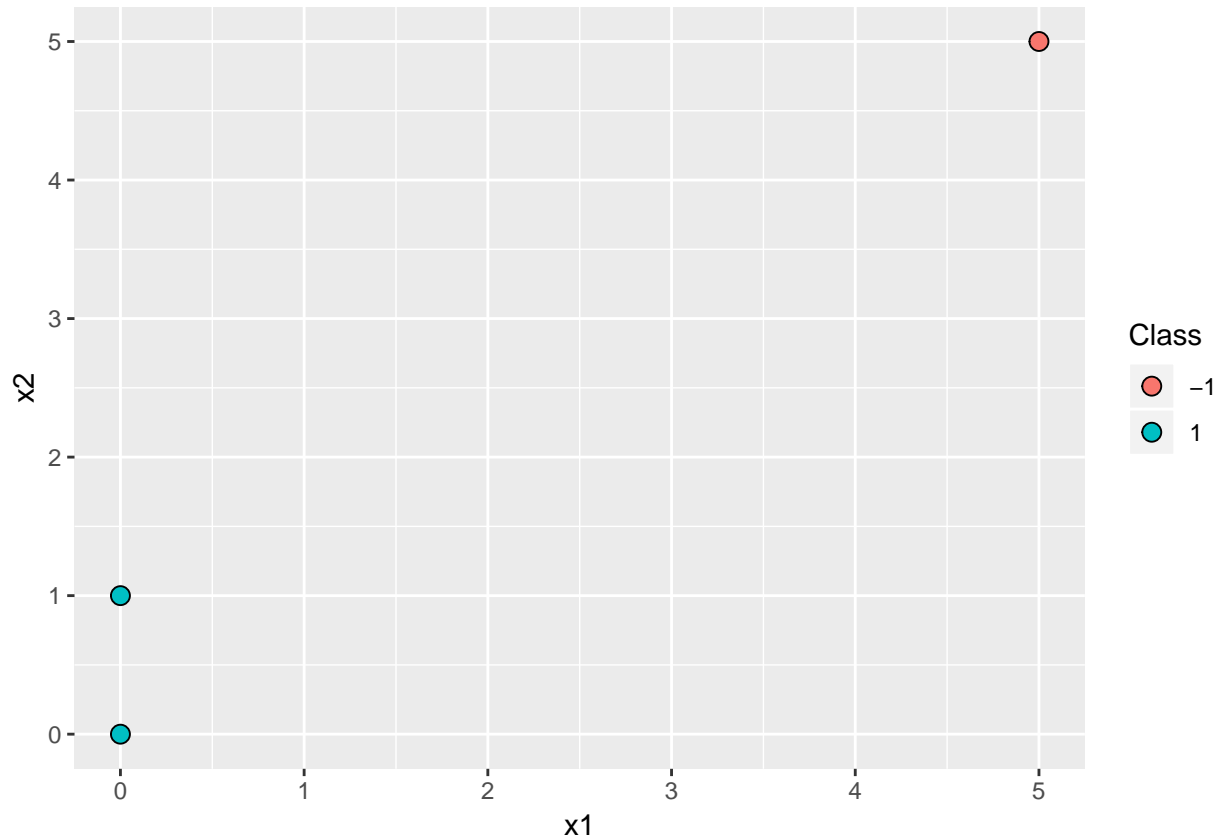
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## Problem 9.1

