Problem Solutions

e-Chapter 9

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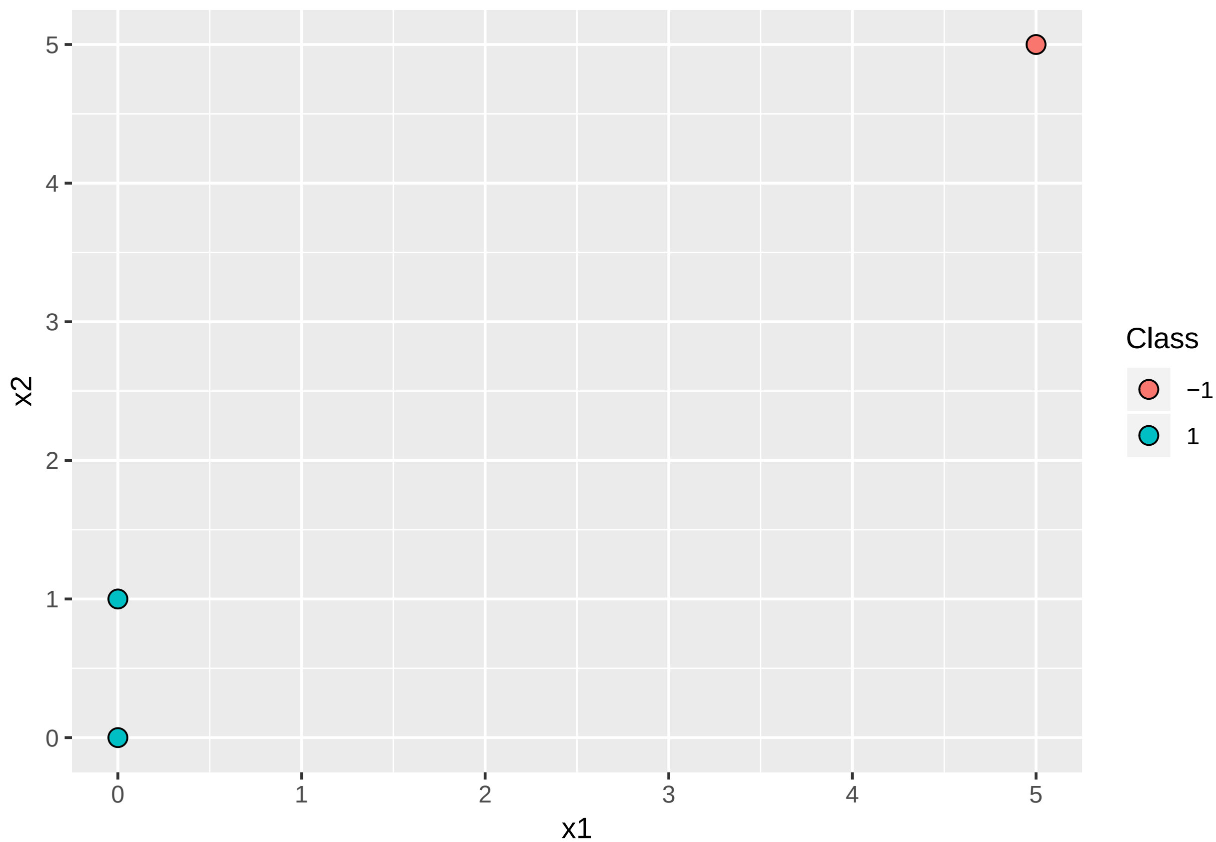
Problem 9.1

