

**Part I:** Pen and paper

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

As a side note, we'll be using the  $k_1$  and  $k_2$  notation to represent clusters 1 and 2 - with that, we'll say that  $\pi_1 = P(C = k_1)$ , with analogous notation for  $\pi_2$ .

EM-Clustering, being an unsupervised learning algorithm intending to calculate the probability of a sample belonging to a certain cluster, is a method that iteratively updates the parameters of the model until convergence is reached (for a given definition of convergence). Here, we'll perform exactly one epoch of the algorithm, which means we'll be going through two steps:

- **E-step:** In this step, our goal is to calculate the **posterior probability** of each sample belonging to each cluster. In order to perform this calculation, we'll be using **Bayes' rule**, of course, to decompose the posterior probability into the product of the **likelihood** and the **prior probability** of the sample belonging to the cluster. Let's try, then, to assign each sample to the cluster that maximizes the posterior probability.

For starters, we must first note that the likelihood of a sample belonging to a cluster is given by the **multivariate Gaussian distribution**, which can be written as (considering  $d = 2$ ):

$$P(x_i | C = k_n) \sim \mathcal{N}(x_i; \mu_n, \Sigma_n) = \frac{1}{\sqrt{(2\pi)^d \det \Sigma_n}} \exp \left( -\frac{1}{2} (x_i - \mu_n)^T \Sigma_n^{-1} (x_i - \mu_n) \right)$$

We'll also use the  $\gamma_{i,j}$  notation to represent the normalized posteriors, where  $i$  matches the  $i$ -th sample and  $j$  the  $j$ -th cluster:

$$\gamma_{i,j} = \frac{\pi_j P(x_i | C = k_j)}{\sum_{k=1}^d \pi_k P(x_i | C = k_k)} = \frac{\pi_j \mathcal{N}(x_i | \mu_j, \Sigma_j)}{\sum_{k=1}^d \pi_k \mathcal{N}(x_i | \mu_k, \Sigma_k)}$$

Moreover, in this step we'll use **teal** to denote the priors and **purple** to denote the likelihoods.

As a given, we have that the priors are (for every sample, of course):

$$P(C = k_1) = P(C = k_2) = \pi_1 = \pi_2 = 0.5$$

Regarding  $x_1$ , we have:

$$\begin{aligned} P(x_1 | C = k_1) &= \frac{1}{\sqrt{(2\pi)^d \det \Sigma_1}} \exp \left( -\frac{1}{2} (x_1 - \mu_1)^T \Sigma_1^{-1} (x_1 - \mu_1) \right) \\ &= \frac{1}{\sqrt{(2\pi)^2 \det \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}}} \exp \left( -\frac{1}{2} \left( \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix} \right)^T \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}^{-1} \left( \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix} \right) \right) \\ &= \frac{e^{-1/3}}{\sqrt{(2\pi)^2 \cdot 3}} \\ &\approx 0.0658407 \end{aligned}$$

$$\begin{aligned} P(x_1 | C = k_2) &= \frac{1}{\sqrt{(2\pi)^d \det \Sigma_2}} \exp \left( -\frac{1}{2} (x_1 - \mu_2)^T \Sigma_2^{-1} (x_1 - \mu_2) \right) \\ &= \frac{1}{\sqrt{(2\pi)^2 \det \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}}} \exp \left( -\frac{1}{2} \left( \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right)^T \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \left( \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right) \right) \\ &\approx 0.0227993 \end{aligned}$$

The (normalized) posteriors can be computed as follows:

$$\begin{aligned} \gamma_{1,1} &= \frac{P(C = k_1)P(x_1 | C = k_1)}{P(C = k_1)P(x_1 | C = k_1) + P(C = k_2)P(x_1 | C = k_2)} \\ &= \frac{0.5 \cdot 0.0658407}{0.5 \cdot 0.0658407 + 0.5 \cdot 0.0227993} \\ &= 0.742788 \\ \gamma_{1,2} &= \frac{P(C = k_2)P(x_1 | C = k_2)}{P(C = k_1)P(x_1 | C = k_1) + P(C = k_2)P(x_1 | C = k_2)} \\ &= \frac{0.5 \cdot 0.0227993}{0.5 \cdot 0.0658407 + 0.5 \cdot 0.0227993} \\ &= 0.257212 \end{aligned}$$

As to avoid presenting here the repetitive calculations for the remaining samples, for which the results in question are calculated in the same manner, we include here only the intermediate values of such calculations, as discussed with Prof. Rui Henriques. The respective Python code is available in this report's appendix.

