

Aprendizagem 2023  
Homework IV – Group 28

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**Part I: Pen and Paper**

Given the following observations,  $\left\{ \begin{pmatrix} 1 \\ 0.6 \\ 0.1 \end{pmatrix}, \begin{pmatrix} 0 \\ -0.4 \\ 0.8 \end{pmatrix}, \begin{pmatrix} 0 \\ 0.2 \\ 0.5 \end{pmatrix}, \begin{pmatrix} 1 \\ 0.4 \\ -0.1 \end{pmatrix} \right\}$ .

Consider a Bayesian clustering that assumes  $\{y_1\} \perp\!\!\!\perp \{y_2, y_3\}$ , two clusters following a Bernoulli distribution on  $y_1$  ( $p_1$  and  $p_2$ ), a multivariate Gaussian on  $\{y_2, y_3\}$  ( $N_1$  and  $N_2$ ), and the following initial mixture:

$$\begin{aligned} \pi_1 &= 0.5 \quad , \quad \pi_2 = 0.5 \\ p_1 &= P(y_1 = 1) = 0.3 \quad , \quad p_2 = P(y_1 = 1) = 0.7 \\ \mathcal{N}_1 \left( \mu_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \Sigma_1 = \begin{pmatrix} 2 & 0.5 \\ 0.5 & 2 \end{pmatrix} \right) \quad , \quad \mathcal{N}_2 \left( \mu_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Sigma_2 = \begin{pmatrix} 1.5 & 1 \\ 1 & 1.5 \end{pmatrix} \right) \end{aligned}$$

1. **Perform one epoch of the EM clustering algorithm and determine the new parameters.**

*Hint:* we suggest you to use numpy and scipy, however disclose the intermediary results step by step.

The EM (Expectation-Maximization) algorithm has four major steps: Initialization, Expectation, Maximization and Verification.

## 1. Initialization

We'll start by labeling each observation:

$$x_1 = \begin{pmatrix} 1 \\ 0.6 \\ 0.1 \end{pmatrix} \quad , \quad x_2 = \begin{pmatrix} 0 \\ -0.4 \\ 0.8 \end{pmatrix} \quad , \quad x_3 = \begin{pmatrix} 0 \\ 0.2 \\ 0.5 \end{pmatrix} \quad , \quad x_4 = \begin{pmatrix} 1 \\ 0.4 \\ -0.1 \end{pmatrix}$$

From the statement we have the following initial parameters,  $p_1, p_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2, \pi_1$  and  $\pi_2$ :

Cluster	$p$	$\mu$	$\Sigma$	$\pi$
Cluster 1	0.3	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0.5 \\ 0.5 & 2 \end{pmatrix}$	0.5
Cluster 2	0.7	$\begin{pmatrix} 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 1.5 & 1 \\ 1 & 1.5 \end{pmatrix}$	0.5

Table 1: Initial parameters for the two clusters

## 2. Expectation (E-step)

Considering  $\{y_1\} \perp\!\!\!\perp \{y_2, y_3\}$  we know the posterior probability,  $P(c_k|x_i)$ , is given by Baye's rule:

$$P(c_k|x_i) = \frac{P(y_1, y_2, y_3|c_k)P(c_k)}{P(y_1, y_2, y_3)} = \frac{P(y_1|c_k)P(y_2, y_3|c_k)P(c_k)}{P(y_1)P(y_2, y_3)} \quad (1)$$

Since we know that  $\sum_j P(c_j|x_i)$  must be equal to 1, we need to normalize the values given by equation (1). Therefore, we get these new normalized values for the posteriors represented by  $\gamma_{k,i}$ :

$$\gamma_{k,i} = \frac{P(c_k|x_i)}{\sum_j P(c_j|x_i)} = \frac{P(y_1|c_k)P(y_2, y_3|c_k)P(c_k)}{\sum_j P(y_1|c_j)P(y_2, y_3|c_j)P(c_j)} \quad (2)$$

The variable  $y_1$  follows a Bernoulli distribution ( $y_1 \sim \text{Bern}(p = p_k)$ ), and so the likelihoods,  $P(y_1 = 0|c_k)$  and  $P(y_1 = 1|c_k)$ , can be calculated for each cluster:

$$\begin{aligned} P(y_1 = 0|c_1) &= 1 - p_1 = 1 - 0.3 = 0.7 & P(y_1 = 0|c_2) &= 1 - p_2 = 1 - 0.7 = 0.3 \\ P(y_1 = 1|c_1) &= p_1 = 0.3 & P(y_1 = 1|c_2) &= p_2 = 0.7 \end{aligned}$$

We know the likelihood,  $P(y_2, y_3|c_k)$ , follows a multivariate Gaussian, and so it is given by (considering  $d = 2$ , since we are working in two dimensions):

$$P(y_2 = a, y_3 = b|c_k) = \mathcal{N}_k(y_2 = a, y_3 = b|\mu_k, \Sigma_k) = \frac{\exp\left(-\frac{1}{2} \left(\begin{bmatrix} a \\ b \end{bmatrix} - \mu_k\right)^T \Sigma_k^{-1} \left(\begin{bmatrix} a \\ b \end{bmatrix} - \mu_k\right)\right)}{(2\pi)^{d/2} \times |\Sigma_k|^{1/2}} \quad (3)$$

We now have all the building blocks to calculate the posterior probabilities for each combination of observation,  $x_i$  and cluster,  $c_k$ .