(*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"))
```



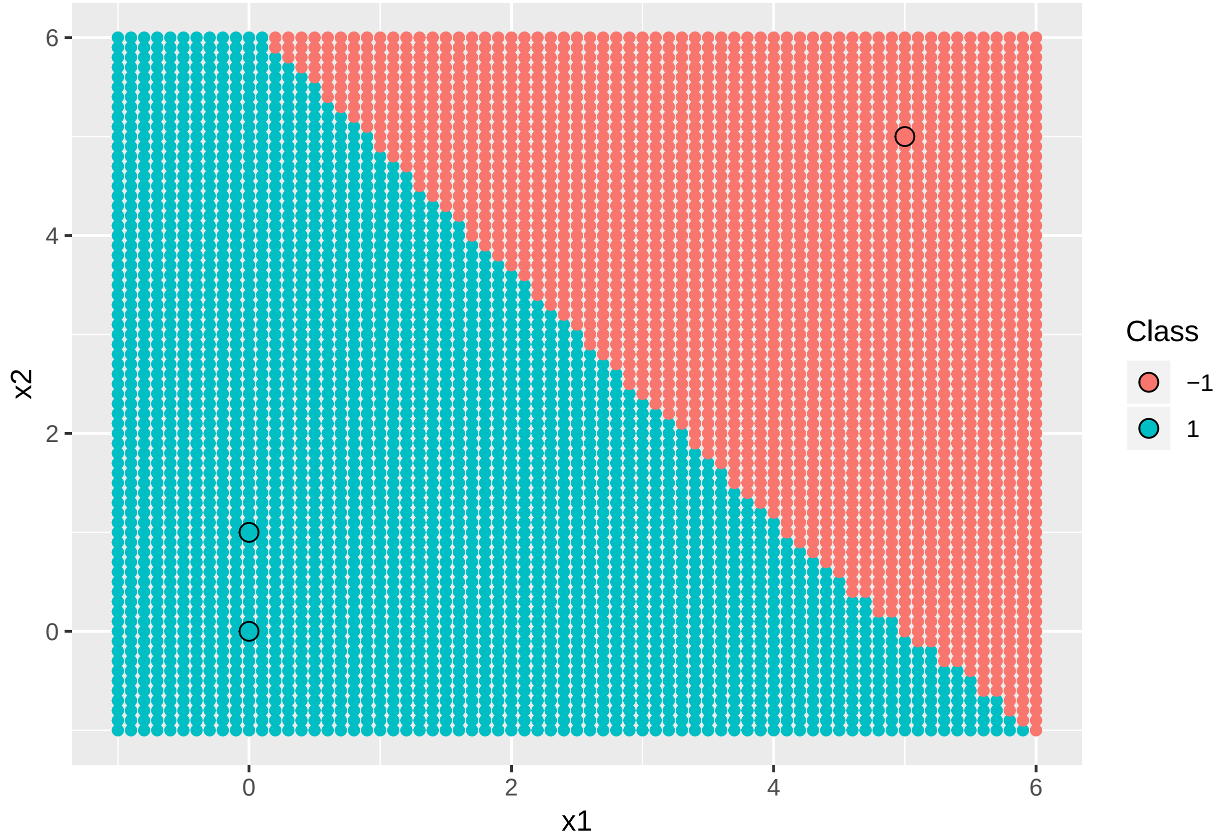

```
grid <- expand.grid(x1 = seq(min(data[, 1] - 1), max(data[, 1] + 1), by = 0.1),
                    x2 = seq(min(data[, 2] - 1), max(data[, 2] + 1), by = 0.1))