(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"))
```



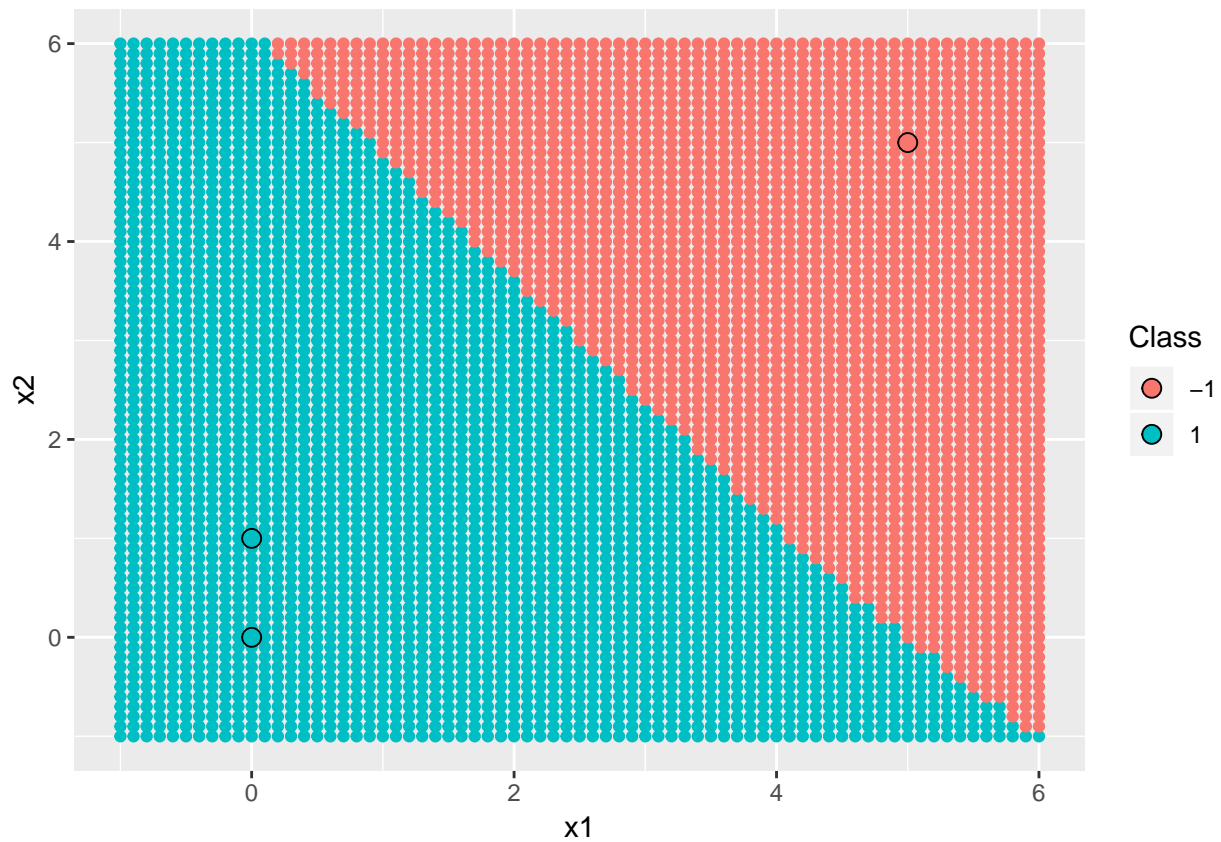
```
grid <- expand.grid(x1 = seq(min(data[, 1] - 1), max(data[, 1] + 1), by = 0.1),
  x2 = seq(min(data[, 2] - 1), max(data[, 2] + 1), by = 0.1))

