Aprendizagem 2023/24

Homework I V– Group 35

(ist1100032, ist1100070)

I. Pen-and-paper

1)

1

E-step: posterior probabilities for each observation

$\boxed{x_1 : (1, 0.6, 0.1)}$

likelihoods:

bernoulli

$$\begin{cases} p(\{y_1\} \mid k=1) = 0.3^{1} \cdot (1-0.3)^{1-1} = 0.3 \\ p(\{y_1\} \mid k=2) = 0.7^{1} \cdot (1-0.7)^{1-1} = 0.7 \end{cases}$$

multivariate gaussian

$$\begin{cases} p(\{y_2, y_3\} \mid k=1) = (0.6, 0.1) \sim N_1(\mu_1, \Sigma_1) = 0.06657 \\ p(\{y_2, y_3\} \mid k=2) = (0.6, 0.1) \sim N_2(\mu_2, \Sigma_2) = 0.11961 \end{cases}$$

- $P(x_1 \mid k=1) = P(\{y_1\} \mid k=1) \times P(\{y_2, y_3\} \mid k=1) = 0.01997$
- $P(x_1 \mid k=2) = P(\{y_1\} \mid k=2) \times P(\{y_2, y_3\} \mid k=2) = 0.083732$

posteriors:

$$p(k=1|x_1) = \frac{P(x_1|k=1) \times \pi_1}{\sum_{i=1}^{2} \pi_i \cdot P(x_1|k=i)} = 0.1926$$

0.05185

$$p(k=2|x_1) = \frac{P(x_1|K_2) \times \pi_2}{\sum_{i=1}^{2} \pi_i \cdot P(x_1|k=i)} = 0.8074$$

$$\boxed{x_2 : (0, -0.4, 0.8)}$$

likelihoods:

bernoulli

$$p(\{y_1\}|k=1) = 0.3^{0} \cdot (1-0.3)^{1-0} = 0.7$$

$$p(\{y_1\}|k=2) = 0.7^{0} \cdot (1-0.7)^{1-0} = 0.3$$

multivariate gaussian

$$p(\{y_2, y_3\}|k=1) = (-0.4, 0.8) \sim N_1(\mu_1, \Sigma_1) = 0.050048$$

$$p(\{y_2, y_3\}|k=2) = (-0.4, 0.8) \sim N_2(\mu_2, \Sigma_2) = 0.06819$$

- $P(x_2|k=1) = P(\{y_1\}|k=1) \times P(\{y_2, y_3\}|k=1) = 0.035034$
- $P(x_2|k=2) = P(\{y_1\}|k=2) \times P(\{y_2, y_3\}|k=2) = 0.020457$

posteriors:

$$P(K=1 \mid x_2) = \frac{P(x_2 \mid K=1) \times \pi_1}{\sum_{i=1}^{2} \pi_i \cdot P(x_2 \mid K=i)} = 0.63134$$

$$P(K=2 \mid x_2) = \frac{P(x_2 \mid K_2) \times \pi_2}{\sum_{i=1}^{2} \pi_i \cdot P(x_2 \mid K=i)} = 0.36865$$

$$\boxed{x_3 : (0, 0.2, 0.5)}$$

likelihoods:

bernoulli

$$p(\{y_1\} \mid K=1) = 0.3^{0} \cdot (1-0.3)^{1-0} = 0.7$$

$$p(\{y_1\} \mid K=2) = 0.7^{0} \cdot (1-0.7)^{1-0} = 0.3$$

multivariate gaussian

$$p(\{y_2, y_3\} \mid K=1) = (0.2, 0.5) \sim N_1(\mu_1, \Sigma_1) = 0.06837$$

$$p(\{y_2, y_3\} \mid K=2) = (0.2, 0.5) \sim N_2(\mu_2, \Sigma_2) = 0.12958$$

- $P(x_3 \mid k=1) = P(\{y_1\} \mid k=1) \times P(\{y_2, y_3\} \mid k=1) = 0.04786$
- $P(x_3 \mid k=2) = P(\{y_1\} \mid k=2) \times P(\{y_2, y_3\} \mid k=2) = 0.03887$

posteriors:

$$P(k=1 \mid x_3) = \frac{P(x_3 \mid k=1) \times \tilde{\pi}_1}{\sum_{i=1}^{2} \tilde{\pi}_i \cdot P(x_3 \mid k=i)} = 0.55181$$

$$P(k=2 \mid x_3) = \frac{P(x_3 \mid k_2) \times \tilde{\pi}_2}{\sum_{i=1}^{2} \tilde{\pi}_i \cdot P(x_3 \mid k=i)} = 0.44819$$