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")) +
```

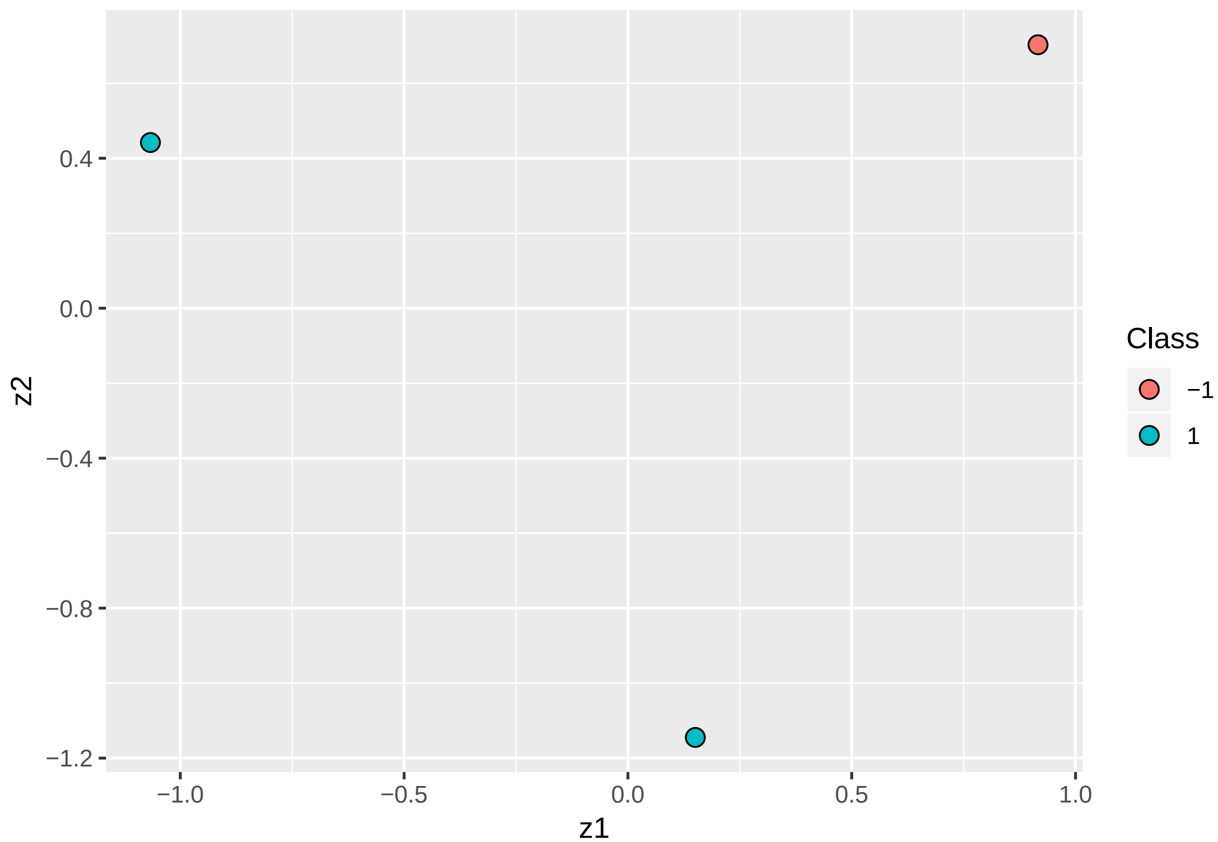
```r
  guides(col = guide_legend(title = "Class"))
```



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

```r
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"))
```

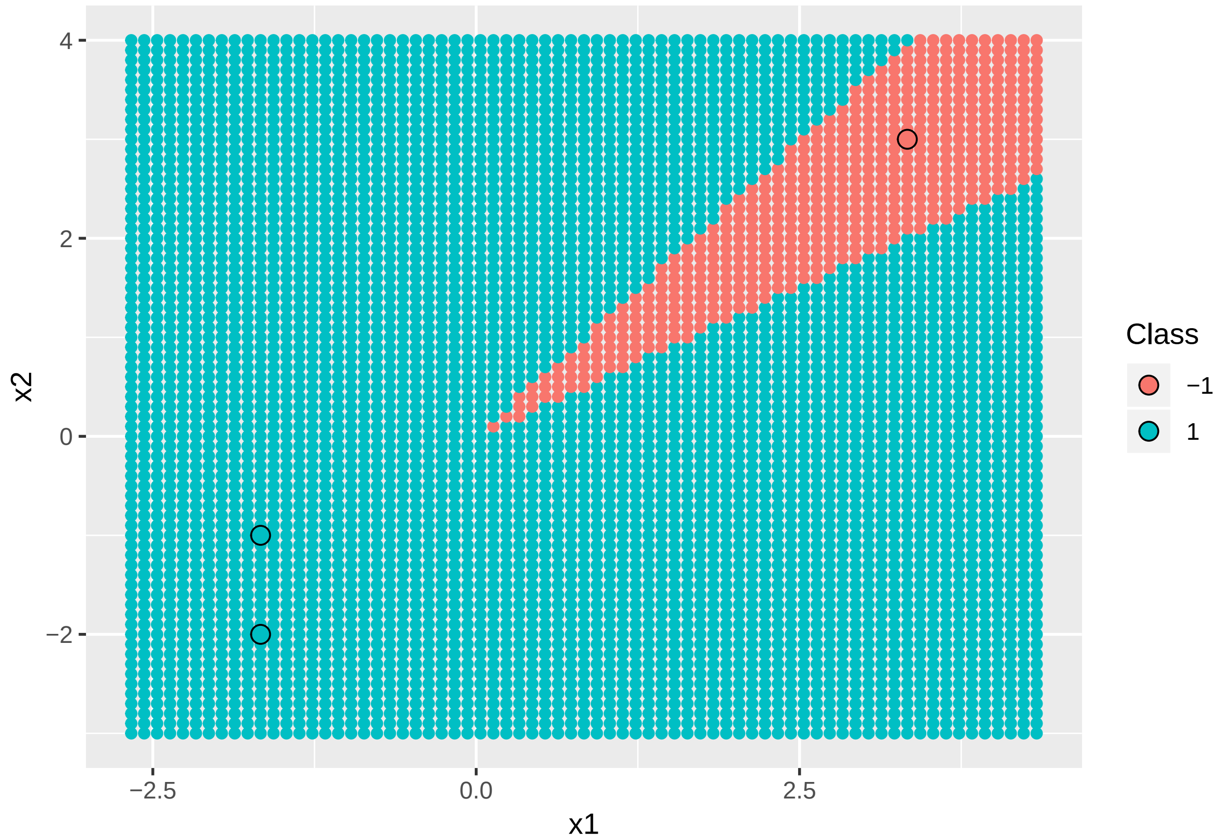