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")) +
```

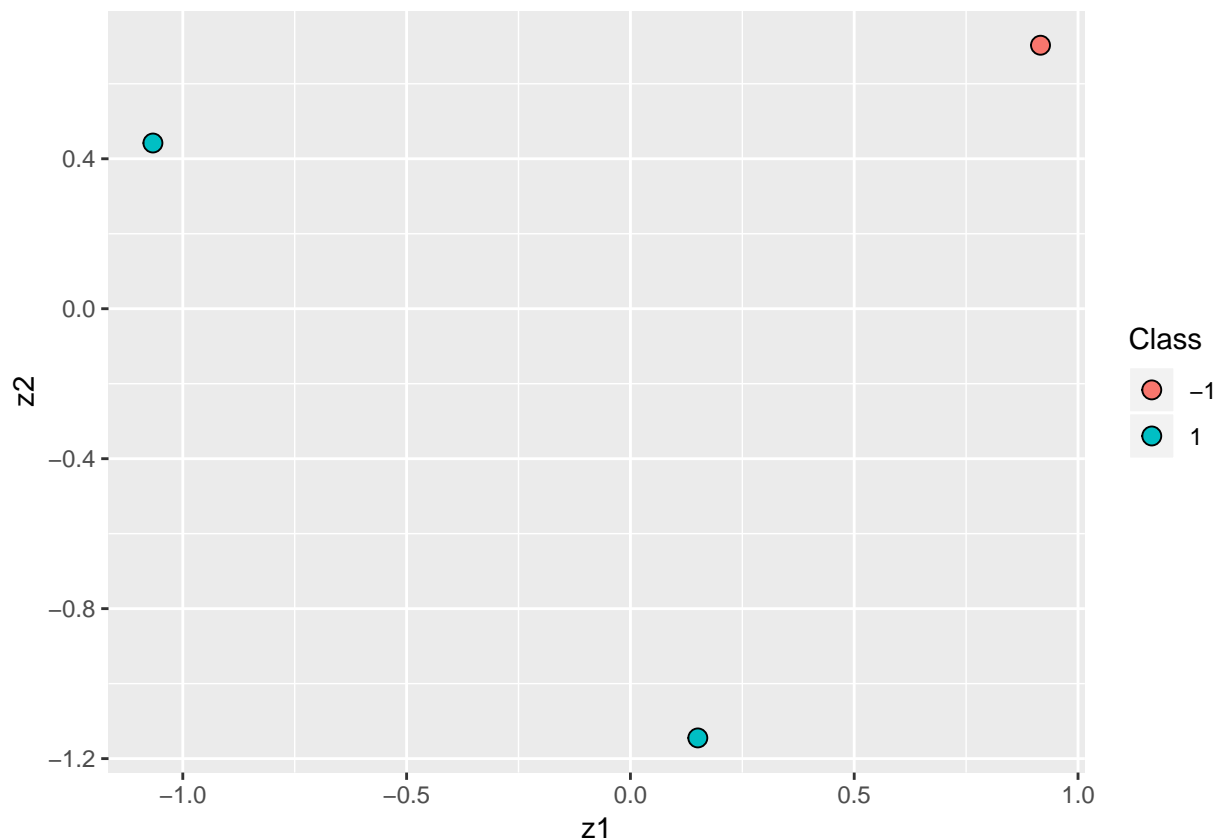
```
guides(col = guide_legend(title = "Class"))
```



(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")

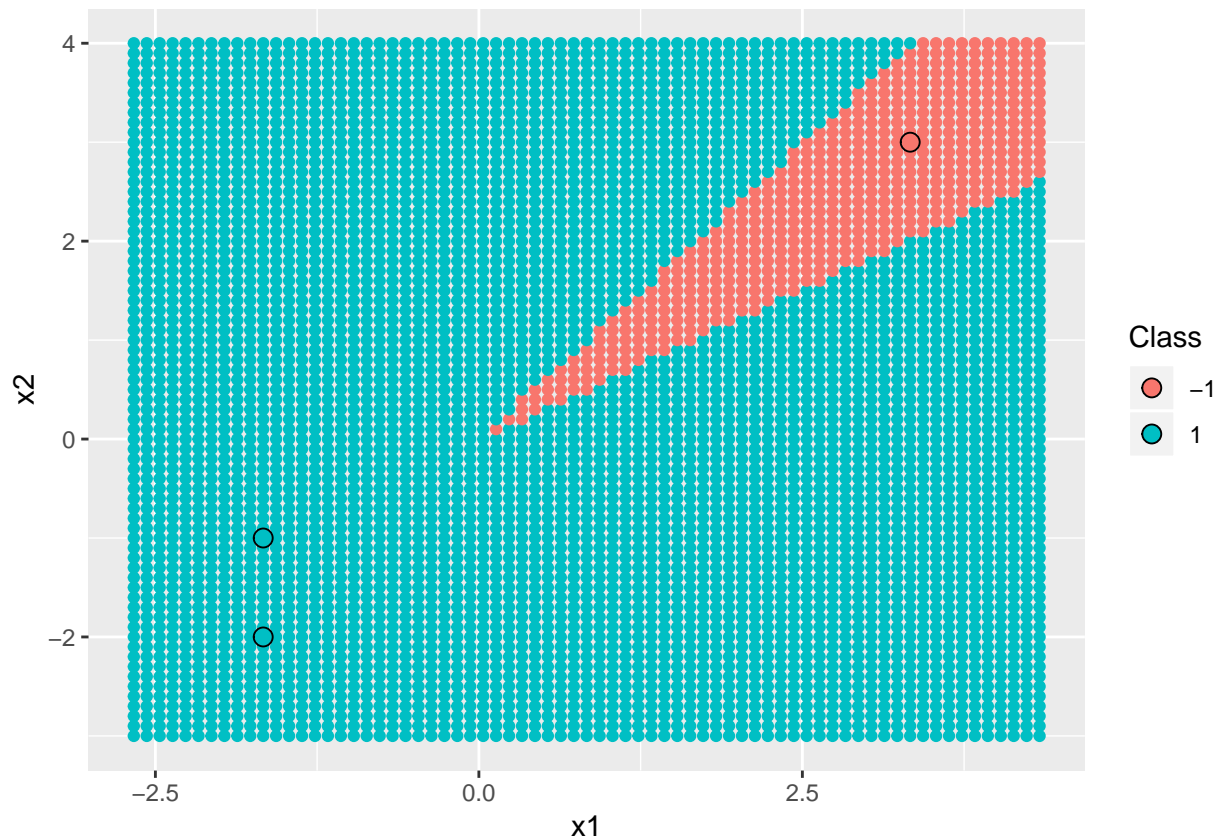
ggplot(data_whitened, aes(x = z1, y = z2, fill = class)) + geom_point(size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class"))
```



```