$\boxed{x_4 : (1, 0.4, -0.1)}$

likelihoods:

bernoulli
$$p(\{y_1\} \mid k=1) = 0.3^1 \cdot (1-0.3)^{1-1} = 0.3$$
$$p(\{y_1\} \mid k=2) = 0.7^1 \cdot (1-0.7)^{1-1} = 0.7$$

multivariate gaussian
$$p(\{y_2, y_3\} \mid k=1) = (0.4, -0.1) \sim N_1(\mu_1, \Sigma_1) = 0.059047$$
$$p(\{y_2, y_3\} \mid k=2) = (0.4, -0.1) \sim N_2(\mu_2, \Sigma_2) = 0.12450$$

- $P(x_4 \mid k=1) = P(\{y_1\} \mid k=1) \times P(\{y_2, y_3\} \mid k=1) = 0.01771$
- $P(x_4 \mid k=2) = P(\{y_1\} \mid k=2) \times P(\{y_2, y_3\} \mid k=2) = 0.08715$

Posteriors:

$$P(k=1 \mid x_4) = \frac{P(x_4 \mid k=1) \times \pi_1}{\sum_{i=1}^{2} \pi_i \cdot P(x_4 \mid k=i)} = 0.1689$$

$$P(k=2 \mid x_4) = \frac{P(x_4 \mid k_2) \times \pi_2}{\sum_{i=1}^{2} \pi_i \cdot P(x_4 \mid k=i)} = 0.8311$$

M-Step : Update parameters

Cluster 1

Prior : $\pi_1 = P(k=1) = \frac{\sum_{i=1}^{4} P(k=1 \mid x_i)}{4} = 0.38617$

Bernoulli Parameters:

$$p_1 = P(y_1 = 1 \mid k=1) = \frac{\sum_{i=1}^{4} P(k=1 \mid y_{1i}) \cdot y_{1i}}{\sum_{i=1}^{4} P(k=1 \mid X_i)} = \frac{0.3615}{1.5447} = 0.2340$$

Gaussian Parameters:

$$\mu_1 = \frac{\sum_{i=1}^{4} P(k=1 \mid X_i) \cdot \{y_2, y_3\}_i}{\sum_{i=1}^{4} P(k=1 \mid X_i)} = \begin{pmatrix} 0.0409 \\ 0.7833 \end{pmatrix} \div 1.5447 = \begin{bmatrix} 0.026509 \\ 0.507129 \end{bmatrix}$$

$$\Sigma^{(i,j)} = \frac{\sum_{m=1}^{4} P(k=1 \mid X_m) \cdot (\{y_2, y_3\}_i - \mu_k) \cdot (\{y_2, y_3\}_i - \mu_k)^T}{\sum_{i=1}^{4} P(k=1 \mid X_i)} =$$

$$\begin{bmatrix} 0.21836 & -0.16282 \\ -0.16282 & 0.14837 \end{bmatrix} \div 1.5447 = \begin{bmatrix} 0.14136 & -0.10541 \\ -0.10541 & 0.09605 \end{bmatrix}$$

Cluster 2

Prior: $\pi_1 = P(k=2) = \dfrac{\sum_{i=1}^{4} P(k=2 \mid x_i)}{4} = 0.61383$

Bernoulli Parameters:

$$p_2 = P(y_1 = 1 \mid k=2) = \frac{\sum_{i=1}^{4} P(k=2 \mid y_{1i}) \cdot y_{1i}}{\sum_{i=1}^{4} P(k=2 \mid X_i)} = \frac{1.6385}{2.4553} = 0.66731$$

Gaussian Parameters:

$$\mu_2 = \frac{\sum_{i=1}^{4} P(k=2 \mid X_i) \cdot \{y_2, y_3\}_i}{\sum_{i=1}^{4} P(k=2 \mid X_i)} = \begin{pmatrix} 0.75905 \\ 0.51665 \end{pmatrix} \div 2.4553 = \begin{bmatrix} 0.30914 \\ 0.21042 \end{bmatrix}$$

$$\Sigma^{(i,j)} = \frac{\sum_{m=1}^{4} P(k=2 \mid X_m) \cdot (\{y_2, y_3\}_i - \mu_k) \cdot (\{y_2, y_3\}_i - \mu_k)^T}{\sum_{i=1}^{4} P(k=2 \mid X_i)} =$$

$$= \begin{bmatrix} 0.26589 & -0.217669 \\ -0.217669 & 0.255657 \end{bmatrix} \div 2.4553 = \begin{bmatrix} 0.10829 & -0.08865 \\ -0.08865 & 0.10412 \end{bmatrix}$$

