Aprendizagem 2023 Homework I — Group 003 (ist1107028, ist1107137)

Part I: Pen and paper

Consider the bivariate observations

$$\{x_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, x_2 = \begin{bmatrix} 0 \\ 2 \end{bmatrix}, x_3 = \begin{bmatrix} 3 \\ -1 \end{bmatrix}\}$$

and the multivariate Gaussian mixture given by

$$\mathbf{u}_1 = \begin{bmatrix} 2 \\ -1 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \Sigma_1 = \begin{bmatrix} 4 & 1 \\ 1 & 4 \end{bmatrix}, \quad \Sigma_2 = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}, \quad \pi_1 = 0.5, \quad \pi_2 = 0.5$$

Answer the following questions by presenting all intermediary steps, and use 3 decimal places in each.

1. Perform two epochs of the EM clustering algorithm and determine the new parameters.

FIRST EM EPOCH

1) Expectation: **E-STEP**

 x_1

 \rightarrow Cluster c=1:

prior:
$$P(c=1) = \pi_1 = \mathbf{0.5}$$

likelihood: $p(x_1|c=1) = \mathcal{N}(x_1|\mu_1, \sigma_1)$ $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{\det(\Sigma_1)} \cdot \exp\left(-\frac{1}{2} \cdot (x_1 - \mu_1)^T \Sigma_1^{-1} \cdot (x_1 - \mu_1)\right)$ $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{15} \cdot \exp\left(-\frac{1}{2} \cdot \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 2 \\ -1 \end{pmatrix}\right)^T \cdot \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 2 \\ -1 \end{pmatrix}\right)\right)$ $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{15} \cdot \exp\left(-\frac{1}{2} \cdot (-1 \quad 1) \cdot \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix} \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix}\right) = \frac{e^{-3}}{2\pi \cdot 15} = \mathbf{0.029}$

joint probability:
$$P(c=1,x_1) = P(c=1)p(x_1|c=1) = \pi_1 \cdot \mathcal{N}(x_1|\mu_1,\sigma_1) = \mathbf{0.015}$$

normalized posterior:
$$P(c = 1|x_1) = \frac{0.015}{0.015 + 0.007} = \mathbf{0.681}$$

1

 \rightarrow Cluster c=2:

prior:
$$P(c=2) = \pi_2 = 0.5$$

likelihood:
$$p(x_1|c=2) = \mathcal{N}(x_1|\mu_2, \sigma_2)$$

$$= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{\det(\Sigma_2)} \cdot \exp\left(-\frac{1}{2} \cdot (x_1 - \mu_2)^T \Sigma_2^{-1} \cdot (x_1 - \mu_2)\right)$$

$$= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{4} \cdot \exp\left(-\frac{1}{2} \cdot \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right)^T \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right)\right)$$

$$= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{4} \cdot \exp\left(-\frac{1}{2} \cdot (0 - 1) \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ -1 \end{pmatrix}\right) = \frac{e^{-1}}{2\pi \cdot 4} = \mathbf{0.015}$$

joint probability: $P(c=2,x_1) = P(c=2)p(x_1|c=2) = \pi_2 \cdot \mathcal{N}(x_1|\mu_2,\sigma_2) = \mathbf{0.007}$

normalized posterior:
$$P(c=2|x_1) = \frac{0.007}{0.007 + 0.015} = \mathbf{0.318}$$

 x_2

 \rightarrow Cluster c = 1:

prior:
$$P(c = 1) = \pi_1 = \mathbf{0.5}$$

likelihood: $p(x_2|c = 1) = \mathcal{N}(x_2|\mu_1, \sigma_1)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{\det(\Sigma_1)} \cdot \exp\left(-\frac{1}{2} \cdot (x_2 - \mu_1)^T \Sigma_1^{-1} \cdot (x_2 - \mu_1)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{15} \cdot \exp\left(-\frac{1}{2} \cdot \left(\begin{pmatrix} 0 \\ 2 \end{pmatrix} - \begin{pmatrix} 2 \\ -1 \end{pmatrix}\right)^T \cdot \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} 0 \\ 2 \end{pmatrix} - \begin{pmatrix} 2 \\ -1 \end{pmatrix}\right)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{15} \cdot \exp\left(-\frac{1}{2} \cdot \left(-2 \quad 3\right) \cdot \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix} \cdot \begin{pmatrix} -2 \\ 3 \end{pmatrix}\right) = \frac{e^{-20}}{2\pi \cdot 15} = \mathbf{0}$