```
grid_centered <- expand.grid(x1 = seq(min(data_centered[, 1] - 1),
                                      max(data_centered[, 1] + 1), by = 0.1),
                             x2 = seq(min(data_centered[, 2] - 1),
                                      max(data_centered[, 2] + 1), by = 0.1))
grid_whitened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

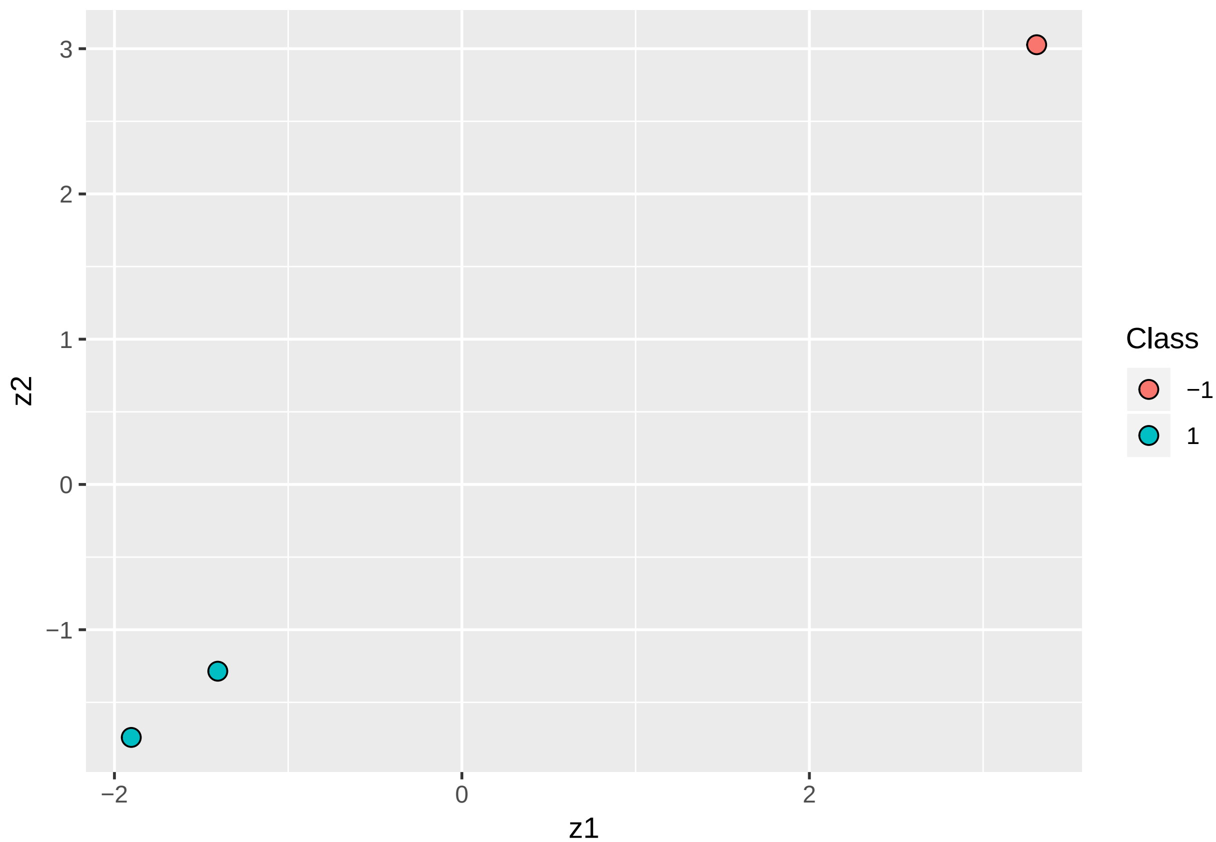
```
ggplot() + geom_point(data = grid_centered, aes(x = x1, y = x2, col = knn_mod_whitened)) +
  geom_point(data = as.data.frame(data_centered), aes(x = x1, y = x2, fill = class),
