Machine Learning - Homework 4

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Pen and Paper Exercises

Dataset

In the following exercise our goal is to consider a Bayesian Clustering model in order to separate the observations into 2 different clusters:

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

We are working with 3 different variables (y_1, y_1, y_3) for each observation. In addition, we are assuming:

1. $\{y_1\} \perp \{y_2, y_3\}$
2. y_1 follows a Bernoulli distribution with parameter p: $y_1 \sim \text{Bernoulli}(p)$

$$P(y_1 = 1) = p \qquad P(y_1 = 0) = 1 - p$$

3. y_2 and y_3 follow a multivariate gaussian distribution with parameters $\vec{\mu}$ and Σ: $y_2, y_3 \sim \mathcal{N}(\vec{\mu}, \Sigma)$

$$P(\vec{x}) = \frac{1}{2\pi\sqrt{|\Sigma|}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu})^T \Sigma^{-1} (\vec{x} - \vec{\mu})\right)$$

$$\vec{x} = (y_2, y_3)$$

1st Question

Computing the Responsibilities

First, we need to compute the responsibility of each cluster for each observation. The responsibility γ_{ki} is defined as the probability of belonging to cluster k for observation i:

$$\gamma_{ki} = P(c_k|\vec{x_i}) =_{\text{Bayes}} \frac{P(\vec{x_i}|c_k)P(c_k)}{P(\vec{x_i})} = \frac{P(\vec{x_i}|c_k)P(c_k)}{\sum_{j=1}^{K} P(\vec{x_i}|c_j)P(c_j)}$$

$$\sum_{j=1}^{K} P(\vec{x_i}|c_j)P(c_j) = P(\vec{x_i})$$

Where c_k is the cluster k, K is the number of clusters and $\vec{x_i}$ is the observation i. In addition, the probability of belonging to cluster k, $P(c_k)$, is represented by the mixing coefficient π_k:

$$P(c_k) = \pi_k$$

In order to compute the responsibilities, we're told to use the following parameters for each cluster's y_1 and y_2, y_3 distributions:

Cluster	π_k	Parameters for $\{y_1\}$	Parameters for $\{y_2, y_3\}$
1 (c_1)	$P(c_1) = \pi_1 = 0.5$	$p_1 = P(y_1 = 1) = 0.3$	$\{y_2, y_3\} \sim \mathcal{N}\left(\vec{\mu}_1 = \begin{bmatrix}1\\1\end{bmatrix}, \Sigma_1 = \begin{bmatrix}2 & 0.5\\0.5 & 2\end{bmatrix}\right)$
2 (c_2)	$P(c_2) = \pi_2 = 0.5$	$p_2 = P(y_1 = 1) = 0.7$	$\{y_2, y_3\} \sim \mathcal{N}\left(\vec{\mu}_2 = \begin{bmatrix}0\\0\end{bmatrix}, \Sigma_2 = \begin{bmatrix}1.5 & 1\\1 & 1.5\end{bmatrix}\right)$

Table 1: Initial Parameters for each cluster

Responsibilities for $\vec{x_1}$

First of all, we will compute $P(\vec{x_1}|c_k)P(c_k)$ for clusters c_1 and c_2:

$$P(\vec{x_1}|c_1)P(c_1) = P(y_1 = 1|c_1)P(\{y_2, y_3\} = \{0.6, 0.1\}|c_1)\pi_1 = 0.3 \cdot 0.06658 \cdot 0.5 = 0.00999$$

$$P(\vec{x_1}|c_2)P(c_2) = P(y_1 = 1|c_2)P(\{y_2, y_3\} = \{0.6, 0.1\}|c_2)\pi_2 = 0.7 \cdot 0.11962 \cdot 0.5 = 0.04187$$

And then, we can compute γ_{ki}:

$$\gamma_{11} = P(c_1|\vec{x_1}) = \frac{P(\vec{x_1}|c_1)P(c_1)}{P(\vec{x_1})} = \frac{P(\vec{x_1}|c_1)P(c_1)}{\sum_{j=1}^{2} P(\vec{x_1}|c_j)P(c_j)} = \frac{0.00999}{0.00999 + 0.04187} = 0.19259$$

$$\gamma_{21} = P(c_2|\vec{x_1}) = \frac{P(\vec{x_1}|c_2)P(c_2)}{P(\vec{x_1})} = \frac{P(\vec{x_1}|c_2)P(c_2)}{\sum_{j=1}^{2} P(\vec{x_1}|c_j)P(c_j)} = \frac{0.04187}{0.00999 + 0.04187} = 0.80741$$

Responsibilities for $\vec{x}_2$

First of all, we will compute $P(\vec{x}_2|c_k)P(c_k)$ for clusters c_1 and c_2:

$$P(\vec{x}_2|c_1)P(c_1) = P(y_1 = 0|c_1)P(\{y_2, y_3\} = \{-0.4, 0.8\}|c_1)\pi_1 = 0.7 \cdot 0.05005 \cdot 0.5 = 0.01752$$

$$P(\vec{x}_2|c_2)P(c_2) = P(y_1 = 0|c_2)P(\{y_2, y_3\} = \{-0.4, 0.8\}|c_2)\pi_2 = 0.3 \cdot 0.06819 \cdot 0.5 = 0.01023$$

And then, we can compute γ_{ki}:

$$\gamma_{12} = P(c_1|\vec{x}_2) = \frac{P(\vec{x}_2|c_1)P(c_1)}{P(\vec{x}_2)} = \frac{P(\vec{x}_2|c_1)P(c_1)}{\sum_{j=1}^{2} P(\vec{x}_2|c_j)P(c_j)} = \frac{0.01752}{0.01752 + 0.01023} = 0.63135$$

$$\gamma_{22} = P(c_2|\vec{x}_2) = \frac{P(\vec{x}_2|c_2)P(c_2)}{P(\vec{x}_2)} = \frac{P(\vec{x}_2|c_2)P(c_2)}{\sum_{j=1}^{2} P(\vec{x}_2|c_j)P(c_j)} = \frac{0.01023}{0.01752 + 0.01023} = 0.36865$$