$x_2$ :	$x_3$ :
$P(x_2 C = k_1) = 0.00891057$	$P(x_3 C = k_1) = 0.0338038$
$P(x_2 C = k_2) = 0.0482662$	$P(x_3 C = k_2) = 0.061975$
$\gamma_{2,1} = 0.155843$	$\gamma_{3,1} = 0.352936$
$\gamma_{2,2} = 0.844157$	$\gamma_{3,2} = 0.647064$

- **M-step: Having calculated the posteriors, we can now update the parameters of the cluster-defining distributions.**

For each cluster, we'll want to find the new distribution parameters: in this case,  $\mu_k$  and  $\Sigma_k$  (for every cluster  $k$ ). For likelihoods, we'll need to update both  $\mu_k$  and  $\Sigma_k$ , using all samples weighted by their respective posteriors, as can be seen below; for priors, we'll need to perform a weighted mean of the posteriors.

$$\mu_\alpha = \frac{\sum_{i=1}^3 P(C = k_\alpha | x_i) x_i}{\sum_{i=1}^3 P(C = k_\alpha | x_i)}$$

$$\Sigma_\alpha = \frac{\sum_{i=1}^3 P(C = k_\alpha | x_i) (x_{i,n} - \mu_{\alpha,n})(x_{i,m} - \mu_{\alpha,m})^T}{\sum_{i=1}^3 P(C = k_\alpha | x_i)}$$

$$P(C = k_\alpha) = \frac{\sum_{i=1}^3 P(C = k_\alpha | x_i)}{\sum_{c=1}^2 \sum_{i=1}^3 P(C = k_c | x_i)}$$

In the equations stated above, we're considering  $x_{i,n}$  as the  $n$ -th feature's value of the  $i$ -th sample, and  $\mu_{k,n}$  as the  $n$ -th index of centroid  $\mu_k$ .

We can now estimate the new parameters of the distributions (and the new priors) as shown in the next page (note that the updated  $\mu_\alpha$ 's are used in the calculation of the new  $\Sigma_\alpha$ 's). The Python code used for these calculations is also available in the appendix.

Regarding  $k_1$ :

$$\begin{aligned}
\mu_1 &= \frac{\sum_{i=1}^3 P(C = k_1 | x_i) x_i}{\sum_{i=1}^3 P(C = k_1 | x_i)} \\
&= \frac{0.742788 \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} + 0.155843 \cdot \begin{bmatrix} -1 \\ 1 \end{bmatrix} + 0.352936 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix}}{0.742788 + 0.155843 + 0.352936} \\
&= \begin{bmatrix} 0.750964 \\ 1.31149 \end{bmatrix} \\
\Sigma_1^{nm} &= \frac{\sum_{i=1}^3 P(C = k_1 | x_i) (x_{i,n} - \mu_{1,n})(x_{i,m} - \mu_{1,m})^T}{\sum_{i=1}^3 P(C = k_1 | x_i)} \\
&= \begin{bmatrix} 0.436053 & 0.0775726 \\ 0.0775726 & 0.778455 \end{bmatrix} \\
\pi_1 = P(C = k_1) &= \frac{\sum_{i=1}^3 P(C = k_1 | x_i)}{\sum_{c=1}^2 \sum_{i=1}^3 P(C = k_c | x_i)} = 0.417189
\end{aligned}$$