             size = 3, shape = 21) +
  guides(fill = guide_legend(title = "Class")) +
  guides(col = guide_legend(title =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

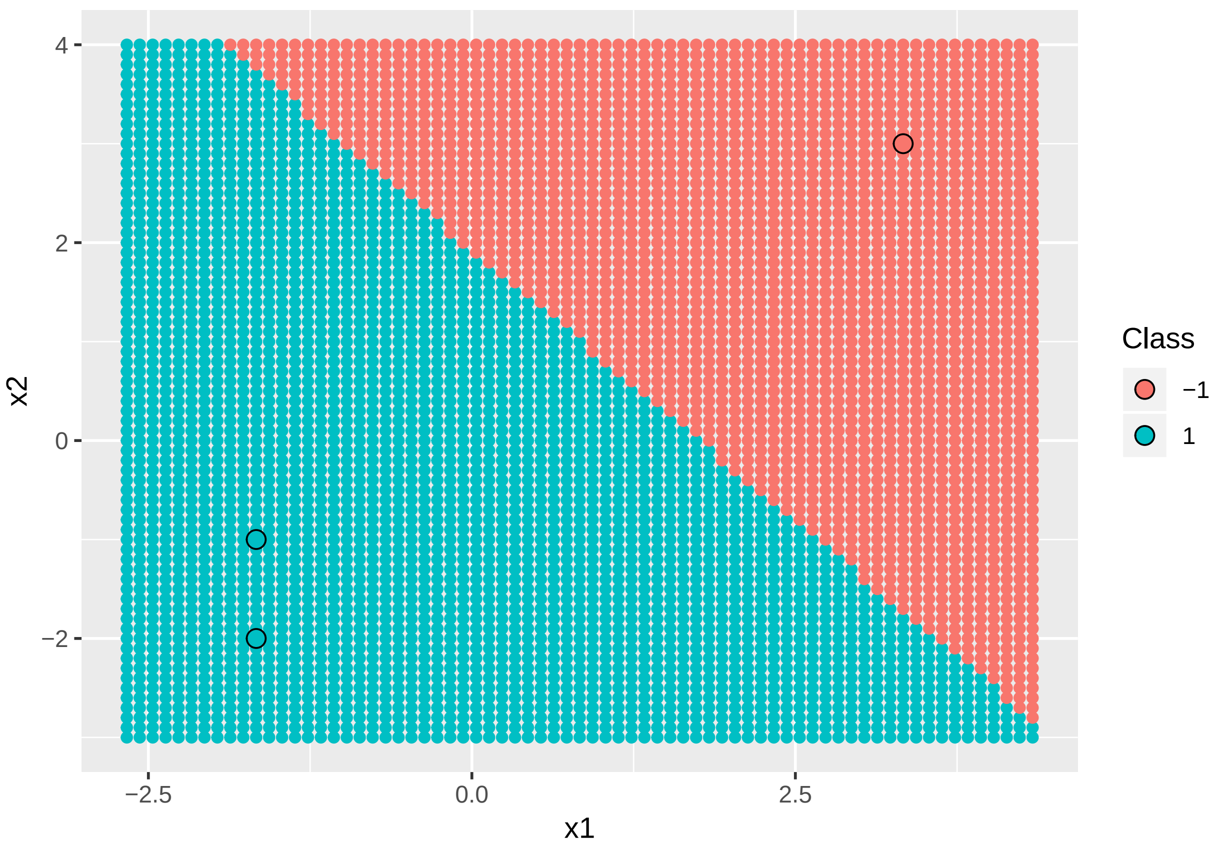



```
grid_pca <- (as.matrix(grid_centered) %*% V1) %*% t(V1)

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

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

  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 $A = \text{diag}(a_1, \cdots, a_d)$ $(a_i \neq 0)$. 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.