joint probability: $P(c = 1, x_2) = P(c = 1)p(x_2|c = 1) = \pi_1 \cdot \mathcal{N}(x_2|\mu_1, \sigma_1) = \mathbf{0}$

normalized posterior:
$$P(c = 1|x_2) = \frac{0}{0 + 0.003} = \mathbf{0}$$

\rightarrow Cluster c=2:

prior:
$$P(c = 2) = \pi_2 = \mathbf{0.5}$$

likelihood: $p(x_2|c = 2) = \mathcal{N}(x_2|\mu_2, \sigma_2)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{\det(\Sigma_2)} \cdot \exp\left(-\frac{1}{2} \cdot (x_2 - \mu_2)^T \Sigma_2^{-1} \cdot (x_2 - \mu_2)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{4} \cdot \exp\left(-\frac{1}{2} \cdot \left(\begin{pmatrix} 0 \\ 2 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right)^T \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} 0 \\ 2 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{4} \cdot \exp\left(-\frac{1}{2} \cdot \left(-1 \quad 1\right) \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix}\right) = \frac{e^{-2}}{2\pi \cdot 4} = \mathbf{0.005}$

joint probability: $P(c=2, x_2) = P(c=2)p(x_2|c=2) = \pi_2 \cdot \mathcal{N}(x_2|\mu_2, \sigma_2) = \mathbf{0.003}$

normalized posterior: $P(c = 2|x_2) = \frac{0.003}{0 + 0.003} = 1$

 x_3

\rightarrow Cluster c=1:

prior:
$$P(c = 1) = \pi_1 = \mathbf{0.5}$$

likelihood: $p(x_3|c = 1) = \mathcal{N}(x_3|\mu_1, \sigma_1)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{\det(\Sigma_1)} \cdot \exp\left(-\frac{1}{2} \cdot (x_3 - \mu_1)^T \Sigma_1^{-1} \cdot (x_3 - \mu_1)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{15} \cdot \exp\left(-\frac{1}{2} \cdot \left(\begin{pmatrix} 3 \\ -1 \end{pmatrix} - \begin{pmatrix} 2 \\ -1 \end{pmatrix}\right)^T \cdot \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} 3 \\ -1 \end{pmatrix} - \begin{pmatrix} 2 \\ -1 \end{pmatrix}\right)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{15} \cdot \exp\left(-\frac{1}{2} \cdot (1 \quad 0) \cdot \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) = \frac{e^{-2}}{2\pi \cdot 15} = \mathbf{0.001}$

joint probability: $P(c = 1, x_3) = P(c = 1)p(x_3|c = 1) = \pi_1 \cdot \mathcal{N}(x_3|\mu_1, \sigma_1) = \mathbf{0.001}$

normalized posterior:
$$P(c = 1|x_3) = \frac{0.001}{0 + 0.001} = \mathbf{1}$$

\rightarrow Cluster c=2:

prior:
$$P(c = 2) = \pi_2 = \mathbf{0.5}$$

likelihood: $p(x_3|c = 2) = \mathcal{N}(x_3|\mu_2, \sigma_2)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{\det(\Sigma_2)} \cdot \exp\left(-\frac{1}{2} \cdot (x_3 - \mu_2)^T \Sigma_2^{-1} \cdot (x_3 - \mu_2)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{4} \cdot \exp\left(-\frac{1}{2} \cdot \left(\begin{pmatrix} 3 \\ -1 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right)^T \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} 3 \\ -1 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right)\right)$
 $= \frac{1}{(2 \cdot \pi)} \cdot \frac{1}{4} \cdot \exp\left(-\frac{1}{2} \cdot (2 - 2) \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ -2 \end{pmatrix}\right) = \frac{e^{-8}}{2\pi \cdot 4} = \mathbf{0}$

joint probability:
$$P(c = 1, x_3) = P(c = 1)p(x_3|c = 1) = \pi_1 \cdot \mathcal{N}(x_3|\mu_1, \sigma_1) = \mathbf{0}$$

normalized posterior:
$$P(c = 2|x_3) = \frac{0}{0 + 0.001} = \mathbf{0}$$

Observations	c = 1	c=2
$\overline{x_1}$	0.681	0.318
x_2	0	1
x_3	1	0

Table 1: Normalized posteriors

2) Maximization: M-STEP

For the recalculation we will use the following formulas (n represents the cluster):