We'll start off by calculating the multivariate likelihood by employing equation (3), for each pair of observation and cluster:

### Cluster 1 Multivariate Likelihoods

$$\begin{aligned} P(y_2 = 0.6, y_3 = 0.1|c_1) &= \mathcal{N}_1(y_2 = 0.6, y_3 = 0.1|\mu_1, \Sigma_1) \approx 0.06658 \\ P(y_2 = -0.4, y_3 = 0.8|c_1) &= \mathcal{N}_1(y_2 = -0.4, y_3 = 0.8|\mu_1, \Sigma_1) \approx 0.05005 \\ P(y_2 = 0.2, y_3 = 0.5|c_1) &= \mathcal{N}_1(y_2 = 0.2, y_3 = 0.5|\mu_1, \Sigma_1) \approx 0.06837 \\ P(y_2 = 0.4, y_3 = -0.1|c_1) &= \mathcal{N}_1(y_2 = 0.4, y_3 = -0.1|\mu_1, \Sigma_1) \approx 0.05905 \end{aligned}$$

### Cluster 2 Multivariate Likelihood

$$\begin{aligned} P(y_2 = 0.6, y_3 = 0.1|c_2) &= \mathcal{N}_2(y_2 = 0.6, y_3 = 0.1|\mu_2, \Sigma_2) \approx 0.11962 \\ P(y_2 = -0.4, y_3 = 0.8|c_2) &= \mathcal{N}_2(y_2 = -0.4, y_3 = 0.8|\mu_2, \Sigma_2) \approx 0.06819 \\ P(y_2 = 0.2, y_3 = 0.5|c_2) &= \mathcal{N}_2(y_2 = 0.2, y_3 = 0.5|\mu_2, \Sigma_2) \approx 0.12958 \\ P(y_2 = 0.4, y_3 = -0.1|c_2) &= \mathcal{N}_2(y_2 = 0.4, y_3 = -0.1|\mu_2, \Sigma_2) \approx 0.12450 \end{aligned}$$

Finally, we can employ equation (2) to calculate the normalized posteriors with the previously calculated values, for each pair of observation and cluster:

### Cluster 1 Posteriors

$$\begin{aligned}\gamma_{1,1} &= \frac{P(y_1 = 1|c_1)P(y_2 = 0.6, y_3 = 0.1|c_1)P(c_1)}{P(y_1 = 1|c_1)P(y_2 = 0.6, y_3 = 0.1|c_1)P(c_1) + P(y_1 = 1|c_2)P(y_2 = 0.6, y_3 = 0.1|c_2)P(c_2)} \\ &= \frac{0.3 \times 0.06658 \times 0.5}{0.3 \times 0.06658 \times 0.5 + 0.7 \times 0.11962 \times 0.5} \approx 0.19259\end{aligned}$$

$$\begin{aligned}\gamma_{1,2} &= \frac{P(y_1 = 0|c_1)P(y_2 = -0.4, y_3 = 0.8|c_1)P(c_1)}{P(y_1 = 0|c_1)P(y_2 = -0.4, y_3 = 0.8|c_1)P(c_1) + P(y_1 = 0|c_2)P(y_2 = -0.4, y_3 = 0.8|c_2)P(c_2)} \\ &= \frac{0.7 \times 0.05005 \times 0.5}{0.7 \times 0.05005 \times 0.5 + 0.3 \times 0.06819 \times 0.5} \approx 0.63135\end{aligned}$$

$$\begin{aligned}\gamma_{1,3} &= \frac{P(y_1 = 0|c_1)P(y_2 = 0.2, y_3 = 0.5|c_1)P(c_1)}{P(y_1 = 0|c_1)P(y_2 = 0.2, y_3 = 0.5|c_1)P(c_1) + P(y_1 = 0|c_2)P(y_2 = 0.2, y_3 = 0.5|c_2)P(c_2)} \\ &= \frac{0.7 \times 0.06837 \times 0.5}{0.7 \times 0.06837 \times 0.5 + 0.3 \times 0.12958 \times 0.5} \approx 0.55181\end{aligned}$$

$$\begin{aligned}\gamma_{1,4} &= \frac{P(y_1 = 1|c_1)P(y_2 = 0.4, y_3 = -0.1|c_1)P(c_1)}{P(y_1 = 1|c_1)P(y_2 = 0.4, y_3 = -0.1|c_1)P(c_1) + P(y_1 = 1|c_2)P(y_2 = 0.4, y_3 = -0.1|c_2)P(c_2)} \\ &= \frac{0.3 \times 0.05905 \times 0.5}{0.3 \times 0.05905 \times 0.5 + 0.7 \times 0.12450 \times 0.5} \approx 0.16892\end{aligned}$$