Responsibilities for $\vec{x}_3$

First of all, we will compute $P(\vec{x}_3|c_k)P(c_k)$ for clusters c_1 and c_2:

$$P(\vec{x}_3|c_1)P(c_1) = P(y_1 = 0|c_1)P(\{y_2, y_3\} = \{0.2, 0.5\}|c_1)\pi_1 = 0.7 \cdot 0.06837 \cdot 0.5 = 0.02393$$

$$P(\vec{x}_3|c_2)P(c_2) = P(y_1 = 0|c_2)P(\{y_2, y_3\} = \{0.2, 0.5\}|c_2)\pi_2 = 0.3 \cdot 0.12958 \cdot 0.5 = 0.01944$$

And then, we can compute γ_{ki}:

$$\gamma_{13} = P(c_1|\vec{x}_3) = \frac{P(\vec{x}_3|c_1)P(c_1)}{P(\vec{x}_3)} = \frac{P(\vec{x}_3|c_1)P(c_1)}{\sum_{j=1}^{2} P(\vec{x}_3|c_j)P(c_j)} = \frac{0.02393}{0.02393 + 0.01944} = 0.55181$$

$$\gamma_{23} = P(c_2|\vec{x}_3) = \frac{P(\vec{x}_3|c_2)P(c_2)}{P(\vec{x}_3)} = \frac{P(\vec{x}_3|c_2)P(c_2)}{\sum_{j=1}^{2} P(\vec{x}_3|c_j)P(c_j)} = \frac{0.01944}{0.02393 + 0.01944} = 0.44819$$

Responsibilities for $\vec{x}_4$

First of all, we will compute $P(\vec{x}_4|c_k)P(c_k)$ for clusters c_1 and c_2:

$$P(\vec{x}_4|c_1)P(c_1) = P(y_1 = 1|c_1)P(\{y_2, y_3\} = \{0.4, -0.1\}|c_1)\pi_1 = 0.3 \cdot 0.05905 \cdot 0.5 = 0.00886$$

$$P(\vec{x}_4|c_2)P(c_2) = P(y_1 = 1|c_2)P(\{y_2, y_3\} = \{0.4, -0.1\}|c_2)\pi_2 = 0.7 \cdot 0.12450 \cdot 0.5 = 0.04358$$

And then, we can compute γ_{ki}:

$$\gamma_{14} = P(c_1|\vec{x}_4) = \frac{P(\vec{x}_4|c_1)P(c_1)}{P(\vec{x}_4)} = \frac{P(\vec{x}_4|c_1)P(c_1)}{\sum_{j=1}^{2} P(\vec{x}_4|c_j)P(c_j)} = \frac{0.00886}{0.00886 + 0.04358} = 0.16892$$

$$\gamma_{24} = P(c_2|\vec{x}_4) = \frac{P(\vec{x}_4|c_2)P(c_2)}{P(\vec{x}_4)} = \frac{P(\vec{x}_4|c_2)P(c_2)}{\sum_{j=1}^{2} P(\vec{x}_4|c_j)P(c_j)} = \frac{0.04358}{0.00886 + 0.04358} = 0.83108$$

Responsibilities

$\gamma_{11} = 0.19259$	$\gamma_{12} = 0.63135$	$\gamma_{13} = 0.55181$	$\gamma_{14} = 0.16892$
$\gamma_{21} = 0.80741$	$\gamma_{22} = 0.36865$	$\gamma_{23} = 0.44819$	$\gamma_{24} = 0.83108$

M-Step

In the M-Step (Maximization Step), we will compute the new parameters for each cluster (we need to update the parameters in the table **??**).

New Parameters for Cluster c_1

$$\vec{\mu}_{1_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{1i} \vec{x}_i}{\sum_{i=1}^{4} \gamma_{1i}} = \begin{bmatrix} 0.02651 & 0.50713 \end{bmatrix}$$

$$\Sigma_{1_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{1i} \left(\vec{x}_i - \vec{\mu}_{1_{\text{new}}}\right) \left(\vec{x}_i - \vec{\mu}_{1_{\text{new}}}\right)^T}{\sum_{i=1}^{4} \gamma_{1i}} = \begin{bmatrix} 0.14137 & -0.10541 \\ -0.10541 & 0.09605 \end{bmatrix}$$

$$p_{1_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{1i} \vec{x}_i}{\sum_{i=1}^{4} \gamma_{1i}} = 0.23404$$

$$\pi_{1_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{1i}}{4} = 0.38617$$

New Parameters for Cluster c_2

$$\vec{\mu}_{2_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{2i} \vec{x}_i}{\sum_{i=1}^{4} \gamma_{2i}} = \begin{bmatrix} 0.30914 & 0.21042 \end{bmatrix}$$

$$\Sigma_{2_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{2i} \left(\vec{x}_i - \vec{\mu}_{2_{\text{new}}}\right) \left(\vec{x}_i - \vec{\mu}_{2_{\text{new}}}\right)^T}{\sum_{i=1}^{4} \gamma_{2i}} = \begin{bmatrix} 0.10829 & -0.08865 \\ -0.08865 & 0.10412 \end{bmatrix}$$

$$p_{2_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{2i} \vec{x}_i}{\sum_{i=1}^{4} \gamma_{2i}} = 0.66732$$

$$\pi_{2_{\text{new}}} = \frac{\sum_{i=1}^{4} \gamma_{2i}}{4} = 0.61383$$

New table with the updated parameters

Cluster	π_k	Parameters for $\{y_1\}$	Parameters for $\{y_2, y_3\}$
1 (c_1)	$P(c_1) = \pi_1 = 0.38617$	$p_1 = 0.23404$	$\{y_2, y_3\} \sim \mathcal{N}\left(\vec{\mu}_1 = \begin{bmatrix} 0.02651 \\ 0.50713 \end{bmatrix}, \Sigma_1 = \begin{bmatrix} 0.14137 & -0.10541 \\ -0.10541 & 0.09605 \end{bmatrix}\right)$
2 (c_2)	$P(c_2) = \pi_2 = 0.61383$	$p_2 = 0.66732$	$\{y_2, y_3\} \sim \mathcal{N}\left(\vec{\mu}_2 = \begin{bmatrix} 0.30914 \\ 0.21042 \end{bmatrix}, \Sigma_2 = \begin{bmatrix} 0.10829 & -0.08865 \\ -0.08865 & 0.10412 \end{bmatrix}\right)$