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.

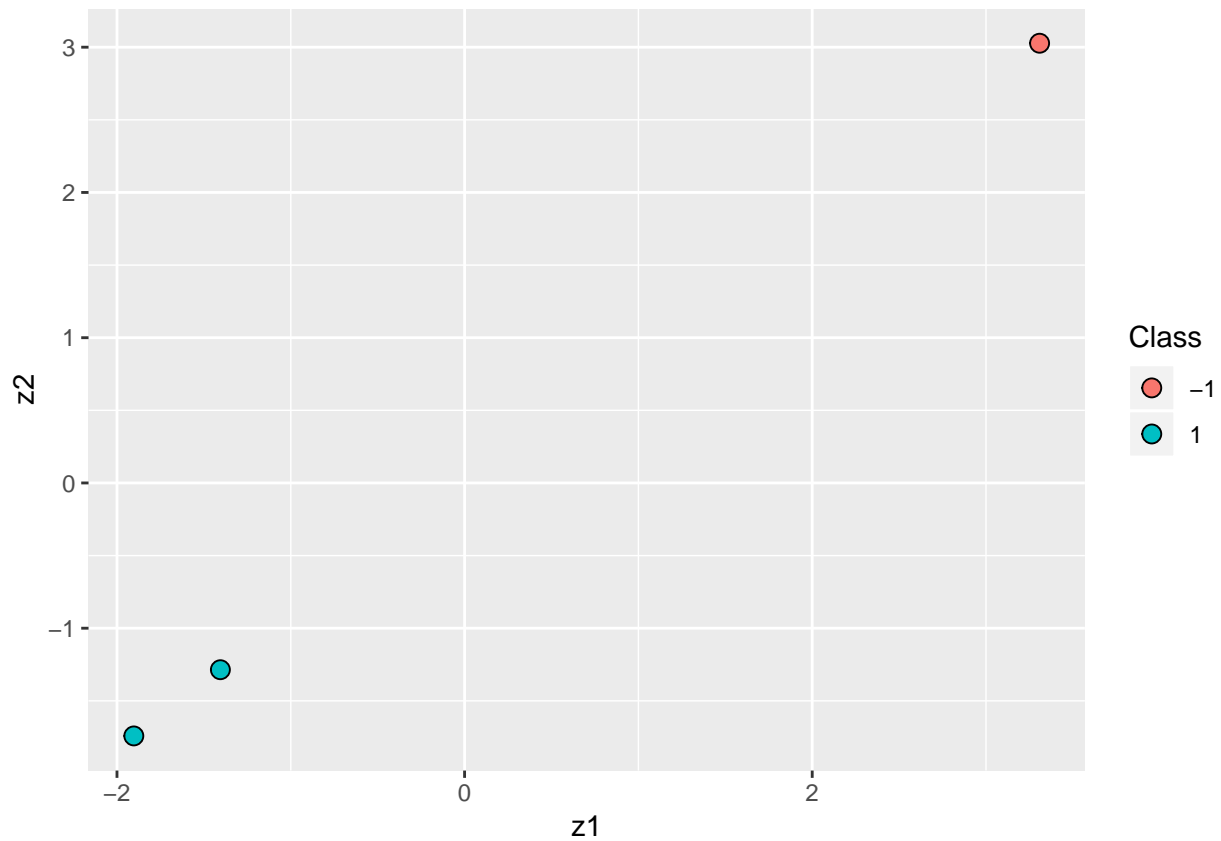
```
ggplot() + geom_point(data = grid_centered, aes(x = x1, y = x2, col = knn_mod_whitened)) +
  geom_point(data = as.data.frame(data_centered), aes(x = x1, y = x2, fill = class),
            size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class")) +
  guides(col = guide_legend(title =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

