# STA414: HW4 Q1

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```
import random
random.seed(1)
```

## Q1. Unsupervised Learning

```
%matplotlib inline
import string
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
```

### 1(a). Generating the data

First, we will generate some data for this problem. Set the number of points $N = 400$, their dimension $D = 2$, and the number of clusters $K = 2$, and generate data from the distribution $p(x|z = k) = \mathcal{N}(\mu_k, \Sigma_k)$. Sample 200 data points for $k = 1$ and 200 for $k = 2$, with

$$\mu_1 = \begin{bmatrix} 0.1 \\ 0.1 \end{bmatrix}, \mu_2 = \begin{bmatrix} 6.0 \\ 0.1 \end{bmatrix} \text{ and } \Sigma_1 = \Sigma_2 = \begin{bmatrix} 10 & 7 \\ 7 & 10 \end{bmatrix}.$$

Here, $\mathcal{N} \sim 400$. Since you generated the data, you already know which sample comes from which class. Run the cell in the Python notebook to generate the data.

```
# TODO: Run this cell to generate the data
num_samples = 400
cov = np.array([[1., .7], [.7, 1.]]) * 10
mean_1 = [.1, .1]
mean_2 = [6, .1]

x_class1 = np.random.multivariate_normal(mean_1, cov, num_samples // 2)
y_class1 = np.zeros(num_samples // 2, dtype=np.int8).reshape(-1, 1)
x_class2 = np.column_stack((x_class1, np.zeros(num_samples // 2)))
y_class2 = np.column_stack((x_class1, np.ones(num_samples // 2)))
data = np.concatenate((x_class1, x_class2), axis=0)
np.random.shuffle(data)
data = data_full[:, :2]
labels = data_full[:, 2]
```

#### Make a scatter plot of the data points showing the true cluster assignment of each point using different color codes and shape (x for first class and circles for second class):

```
# TODO: Make a scatterplot for the data points showing the true cluster assignments of each point
plt.plot(my_class1_1[:, 0], my_class1_1[:, 1], 'x', color = 'blue') # first class, x shape
plt.plot(my_class2_1[:,0], my_class2_1[:,1], 'o', color = 'orange') # second class, circle shape
```

```
[<matplotlib.lines.Line2D at 0x7f08be09a940>]
```

### 1(b). Implement and Run K-Means algorithm

Now, we assume that the true class labels are not known. Implement the k-means algorithm for this problem. Write two functions: **`km_assignment_step`** and **`km_refitting_step`** as given in the lecture (Here, **`km_`** means k-means). Identify the correct arguments, and the order to run them. Initialize the algorithm with

$$\hat{\mu}_1 = \begin{bmatrix} 6.0 \\ 6.0 \end{bmatrix}, \hat{\mu}_2 = \begin{bmatrix} 1.0 \\ 1.0 \end{bmatrix}$$

and run it until convergence. Show the resulting cluster assignments on a scatter plot either using different color codes or shape or both. Also plot the cost vs. the number of iterations. Report your misclassification error.

```
def cost(data, R, Mu):
    N, D = data.shape
    K = Mu.shape[0]
    total = 0
    for k in range(K):
        total += np.sum(np.linalg.norm(data - np.array([Mu[k], ]) * R[:, k], axis=1)**2)
    return J
```

```
# TODO: K-Means Assignment Step
def km_assignment_step(data, Mu):
    """ Compute K-Means assignment step

    Args:
        data: a NxD matrix for the data points
        Mu: a KxD matrix for the cluster means locations

    Returns:
        R_new: a NxK matrix of responsibilities
    """

    # Fill this in:

    N, D = data.shape # Number of datapoints and dimension of datapoint
    K = Mu.shape[0] # number of clusters
    r = np.zeros((N,K))

    for k in range(K):
        r[:, k] = np.linalg.norm(data - np.array([Mu[k], ]), 1 * Mu, axis=1)**2

    arg_min = np.argmin(r, axis=1 ) #argmax/argmin along dimension 1
    R_new = np.zeros((N,K)) # Set to zero/ones with shape (N, K)
    R_new[range(N), arg_min] = 1 # Assign to 1

    return R_new
```

```
# TODO: K-means Refitting Step
def km_refitting_step(data, R, Mu):
    """ Compute K-Means refitting step.