Table 2: New Parameters for each cluster

2nd Question

We now have a new observation $\vec{x}_{\text{new}}$ and want to compute the probability of belonging to each cluster using a ML approach. The new observation is:

$$\vec{x}_{\text{new}} = \begin{bmatrix} 1 \\ 0.3 \\ 0.7 \end{bmatrix}$$

First, we will compute $P(\vec{x}_{\text{new}}|c_k)P(c_k)$ for clusters c_1 and c_2:

$$P(\vec{x}_{\text{new}}|c_1)P(c_1) = P(y_1 = 1|c_1)P(\{y_2, y_3\}\pi_1 = \{0.3, 0.7\}|c_1) = 0.23404 \cdot 0.02708 \cdot 0.38617 = 0.00245$$

$$P(\vec{x}_{\text{new}}|c_2)P(c_2) = P(y_1 = 1|c_2)P(\{y_2, y_3\}\pi_2 = \{0.3, 0.7\}|c_2) = 0.66732 \cdot 0.06843 \cdot 0.61383 = 0.02803$$

And then, we can compute γ_{ki}:

$$\gamma_{1_{\text{new}}} = P(c_1|\vec{x}_{\text{new}}) = \frac{P(\vec{x}_{\text{new}}|c_1)P(c_1)}{P(\vec{x}_{\text{new}})} = \frac{0.00245}{0.00245 + 0.02803} = 0.08029$$

$$\gamma_{2_{\text{new}}} = P(c_2|\vec{x}_{\text{new}}) = \frac{P(\vec{x}_{\text{new}}|c_2)P(c_2)}{P(\vec{x}_{\text{new}})} = \frac{0.02803}{0.00245 + 0.02803} = 0.91971$$

Answer We can conclude that the observation $\vec{x}_{\text{new}}$ belongs to cluster c_2 with a probability of 0.91971 and to cluster c_1 with a probability of 0.08029.

3rd Question

Along the first and second questions, we have worked under a soft assignment approach. In this question, we will work under a hard assignment approach: we will assign each observation to the cluster with the highest probability instead of assigning each observation to each cluster with a certain probability. Beyond that, we are asked to use a ML approach to compute the responsibilities. Hence, we will compute $P(\vec{x}_{\text{new}}|c_k)$ for clusters c_1 and c_2, using the parameters from table **??**:

Cluster for $\vec{x}_1$

$$P(\vec{x}_1|c_1) = P(y_1 = 1|c_1)P(\{y_2, y_3\} = \{0.6, 0.1\}|c_1) = 0.23404 \cdot 0.98904 = 0.23147$$

$$P(\vec{x}_1|c_2) = P(y_1 = 1|c_2)P(\{y_2, y_3\} = \{0.6, 0.1\}|c_2) = 0.66732 \cdot 1.42292 = 0.94954$$

$$\gamma_{11} = P(c_1|\vec{x}_1) = \frac{P(\vec{x}_1|c_1)}{P(\vec{x}_1)} = \frac{0.23147}{0.23147 + 0.94954} = 0.19600$$

$$\gamma_{21} = P(c_2|\vec{x}_1) = \frac{P(\vec{x}_1|c_2)}{P(\vec{x}_1)} = \frac{0.94954}{0.23147 + 0.58286} = 0.80400$$

We can conclude that the observation $\vec{x}_1$ belongs to cluster c_2 because $\gamma_{21} > \gamma_{11}$.

Cluster for $\vec{x}_2$

$$P(\vec{x}_2|c_1) = P(y_1 = 0|c_1)P(\{y_2, y_3\} = \{-0.4, 0.8\}|c_1) = 0.76596 \cdot 1.65326 = 1.26633$$

$$P(\vec{x}_2|c_2) = P(y_1 = 0|c_2)P(\{y_2, y_3\} = \{-0.4, 0.8\}|c_2) = 0.33268 \cdot 0.26673 = 0.08874$$

$$\gamma_{12} = P(c_1|\vec{x}_2) = \frac{P(\vec{x}_2|c_1)}{P(\vec{x}_2)} = \frac{1.26633}{1.26633 + 0.08874} = 0.93451$$

$$\gamma_{22} = P(c_2|\vec{x}_2) = \frac{P(\vec{x}_2|c_2)}{P(\vec{x}_2)} = \frac{0.08874}{1.26633 + 0.08874} = 0.06549$$

We can conclude that the observation $\vec{x}_2$ belongs to cluster c_1 because $\gamma_{12} > \gamma_{22}$.

Cluster for $\vec{x}_3$

$$P(\vec{x}_3|c_1) = P(y_1 = 0|c_1)P(\{y_2, y_3\} = \{0.2, 0.5\}|c_1) = 0.76596 \cdot 1.87753 = 1.43811$$

$$P(\vec{x}_3|c_2) = P(y_1 = 0|c_2)P(\{y_2, y_3\} = \{0.2, 0.5\}|c_2) = 0.33268 \cdot 1.36519 = 0.45417$$

$$\gamma_{13} = P(c_1|\vec{x}_3) = \frac{P(\vec{x}_3|c_1)}{P(\vec{x}_3)} = \frac{1.43811}{1.43811 + 0.45417} = 0.75999$$

$$\gamma_{23} = P(c_2|\vec{x}_3) = \frac{P(\vec{x}_3|c_2)}{P(\vec{x}_3)} = \frac{0.45417}{1.43811 + 0.45417} = 0.24001$$

We can conclude that the observation $\vec{x}_3$ belongs to cluster c_1 because $\gamma_{13} > \gamma_{23}$.

Cluster for $\vec{x}_4$

$$P(\vec{x}_4|c_1) = P(y_1 = 1|c_1)P(\{y_2, y_3\} = \{0.4, -0.1\}|c_1) = 0.23404 \cdot 0.08873 = 0.02077$$

$$P(\vec{x}_4|c_2) = P(y_1 = 1|c_2)P(\{y_2, y_3\} = \{0.4, -0.1\}|c_2) = 0.66732 \cdot 1.08391 = 0.72331$$

$$\gamma_{14} = P(c_1|\vec{x}_4) = \frac{P(\vec{x}_4|c_1)}{P(\vec{x}_4)} = \frac{0.02077}{0.02077 + 0.72331} = 0.02791$$

$$\gamma_{24} = P(c_2|\vec{x}_4) = \frac{P(\vec{x}_4|c_2)}{P(\vec{x}_4)} = \frac{0.72331}{0.02077 + 0.72331} = 0.97209$$

We can conclude that the observation $\vec{x}_4$ belongs to cluster c_2 because $\gamma_{24} > \gamma_{14}$.