For the means:

$$\mu_{n} = \frac{P(c=n|x_{1}) \cdot x_{1} + P(c=n|x_{2}) \cdot x_{2} + P(c=n|x_{3}) \cdot x_{3}}{P(c=n|x_{1}) + P(c=n|x_{2}) + P(c=n|x_{3})}$$
(1)

For the covariance matrices:

$$\Sigma_n = \begin{pmatrix} \Sigma_{11} & \Sigma_{21} \\ \Sigma_{12} & \Sigma_{22} \end{pmatrix} \tag{2}$$

Where

$$\Sigma_{ij} = \frac{P(c=n|x_1)((x_{1i}-\mu_{1i})(x_{1j}-\mu_{1j})) + P(c=n|x_2)((x_{2i}-\mu_{2i})(x_{2j}-\mu_{2j})) + P(c=n|x_3)((x_{3i}-\mu_{3i})(x_{3j}-\mu_{3j}))}{P(c=n|x_1) + P(c=n|x_2) + P(c=n|x_3)}$$

 \rightarrow Cluster c=1:

$$\mu_{1} = \frac{0.681 \cdot x_{1} + 0 \cdot x_{2} + 1 \cdot x_{3}}{0.681 + 0 + 1} = \frac{0.681 \cdot {1 \choose 0} + 0 \cdot {0 \choose 2} + 1 \cdot {3 \choose -1}}{1.681} = {2.190 \choose -0.595}$$

$$\Sigma_{1} = {\Sigma_{11} \quad \Sigma_{21} \choose \Sigma_{12} \quad \Sigma_{22}} = {0.964 \quad -0.482 \choose -0.482 \quad 0.241}$$

$$\Sigma_{11} = \frac{0.681 \cdot ((x_{11} - \mu_{11}) \cdot (x_{11} - \mu_{11})) + 0 \cdot ((x_{21} - \mu_{11}) \cdot (x_{21} - \mu_{11})) + 1 \cdot ((x_{31} - \mu_{11}) \cdot (x_{31} - \mu_{11}))}{1.681}$$

$$= \frac{0.681 \cdot ((1 - 2.190) \cdot (1 - 2.190)) + 1 \cdot ((3 - 2.190) \cdot (3 - 2.190))}{1.681} = \frac{0.964 + 0.656}{1.681} = 0.964$$

$$\Sigma_{21} = \frac{0.681 \cdot ((x_{12} - \mu_{12}) \cdot (x_{11} - \mu_{11})) + 0 \cdot ((x_{22} - \mu_{12}) \cdot (x_{21} - \mu_{11})) + 1 \cdot ((x_{32} - \mu_{12}) \cdot (x_{31} - \mu_{11}))}{1.681}$$

$$= \frac{0.681 \cdot ((0 - (-0.595)) \cdot (1 - 2.190)) + 1 \cdot ((-1 - (-0.595)) \cdot (3 - 2.190))}{1.681} = \frac{-0.482 + -0.328}{1.681}$$

$$= -0.482$$

$$\Sigma_{12} = \Sigma_{21} = -0.482$$

$$\Sigma_{22} = \frac{0.681 \cdot ((x_{12} - \mu_{12}) \cdot (x_{12} - \mu_{12})) + 0 \cdot ((x_{22} - \mu_{12}) \cdot (x_{22} - \mu_{12})) + 1 \cdot ((x_{32} - \mu_{12}) \cdot (x_{32} - \mu_{12}))}{1.681}$$

$$= \frac{0.681 \cdot ((0 - (-0.595)) \cdot (0 - (-0.595))) + 1 \cdot ((-1 - (-0.595)) \cdot (-1 - (-0.595)))}{1.681} = \frac{0.241 + 0.164}{1.681}$$

$$= 0.241$$

\rightarrow cluster c=2

$$\mu_2 = \frac{0.318 \cdot x_1 + 1 \cdot x_2 + 0 \cdot x_3}{0.318 + 1 + 0} = \frac{0.318 \cdot \binom{1}{0} + 0 \cdot \binom{0}{2} + 1 \cdot \binom{3}{-1}}{1.318} = \binom{2.517}{-0.759}$$
$$\Sigma_2 = \binom{\Sigma_{11} \quad \Sigma_{21}}{\Sigma_{12} \quad \Sigma_{22}} = \binom{5.362 \quad -5.546}{-5.546 \quad 7.795}$$