Código auxiliar:

```python
import numpy as np
from scipy.stats import bernoulli, multivariate_normal

# Given data points
data = np.array([
    [1, 0.6, 0.1],
    [0, -0.4, 0.8],
    [0, 0.2, 0.5],
    [1, 0.4, -0.1]
])

# Given parameters
pi = np.array([0.5, 0.5])
p = np.array([0.3, 0.7])
N1 = {
    'mean': np.array([1, 1]),
    'cov': np.array([[2, 0.5], [0.5, 2]])
}
N2 = {
    'mean': np.array([0, 0]),
    'cov': np.array([[1.5, 1], [1, 1.5]])
}
```

```python
# Initialize arrays to store posterior probabilities
posterior_probs = np.zeros((len(data), 2))

# E-step: Compute posterior probabilities
for i in range(len(data)):
    print(f"\n\nX{ i }\n")
    likelihood_bernoulli_1 = p[0]**data[i, 0] * (1-p[0])**(1-data[i, 0])
    likelihood_bernoulli_2 = p[1]**data[i, 0] * (1-p[1])**(1-data[i, 0])
    print(f"Bernoulli Likelihood (Cluster 1): {likelihood_bernoulli_1}")
    print(f"Bernoulli Likelihood (Cluster 2): {likelihood_bernoulli_2}")

    likelihood_gaussian_1 = multivariate_normal.pdf(data[i, 1:], mean=N1['mean'], cov=N1['cov'])
    likelihood_gaussian_2 = multivariate_normal.pdf(data[i, 1:], mean=N2['mean'], cov=N2['cov'])
    print(f"Gaussian Likelihood (Cluster 1): {likelihood_gaussian_1}")
    print(f"Gaussian Likelihood (Cluster 2): {likelihood_gaussian_2}")

    likelihood_1 = likelihood_bernoulli_1 * likelihood_gaussian_1
    likelihood_2 = likelihood_bernoulli_2 * likelihood_gaussian_2
    print(f"likelihood (Cluster 1): {likelihood_1}")
    print(f"likelihood (Cluster 2): {likelihood_2}")

    denominator = pi[0] * likelihood_1 + pi[1] * likelihood_2
    print(f"Denominator): {denominator}")

    posterior_probs[i, 0] = (pi[0] * likelihood_bernoulli_1 * likelihood_gaussian_1) / denominator
    posterior_probs[i, 1] = (pi[1] * likelihood_bernoulli_2 * likelihood_gaussian_2) / denominator

print("Posterior Probabilities:\n", posterior_probs)
```

```
X0

Bernoulli Likelihood (Cluster 1): 0.3
Bernoulli Likelihood (Cluster 2): 0.7
Gaussian Likelihood (Cluster 1): 0.06657529920303393
Gaussian Likelihood (Cluster 2): 0.11961837142058572
likelihood (Cluster 1): 0.019972589760910178
likelihood (Cluster 2): 0.08373285999441
Denominator): 0.05185272487766009


X1

Bernoulli Likelihood (Cluster 1): 0.7
Bernoulli Likelihood (Cluster 2): 0.30000000000000004
Gaussian Likelihood (Cluster 1): 0.05004888824270901
Gaussian Likelihood (Cluster 2): 0.0681905803254947
likelihood (Cluster 1): 0.035034221769896304
likelihood (Cluster 2): 0.020457174097648412
Denominator): 0.027745697933772358
```

```
X2

Bernoulli Likelihood (Cluster 1): 0.7
Bernoulli Likelihood (Cluster 2): 0.30000000000000004
Gaussian Likelihood (Cluster 1): 0.06837452355368487
Gaussian Likelihood (Cluster 2): 0.12958103481626038
likelihood (Cluster 1): 0.047862166487579405
likelihood (Cluster 2): 0.038874310444878116