Clusters for each observation

Observation	$\vec{x}_1$	$\vec{x}_2$	$\vec{x}_3$	$\vec{x}_4$
Cluster	c_2	c_1	c_1	c_2

Table 3: Cluster for each observation

Silhouette Coefficient of the Clustering

The silhouette coefficient of the clustering is defined as the mean of the silhouette coefficients of each cluster. The silhouette coefficient of each cluster is defined as the mean of the silhouette coefficients of each observation in the cluster. The silhouette coefficient of each observation is defined as:

$$S(\text{clustering}) = \frac{1}{K}\sum_{i=1}^{K} S(c_i)$$

$$S(c_i) = \frac{1}{N_i}\sum_{j=1}^{N_i} S(\vec{x}_j)$$

$$S(\vec{x}_i) = \frac{b(\vec{x}_i) - a(\vec{x}_i)}{\max\{a(\vec{x}_i), b(\vec{x}_i)\}}$$

Where $a(\vec{x}_i)$ is the mean distance between $\vec{x}_i$ and the other observations in the same cluster and $b(\vec{x}_i)$ is the mean distance between $\vec{x}_i$ and the observations in the other clusters. N_i is the number of observations in the cluster c_i and K is the number of clusters.

Distances between Observations

In this exercise we are considering the Manhattan distance between observations:

$$d(\vec{x}_i, \vec{x}_j) = \sum_{k=1}^{3} |x_{ik} - x_{jk}|$$

We computed the distances between each observation in the following table:

Observation	$\vec{x}_1$	$\vec{x}_2$	$\vec{x}_3$	$\vec{x}_4$
$\vec{x}_1$	0	2.7	1.8	0.4
$\vec{x}_2$	2.7	0	0.9	2.7
$\vec{x}_3$	1.8	0.9	0	1.8
$\vec{x}_4$	0.4	2.7	1.8	0

Table 4: Distances between observations

Computing $\vec{a}$

We will now compute $\vec{a}$ for each observation. $\vec{a}$ is the mean distance between $\vec{x}_i$ and the other observations in the same cluster:

$$\vec{a} = \begin{bmatrix} a(\vec{x}_1) \\ a(\vec{x}_2) \\ a(\vec{x}_3) \\ a(\vec{x}_4) \end{bmatrix} = \begin{bmatrix} \frac{0.4}{1} \\ \frac{0.9}{1} \\ \frac{0.9}{1} \\ \frac{0.4}{1} \end{bmatrix} = \begin{bmatrix} 0.4 \\ 0.9 \\ 0.9 \\ 0.4 \end{bmatrix}$$

Computing $\vec{b}$

We will now compute $\vec{b}$ for each observation. $\vec{b}$ is the mean distance between $\vec{x}_i$ and the observations in the other clusters:

$$\vec{b} = \begin{bmatrix} b(\vec{x}_1) \\ b(\vec{x}_2) \\ b(\vec{x}_3) \\ b(\vec{x}_4 \end{bmatrix} = \begin{bmatrix} \frac{2.7+1.8}{2} \\ \frac{2.7+2.7}{2} \\ \frac{1.8+1.8}{2} \\ \frac{2.7+1.8}{2} \end{bmatrix} = \begin{bmatrix} 2.25 \\ 2.7 \\ 1.8 \\ 2.25 \end{bmatrix}$$

Silhouette Coefficient of each Observation

$$S(\vec{x}_1) = \frac{b(\vec{x}_1) - a(\vec{x}_1)}{\max\{a(\vec{x}_1), b(\vec{x}_1)\}} = \frac{2.25 - 0.4}{\max\{0.4, 2.25\}} = 0.82222$$
$$S(\vec{x}_2) = \frac{b(\vec{x}_2) - a(\vec{x}_2)}{\max\{a(\vec{x}_2), b(\vec{x}_2)\}} = \frac{2.7 - 0.9}{\max\{0.9, 2.7\}} = 0.66667$$
$$S(\vec{x}_3) = \frac{b(\vec{x}_3) - a(\vec{x}_3)}{\max\{a(\vec{x}_3), b(\vec{x}_3)\}} = \frac{1.8 - 0.9}{\max\{0.9, 1.8\}} = 0.5$$
$$S(\vec{x}_4) = \frac{b(\vec{x}_4) - a(\vec{x}_4)}{\max\{a(\vec{x}_4), b(\vec{x}_4)\}} = \frac{2.25 - 0.4}{\max\{0.4, 2.25\}} = 0.82222$$

Silhouette Coefficient of each Cluster

$$S(c_1) = \frac{1}{N_1}\sum_{j=1}^{N_1} S(\vec{x_j}) = \frac{1}{2}(S(\vec{x_2}) + S(\vec{x_3})) = \frac{1}{2}(0.66667 + 0.5) = 0.58333$$

$$S(c_2) = \frac{1}{N_2}\sum_{j=1}^{N_2} S(\vec{x_j}) = \frac{1}{2}(S(\vec{x_1}) + S(\vec{x_4})) = \frac{1}{2}(0.82222 + 0.82222) = 0.82222$$

Silhouette Coefficient of the Clustering

$$S(\text{clustering}) = \frac{1}{K}\sum_{i=1}^{K} S(c_i) = \frac{1}{2}(S(c_1) + S(c_2)) = \frac{1}{2}(0.58333 + 0.82222) = 0.70278$$

Answer The silhouette coefficient of the clustering is 0.70278.

4th Question

The purity of a clustering is defined as:

$$\text{purity} = \frac{1}{N}\sum_{k=1}^{K}\max_{j}(\#(c_k \cap l_j))$$

Where N is the number of observations, K is the number of clusters, c_k is the cluster k and l_j is the class j. $\#(c_k \cap l_j)$ is the number of observations in the cluster c_k and in the class l_j.

We are told that the purity of our clustering is 0.75, therefore:

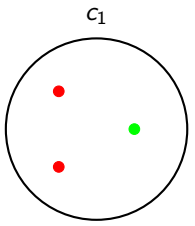
$$0.75 = \frac{1}{4}(\max_{j}(\#(c_1 \cap l_j)) + \max_{j}(\#(c_2 \cap l_j))) \Leftrightarrow$$
$$\Leftrightarrow 3 = \max_{j}(\#(c_1 \cap l_j)) + \max_{j}(\#(c_2 \cap l_j))$$

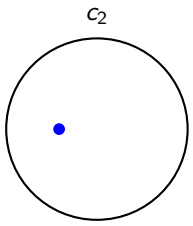
Therefore, we have two options, either $\max_j(\#(c_1 \cap l_j)) = 3$ and $\max_j(\#(c_2 \cap l_j)) = 0$ or $\max_j(\#(c_1 \cap l_j)) = 2$ and $\max_j(\#(c_2 \cap l_j)) = 1$.