### Cluster 2 Posteriors

$$\begin{aligned}\gamma_{2,1} &= \frac{P(y_1 = 1|c_2)P(y_2 = 0.6, y_3 = 0.1|c_2)P(c_2)}{P(y_1 = 1|c_1)P(y_2 = 0.6, y_3 = 0.1|c_1)P(c_1) + P(y_1 = 1|c_2)P(y_2 = 0.6, y_3 = 0.1|c_2)P(c_2)} \\ &= \frac{0.7 \times 0.11962 \times 0.5}{0.3 \times 0.06658 \times 0.5 + 0.7 \times 0.11962 \times 0.5} \approx 0.80741\end{aligned}$$

$$\begin{aligned}\gamma_{2,2} &= \frac{P(y_1 = 0|c_2)P(y_2 = -0.4, y_3 = 0.8|c_2)P(c_2)}{P(y_1 = 0|c_1)P(y_2 = -0.4, y_3 = 0.8|c_1)P(c_1) + P(y_1 = 0|c_2)P(y_2 = -0.4, y_3 = 0.8|c_2)P(c_2)} \\ &= \frac{0.3 \times 0.06819 \times 0.5}{0.7 \times 0.05005 \times 0.5 + 0.3 \times 0.06819 \times 0.5} \approx 0.36865\end{aligned}$$

$$\begin{aligned}\gamma_{2,3} &= \frac{P(y_1 = 0|c_2)P(y_2 = 0.2, y_3 = 0.5|c_2)P(c_2)}{P(y_1 = 0|c_1)P(y_2 = 0.2, y_3 = 0.5|c_1)P(c_1) + P(y_1 = 0|c_2)P(y_2 = 0.2, y_3 = 0.5|c_2)P(c_2)} \\ &= \frac{0.3 \times 0.12958 \times 0.5}{0.7 \times 0.06837 \times 0.5 + 0.3 \times 0.12958 \times 0.5} \approx 0.44819\end{aligned}$$

$$\begin{aligned}\gamma_{2,4} &= \frac{P(y_1 = 1|c_2)P(y_2 = 0.4, y_3 = -0.1|c_2)P(c_2)}{P(y_1 = 1|c_1)P(y_2 = 0.4, y_3 = -0.1|c_1)P(c_1) + P(y_1 = 1|c_2)P(y_2 = 0.4, y_3 = -0.1|c_2)P(c_2)} \\ &= \frac{0.7 \times 0.12450 \times 0.5}{0.3 \times 0.05905 \times 0.5 + 0.7 \times 0.12450 \times 0.5} \approx 0.83108\end{aligned}$$

### 3. Maximization (M-step)

Below we will use  $x_{i[y_1]}$  to refer to the variable  $\{y_1\}$  of observation  $x_i$  and  $x_{i[y_2 \wedge y_3]}$  to refer to the variables  $\{y_2, y_3\}$  of observation  $x_i$ .

For each cluster,  $c_k$ , we will calculate the following in order to update the parameters:

$$N_k = \sum_i \gamma_{k,i} \quad (4)$$

$$p'_k = \frac{1}{N_k} \sum_i \gamma_{k,i} \cdot x_{i[y_1]} \quad (5)$$

$$\mu'_k = \frac{1}{N_k} \sum_i \gamma_{k,i} \cdot x_{i[y_2 \wedge y_3]} \quad (6)$$

$$\Sigma'_k = \frac{1}{N_k} \sum_i \gamma_{k,i} \cdot (x_{i[y_2 \wedge y_3]} - \mu'_k) \cdot (x_{i[y_2 \wedge y_3]} - \mu'_k)^T \quad (7)$$

Considering  $N = \sum_k N_k$ , we can also update the priors:

$$\pi'_k = \frac{N_k}{N} \quad (8)$$

We can now update the values for both clusters using the previous equations.