Regarding  $k_2$ :

$$\begin{aligned}
\mu_2 &= \frac{\sum_{i=1}^3 P(C = k_2 | x_i) x_i}{\sum_{i=1}^3 P(C = k_2 | x_i)} \\
&= \frac{0.257212 \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} + 0.844157 \cdot \begin{bmatrix} -1 \\ 1 \end{bmatrix} + 0.647064 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix}}{0.257212 + 0.844157 + 0.647064} \\
&= \begin{bmatrix} 0.0343846 \\ 0.777028 \end{bmatrix} \\
\Sigma_2^{nm} &= \frac{\sum_{i=1}^3 P(C = k_2 | x_i) (x_{i,n} - \mu_{2,n})(x_{i,m} - \mu_{2,m})^T}{\sum_{i=1}^3 P(C = k_2 | x_i)} \\
&= \begin{bmatrix} 0.998818 & -0.215305 \\ -0.215305 & 0.467476 \end{bmatrix} \\
\pi_2 = P(C = k_2) &= \frac{\sum_{i=1}^3 P(C = k_2 | x_i)}{\sum_{c=1}^2 \sum_{i=1}^3 P(C = k_c | x_i)} = 0.582811
\end{aligned}$$

## 2. Given the updated parameters computed in previous question:

### (a) Perform a hard assignment of observations to clusters under a MAP assumption.

*Note that, since all calculations follow the same general expressions used in the previous question's **E-Step**, we have opted not to repeat them here, showing just the final results for each intermediate step instead. The code required for these calculations is, once again, available in the appendix.*

Just like in the first question's answer, we'll need to compute the posterior probabilities of each sample belonging to each cluster (now utilizing the newly updated parameters); however, instead of proceeding to the **M-Step**, we'll just assign each sample to the cluster with the highest posterior probability.

The priors have been updated in the previous question's answer to:

$$\pi_1 = 0.417189, \quad \pi_2 = 0.582811$$

Moreover, we've also updated the means and covariances of the distributions to:

$$\begin{aligned} \mu_1 &= \begin{bmatrix} 0.750964 \\ 1.31149 \end{bmatrix} & \Sigma_1 &= \begin{bmatrix} 0.436053 & 0.0775726 \\ 0.0775726 & 0.778455 \end{bmatrix} \\ \mu_2 &= \begin{bmatrix} 0.0343846 \\ 0.777028 \end{bmatrix} & \Sigma_2 &= \begin{bmatrix} 0.998818 & -0.215305 \\ -0.215305 & 0.467476 \end{bmatrix} \end{aligned}$$

Therefore, for each sample, we'll have:

$x_1$ :	$x_2$ :	$x_3$ :
$P(x_1 C = k_1) = 0.195695$	$P(x_2 C = k_1) = 0.00819528$	$P(x_3 C = k_1) = 0.0771661$
$P(x_1 C = k_2) = 0.0135196$	$P(x_2 C = k_2) = 0.143645$	$P(x_3 C = k_2) = 0.104784$
$\gamma_{1,1} = \underline{0.911983}$	$\gamma_{2,1} = 0.0392368$	$\gamma_{3,1} = 0.345186$
$\gamma_{1,2} = 0.0880168$	$\gamma_{2,2} = \underline{0.960763}$	$\gamma_{3,2} = \underline{0.654814}$

After performing these calculations, under a MAP (*Maximum A Posteriori*) assumption, we'll assign each sample to the cluster with the highest posterior probability, as underlined above:

$x_1$ :	$x_2$ :	$x_3$ :
MAP( $x_1$ ) $\mapsto$ $k_1$	MAP( $x_2$ ) $\mapsto$ $k_2$	MAP( $x_3$ ) $\mapsto$ $k_2$

(b) **Compute the silhouette of the larger cluster using the Euclidean distance.**

As we know, the silhouette of a given sample  $x_i$  is defined as

$$s_i = \frac{b_i - a_i}{\max \{a_i, b_i\}},$$

where  $a_i$  is the average distance between  $x_i$  and all other samples in the same cluster, and  $b_i$  is the average distance between  $x_i$  and all other samples in its **neighboring cluster** - the neighboring cluster being, therefore, the cluster minimizing such average distance.