1st Option

Considering the case where the maximum number of observations in a class in one cluster is 2 and the maximum number of observations in a class in the other cluster is 1, we have the following options:

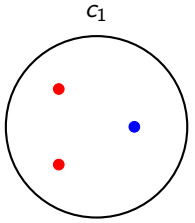
Option 1

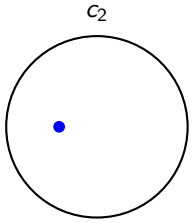




3 classes

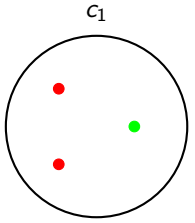
Option 2

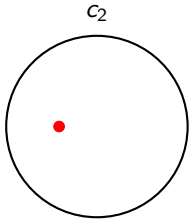




2 classes

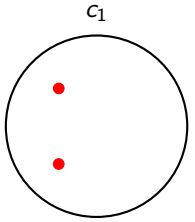
Option 3

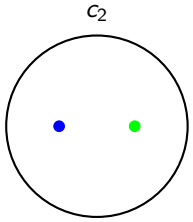




2 classes

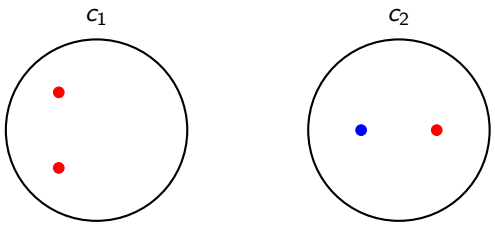
Option 4





3 classes

Option 5



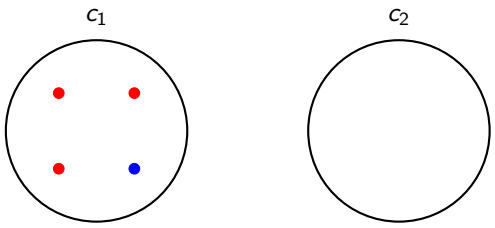
2 classes

In each of these diagrams, different colors represent different classes.

2nd Option

Considering the case where the maximum number of observations in a class in one cluster is 3 and the maximum number of observations in a class in the other cluster is 0, we have the following options:

Option 1



2 classes

Answer: We can conclude that a purity of 0.75 can be obtained if our data is classified in 2 or 3 classes.

Programming and Critical Analysis

Imports

```
import pandas as pd
from scipy.io.arff import loadarff
from sklearn.cluster import KMeans
from sklearn.preprocessing import MinMaxScaler
from sklearn.decomposition import PCA
import matplotlib.pyplot as plt
import numpy as np
from sklearn.metrics import silhouette_score, silhouette_samples
from pathlib import Path
import math
```

Listing 1:

Loading Data Set

```
IMAGES_DIR = Path('images')
IMAGES_DIR.mkdir(parents=True, exist_ok=True)
DATA_DIR = Path('data')
DATA_DIR.mkdir(parents=True, exist_ok=True)
DATA_FILE = 'column_diagnosis.arff'
DATA_PATH = DATA_DIR / DATA_FILE
data = loadarff(DATA_PATH)
df = pd.DataFrame(data[0])
df['class'] = df['class'].str.decode('utf-8')
# Show the first 5 rows
df.head()
```

Listing 2:

Pre Processing

```
# Make the data unsupervised
X = df.drop('class', axis=1)

# Ground truth
y = df['class']

# Normalize the data using MinMaxScaler
scaler = MinMaxScaler()
X_scaled = scaler.fit_transform(X)
```

Listing 3:

Question 1

```
# Apply K-means clustering for k {2, 3, 4, 5}
k_values = [2, 3, 4, 5]
silhouette_scores = []
purity_scores = []

for k in k_values:
    kmeans = KMeans(n_clusters=k,
                    random_state=0)
```

```
        cluster_labels = kmeans.fit_predict(X_scaled)

        # Calculate silhouette score for each sample
        silhouette = silhouette_samples(X_scaled, cluster_labels)

        # Split the silhouette scores by cluster
        silhouette_per_cluster = [silhouette[cluster_labels == i] for i in range(k)]

        # Calculate the average silhouette score for each cluster
        silhouette_per_cluster_avg = [np.mean(silhouette_per_cluster[i]) for i in range(k)]

        # Calculate the average silhouette score for all clusters
        silhouette_avg = np.mean(silhouette_per_cluster_avg)
        print(f'Silhouette score for {k} clusters: {silhouette_avg:.5f}')
        silhouette_scores.append(silhouette_avg)

        # Purity
        clusters = {i: [] for i in range(k)}
        for i in range(len(cluster_labels)):
            clusters[cluster_labels[i]].append(y[i])

        # Count the most frequent class in each cluster
        cluster_purities = [clusters[i].count(max(clusters[i], key=clusters[i].count)) for i
    in range(k)]

        # Calculate purity
        purity = sum(cluster_purities) / len(y)
        purity_scores.append(purity)
        print(f'Purity score for {k} clusters: {purity:.5f}')

    # Plot the silhouette scores
    plt.figure(figsize=(10, 6))
    plt.plot(k_values, silhouette_scores, marker='o')
    plt.xlabel('Number of clusters')
    plt.xticks(k_values)
    plt.ylabel('Silhouette score')
    plt.title('Silhouette score for different number of clusters')
    # Write the silhouette scores on the plot
    for i, score in enumerate(silhouette_scores):
        plt.text(k_values[i] + 0.02, score + 0.001, f'{score:.5f}', bbox=dict(facecolor='
      white', alpha=0.8))
    plt.savefig(IMAGES_DIR / 'silhouette.png')
    plt.show()

    # Plot the purity scores
    plt.figure(figsize=(10, 6))
    plt.plot(k_values, purity_scores, marker='o')
    plt.xlabel('Number of clusters')
    plt.xticks(k_values)
    plt.ylabel('Purity score')
    plt.title('Purity score for different number of clusters')
    # Write the purity scores on the plot
    for i, score in enumerate(purity_scores):
        plt.text(k_values[i] + 0.02, score + 0.001, f'{score:.5f}', bbox=dict(facecolor='
      white', alpha=0.5))
    plt.savefig(IMAGES_DIR / 'purity.png')
    plt.show()
```

