Aprendizagem 2024 Homework IV – Group 016 (ist1106022, ist1106720)

Part I: Pen and paper

1.) E-step

a)
$$P(x_i \mid c_k) = N(x_i \mid \mu_k, \Sigma_k) = \frac{1}{(2\pi)^{d/2} |\Sigma_k|^{1/2}} e^{-\frac{1}{2}(x_i - u_k)^T \Sigma_k^{-1}(x_i - u_k)}$$

b)
$$P(c_k, x_i) = \pi_k \cdot N(x_i \mid \mu_k, \Sigma_k)$$

c)
$$P(x_i) = \sum_k (P(c_k, x_i))$$
$$\gamma(c_{ki}) = P(c_k \mid x_i) = \frac{P(c_k, x_i)}{P(x_i)}$$

a)-c)
$$\gamma(c_{ki}) = P(c_k \mid x_i) = \frac{P(x_i \mid c_k) \cdot P(c_k)}{P(x_i)} = \frac{N(x_i \mid \mu_k, \Sigma_k) \cdot \pi_k}{\sum_k (\pi_k \cdot N(x_i \mid \mu_k, \Sigma_k))}$$

M-step

$$N_k = \sum_{i=1}^N \gamma(c_{ki})$$

$$\mu_k = \frac{1}{N_k} \sum_{i=1}^N \gamma(c_{ki}) \cdot \mathbf{x}_i$$

$$\Sigma_k = \frac{1}{N_k} \sum_{i=1}^N \left(\gamma(c_{ki}) \cdot (\mathbf{x}_i - \mu_k) (\mathbf{x}_i - \mu_k)^T \right)$$

$$\pi_k = P(c_k) = \frac{N_k}{N}$$

First Epoch

E-step Calculations

a)
$$p(\mathbf{x}_1 \mid c_1) = 0.029$$
, $p(\mathbf{x}_1 \mid c_2) = 0.062$
 $p(\mathbf{x}_2 \mid c_1) = 0.005$, $p(\mathbf{x}_2 \mid c_2) = 0.048$
 $p(\mathbf{x}_3 \mid c_1) = 0.036$, $p(\mathbf{x}_3 \mid c_2) = 0.011$

b)
$$p(\mathbf{x}_1, c_1) = 0.015$$
, $p(\mathbf{x}_1, c_2) = 0.031$
 $p(\mathbf{x}_2, c_1) = 0.002$, $p(\mathbf{x}_2, c_2) = 0.024$
 $p(\mathbf{x}_3, c_1) = 0.018$, $p(\mathbf{x}_3, c_2) = 0.005$

c)
$$\gamma(c_{11}) = p(c_1 \mid \mathbf{x}_1) = 0.322$$
, $\gamma(c_{21}) = p(c_2 \mid \mathbf{x}_1) = 0.678$
 $\gamma(c_{12}) = p(c_1 \mid \mathbf{x}_2) = 0.092$, $\gamma(c_{22}) = p(c_2 \mid \mathbf{x}_2) = 0.908$
 $\gamma(c_{13}) = p(c_1 \mid \mathbf{x}_3) = 0.770$, $\gamma(c_{23}) = p(c_2 \mid \mathbf{x}_3) = 0.230$

M-step Calculations

$$N_1 = 1.184$$
 $N_2 = 1.816$

Updated Means:
$$\mu_1 = \begin{pmatrix} 2.223 \\ -0.496 \end{pmatrix}$$
 $\mu_2 = \begin{pmatrix} 0.754 \\ 0.873 \end{pmatrix}$

Updated Covariance Matrices:
$$\Sigma_1 = \begin{pmatrix} 1.182 & -0.849 \\ -0.849 & 0.714 \end{pmatrix}$$
 $\Sigma_2 = \begin{pmatrix} 0.947 & -1.039 \\ -1.039 & 1.364 \end{pmatrix}$

Updated Priors: $\pi_1 = 0.394$ $\pi_2 = 0.606$

Second Epoch

E-step Calculations

a)
$$p(\mathbf{x}_1 \mid c_1) = 0.119$$
, $p(\mathbf{x}_1 \mid c_2) = 0.149$
 $p(\mathbf{x}_2 \mid c_1) = 0.001$, $p(\mathbf{x}_2 \mid c_2) = 0.209$
 $p(\mathbf{x}_3 \mid c_1) = 0.346$, $p(\mathbf{x}_3 \mid c_2) = 0.011$

b)
$$p(\mathbf{x}_1, c_1) = 0.047$$
, $p(\mathbf{x}_1, c_2) = 0.090$
 $p(\mathbf{x}_2, c_1) = 0.000$, $p(\mathbf{x}_2, c_2) = 0.127$
 $p(\mathbf{x}_3, c_1) = 0.136$, $p(\mathbf{x}_3, c_2) = 0.007$