We start off by calculating the sum of the weights, for each cluster,  $N_k$ , by employing equation (4):

$$N_1 = \sum_i \gamma_{1,i} = \gamma_{1,1} + \gamma_{1,2} + \gamma_{1,3} + \gamma_{1,4} = 1.54467$$

$$N_2 = \sum_i \gamma_{2,i} = \gamma_{2,1} + \gamma_{2,2} + \gamma_{2,3} + \gamma_{2,4} = 2.45533$$

#### Cluster 1 Updates

Now for cluster 1 we can update  $p_1$ ,  $\mu_1$ ,  $\Sigma_1$  and  $\pi_1$ , by employing, (5), (6), (7) and (8), respectively:

$$p'_1 = \frac{1}{N_1} \sum_i \gamma_{1,i} \cdot x_{i[y_1]} = \frac{\gamma_{1,1} \cdot 1 + \gamma_{1,2} \cdot 0 + \gamma_{1,3} \cdot 0 + \gamma_{1,4} \cdot 1}{1.54467} = 0.23404$$

$$\mu'_1 = \frac{1}{N_1} \sum_i \gamma_{1,i} \cdot x_{i[y_2 \wedge y_3]} = \frac{\gamma_{1,1} \cdot \begin{pmatrix} 0.6 \\ 0.1 \end{pmatrix} + \gamma_{1,2} \cdot \begin{pmatrix} -0.4 \\ 0.8 \end{pmatrix} + \gamma_{1,3} \cdot \begin{pmatrix} 0.2 \\ 0.5 \end{pmatrix} + \gamma_{1,4} \cdot \begin{pmatrix} 0.4 \\ -0.1 \end{pmatrix}}{1.54467} = \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix}$$

$$\Sigma'_1 = \frac{1}{N_1} \sum_i \gamma_{1,i} \cdot (x_{i[y_2 \wedge y_3]} - \mu'_1) \cdot (x_{i[y_2 \wedge y_3]} - \mu'_1)^T$$

$$\begin{aligned}
&= \frac{1}{1.54467} \times \left[ \gamma_{1,1} \cdot \left( \begin{pmatrix} 0.6 \\ 0.1 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} 0.6 \\ 0.1 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right)^T \\
&+ \gamma_{1,2} \cdot \left( \begin{pmatrix} -0.4 \\ 0.8 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} -0.4 \\ 0.8 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right)^T \\
&+ \gamma_{1,3} \cdot \left( \begin{pmatrix} 0.2 \\ 0.5 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} 0.2 \\ 0.5 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right)^T \\
&+ \gamma_{1,4} \cdot \left( \begin{pmatrix} 0.4 \\ -0.1 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} 0.4 \\ -0.1 \end{pmatrix} - \begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix} \right)^T \Big] \\
&= \begin{pmatrix} 0.14137 & -0.10541 \\ -0.10541 & 0.09605 \end{pmatrix}
\end{aligned}$$

$$\pi'_1 = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2} = \frac{1.54467}{1.54467 + 2.45533} = 0.38617$$

### Cluster 2 Updates

Finally, for cluster 2 we can update  $p_2$ ,  $\mu_2$ ,  $\Sigma_2$  and  $\pi_2$ , by employing, (5), (6), (7) and (8), respectively:

$$p'_2 = \frac{1}{N_2} \sum_i \gamma_{2,i} \cdot x_{i[y_1]} = \frac{\gamma_{2,1} \cdot 1 + \gamma_{2,2} \cdot 0 + \gamma_{2,3} \cdot 0 + \gamma_{2,4} \cdot 1}{2.45533} = 0.66732$$

$$\mu'_2 = \frac{1}{N_2} \sum_i \gamma_{2,i} \cdot x_{i[y_2 \wedge y_3]} = \frac{\gamma_{2,1} \cdot \begin{pmatrix} 0.6 \\ 0.1 \end{pmatrix} + \gamma_{2,2} \cdot \begin{pmatrix} -0.4 \\ 0.8 \end{pmatrix} + \gamma_{2,3} \cdot \begin{pmatrix} 0.2 \\ 0.5 \end{pmatrix} + \gamma_{2,4} \cdot \begin{pmatrix} 0.4 \\ -0.1 \end{pmatrix}}{2.45533} = \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix}$$

$$\begin{aligned}
\Sigma'_2 &= \frac{1}{N_2} \sum_i \gamma_{2,i} \cdot (x_{i[y_2 \wedge y_3]} - \mu'_2) \cdot (x_{i[y_2 \wedge y_3]} - \mu'_2)^T \\
&= \frac{1}{2.45533} \times \left[ \gamma_{2,1} \cdot \left( \begin{pmatrix} 0.6 \\ 0.1 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} 0.6 \\ 0.1 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right)^T \\
&+ \gamma_{2,2} \cdot \left( \begin{pmatrix} -0.4 \\ 0.8 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} -0.4 \\ 0.8 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right)^T \\
&+ \gamma_{2,3} \cdot \left( \begin{pmatrix} 0.2 \\ 0.5 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} 0.2 \\ 0.5 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right)^T \\
&+ \gamma_{2,4} \cdot \left( \begin{pmatrix} 0.4 \\ -0.1 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right) \cdot \left( \begin{pmatrix} 0.4 \\ -0.1 \end{pmatrix} - \begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix} \right)^T \Big] \\
&= \begin{pmatrix} 0.10829 & -0.08865 \\ -0.08865 & 0.10412 \end{pmatrix}
\end{aligned}$$

$$\pi'_2 = \frac{N_2}{N} = \frac{N_2}{N_1 + N_2} = \frac{2.45533}{1.54467 + 2.45533} = 0.61383$$

#### 4. Verify the log likelihood

Since we are only performing one epoch of the EM clustering algorithm, we can skip this step.