Denominator): 0.04336823846622876


X3

Bernoulli Likelihood (Cluster 1): 0.3
Bernoulli Likelihood (Cluster 2): 0.7
Gaussian Likelihood (Cluster 1): 0.059046993443730274
Gaussian Likelihood (Cluster 2): 0.12450008976589248
likelihood (Cluster 1): 0.01771409803311908
likelihood (Cluster 2): 0.08715006283612474
Denominator): 0.052432080434621914
Posterior Probabilities:
 [[0.19258959 0.80741041]
 [0.63134512 0.36865488]
 [0.55181128 0.44818872]
 [0.16892423 0.83107577]]
```

```python
# M-step: Update model parameters
new_pi = np.mean(posterior_probs, axis=0)
print("PI:", new_pi)
print("\n\n")

# Update p
print("BERNOULLI")

new_p = np.zeros(2)
for j in range(2): # 2 clusters
    print("cluster:", j)
    p_sum = 0
    for i in range(len(data)):
        p_sum += data[i, 0] * posterior_probs[i, j]
    print("p_sum:", p_sum)
    denominator = np.sum(posterior_probs[:, j])
    print("denominator:", denominator)
    new_p[j] = p_sum / denominator
print("p:", new_p)
print("\n\n")
```

```python
# Update N1 and N2
new_N1_mean = np.zeros(2)
new_N2_mean = np.zeros(2)
new_N1_cov = np.zeros((2, 2))
new_N2_cov = np.zeros((2, 2))

print("\nGAUSS")
for j in range(2): # 2 clusters
    print("\ncluster:", j)
    mean_sum = np.zeros(2)
    cov_sum = np.zeros((2, 2))
    for i in range(len(data)):
        mean_sum += posterior_probs[i, j] * data[i, 1:]
        cov_sum += posterior_probs[i, j] * np.outer(data[i, 1:] - [N1['mean'], N2['mean']][j], data[i, 1:] - [N1['mean'], N2['mean']][j])
    print("mean_sum:", mean_sum)
    print("cov_sum:", cov_sum)
    if j == 0:
        new_N1_mean = mean_sum / np.sum(posterior_probs[:, j])
        new_N1_cov = cov_sum / np.sum(posterior_probs[:, j])
    else:
        new_N2_mean = mean_sum / np.sum(posterior_probs[:, j])
        new_N2_cov = cov_sum / np.sum(posterior_probs[:, j])
```

```python
# Update the model parameters
pi = new_pi
p = new_p

N1['mean'] = new_N1_mean
N2['mean'] = new_N2_mean
N1['cov'] = new_N1_cov
N2['cov'] = new_N2_cov

print("\n")
print("N1 mean:", N1['mean'])
print("N1 cov:\n", N1['cov'])
print("\n")
print("N2 mean:", N2['mean'])
print("N2 cov:\n", N2['cov'])
```

```
PI: [0.38616755 0.61383245]
```

```
BERNOULLI
cluster: 0
p_sum: 0.36151382107026986
denominator: 1.5446702187154808
cluster: 1
p_sum: 1.63848617892973
denominator: 2.455329781284519
p: [0.23403948 0.66731817]
```

```
GAUSS

cluster: 0
mean_sum: [0.04094766 0.78334827]
cov_sum: [[ 0.21836232 -0.16281668]
 [-0.16281668  0.1483696 ]]

cluster: 1
mean_sum: [0.75905234 0.51665173]
cov_sum: [[ 0.26589514 -0.21766927]
 [-0.21766927  0.25565705]]


N1 mean: [0.026509   0.50712978]
N1 cov:
 [[ 0.14136501 -0.10540546]
 [-0.10540546  0.0960526 ]]


N2 mean: [0.30914476 0.2104205 ]
N2 cov:
 [[ 0.10829305 -0.08865175]
 [-0.08865175  0.1041233 ]]
```