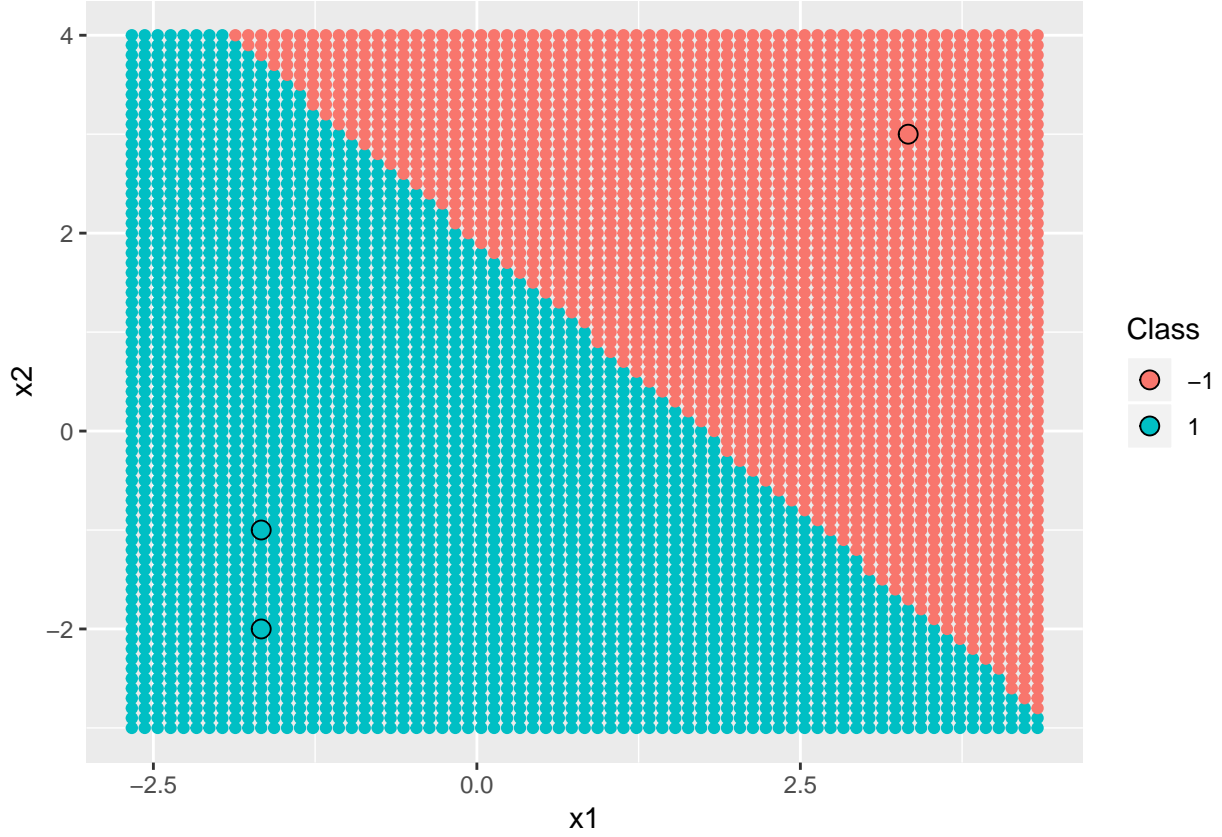
ggplot(data_pca, aes(x = z1, y = z2, fill = class)) + geom_point(size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class"))
```