Moreover, the silhouette of a given cluster  $k_n$ , with  $m$  assigned samples, is defined as:

$$s(k_n) = \frac{\sum_{i=1}^m s_i}{m}$$

Here, the **largest cluster** will be the cluster with the greatest associated prior value ( $\pi_k$ ). As we computed in 1.,  $\pi_2 = 0.582811 > 0.417189 = \pi_1$ , hence the larger cluster will be  $k_2$ . Its assigned samples, considering a MAP assumption, are  $x_2$  and  $x_3$  (as asserted in the previous question's answer), so we'll have the following:

$x_2$ :		$x_3$ :
$a_2 = \frac{\ x_2 - x_3\ _2}{2 - 1}$ $= \left\  \begin{bmatrix} -1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right\ _2 = 2.23607$ $b_2 = \min \left\{ \frac{\ x_2 - x_1\ _2}{1} \right\}$ $= \left\  \begin{bmatrix} -1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\ _2 = 2.23607$ $s_2 = \frac{b_2 - a_2}{\max \{a_2, b_2\}}$ $= \frac{2.23607 - 2.23607}{\max \{2.23607, 2.23607\}} = 0$		$a_3 = \frac{\ x_3 - x_2\ _2}{2 - 1}$ $= \left\  \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} -1 \\ 1 \end{bmatrix} \right\ _2 = 2.23607$ $b_3 = \min \left\{ \frac{\ x_3 - x_1\ _2}{1} \right\}$ $= \left\  \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\ _2 = 2$ $s_3 = \frac{b_3 - a_3}{\max \{a_3, b_3\}}$ $= \frac{2 - 2.23607}{\max \{2.23607, 2\}} = -0.105573$

With this, we can compute the silhouette of the larger cluster:

$$s(k_2) = \frac{s_2 + s_3}{2} = -0.052786$$

## Part II: Programming and critical analysis

The code utilized to answer the following questions is available in this report's appendix.

---

Recall the `pd.speech.arff` dataset from earlier homeworks, centered on the Parkinson diagnosis from speech features. For the following exercises, normalize the data using `sklearn`'s `MinMaxScaler`.

3. **Using `sklearn`, apply  $k$ -means clustering fully unsupervisedly (without targets) on the normalized data with  $k = 3$  and three different seeds (using `random \in \{0, 1, 2\}`). Assess the silhouette and purity of the produced solutions.**

`sklearn.metrics` offers us the `silhouette_score` method, which computes the silhouette of a given clustering solution. `purity_score` is a custom method defined in the appendix of this report, which computes the purity of a given clustering solution.

Regarding the  $k$ -means clustering solutions for  $k = 3$ , for each of the given seeds, we were able to gather the following scores:

<code>random_state</code>	Silhouette score	Purity score
0	0.11362028	0.76719577
1	0.11403554	0.76322751
2	0.11362028	0.76719577

Table 1: Silhouette and Purity scores for each clustering solution

4. **What is causing the non-determinism?**

The non-determinism present in the  $k$ -means clustering solutions gathered in the previous exercise is caused by the fact that the algorithm is inherently random: `sklearn`'s `KMeans` class sets up the centroids' initial positions in a randomly generated fashion, thus leading to possible different convergence points for the same data and number of clusters. `random_state`, here, works as a mere manner of controlling the random seed used to generate the initial centroid positions: for the same seed, the same initial centroids' positions will be generated, thus leading to the same convergence point. For different seeds, different initial centroid positions will be generated, which will generally lead to different convergence points. In the case seen above, with seeds 0 and 2, the convergence point reached was practically the same (in terms of evaluated), even though the final centroids' positions were different.

5. **Using a scatter plot, visualize side-by-side the labeled data using as labels: i) the original Parkinson diagnoses, and ii) the previously learned  $k = 3$  clusters (random = 0). To this end, select the two most informative features as axes and color observations according to their label. For feature selection, select the two input variables with highest variance on the MinMax normalized data.**

In order to select the two most informative features, we'll use the custom method `select_most_informative_features` defined in the appendix of this report. After gathering that the two input variables presenting the highest variance are both `tqwt_entropy_shannon_dec_16` and `tqwt_kurtosisValue_dec_34`, we were able to gather the scatter plots present in Figure 1.

6. **The fraction of variance explained by a principal component is the ratio between the variance of that component (i.e., its eigenvalue) and total variance (i.e., sum of all eigenvalues). How many principal components are necessary to explain more than 80% of variability?**

The PCA class from `sklearn.decomposition` can be used to compute the **principal components** of a dataset. Moreover, its `n_components` parameter, if set to a value between 0 and 1, will automatically select the number of components necessary to explain a fraction of variability greater than the given value - in our case, 0.8 - which can be consulted in the `n_components_` attribute.