#### 5. Conclusion

After performing one epoch of the EM clustering algorithm, we end up with the following updated parameters for each cluster:

Cluster	$p'$	$\mu'$	$\Sigma'$	$\pi'$
Cluster 1	0.23404	$\begin{pmatrix} 0.02651 \\ 0.50713 \end{pmatrix}$	$\begin{pmatrix} 0.14137 & -0.10541 \\ -0.10541 & 0.09605 \end{pmatrix}$	0.38617
Cluster 2	0.66732	$\begin{pmatrix} 0.30914 \\ 0.21042 \end{pmatrix}$	$\begin{pmatrix} 0.10829 & -0.08865 \\ -0.08865 & 0.10412 \end{pmatrix}$	0.61383

Table 2: Updated parameters for the two clusters after one epoch of the EM clustering algorithm

2. **Given the new observation,  $x_{new} = [1 \ 0.3 \ 0.7]^T$ , determine the cluster memberships (posteriors).**

**Note:** As per the *FAQ*, we will be using the updated values obtained in exercise 1.

Using the equation on (3), we can compute, for each cluster,  $c_k$ , the value of  $P(y_2, y_3|c_k)$  for the new observation,  $x_{new}$ :

$$P(y_2 = 0.3, y_3 = 0.7|c_1) = \mathcal{N}_1(y_2 = 0.3, y_3 = 0.7|\mu'_1, \Sigma'_1) \approx 0.02708$$

$$P(y_2 = 0.3, y_3 = 0.7|c_2) = \mathcal{N}_2(y_2 = 0.3, y_3 = 0.7|\mu'_2, \Sigma'_2) \approx 0.06843$$

Now, by using the equation on (2), we can compute the normalized posteriors:

$$\begin{aligned} \gamma_{1,new} &= \frac{P(y_1 = 1|c_1)P(y_2 = 0.3, y_3 = 0.7|c_1)P(c_1)}{P(y_1 = 1|c_1)P(y_2 = 0.3, y_3 = 0.7|c_1)P(c_1) + P(y_1 = 1|c_2)P(y_2 = 0.3, y_3 = 0.7|c_2)P(c_2)} \\ &= \frac{p'_1 \times 0.02708 \times \pi'_1}{p'_1 \times 0.02708 \times \pi'_1 + p'_2 \times 0.06843 \times \pi'_2} \\ &= \frac{0.23404 \times 0.02708 \times 0.38617}{0.23404 \times 0.02708 \times 0.38617 + 0.66732 \times 0.06843 \times 0.61383} \approx 0.08029 \\ \gamma_{2,new} &= \frac{P(y_1 = 1|c_2)P(y_2 = 0.3, y_3 = 0.7|c_2)P(c_2)}{P(y_1 = 1|c_1)P(y_2 = 0.3, y_3 = 0.7|c_1)P(c_1) + P(y_1 = 1|c_2)P(y_2 = 0.3, y_3 = 0.7|c_2)P(c_2)} \\ &= \frac{p'_2 \times 0.06843 \times \pi'_2}{p'_1 \times 0.02708 \times \pi'_1 + p'_2 \times 0.06843 \times \pi'_2} \\ &= \frac{0.66732 \times 0.06843 \times 0.61383}{0.23404 \times 0.02708 \times 0.38617 + 0.66732 \times 0.06843 \times 0.61383} \approx 0.91971 \end{aligned}$$

3. **Performing a hard assignment of observations to clusters under a ML assumption, identify the silhouette of both clusters under a Manhattan distance.**

**Note:** As per the *FAQ*, we will be using the updated values obtained in exercise 1 and only show the calculus for the observation  $x_2$ , only presenting the remaining results in Table 3.

Firstly, we need to calculate the updated likelihoods. For that, we consider  $\{y_1\} \perp\!\!\!\perp \{y_2, y_3\}$  and multiply  $P(y_1|c_k)$  by  $P(y_2, y_3|c_k)$ , which is given by the equation (3):

$$\begin{aligned} P(x_2|c_1) &= P(y_1 = 0|c_1) \times P(y_2 = -0.4, y_3 = 0.8|c_1) = (1 - p'_1) \times \mathcal{N}_1(y_2 = -0.4, y_3 = 0.8|\mu'_1, \Sigma'_1) \\ &= 0.76596 \times 1.65326 \approx 1.26633 \end{aligned}$$

$$\begin{aligned} P(x_2|c_2) &= P(y_1 = 0|c_2) \times P(y_2 = -0.4, y_3 = 0.8|c_2) = (1 - p'_2) \times \mathcal{N}_2(y_2 = -0.4, y_3 = 0.8|\mu'_2, \Sigma'_2) \\ &= 0.33268 \times 0.26673 \approx 0.08874 \end{aligned}$$