c)
$$\gamma(c_{11}) = p(c_1 \mid \mathbf{x}_1) = 0.343$$
, $\gamma(c_{21}) = p(c_2 \mid \mathbf{x}_1) = 0.657$
 $\gamma(c_{12}) = p(c_1 \mid \mathbf{x}_2) = 0.004$, $\gamma(c_{22}) = p(c_2 \mid \mathbf{x}_2) = 0.996$
 $\gamma(c_{13}) = p(c_1 \mid \mathbf{x}_3) = 0.953$, $\gamma(c_{23}) = p(c_2 \mid \mathbf{x}_3) = 0.047$

M-step Calculations

$$N_1 = 1.300$$
 $N_2 = 1.700$
Updated Means: $\mu_1 = \begin{pmatrix} 2.464 \\ -0.728 \end{pmatrix}$ $\mu_2 = \begin{pmatrix} 0.469 \\ 1.145 \end{pmatrix}$
Updated Covariance Matrices: $\Sigma_1 = \begin{pmatrix} 0.793 & -0.407 \\ -0.407 & 0.215 \end{pmatrix}$ $\Sigma_2 = \begin{pmatrix} 0.414 & -0.619 \\ -0.619 & 1.062 \end{pmatrix}$
Updated Priors: $\pi_1 = 0.433$ $\pi_2 = 0.567$

2.) a. Hard assignment of observations to clusters under a MAP assumption

Using the same formulas as the first exercise and the updated means, covarience matrices and priors of the same exercise:

2

$$p(c_1|\mathbf{x}_1) = 0.588, \quad p(c_2|\mathbf{x}_1) = 0.412$$

 $p(c_1|\mathbf{x}_2) = 0.000, \quad p(c_2|\mathbf{x}_2) = 1.000$
 $p(c_1|\mathbf{x}_3) = 1.000, \quad p(c_2|\mathbf{x}_3) = 0.000$
Clusters: $\{c_1 = \{\mathbf{x}_1, \mathbf{x}_3\}, c_2 = \{\mathbf{x}_2\}\}$

b. Silhouette of the larger cluster using Euclidean distance

Using the following formulas:

 $a(x_i)$ = average distance of x_i to the points in its cluster $b(x_i)$ = min(average distance of x_i to points in another cluster)

$$s(x_i) = \begin{cases} 1 - \frac{a(x_i)}{b(x_i)}, & \text{if } a(x_i) < b(x_i), \\ \frac{b(x_i)}{a(x_i)} - 1, & \text{if } a(x_i) \ge b(x_i). \end{cases}$$

We can calculate the silhouette of the larger cluster:

$$s(x_1) = \frac{b(x_1)}{a(x_1)} - 1 = \frac{\|x_1 - x_2\|_2}{\|x_1 - x_3\|_2} - 1 = \frac{\sqrt{5}}{\sqrt{5}} - 1 = 0.000$$

$$s(x_3) = 1 - \frac{a(x_3)}{b(x_3)} = 1 - \frac{\|x_3 - x_1\|_2}{\|x_3 - x_2\|_2} = 1 - \frac{\sqrt{5}}{\sqrt{18}} = 0.473$$

$$s(c_1) = \frac{s(x_1) + s(x_3)}{2} = 0.237$$

Part II: Programming

Before any exercise, a dataset preprocess was made, shortening the dataset to accommodate only the first 8 features and any categoric feature changed to numeric. All duplicates and null values were also removed.

- 1.) The 3 next exercises work upon the dataset data normalized according to MinMaxScaler
- **a.)** To pick how many clusters there should be, k-means was performed on the data with increasing values of k. The resulting inertia was plotted against the number of cluster, giving the following results:

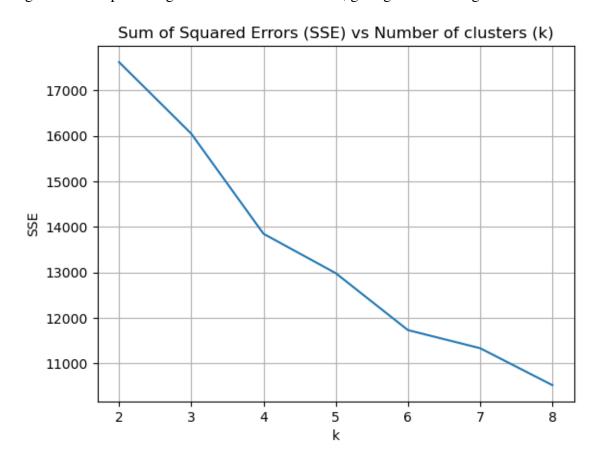


Figure 1: Inertia vs. Number of Clusters

b.) MISSING EXPLANATION

c.) MISSING EXPLANATION

- 2.) The 3 next exercises work upon the dataset data normalized according to **StandardScaler**
- **a.**) After performing the **PCA** on the data, the top 2 components correspond to the features 'age' and 'balance' with the variance ratios of 0.11679024 (aprox. 11,68%) and 0.11075988 (aprox. 11,08%), respectively. This means that the top 2 components explain 22,76% of the variance in the data.
- **b.**) After performing k-means, considering k = 3, and plotting the results according to the first 2 principal components, the following plot was obtained:

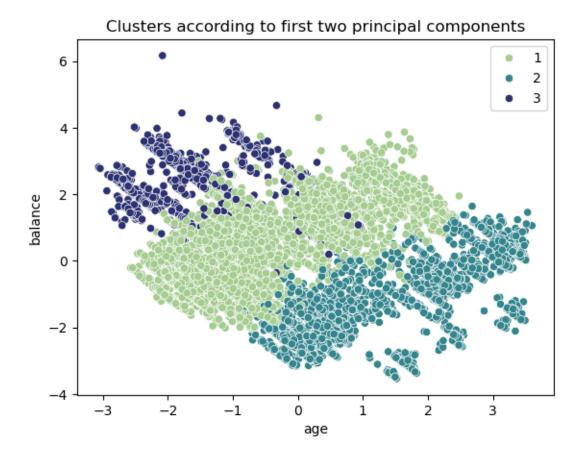


Figure 2: Clusters according to the first 2 principal components

We can conclude, by observing the plot, these 2 components aren't enough to clearly separate the clusters, as they overlap in some regions. This can be explained by the fact that, together, these components only explain 22.76% of the variance in the data.

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c.) When looking at the cluster conditional features for the original features 'job' and 'education', we get the following results:

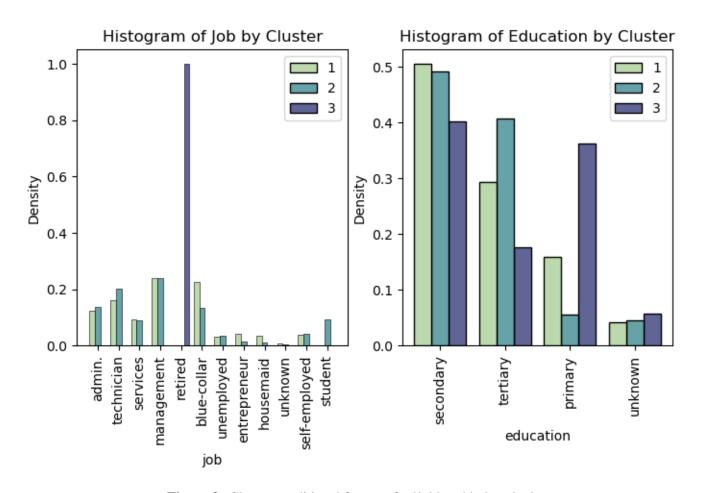


Figure 3: Cluster conditional features for 'job' and 'education'