```
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  $\bar{x}'$ ,  $\sigma_i'^2$  and  $\Sigma'$ . We have

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

moreover, we have

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

and finally

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

- **Centering.** We may write that

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

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

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

where

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

In that case, we have

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

- **Whitening.** We have

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

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

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

moreover, we have

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

and finally

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

- **Centering.** We may write that

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

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

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

where

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

In that case, we have

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

- **Whitening.** We have

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

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

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

moreover, we have

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

and finally

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

- **Centering.** We may write that

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

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

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

where

$$D' = \text{diag}(1/\sigma'_1, \dots, 1/\sigma'_d) = \text{diag}(1/(a_1\sigma_1), \dots, 1/(a_d\sigma_d));$$

which means that  $D'A = D$ . In that case, we have

$$z'_n = D'(x'_n - \bar{x}') = D'A(x_n - \bar{x}) = D(x_n - \bar{x}) = z_n.$$

- **Whitening.** We have

$$z'_n = \Sigma'^{-1/2}(x'_n - \bar{x}') = (A\Sigma A^T)^{-1/2}A(x_n - \bar{x}) \neq z_n.$$

(d) Here, we have  $x'_n = Ax_n$  with  $\det(A) \neq 0$ . Let us compute  $\bar{x}'$ ,  $\sigma_i'^2$  and  $\Sigma'$ . We have

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

moreover, we have

$$\sigma_i'^2 = \frac{1}{N} \sum_{n=1}^N (x'_{ni} - \bar{x}'_i)^2 = \frac{1}{N} \sum_{n=1}^N (l_i^T x_n - l_i^T \bar{x})^2 = \frac{1}{N} \sum_{n=1}^N l_i^T (x_n - \bar{x})(x_n - \bar{x})^T l_i = l_i^T \Sigma l_i$$

where  $l_i$  is the  $i$ th row of  $A$ ; and finally

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

- **Centering.** We may write that

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

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

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

where

$$D' = \text{diag}(1/\sigma'_1, \dots, 1/\sigma'_d) = \text{diag}(1/(l_1^T \Sigma l_1), \dots, 1/(l_d^T \Sigma l_d)).$$

In that case, we have

$$z'_n = D'(x'_n - \bar{x}') = D'A(x_n - \bar{x}) = D'Az_n \neq z_n.$$

- **Whitening.** We have

$$z'_n = \Sigma'^{-1/2}(x'_n - \bar{x}') = (A\Sigma A^T)^{-1/2}A(x_n - \bar{x}) \neq z_n.$$

### Problem 9.3

We may write

$$\Gamma = \text{diag}(\lambda_1, \dots, \lambda_d)$$

where  $\lambda_i > 0$ . With this in mind, it is easy to describe  $\Gamma^{1/2}$  and  $\Gamma^{-1/2}$ ; we have

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



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

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

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

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

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

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

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

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

#### Problem 9.4

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

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

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

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

since  $A$  is an orthogonal matrix as well; this means that  $\psi$  is also an orthogonal matrix.