Listing 4:

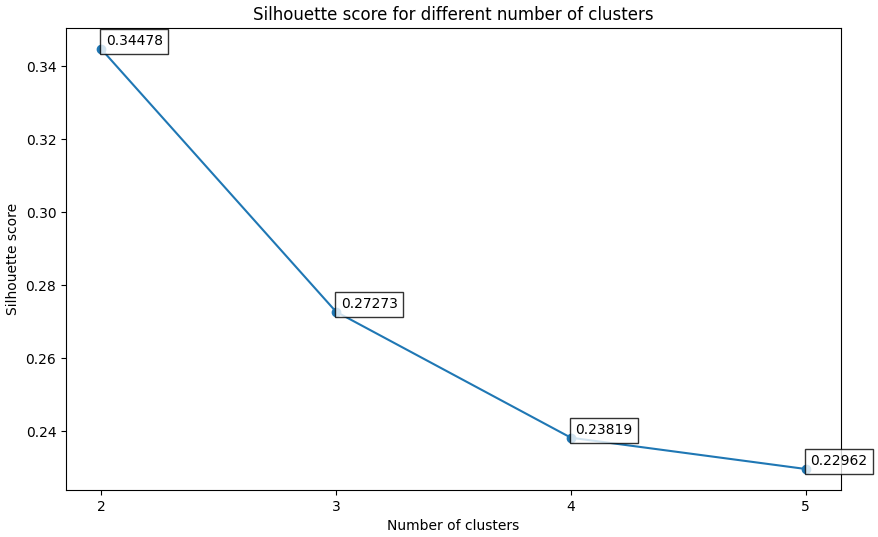


Figure 1: Silhouette score for different number of clusters

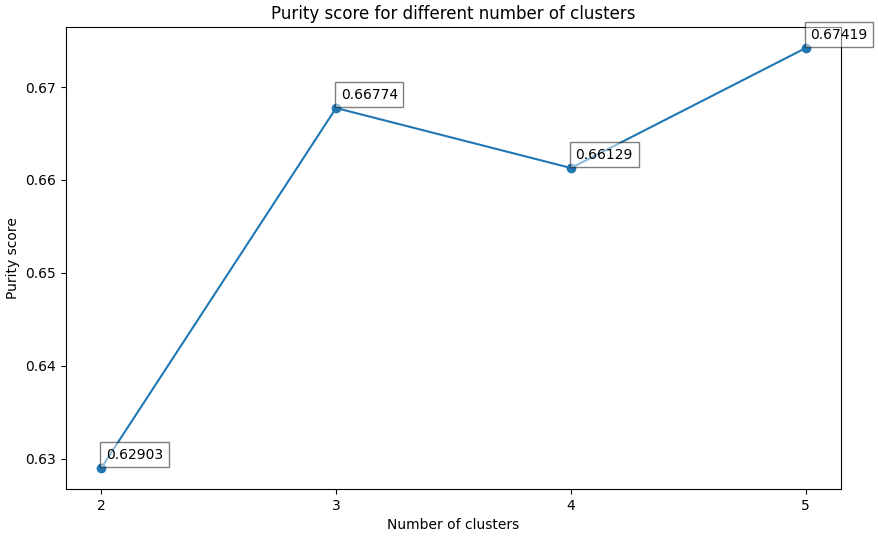


Figure 2: Purity score for different number of clusters

Comment

- For k=2, the silhouette score is 0.34478 and the purity score is 0.62903. Indicating that the clustering with two clusters has relatively good cohesion and separation, with data points well-matched to their own clusters and somewhat distant from other clusters. The purity score suggests that the majority of data points within each cluster belong to the same class, but there is some mixing of classes.
- For k=3, the silhouette score decreases to 0.27273, which may indicate some overlap or less distinct clusters. However, the purity score improves to 0.66774, indicating that each cluster contains a higher proportion of data points from a single class. This suggests a trade-off between silhouette and purity.

- For k=4, the silhouette score further decreases to 0.23819, indicating more overlap or less distinct clusters. The purity score remains relatively high at 0.66129, indicating good consistency with class labels.
- For k=5, the silhouette score decreases to 0.22962, indicating more overlap or less distinct clusters. The purity score remains relatively high at 0.67419, indicating good consistency with class labels.

Overall, these results show that the choice of the number of clusters (k) affects the quality of the clustering solution. A smaller k (k=2) results in better silhouette scores but lower purity, indicating that clusters are more distinct but not as pure in terms of class membership. A larger k (k=5) provides higher purity but lower silhouette scores, suggesting more class consistency but potentially less distinct clusters. The choice of k should be made based on the specific aim of the clustering task, considering the trade-off between silhouette and purity.

Question 2

```python
# Apply PCA to reduce the dimensionality to 2
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_scaled)

# Plot the data
plt.figure(figsize=(10, 6))
plt.scatter(X_pca[:, 0], X_pca[:, 1])
plt.xlabel('First principal component')
plt.ylabel('Second principal component')
plt.title('Data after PCA')
plt.savefig(IMAGES_DIR / 'pca.png')
plt.show()
```

Listing 5:

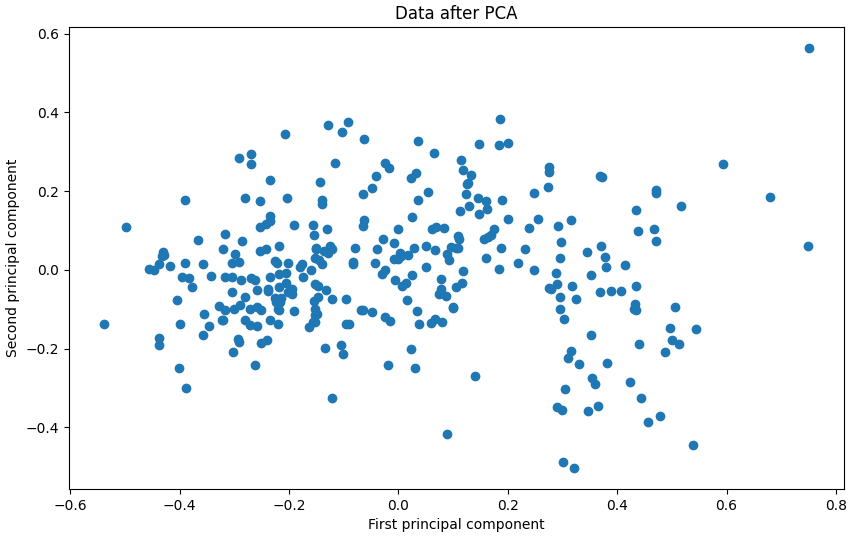


Figure 3: Data after PCA

i)

```python
print(f'Explained variance: {pca.explained_variance_ratio_}')
```

Listing 6:

```
Explained variance: [0.56181445 0.20955953]
```

Listing 7:

Comment

When considering the variability explained by the top two principal components in a PCA (Principal Component Analysis), the values represent the proportion of total variance in the data that is captured by each of these components.