Aprendizagem 2023/24

Homework I V– Group 35

(ist1100032, ist1100070)

2)

2) $x_{new} = \begin{pmatrix} 1 \\ 0,3 \\ 0,7 \end{pmatrix}$

After EM update

$\pi_1 = 0,38617$ $\qquad \pi_2 = 0,61383$

$p_1 = 0,23404$ $\qquad p_2 = 0,66732$

$N_1\left(\mu_1 = \begin{pmatrix} 0,02651 \\ 0,50713 \end{pmatrix}, \Sigma_1 = \begin{pmatrix} 0,14137 & -0,10541 \\ -0,10541 & 0,09605 \end{pmatrix} \right)$

$N_2\left(\mu_2 = \begin{pmatrix} 0,30914 \\ 0,21042 \end{pmatrix}, \Sigma_2 = \begin{pmatrix} 0,10829 & -0,08865 \\ -0,08865 & 0,10412 \end{pmatrix} \right)$

likelihood cluster 1 $= p(\{y_1\} \mid k=1) \times p(\{y_2, y_3\} \mid k=1) =$

$= 0,006337$

likelihood cluster 2 $= p(\{y_1\} \mid k=2) \times p(\{y_2, y_3\} \mid k=2) =$

$= 0,04567$

posteriors:

$$p(k=1 \mid x_{new}) = \frac{P(x_{new} \mid k=1) \times \pi_1}{\sum_{i=1}^{2} \pi_i \cdot P(x_{new} \mid k=i)} = 0{,}08029$$

$$p(k=2 \mid x_{new}) = \frac{P(x_{new} \mid k=2) \times \pi_2}{\sum_{i=1}^{2} \pi_i \cdot P(x_{new} \mid k=i)} = 0{,}91971$$

Código auxiliar:

```
import numpy as np
from scipy.stats import multivariate_normal

# Given initial values
pi1 = new_pi[0]
pi2 = new_pi[1]
p1 = new_p[0]
p2 = new_p[1]
mu1 = new_N1_mean
sigma1 = new_N1_cov
mu2 = new_N2_mean
sigma2 = new_N2_cov
x_new = np.array([1, 0.3, 0.7])
```

```python
# Likelihood of x_new under each cluster
likelihood_c1 = (p1**x_new[0]) * ((1 - p1)**(1 - x_new[0])) * multivariate_normal.pdf(x_new[1:], mean=mu1, cov=sigma1)
likelihood_c2 = (p2**x_new[0]) * ((1 - p2)**(1 - x_new[0])) * multivariate_normal.pdf(x_new[1:], mean=mu2, cov=sigma2)

print("Likelihood for Cluster 1: ",likelihood_c1)
print("Likelihood for Cluster 2: ",likelihood_c2)

# Posterior probabilities
posterior_c1 = (likelihood_c1 * pi1) / (likelihood_c1 * pi1 + likelihood_c2 * pi2)
posterior_c2 = (likelihood_c2 * pi2) / (likelihood_c1 * pi1 + likelihood_c2 * pi2)

print("Posterior Probability for Cluster 1:", posterior_c1)
print("Posterior Probability for Cluster 2:", posterior_c2)
```

```
Likelihood for Cluster 1:  0.006336753293816409
Likelihood for Cluster 2:  0.045665170414993406
Posterior Probability for Cluster 1: 0.08028950846197516
Posterior Probability for Cluster 2: 0.9197104915380249
```

3)

3)

likelihoods for x_1

$$P(x_1 \mid K=1) = P(\{y_1\} \mid K=1) \times P(\{y_2, y_3\} \mid k=1) =$$

$$= p_1^{\,1} \cdot (1-p_1)^{1-1} \times N((0{,}6; 0{,}1) \mid \mu_1, \Sigma_1) =$$

$$= 0{,}23147$$

$$P(x_1 \mid K=2) = p_2^{\,1} \cdot (1-p_1)^{1-1} \times N((0{,}6; 0{,}1) \mid \mu_1, \Sigma_1) =$$

$$= 0{,}333$$

x_1 belongs to the second cluster

likelihoods for x_2

$$P(x_2 \mid K=1) = 1{,}3$$

$$P(x_2 \mid K=2) = 0{,}2$$

x_2 belongs to the first cluster

likelihoods for x_3

$$P(x_3 \mid k=1) = 1{,}4$$

$$P(x_3 \mid K=2) = 1{,}05$$

x_3 belongs to the second cluster

likelihoods for x_4:

$P(x_4 | k=1) = 0{,}02$

$P(x_4 | k=2) = 0{,}25$

x_4 belongs to the second cluster

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

Manhattan distances:

x_1: $\|x_1 - x_2\|_2 = |1-0| + |0{,}6-(-0{,}4)| + |0{,}1-0{,}8| =$
$= 2{,}7$

$\|x_1 - x_3\|_2 = |1-0| + |0{,}6-0{,}2| + |0{,}1-0{,}5| =$
$= 1{,}8$

$\|x_1 - x_4\| = |1-1| + |0{,}6-0{,}4| + |0{,}1-(-0{,}1)| =$
$= 0{,}4$

x_2: $\|x_2 - x_1\| = 2{,}7$ $\quad$ $\|x_2 - x_3\| = 0{,}9$

$\|x_2 - x_4\| = 2{,}7$

x_3: $\|x_3 - x_1\| = 1{,}8$ $\quad$ $\|x_3 - x_2\| = 0{,}9$

$\|x_3 - x_4\| = 1{,}8$

x_4: $\|x_4 - x_1\| = 0{,}4$ $\quad$ $\|x_4 - x_2\| = 2{,}7$

$\|x_4 - x_3\| = 1{,}8$

Aprendizagem 2023/24

Homework I V– Group 35

(ist1100032, ist1100070)