MISSING EXPLANATION

A Numpy Code for Exercise 1 - Pen and Paper

Listing 1: Python code for Exercise 1

```
import numpy as np
# Initializing the observations, means, covariances, and mixture probabilities
observations = np.array([[1, 0], [0, 2], [3, -1]])
means = [np.array([2, -1]), np.array([1, 1])]
covariances = [np.array([[4, 1], [1, 4]]), np.array([[2, 0], [0, 2]])]
pis = [0.5, 0.5]
def multivariate_gaussian(x, mean, cov):
    d = len(mean)
    cov_det = np.linalg.det(cov)
    cov_inv = np.linalg.inv(cov)
    factor = 1 / ((2 * np.pi) ** (d / 2) * cov_det ** 0.5)
    exponent = -0.5 * (x - mean).T @ cov_inv @ (x - mean)
    return factor * np.exp(exponent)
def e_step(observations, means, covariances, pis):
    gammas = np. zeros ((len (observations), len (means)))
    print("E-step:")
    # Step a
    p_x = given_c = []
    for i, x_i in enumerate (observations):
        p_{-}x_{-}k = []
        for k in range(len(means)):
            prob = multivariate_gaussian(x_i, means[k], covariances[k])
            p_x_k. append (prob)
            print (f"p(x{i + 1}|c{k + 1}) = \{prob.round(3)\}")
        p_x_given_c.append(p_x_k)
    # Step b
    p_c_and_x = []
    for i, x_i in enumerate (observations):
        p_c_x_k = []
        for k in range(len(means)):
            p_c_x = p_x_given_c[i][k] * pis[k]
            p_c_x_k . append ( p_c_x
            print (f"p(x\{i+1\}, c\{k+1\}) = \{p_c_x.round(3)\}")
        p_c_and_x.append(p_c_x_k)
    # Step c
    p_x = [sum(p_c_and_x[i]) \text{ for } i \text{ in } range(len(observations))]
    for i in range(len(observations)):
        for k in range(len(means)):
```

```
gammas[i, k] = p_c_and_x[i][k] / p_x[i]
            print(f'' \setminus gamma(c\{k+1\}\{i+1\})) = p(c\{k+1\}|x\{i+1\}) =
            {gammas[i, k].round(3)}")
    return gammas
def m_step(observations, gammas):
    n_clusters = gammas.shape[1]
    N_k = gammas.sum(axis=0)
    new_means = []
    new_covariances = []
    new_pis = []
    print("\nM\text{-Step:")
    for k in range(n_clusters):
        # Update mean
        weighted_sum = sum(gammas[i, k] * observations[i]
            for i in range(len(observations)))
        new_mean = weighted_sum / N_k[k]
        new_means.append(new_mean.round(3))
        print(f"\backslash mu\{k+1\} = \{new\_mean.round(3)\}")
        # Update covariance
        weighted_cov_sum = sum(gammas[i, k] * np.outer(observations[i])
            - new_mean, observations[i] - new_mean) for i in
            range(len(observations)))
        new_covariance = weighted_cov_sum / N_k[k]
        new_covariances.append(new_covariance.round(3))
        print(f"Sigma{k + 1} = {new_covariance.round(3)}")
        # Update pi
        new_pi = (N_k[k] / len(observations)). round(3)
        new_pis.append(new_pi)
        print(f" \setminus pi\{k + 1\} = \{new_pi:.3f\}")
    return new_means, new_covariances, new_pis
# Run EM steps
for iteration in range(2): # specify number of iterations
    print(f"\nIteration {iteration + 1}:")
    gammas = e_step(observations, means, covariances, pis)
    means, covariances, pis = m_step(observations, gammas)
    print("Updated Means:", means)
    print("Updated Covariances:", covariances)
    print("Updated Pis:", pis)
```

B Numpy Code for Exercise 2a - Pen and Paper

Listing 2: Python code for Exercise 2a

```
import numpy as np
# Updated parameters from Iteration 2
mu_{-1} = np. array([2.464, -0.728])
mu_2 = np. array([0.469, 1.145])
sigma_1 = np. array([[0.793, -0.407], [-0.407, 0.215]])
sigma_2 = np. array([[0.414, -0.619], [-0.619, 1.062]])
pi_1 = 0.433
pi_{-}2 = 0.567
# Observations
x1 = np.array([1, 0])
x2 = np.array([0, 2])
x3 = np.array([3, -1])
observations = [x1, x2, x3]
# Multivariate Gaussian function
def multivariate_gaussian(x, mean, cov):
    d = len(mean)
    cov_det = np.linalg.det(cov)
    cov_inv = np.linalg.inv(cov)
    term1 = 1 / ((2 * np.pi) ** (d / 2) * np.sqrt(cov_det))
    term2 = np.exp(-0.5 * (x - mean).T @ cov_inv @ (x - mean))
    return term1 * term2
# Step 2a: Calculate the posterior probabilities for
#each observation and cluster
posteriors = []
for x in observations:
    p_x_given_c1 = multivariate_gaussian(x, mu_1, sigma_1)
    p_x_given_c2 = multivariate_gaussian(x, mu_2, sigma_2)
    p_c1_x = p_x_given_c1 * pi_1
    p_c2_x = p_x_given_c2 * pi_2
    p_x = p_c 1_x + p_c 2_x
    posterior_c1 = p_c1_x / p_x
    posterior_c2 = p_c2_x / p_x
    posteriors.append((posterior_c1, posterior_c2))
print("Posterior probabilities (question 2a):")
for i, (p_c1, p_c2) in enumerate(posteriors, 1):
    print(f"p(c1 | x{i})) = {p_c1.round(3)}, p(c2 | x{i}) = {p_c2.round(3)}")
```

```
# Hard assignments based on MAP
clusters = {1: [], 2: []}
for i, (p_c1, p_c2) in enumerate(posteriors, 1):
    if p_c1 > p_c2:
        clusters [1]. append(observations [i - 1])
    else:
        clusters [2]. append(observations [i - 1])

print("\nClusters after hard assignment (question 2a):")
for cluster, points in clusters.items():
    print(f"Cluster {cluster}: {points}")
```