#### Problem 9.5

(a) if  $A$  is a diagonal matrix ( $N = d$ ), it suffices to define  $U$ ,  $\Gamma$  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

$$A^T A = \text{diag}(a_1, \dots, a_d)$$

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

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

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

$$U^T U = D^T A^T A D = I_d.$$

In this case, we have

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

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

(d) If  $A$  has SVD  $UTV^T$  and  $Q^T Q = I$ , we may write that

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

with  $QU$  a matrix with orthonormal columns since

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

(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  $U$ ,  $\Gamma$ , 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

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

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

and  $\Gamma$  diagonal.

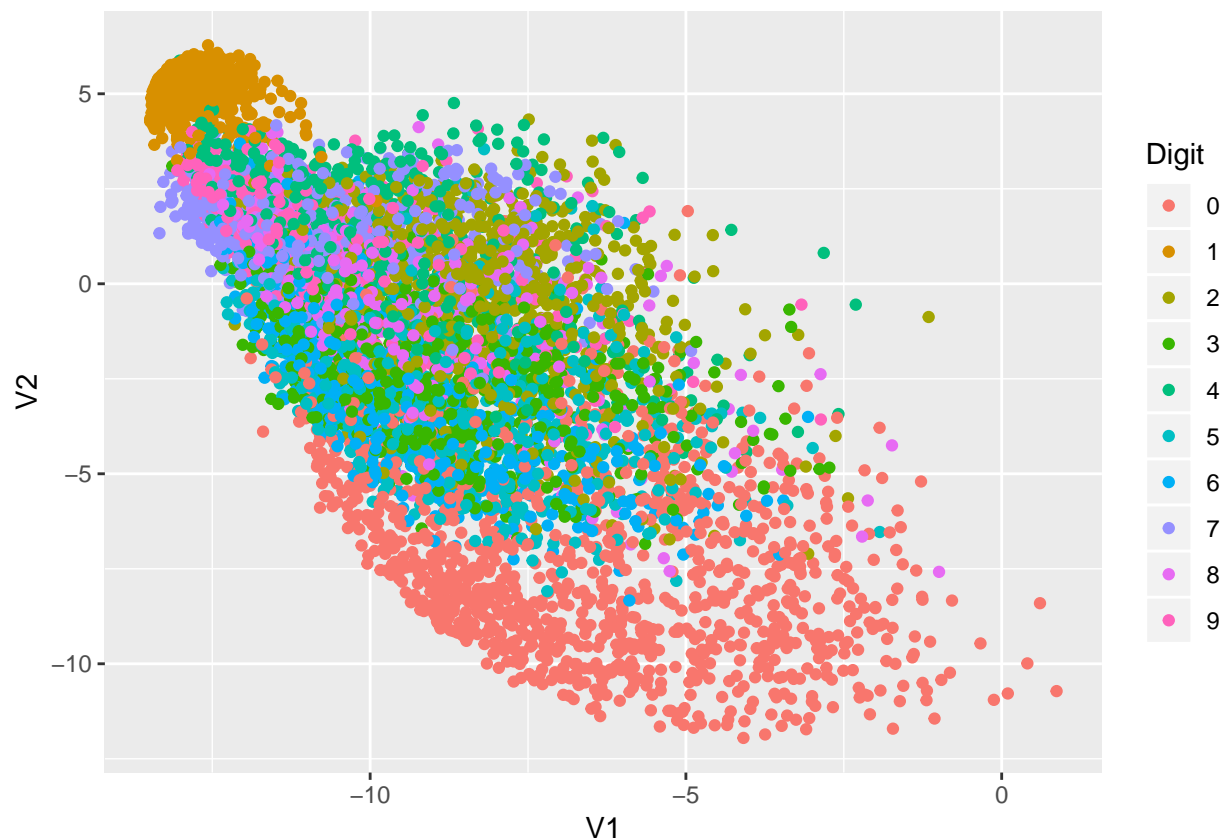
## Problem 9.6

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

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

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

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

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

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

We also have that

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

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.