$$\text{silhouette} = \frac{b - a}{\max\{a, b\}}$$

a representa a distância média de x_i aos pontos do mesmo cluster

b representa o mínimo da distância média de x_i aos pontos de um outro cluster

$$s(x_1) = \frac{\frac{2{,}7+1{,}8}{2} - 0{,}4}{\frac{2{,}7+1{,}8}{2}} = 0{,}8(2)$$

$$s(x_4) = \frac{\frac{2{,}7+1{,}8}{2} - 0{,}4}{\frac{2{,}7+1{,}8}{2}} = 0{,}8(2)$$

$$s(c_2) = \frac{s(x_1) + s(x_4)}{2} = 0{,}8(2)$$

$$s(x_2) = \frac{\frac{\|x_2 - x_1\| + \|x_2 - x_4\|}{2} - \|x_2 - x_3\|_2}{\max\left(\frac{\|x_2 - x_1\| + \|x_2 - x_4\|}{2}, \|x_2 - x_3\|\right)} =$$

$$= \frac{\frac{2{,}7+2{,}7}{2} - 0{,}9}{\frac{2{,}7+2{,}7}{2}} = \frac{2{,}7 - 0{,}9}{2{,}7} = \frac{1{,}8}{2{,}7} = 0{,}66(6)$$

$$s(x_3) = \frac{\frac{1{,}8+1{,}8}{2} - 0{,}9}{\frac{1{,}8+1{,}8}{2}} = \frac{1{,}8 - 0{,}9}{1{,}8} =$$

$$= \frac{0{,}9}{1{,}8} = 0{,}5$$

$$s(c_1) = \frac{s(x_2) + s(x_3)}{2} = 0{,}58(3)$$

Código auxiliar:

```
# Given parameters
pi = new_pi
p = new_p
mean = np.array([new_N1_mean, new_N2_mean])
cov = np.array([new_N1_cov, new_N2_cov])

# Step 1: Calculate the likelihood of each observation belonging to each cluster
likelihoods = np.zeros((len(observations), len(pi)))
for i in range(len(observations)):
    for j in range(len(pi)):
        likelihoods[i, j] = p[0]**observations[i, 0] * (1-p[0])**(1-observations[i, 0]) * \
                            multivariate_normal.pdf(observations[i, 1:], mean[j], cov[j])

print("Likelihoods: ", likelihoods)

# Step 2: Assign each observation to the cluster with the highest likelihood
assignments = np.argmax(likelihoods, axis=1)

print("Clusters assigned: ", assignments)

# Now, we have assigned each observation to a cluster (0 or 1).

from scipy.spatial.distance import cityblock

# Step 3: Calculate the Manhattan distance between each observation and all other observations
manhattan_distances = np.zeros((len(observations), len(observations)))
for i in range(len(observations)):
    for j in range(len(observations)):
        manhattan_distances[i, j] = cityblock(observations[i],observations[j])

print("Distances: ", manhattan_distances)
```

```
Likelihoods:  [[0.23147434 0.33302022]
 [1.26633248 0.20430579]
 [1.4381104  1.045683  ]
 [0.02076523 0.25367744]]
Clusters assigned:  [1 0 0 1]
Distances:  [[0.  2.7 1.8 0.4]
 [2.7 0.  0.9 2.7]
 [1.8 0.9 0.  1.8]
 [0.4 2.7 1.8 0. ]]
```

4) We have 2 clusters: c1 = {x2, x3} and c2 = {x1, x4}.
According to the exercise, the purity is 0,75 which means that 75% of the observations are on the right class. In order to achieve this, we can have 2 or 3 classes.

If we have 2 classes, 3 of the observations have to be on one of the classes and the remaining observation has to be on another class.

Example:
Class 1 = {x2, x3, x4}
Class 2 = {x1}

In this case, x2, x3 and x1 are on the right class, leaving us with a purity of 0,75.

If we have 3 classes, 2 of the observations have to be on one of the classes and the 2 remaing observations are split between the remaining 2 classes. The 2 observations that are on the same class must belong to the same cluster in order to guarantee a purity of 0,75.

Example:
Class 1={x2}
Class 2 = {x1, x4}
Class 3 = {x3}

In this case, x2, x1 and x4 are on the right class, leaving us with a purity of 0,75.