After running the `calculate_pca` method, present in the latter section of this report's appendix, we were able to gather that the number of principal components necessary to explain 80% of variability is 31.



## Appendix

Code utilized to answer the questions in the Pen-and-Paper section:

```
1 import numpy as np
2
3 ### Question 1 ###
4
5 # Initial data
6
7 x_1 = np.array([[1], [2]])
8 x_2 = np.array([[-1], [1]])
9 x_3 = np.array([[1], [0]])
10
11 mu_1 = np.array([[2], [2]])
12 mu_2 = np.array([[0], [0]])
13
14 Sigma_1 = np.array([[2, 1], [1, 2]])
15 Sigma_2 = np.array([[2, 0], [0, 2]])
16
17 from scipy.stats import multivariate_normal
18
19 def calc_likelihoods(x, mu_1, mu_2, Sigma_1, Sigma_2):
20     likelihood_1 = multivariate_normal(mu_1, Sigma_1).pdf(x.T)
21     likelihood_2 = multivariate_normal(mu_2, Sigma_2).pdf(x.T)
22     return np.array([likelihood_1, likelihood_2])
23
24 def calc_posteriors(priors, likelihoods):
25     posteriors = np.array([])
26     for i in range(len(priors)):
27         posteriors = np.append(posteriors, priors[i] * likelihoods[i])
28
29     return posteriors / np.sum(posteriors) # normalize
30
31 def update_means(k1_posteriors, k2_posteriors):
32     mu_1 = np.zeros((2, 1), dtype=float)
33     mu_2 = np.zeros((2, 1), dtype=float)
34
35     for i in range(len(k1_posteriors)):
36         x = eval(f'x_{i+1}')
37         mu_1 += k1_posteriors[i] * x
38         mu_2 += k2_posteriors[i] * x
39
40     return mu_1 / np.sum(k1_posteriors), mu_2 / np.sum(k2_posteriors)
41
42 def update_covs(k1_posteriors, k2_posteriors, mu_1, mu_2):
43     Sigma_1 = np.zeros((2, 2), dtype=float)
44     Sigma_2 = np.zeros((2, 2), dtype=float)
45
46     for i in range(len(k1_posteriors)):
47         x = eval(f'x_{i+1}')
48         Sigma_1 += k1_posteriors[i] * (x - mu_1) @ (x - mu_1).T
49         Sigma_2 += k2_posteriors[i] * (x - mu_2) @ (x - mu_2).T
50
51     return Sigma_1 / np.sum(k1_posteriors), Sigma_2 / np.sum(k2_posteriors)
52
53 def update_priors(k1_posteriors, k2_posteriors):
```

```

54     total = np.sum(k1_posteriors) + np.sum(k2_posteriors)
55     return np.sum(k1_posteriors) / total, np.sum(k2_posteriors) / total
56
57 mu_1_vector = mu_1.transpose()[0]
58 mu_2_vector = mu_2.transpose()[0]
59
60 priors = np.array([0.5, 0.5])
61
62 p_x_1_given_k_1, p_x_1_given_k_2 = calc_likelihoods(x_1, mu_1_vector, mu_2_vector,
63     Sigma_1, Sigma_2)
64 p_x_2_given_k_1, p_x_2_given_k_2 = calc_likelihoods(x_2, mu_1_vector, mu_2_vector,
65     Sigma_1, Sigma_2)
66 p_x_3_given_k_1, p_x_3_given_k_2 = calc_likelihoods(x_3, mu_1_vector, mu_2_vector,
67     Sigma_1, Sigma_2)
68
69 posteriors_x_1 = calc_posteriors(priors, [p_x_1_given_k_1, p_x_1_given_k_2])
70 posteriors_x_2 = calc_posteriors(priors, [p_x_2_given_k_1, p_x_2_given_k_2])
71 posteriors_x_3 = calc_posteriors(priors, [p_x_3_given_k_1, p_x_3_given_k_2])
72
73 # update parameters
74
75 mu_1_after_update, mu_2_after_update = update_means(k1_posteriors, k2_posteriors)
76 Sigma_1_after_update, Sigma_2_after_update = update_covs(k1_posteriors,
77     k2_posteriors, mu_1_after_update, mu_2_after_update)
78
79 # update the priors
80
81 priors_after_update = update_priors(k1_posteriors, k2_posteriors)
82 prior_1_update, prior_2_update = priors_after_update
83
84 ### Question 2a ###
85
86 mu_1_after_update_vector = mu_1_after_update.transpose()[0]
87 mu_2_after_update_vector = mu_2_after_update.transpose()[0]
88
89 updated_p_x_1_given_k_1, updated_p_x_1_given_k_2 = calc_likelihoods(x_1,
90     mu_1_after_update_vector, mu_2_after_update_vector, Sigma_1_after_update,
91     Sigma_2_after_update)
92 updated_p_x_2_given_k_1, updated_p_x_2_given_k_2 = calc_likelihoods(x_2,
93     mu_1_after_update_vector, mu_2_after_update_vector, Sigma_1_after_update,
94     Sigma_2_after_update)
95 updated_p_x_3_given_k_1, updated_p_x_3_given_k_2 = calc_likelihoods(x_3,
96     mu_1_after_update_vector, mu_2_after_update_vector, Sigma_1_after_update,
97     Sigma_2_after_update)
98
99 updated_posteriors_x_1 = calc_posteriors(priors_after_update, [
100     updated_p_x_1_given_k_1, updated_p_x_1_given_k_2])
101 updated_posteriors_x_2 = calc_posteriors(priors_after_update, [
102     updated_p_x_2_given_k_1, updated_p_x_2_given_k_2])
103 updated_posteriors_x_3 = calc_posteriors(priors_after_update, [
104     updated_p_x_3_given_k_1, updated_p_x_3_given_k_2])
105
106 hard_assignments = np.argmax(np.array([updated_posteriors_x_1,