Cluster		$P(x_1 c_k)$	$P(x_2 c_k)$	$P(x_3 c_k)$	$P(x_4 c_k)$
Cluster 1	$(c_1)$	0.23147	1.26633	1.43811	0.02077
Cluster 2	$(c_2)$	0.94954	0.08874	0.45417	0.72331

Table 3: Updated likelihoods for the two clusters

Based on the calculated likelihoods, we can infer that  $x_1$  and  $x_4$  are assigned to Cluster 2, while  $x_2$  and  $x_3$  are assigned to Cluster 1:

$$C_1 = \{x_2, x_3\} \quad C_2 = \{x_1, x_4\}$$

The Manhattan distance is given by the following equation:

$$d(P, Q) = d((a_1, b_1, c_1), (a_2, b_2, c_2)) = |a_2 - a_1| + |b_2 - b_1| + |c_2 - c_1| \quad (9)$$

By employing equation (9), we can create the Table 4 that has the manhattan distances between every pair of observations. Only the upper diagonal entries are filled, because the distance function is commutative.

$d(x_i, x_j)$	$x_1$	$x_2$	$x_3$	$x_4$
$x_1$	0	2.7	1.8	0.4
$x_2$	-	0	0.9	2.7
$x_3$	-	-	0	1.8
$x_4$	-	-	-	0

Table 4: Manhattan distances between every pair of observations

The Cohesion ( $a(x_i)$ ), Separation ( $b(x_i)$ ) and Silhouette ( $S(x_i)$ ), for a given observation  $x_i$ , are given by:

$a(x_i)$  = average distance of  $x_i$  to the other points in its cluster

$b(x_i) = \min_j \{\text{average distance of } x_i \text{ to the points of cluster } C_j \text{ such that } x_i \notin C_j\}$

$$S(x_i) = \frac{b(x_i) - a(x_i)}{\max\{b(x_i), a(x_i)\}} \quad (10)$$

The silhouette for a cluster  $C_k$  is given by:

$$S(C_k) = \frac{\sum_{x_i \in C_k} S(x_i)}{|C_k|} \quad (11)$$

By replacing the values on the equation (10), we get the following values:

$$\begin{aligned} S(x_1) &= \frac{\frac{d(x_1, x_2) + d(x_1, x_3)}{2} - d(x_1, x_4)}{\max \left\{ \frac{d(x_1, x_2) + d(x_1, x_3)}{2}, d(x_1, x_4) \right\}} \approx 0.82222 \\ S(x_2) &= \frac{\frac{d(x_2, x_1) + d(x_2, x_4)}{2} - d(x_2, x_3)}{\max \left\{ \frac{d(x_2, x_1) + d(x_2, x_4)}{2}, d(x_2, x_3) \right\}} \approx 0.66667 \\ S(x_3) &= \frac{\frac{d(x_3, x_1) + d(x_3, x_4)}{2} - d(x_3, x_2)}{\max \left\{ \frac{d(x_3, x_1) + d(x_3, x_4)}{2}, d(x_3, x_2) \right\}} \approx 0.49999 \\ S(x_4) &= \frac{\frac{d(x_4, x_2) + d(x_4, x_3)}{2} - d(x_4, x_1)}{\max \left\{ \frac{d(x_4, x_2) + d(x_4, x_3)}{2}, d(x_4, x_1) \right\}} \approx 0.82222 \end{aligned}$$

Therefore the values of the silhouette for the clusters are given by (11):

$$S(C_1) = \frac{S(x_2) + S(x_3)}{2} = 0.58333 \quad S(C_2) = \frac{S(x_1) + S(x_4)}{2} = 0.82222$$

**4. Knowing the purity of the clustering solution is 0.75, identify the number of possible classes (ground truth).**

Since we know that the purity of the clustering solution is 0.75, we can deduce the number of correctly labeled observations:

$$\begin{aligned} \text{purity} &= \frac{1}{n} \sum_{k=1}^K \max_j \{|C_k \cap L_j|\} = \frac{1}{4} (\max_j \{|C_1 \cap L_j|\} + \max_j \{|C_2 \cap L_j|\}) = 0.75 \\ \Rightarrow \max_j \{|C_1 \cap L_j|\} + \max_j \{|C_2 \cap L_j|\} &= 4 \times 0.75 = 3 \end{aligned}$$

We know that the number of observations correctly assigned to a cluster is 3. Since there are 4 observations in total, we can conclude that one observation was misclassified.

The number of possible classes needs to be greater than or equal to the number of clusters. If we assume the minimum number of classes, which is two ( $L_1$  and  $L_2$ ), we know that the misclassified observation is in the opposing class. But there is also a possibility that there is a class ( $L_3$ ), that wasn't initially considered, where the misclassified observation should be.