- PC1 captures the largest portion of variance in the data, about 57%. This suggests that PC1 is a significant component that summarizes the primary patterns in the data. A high value for PC1 indicates that it carries substantial information about the relationships between the original features.
- PC2 explains the next largest portion of variance after PC1. It captures approximately 20.96

When summing the explained variances of PC1 and PC2 (0.56181445 + 0.20955953), you get a total explained variance of approximately 77.14

The proportion of variance explained by the top principal components informs about the dimensionality reduction achieved by the PCA. In this case, a significant amount of variability is retained by considering only the top two principal components, which can be beneficial for simplifying the data while preserving the most essential information. However, one may need to perform a deeper analysis of the eigenvectors associated with these components to help identify which original features contribute the most to each principal component.

ii)

```python
# Compute Column Importance for each component
xvector = pca.components_[0] * max(X_pca[:,0])
yvector = pca.components_[1] * max(X_pca[:,1])

columns = X.columns
impt_features = {columns[i] : math.sqrt(xvector[i]**2) for i in range(len(columns))}
sorted_features = sorted(zip(impt_features.values(),impt_features.keys()),reverse=True)
print("Features by importance for first component:\n")
for i in range(len(sorted_features)):
    print(f'{sorted_features[i][1]} : {sorted_features[i][0]:.5f}')

impt_features = {columns[i] : math.sqrt(yvector[i]**2) for i in range(len(columns))}
sorted_features = sorted(zip(impt_features.values(),impt_features.keys()),reverse=True)
print("\nFeatures by importance for second component:\n")
for i in range(len(sorted_features)):
    print(f'{sorted_features[i][1]} : {sorted_features[i][0]:.5f}')

# Compute Column Importance and Sort
columns = X.columns
impt_features = {columns[i] : math.sqrt(xvector[i]**2 + yvector[i]**2) for i in range(len
  (columns))}
sorted_features = sorted(zip(impt_features.values(),impt_features.keys()),reverse=True)
print("\nFeatures by importance:\n")
for i in range(len(sorted_features)):
    print(f'{sorted_features[i][1]} : {sorted_features[i][0]:.5f}')
```

Listing 8:

```
Features by importance for first component:

pelvic_incidence : 0.44394
lumbar_lordosis_angle : 0.38651
pelvic_tilt : 0.35046
sacral_slope : 0.24439
degree_spondylolisthesis : 0.16278
pelvic_radius : 0.08691

Features by importance for second component:
```

```
pelvic_tilt : 0.37797
pelvic_radius : 0.32762
sacral_slope : 0.24994
pelvic_incidence : 0.05640
lumbar_lordosis_angle : 0.04513
degree_spondylolisthesis : 0.00258

Features by importance:

pelvic_tilt : 0.51544
pelvic_incidence : 0.44751
lumbar_lordosis_angle : 0.38913
sacral_slope : 0.34957
pelvic_radius : 0.33895
degree_spondylolisthesis : 0.16280
```

Listing 9:

Comment The first principal component (PC1) is mainly influenced by features related to pelvic and lumbar angles and tilts. This suggests that PC1 might represent a combination of characteristics related to the angles and tilts of the pelvis and lumbar spine. The second principal component (PC2) is primarily associated with pelvic tilt and pelvic radius. It may capture variations in the tilt and radius of the pelvic region. Understanding the feature importance in each principal component can help interpret and use the components for dimensionality reduction or feature selection while preserving the most relevant information in the data.

Question 3

```python
# K-means clustering with k = 3
k = 3
kmeans = KMeans(n_clusters=k,
                random_state=0)
cluster_labels = kmeans.fit_predict(X_scaled)

# Plot the data with y = ground truth
target_names = y.unique()
colors = ['navy', 'turquoise', 'darkorange']
plt.figure(figsize=(10, 6))

for i, targets in enumerate(target_names):
    plt.scatter(X_pca[y==targets,0],
                X_pca[y==targets,1],
                color=colors[i],
                alpha=.8,
                lw=2,
                label=targets)

plt.legend(loc='best', shadow=False, scatterpoints=1)
plt.title('Points with Ground truth')
plt.savefig(IMAGES_DIR / 'ground_truth.png')
plt.show()

# Plot the data with y = cluster labels
plt.figure(figsize=(10, 6))



for i, targets in enumerate(target_names):
    plt.scatter(X_pca[cluster_labels==i,0],
                X_pca[cluster_labels==i,1],
                color=colors[i],
                alpha=.8,
                lw=2)

```

```
plt.title('Clusters for k = 3 using K-means')
plt.savefig(IMAGES_DIR / 'clusters.png')
plt.show()

# Clusters if we assigned the max ground truth class to each cluster
# Attribute Cluster label to a ground truth class
clusters = {i: [] for i in range(3)}
for i in range(len(cluster_labels)):
    clusters[cluster_labels[i]].append(y[i])
for i in range(len(clusters)):
    print(f'cluster {i}')
    print(f'Normal: {clusters[i].count("Normal")}')
    print(f'Hernia: {clusters[i].count("Hernia")}')
    print(f'Spondylolisthesis: {clusters[i].count("Spondylolisthesis")}\n')
lista = [max(clusters[i], key=clusters[i].count) for i in range(3)]
print(lista)

plt.figure(figsize=(10, 6))
for i, targets in enumerate(target_names):
    plt.scatter(X_pca[cluster_labels==i,0],
                X_pca[cluster_labels==i,1],
                color=colors[i],
                alpha=.8,
                lw=2,
                label=lista[i])
plt.legend(loc='best', shadow=False, scatterpoints=1)
plt.title('Clusters for k = 3 using K-means and labelled with the most frequent class')
plt.savefig(IMAGES_DIR / 'clusters_frequency.png')
plt.show()
```