```

```

    updated_posteriors_x_2, updated_posteriors_x_3]), axis=1) + 1
97
98 ### Question 2b ###
99
100 # Calculate the norm between x1 and x2, x2 and x3, x1 and x3
101
102 norm_x1_x2 = np.linalg.norm(x_1 - x_2)
103 norm_x2_x3 = np.linalg.norm(x_2 - x_3)
104 norm_x1_x3 = np.linalg.norm(x_1 - x_3)

```

Code utilized to answer the questions in the Programming and critical analysis section:

```

1 import numpy as np
2 import pandas as pd
3 from matplotlib import rc
4 import matplotlib.pyplot as plt
5 import seaborn as sns
6 from scipy.io.arff import loadarff
7 from sklearn.cluster import KMeans
8 from sklearn.metrics import silhouette_score
9 from sklearn.metrics.cluster import contingency_matrix
10 from sklearn.preprocessing import MinMaxScaler
11 from sklearn.decomposition import PCA
12 sns.set_style('darkgrid')
13 rc('font', **{'family': 'serif', 'serif': ['Computer Modern']})
14 rc('text', usetex=True)
15
16 # Load the data
17 data = loadarff('data/pd_speech.arff')
18 df = pd.DataFrame(data[0])
19 df['class'] = df['class'].str.decode('utf-8')
20
21 def calculate_scores(kmeans):
22     def purity_score(y_true, y_pred):
23         confusion_matrix = contingency_matrix(y_true, y_pred)
24         return np.sum(np.amax(confusion_matrix, axis=0)) / np.sum(confusion_matrix)
25
26     silhouette_scores = np.array([])
27     purity_scores = np.array([])
28     for k in kmeans:
29         silhouette_scores = np.append(silhouette_scores, silhouette_score(X_scaled,
30                                     k.labels_))
31         purity_scores = np.append(purity_scores, purity_score(labels, k.labels_))
32     print(f'Silhouette scores: {silhouette_scores}')
33     print(f'Purity scores: {purity_scores}')
34
35 X = df.iloc[:, :-1].values
36 labels = df.iloc[:, -1].values
37
38 # Normalize the data
39 scaler = MinMaxScaler()
40 X_scaled = scaler.fit_transform(X)
41
42 kmeans = [KMeans(n_clusters=3, random_state=seed).fit(X_scaled) for seed in range
43           (3)]
44
45 calculate_scores(kmeans)