II. Programming and critical analysis

1)

```
from scipy.io import arff
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn import metrics
from sklearn.preprocessing import MinMaxScaler
from sklearn.cluster import KMeans
from sklearn.decomposition import PCA
import warnings

warnings.filterwarnings("ignore", category=FutureWarning) # Ignore FutureWarnings


data = arff.loadarff('column_diagnosis.arff')
df = pd.DataFrame(data[0])

# Features
X = df.drop(columns='class').values

# Normalization
scaler = MinMaxScaler()
X_normalized = scaler.fit_transform(X)
```

```python
def purity_score(y_true, y_pred):
    confusion_matrix = metrics.cluster.contingency_matrix(y_true, y_pred)
    return np.sum(np.amax(confusion_matrix, axis=0)) / np.sum(confusion_matrix)


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_normalized)

    silhouette = metrics.silhouette_score(X_normalized, cluster_labels)
    silhouette_scores[k] = silhouette

    purity = purity_score(df['class'], cluster_labels)
    purity_scores[k] = purity

for k, silhouette in silhouette_scores.items():
    print(f"K = {k}, Silhouette Score: {silhouette}")
for k, purity in purity_scores.items():
    print(f"K = {k}, Purity Score: {purity}")
```

```
K = 2, Silhouette Score: 0.36044124340441114
K = 3, Silhouette Score: 0.29579055730002257
K = 4, Silhouette Score: 0.27442402122340176
K = 5, Silhouette Score: 0.23823928397844843
K = 2, Purity Score: 0.632258064516129
K = 3, Purity Score: 0.667741935483871
K = 4, Purity Score: 0.6612903225806451
K = 5, Purity Score: 0.6774193548387096
```

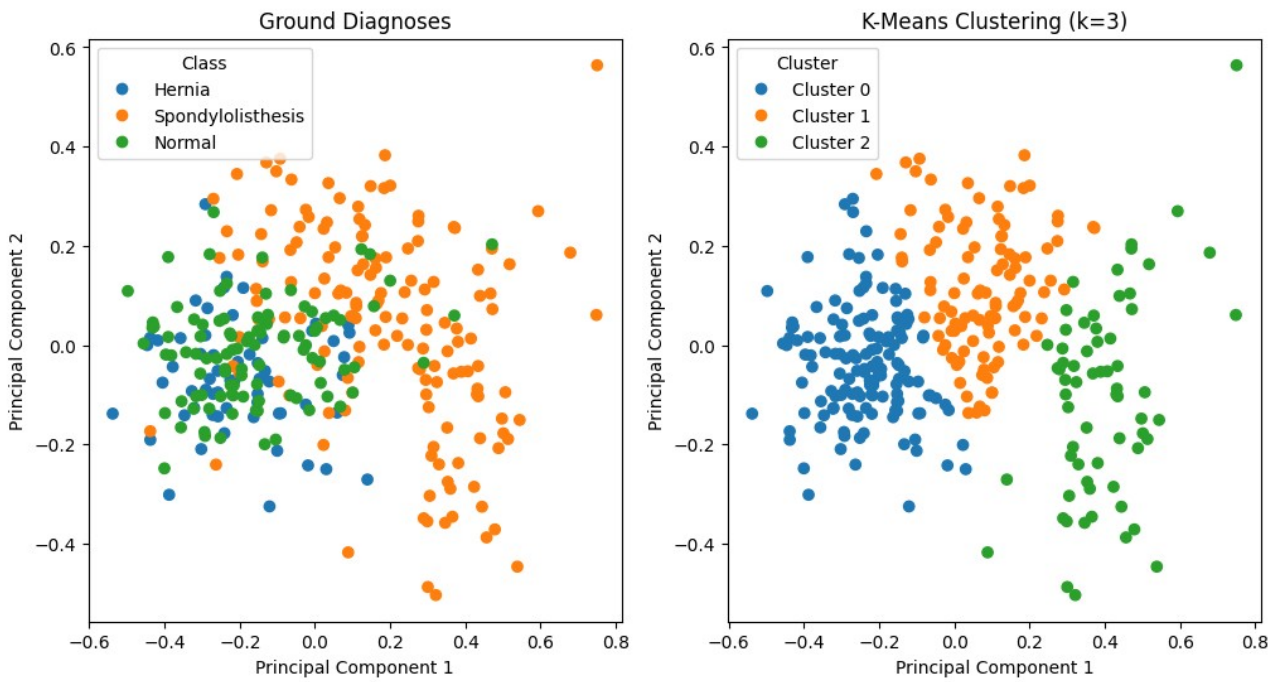
2)

```
n_components = 2

pca = PCA(n_components=n_components)
principal_components = pca.fit_transform(X_normalized)

explained_variance = pca.explained_variance_ratio_
print("Explained Variance for Top Two Components:", explained_variance)

for i, component in enumerate(range(1, n_components + 1)):
    print(f"\nTop Variables for Principal Component {component} (sorted by relevance):")
    component_weights = pca.components_[i]
    sorted_indices = np.argsort(np.abs(component_weights))[::-1]

    for idx in sorted_indices:
        print(f"Variable: {df.columns[idx]}, Weight: {component_weights[idx]}")
```

```
Explained Variance for Top Two Components: [0.56181445 0.20955953]

Top Variables for Principal Component 1 (sorted by relevance):
Variable: pelvic_incidence, Weight: 0.5916206177372234
Variable: lumbar_lordosis_angle, Weight: 0.5150847620730926
Variable: pelvic_tilt, Weight: 0.46703943896727157
Variable: sacral_slope, Weight: 0.3256888625569196
Variable: degree_spondylolisthesis, Weight: 0.21692963450485403
Variable: pelvic_radius, Weight: -0.11582397626328887

Top Variables for Principal Component 2 (sorted by relevance):
Variable: pelvic_tilt, Weight: -0.6703727595553627
Variable: pelvic_radius, Weight: -0.5810738370953603
Variable: sacral_slope, Weight: 0.4433029949470745
Variable: pelvic_incidence, Weight: 0.10003707489152235
Variable: lumbar_lordosis_angle, Weight: 0.08004745059088263
Variable: degree_spondylolisthesis, Weight: 0.004582909709399325
```