Below are all the possible cases for only one misclassified observation, knowing that  $C_1 = \{x_2, x_3\}$  and  $C_2 = \{x_1, x_4\}$  from the previous exercise:



$$\begin{array}{c|c|c|c} L_1 = \{x_2, x_3, x_4\} & L_1 = \{x_2, x_3, x_1\} & L_1 = \{x_2\} & L_1 = \{x_3\} \\ L_2 = \{x_1\} & L_2 = \{x_4\} & L_2 = \{x_1, x_4, x_3\} & L_2 = \{x_1, x_4, x_2\} \end{array} \quad (12)$$

$$\begin{array}{c|c|c|c} L_1 = \{x_2, x_3\} & L_1 = \{x_2, x_3\} & L_1 = \{x_2\} & L_1 = \{x_3\} \\ L_2 = \{x_1\} & L_2 = \{x_4\} & L_2 = \{x_1, x_4\} & L_2 = \{x_1, x_4\} \\ L_3 = \{x_4\} & L_3 = \{x_1\} & L_3 = \{x_3\} & L_3 = \{x_2\} \end{array} \quad (13)$$

**Therefore**, the number of possible classes (ground truth) is either two (12) or three (13).

## Part II: Programming and critical analysis

Recall the `column_diagnosis.arff` dataset from previous homeworks. For the following exercises, normalize the data using sklearn's `MinMaxScaler`.

1. Using **sklearn**, apply ***k*-means clustering fully unsupervisedly on the normalized data with  $k \in \{2, 3, 4, 5\}$  (random = 0 and remaining parameters as default). Assess the silhouette and purity of the produced solutions.**

Using sklearn's `cluster.KMeans` class, we can apply a *k*-means clustering algorithm for each  $k \in \{2, 3, 4, 5\}$  with `random = 0` and remaining parameters as default.

We opted for the default parameters in the `metric.silhouette_score` function.

To calculate the purity score, we used the code in the `purity_score` function from the course's N5 (Clustering) Notebook available in [Fénix](#).

```
1 import numpy as np, pandas as pd
2 from scipy.io.arff import loadarff
3 from sklearn.preprocessing import MinMaxScaler
4 from sklearn import cluster, metrics
5
6 # Read the ARFF file, prepare data and normalize it
7 data = loadarff("./data/column_diagnosis.arff")
8 df = pd.DataFrame(data[0])
9 df["class"] = df["class"].str.decode("utf-8")
10 X, y = df.drop("class", axis=1), df["class"]
11 X_scaled = MinMaxScaler().fit_transform(X)
12
13 # Parametrize the clustering and learn the model
14 k_means_models = []
15 for n_clusters in [2, 3, 4, 5]:
16     k_means = cluster.KMeans(n_clusters=n_clusters, random_state=0)
17     k_means_models.append(k_means.fit(X_scaled))
18
19 for model in k_means_models:
20     n_clusters = model.n_clusters
21     y_pred = model.labels_
22
23     # Calculate the silhouette
24     silhouette = metrics.silhouette_score(X_scaled, y_pred)
25
26     # Calculate the purity
```

```

27 conf_matrix = metrics.cluster.contingency_matrix(y, y_pred)
28 purity = np.sum(np.amax(conf_matrix, axis=0)) / np.sum(conf_matrix)
29
30 # Print the results for each number of clusters
31 print(f"Clustering with n_clusters = {n_clusters}")
32 print(f"\tSilhouette = {silhouette:6.5f}")
33 print(f"\tPurity = {purity:6.5f}")
34 print()

```

n_clusters	2	3	4	5
Silhouette	0.36044	0.29579	0.27442	0.23824
Purity	0.63226	0.66774	0.66129	0.67742

Table 5: Silhouette and purity scores (rounded to 5 decimal places) for  $n\_clusters \in \{2, 3, 4, 5\}$

## 2. Consider the application of PCA after the data normalization:

### (a) Identify the variability explained by the top two principal components.

```

1 from sklearn.decomposition import PCA
2
3 # Apply PCA to the normalized data
4 pca = PCA(n_components=2)
5 X_pca = pca.fit_transform(X_scaled)
6
7 # Variability explained by the top two principal components
8 explained_variance_ratio = pca.explained_variance_ratio_
9 print(f"Explained Variance Ratio for Top 2 PCs: {explained_variance_ratio}")
10 print(f"Total variability: {explained_variance_ratio[0] +
    explained_variance_ratio[1]}")

```

The explained variability for the top 2 PCs is 56.181445% and 20.955953% respectively.

And the total explained variability is 77.1374%.