```

```

44
45 # Exercise 4 below
46
47 def select_most_informative_features(kmeans, n):
48     variances = np.var(X_scaled, axis=0)
49     variance_indexes = np.argsort(variances)[::-1][:n]
50     return variance_indexes, [df.columns[i] for i in variance_indexes]
51
52 variance_indexes, most_informative_features = select_most_informative_features(
53     kmeans, 2)
54
55 # Plot the data
56 fig, axes = plt.subplots(1, 2, figsize=(12, 6))
57 x = X_scaled[:, variance_indexes[0]]
58 y = X_scaled[:, variance_indexes[1]]
59
60 print(most_informative_features)
61
62 plt.suptitle('Ground truth vs $k$-means clustering of Parkinson\'s dataset',
63     fontsize=15)
64
65 # TODO: change legend to show the actual class names/clusters
66
67 for i, ax in enumerate(axes):
68     if i == 0:
69         sns.scatterplot(x=x, y=y, hue=labels, ax=ax, palette='Set2')
70         ax.set_title('Original labels')
71     else:
72         sns.scatterplot(x=x, y=y, hue=kmeans[0].labels_, ax=ax, palette='Set2')
73         ax.set_title("Cluster labels")
74         ax.set_xlabel(f'Feature: {most_informative_features[0]}')
75         ax.set_ylabel(f'Feature: {most_informative_features[1]}')
76
77 plt.savefig('assets/parkinsons.png')
78 plt.show()
79
80 # Exercise 6 below
81
82 def calculate_pca(X, n_components):
83     pca = PCA(n_components=n_components)
84     X_pca = pca.fit(X)
85     return X_pca
86
87 pca = calculate_pca(X_scaled, 0.8)
88 print(f"Number of principal components: {pca.n_components}")

```

Ground truth vs  $k$ -means clustering of Parkinson's dataset

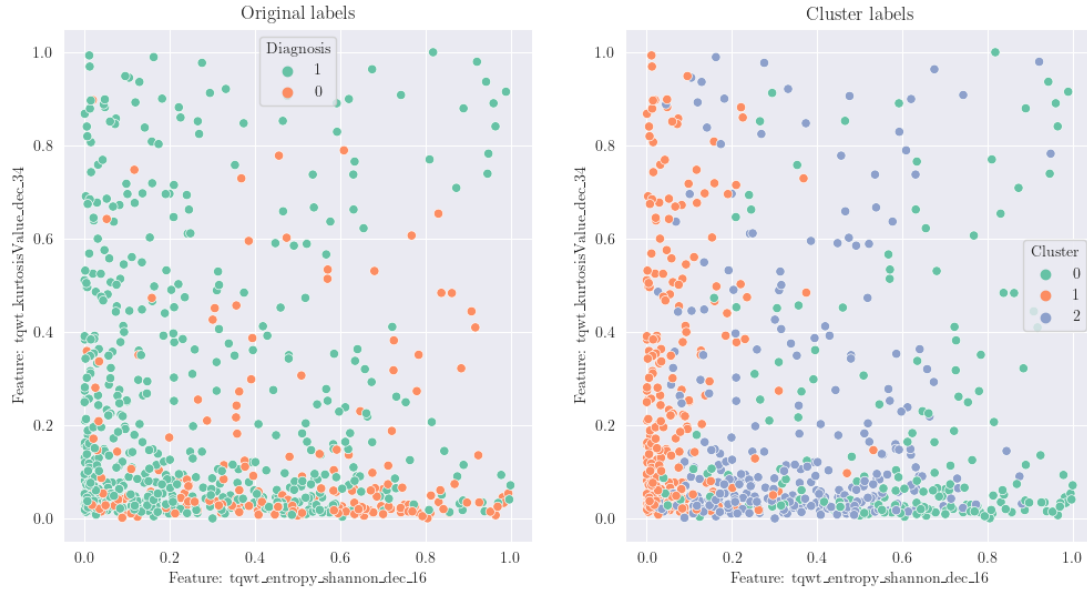


Figure 1: Ground truth vs  $k$ -means clustering of Parkinson's dataset