Listing 10:

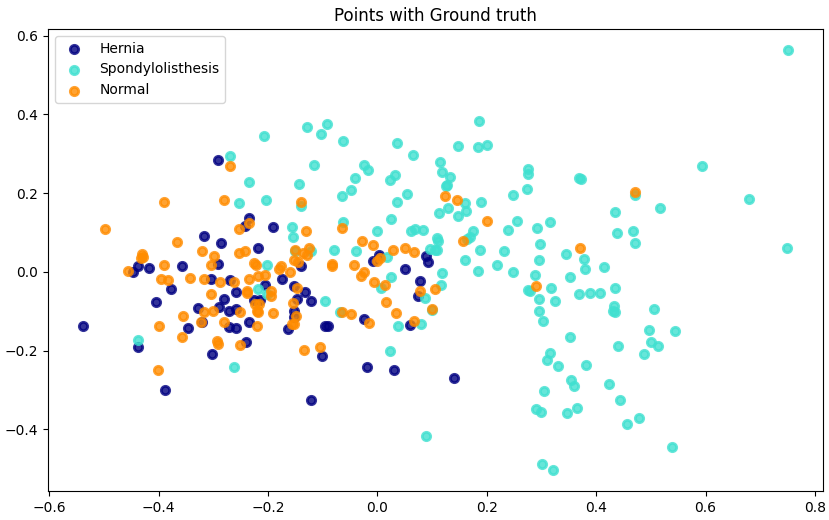


Figure 4: Points with Ground truth

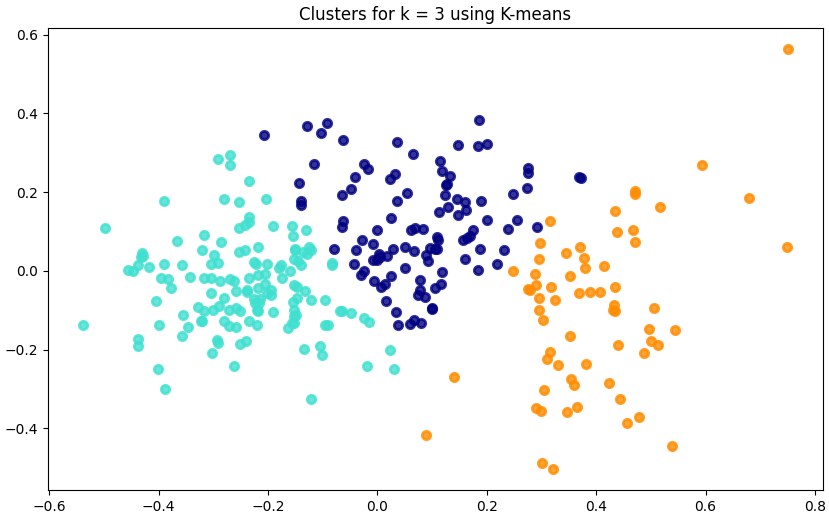


Figure 5: Clusters for k = 3 using K-means

Label the clusters with the most frequent class for visualization

```
cluster 0
Normal: 24
Hernia: 8
Spondylolisthesis: 73

cluster 1
Normal: 73
Hernia: 51
Spondylolisthesis: 16

cluster 2
Normal: 3
Hernia: 1
Spondylolisthesis: 61

['Spondylolisthesis', 'Normal', 'Spondylolisthesis']
```

Listing 11:

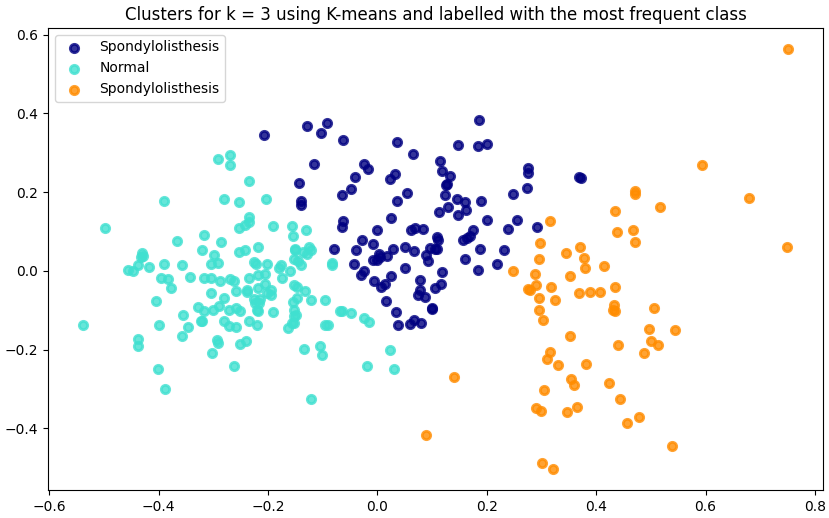


Figure 6: Clusters for k = 3 using K-means and labelled with the most frequent class

Question 4

Using the results we obtained for Question 1 and Question 3, we conclude that one may use clustering to identify groups of patients with similar characteristics to perform a potential diagnosis on a new patient or even to subtype groups inside a major one for specific treatments. However, one need to be careful while fine-tuning the clusters, due to the trade-off we observed between silhouette and purity scores. In addition, one may use PCA to reduce the dimensionality of the data and identify the most relevant features for the clustering task. However, one need to be careful while selecting the number of principal components to retain, as this may affect the amount of information retained in the data. Also, we need to be careful, since the clusters might not represent quite well the classes of the patients. It's important to recognize that the clusters generated through clustering may not perfectly align with the known classes of patients. For instance, in Question 3, where we plotted three clusters and have three ground truth classes, the cluster-class mapping is not straightforward, since the clusters do not represent the classes in a one-to-one fashion. Two clusters may correspond to the same class, as we can see in the labelled clusters using the most frequent class. Suggestions for merging these clusters into one may be considered in further post-processing steps. The third cluster, representing a mix of about 50In light of these considerations, the application of clustering for diagnosis requires careful attention. While it can be a valuable tool for identifying patient groups with similar characteristics, it should be complemented with domain knowledge and a thorough understanding of the data.