3)

```
from matplotlib.colors import ListedColormap

kmeans = KMeans(n_clusters=3, random_state=0)
cluster_labels = kmeans.fit_predict(X_normalized)

# Mapping of class labels to numerical values
y = df['class']
y = y.astype(str)
class_mapping = {'Hernia': 0, 'Spondylolisthesis': 1, 'Normal': 2}
class_numerical = y.map(class_mapping)

# Define colormap and legend labels
cmap = ListedColormap(['#1f77b4', '#ff7f0e', '#2ca02c'])
legend_labels = ['Hernia', 'Spondylolisthesis', 'Normal']


# Create a scatter plot for ground diagnoses
plt.figure(figsize=(12, 6))
plt.subplot(1, 2, 1)
scatter = plt.scatter(principal_components[:, 0], principal_components[:, 1], c=class_numerical, cmap=cmap)
plt.title("Ground Diagnoses")
plt.xlabel("Principal Component 1")
plt.ylabel("Principal Component 2")
plt.legend(handles=scatter.legend_elements()[0], title="Class", labels=legend_labels)

# Create a scatter plot for k-means clustering
plt.subplot(1, 2, 2)
scatter = plt.scatter(principal_components[:, 0], principal_components[:, 1], c=cluster_labels, cmap=cmap)
plt.title("K-Means Clustering (k=3)")
plt.xlabel("Principal Component 1")
plt.ylabel("Principal Component 2")
plt.legend(handles=scatter.legend_elements()[0], title="Cluster", labels=['Cluster 0', 'Cluster 1', 'Cluster 2'])

plt.show()
```



4) The Silhouette Score measures the quality of the clustering results. Higher Silhouette Scores indicate better separation of clusters, in this case, a higher Silhouette Score for K=2 suggests that there may be a clear separation between two groups of individuals, which as we will se could correspond to Hernia and Normal Classes versus the Spondylolisthesis class.
The Purity Score assesses how accurately the clustering corresponds to the true labels. A higher Purity Score for K=3 suggests that the clustering does a good job of assigning individuals to one of three clusters, which corresponds to the different classes of dignostics provided.
In the Ground Diagnoses Plot data points are color-coded based on the ground diagnoses we can see how the different diagnostic categories are distributed in the two-dimensional space created by PCA. There is not a strong separation between the Normal and Hernia Classes, however the Spondylolisthesis class is noticably distanced from the other two classes. This suggests that while PCA is able to capture some structure in the data, there might be significant overlap between the "Normal" and "Hernia" classes, making it challenging to distinguish between them based on the considered features.The clear separation of the "Spondylolisthesis" class from the others indicates that this condition has distinct features or patterns that can be captured by PCA.
When it comes to the K-Means Clustering Plot: data points are color-coded based on the K-Means clustering results with k=3. We see that PCA is effectively capturing the structure of the data new classes assigned by the K-means clustering algorithm as we see a clear separation between classes.This suggests that K-Means has identified underlying structure in the data that might not be entirely related to the known diagnostic categories.

END