$$\Sigma_{11} = \frac{0.318 \cdot ((x_{11} - \mu_{21}) \cdot (x_{11} - \mu_{21})) + 1 \cdot ((x_{21} - \mu_{21}) \cdot (x_{21} - \mu_{21})) + 0 \cdot ((x_{31} - \mu_{21}) \cdot (x_{31} - \mu_{21}))}{1.318}$$

$$= \frac{0.318 \cdot ((1 - 2.517) \cdot (1 - 2.517)) + 1 \cdot ((0 - 2.517) \cdot (0 - 2.517))}{1.318} = \frac{0.732 + 6.335}{1.318} = 5.362$$

$$\Sigma_{21} = \frac{0.318 \cdot ((x_{12} - \mu_{22}) \cdot (x_{11} - \mu_{21})) + 1 \cdot ((x_{22} - \mu_{22}) \cdot (x_{21} - \mu_{21})) + 0 \cdot ((x_{32} - \mu_{22}) \cdot (x_{31} - \mu_{21}))}{1.318}$$

$$= \frac{0.318 \cdot ((0 - (-0.759)) \cdot (1 - 2.517)) + 1 \cdot ((2 - (-0.759)) \cdot (0 - 2.517))}{1.318} = \frac{-0.366 + (-6.944)}{1.318}$$

$$= -5.546$$

$$\Sigma_{12} = \Sigma_{21} = -5.546$$

$$\begin{split} \Sigma_{22} &= \frac{0.318 \cdot ((x_{12} - \mu_{22}) \cdot (x_{12} - \mu_{22})) + 1 \cdot ((x_{22} - \mu_{22}) \cdot (x_{22} - \mu_{22})) + 0 \cdot ((x_{32} - \mu_{22}) \cdot (x_{32} - \mu_{22}))}{1.318} \\ &= \frac{0.318 \cdot ((0 - (-0.759)) \cdot (0 - (-0.759))) + 1 \cdot ((2 - (-0.759)) \cdot (2 - (-0.759)))}{1.318} \\ &= \frac{0.183 + 7.612}{1.318} = 7.795 \end{split}$$

Normalized priors:

$$P(c=1) = \frac{0.681 + 0 + 1}{(0.681 + 0 + 1) + (0.318 + 1 + 0)} = 0.561$$
$$P(c=2) = \frac{0.318 + 1 + 0}{(0.681 + 0 + 1) + (0.318 + 1 + 0)} = 0.439$$

- 2. Using the final parameters computed in previous question:
 - a) perform a hard assignment of observations to clusters under a MAP assumption.
 - b) compute the silhouette of the larger cluster (the one that has more observations assigned to it) using the Euclidean distance.

Part II: Programming

In the next exercise you will use the accounts.csv dataset. This dataset contains account details of bank clients, and the target variable y is binary ('has the client subscribed a term deposit?').

1. Select the first 8 features and remove duplicates and null values. Normalize the data using MinMaxScaler. Using sklearn, apply k-means clustering (without targets) on the normalized data with $k = \{2, 3, 4, 5, 6, 7, 8\}$. Apply k-means randomly initialized, using max_iter = 500 and random_state = 42. Plot the different sum of squared errors (SSE) using the _inertia attribute of k-means according to the number of clusters.

Hint: You can use get_dummies() to change the feature type from categorical to numerical
(e.g. pd.get_dummies(data, drop_first=True))

- 2. According to the previous plot, how many underlying customer segments (clusters) should there be? Explain based on the trade off between the clusters and inertia.
- 3. Would k-modes be a better clustering approach? Explain why based on the dataset features.
- 4. Apply PCA to the data:
 - a) Use StandardScaler to scale the data before you apply fit_transform. How much variability is explained by the top 2 components?
 - b) Provide a scatterplot according to the first 2 principal components and color the points according to k=3 clusters. Can we clearly separate the clusters ? Justify.

5. Plot the cluster conditional features of the frequencies of 'job" and 'education" according to k-means, with multiple='dodge', stat='density', shrink=0.8, common_norm=False. Analyze the frequency plots using sns.displot, (see Data Exploration notebook). Describe the main differences between the clusters in no more than half page.