### (b) For each one of these two components, sort the input variables by relevance by inspecting the absolute weights of the linear projection.

```

1 # Get the absolute weights (loadings) of the top two principal components
2 pc_weights = np.abs(pca.components_[:2, :])
3
4 # Get the feature names
5 feature_names = X.columns
6
7 # Sort the feature names by relevance for each PC
8 sorted_features_pc1 = [feature_names[i] for i in np.argsort(pc_weights[0])
    [::-1]]
9 sorted_features_pc2 = [feature_names[i] for i in np.argsort(pc_weights[1])
    [::-1]]
10
11 print(f"Top Variables for PC1: {sorted_features_pc1}")
12 print(f"Top Variables for PC2: {sorted_features_pc2}")

```

### Top Variables for PC1:

1. pelvic\_incidence
2. lumbar\_lordosis\_angle
3. pelvic\_tilt
4. sacral\_slope
5. degree\_spondylolisthesis
6. pelvic\_radius

### Top Variables for PC2:

1. pelvic\_tilt
2. pelvic\_radius
3. sacral\_slope
4. pelvic\_incidence
5. lumbar\_lordosis\_angle
6. degree\_spondylolisthesis

3. **Visualize side-by-side the data using: i) the ground diagnoses, and ii) the *previously* learned  $k = 3$  clustering solution. To this end, projected the normalized data onto a 2-dimensional data space using PCA and then color observations using the reference and cluster annotations.**

```
1 import matplotlib.pyplot as plt
2 from matplotlib.colors import ListedColormap
3 from sklearn.preprocessing import LabelEncoder
4
5 # Apply PCA to the normalized data
6 pca = PCA(n_components=2)
7 X_pca = pca.fit_transform(X_scaled)
8
9 # Convert labels to numerical format
10 le = LabelEncoder()
11 y_numerical = le.fit_transform(y)
12
13 # Create a figure with two subplots
14 fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 5))
15
16 # Plot the ground diagnoses
17 scatter1 = ax1.scatter(X_pca[:, 0], X_pca[:, 1], c=y_numerical, cmap='viridis')
18 ax1.set_title('Ground Diagnoses')
19 ax1.legend(handles=scatter1.legend_elements()[0], labels=list(set(y)))
20
21 # Plot the k-means clustering solution (k=3)
22 k_means = cluster.KMeans(n_clusters=3, random_state=0)
23 y_pred = k_means.fit_predict(X_scaled)
24
25 scatter2 = ax2.scatter(X_pca[:, 0], X_pca[:, 1], c=y_pred, cmap='viridis')
26 ax2.set_title('K-Means Clustering (k=3)')
27 ax2.legend(handles=scatter2.legend_elements()[0], labels=['Cluster 0', 'Cluster 1',
28     , 'Cluster 2'])
29 plt.show()
```

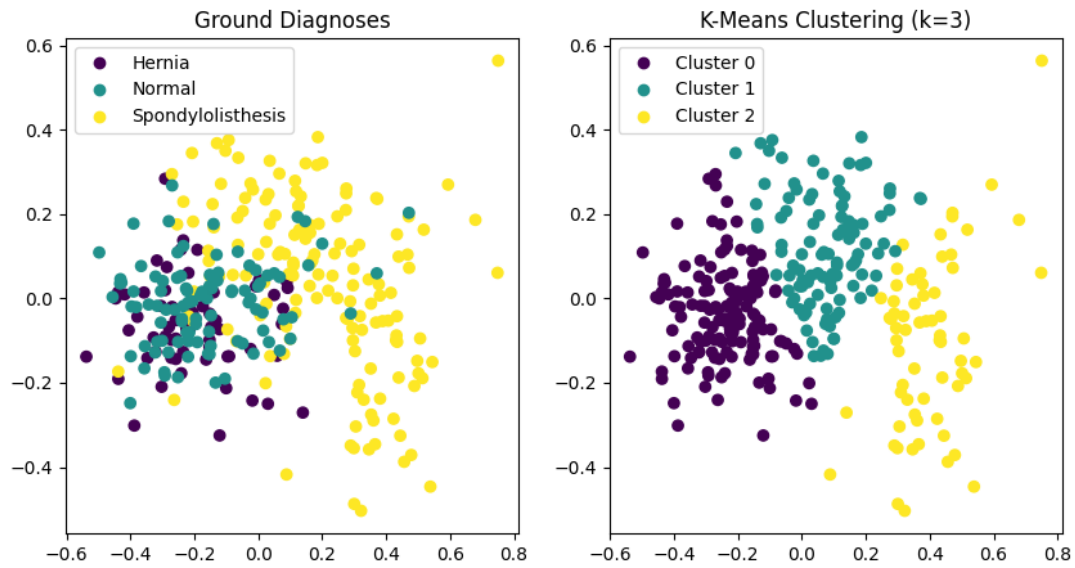


Figure 1: Projected data

4. **Considering the results from questions (1) and (3), identify two ways on how clustering can be used to characterize the population of ill and healthy individuals.**

Raquel