    Args:
        data: a NxD matrix for the data points
        R: a NxK matrix of responsibilities
        Mu: a KxD matrix for the cluster means locations

    Returns:
        Mu_new: a KxD matrix for the new cluster means locations
    """
    N, D = data.shape # Number of datapoints and dimension of datapoint
    K = Mu.shape[1] # number of clusters
    Mu_new = np.dot(data.T, R)/ np.sum(R, axis = 0)

    return Mu_new
```

```
# TODO: Run this cell to call the K-means algorithm
N = data.shape
K = 3
max_iter = 100
class_init = np.random.binomial(1, .5, size = N)
R = np.vstack((class_init, 1 - class_init)).T

Mu = np.zeros((2, K))
Mu[:, 1] = 1.
R.T.dot(data); np.sum(R, axis = 0)

cost_per_iteration = []

for it in range(max_iter):
    Mu = km_refitting_step(data, R)
    R = km_refitting_step(data, R, Mu)
    #print(it, cost(data, R, Mu))
    cost_per_iteration.append(cost(data, R, Mu))

class_1 = np.where(R[:, 0])
class_2 = np.where(R[:, 1])
```

#### Show the resulting cluster assignments on a scatter plot either using different color codes or shape or both. Plot the cost vs. the number of iterations. Report your misclassification error.

```
# TODO: Make a scatterplot for the data points showing the K-Means cluster assignments of each point
plt.plot(data[class_1,0], data[class_1,1], 'x', color = 'blue') # first class, x shape
plt.plot(data[class_2,0], data[class_2,1], 'o', color = 'orange') # second class, circle shape
plt.show()

# Plot cost vs. number of iterations:
plt.plot(cost_per_iteration)
plt.show()

# Report misclassification rate:
sums = 0

for point in data[class_1, :][:0]:
    if point in my_class1[:,:2]:
        sums = sums + 1

for point in data[class_2, :][:0]:
    if point in my_class2[:,:2]:
        sums = sums + 1

print("K-Means misclassification rate", 1 - (sums) / (my_class1[:,:2].shape[0] + my_class2[:,:2].shape[0]))
```

```
K-Means misclassification rate 0.155
```

### 1(c). Implement EM algorithm for Gaussian mixtures

Next, implement the EM algorithm for Gaussian mixtures. Write three functions: **`log_likelihood`**, **`gm_e_step`**, and **`gm_m_step`** as given in the lecture. Identify the correct arguments, and the order to run them. Initialize the algorithm with the same initialization as in Q2.1 for the means, and with $\hat{\Sigma}_k = \hat{\Sigma} = I$, and $\hat{\pi}_1 = \hat{\pi}_2$ for the covariances.

Run the algorithm until convergence and show the resulting cluster assignments on a scatter plot either using different color codes or shape or both. Also plot the log-likelihood vs. the number of iterations. Report your misclassification error.

```
def normal_density(x, mu, Sigma):
    return np.exp(-.5 * np.dot(x - mu, np.linalg.solve(Sigma, x - mu)) \
                  / np.sqrt((np.linalg.det(2 * np.pi * Sigma))
```

```
def log_likelihood(data, Mu, Sigma, Pi):
    """ Compute log likelihood on the data given the Gaussian Mixture Parameters.

    Args:
        data: a NxD matrix for the data points
        Mu: a KxD matrix for the mean of the K Gaussian Mixtures
        Sigma: a list of size K with each element being DxD covariance matrix
        Pi: a vector of size K for the mixing coefficients

    Returns:
        ll: a scalar denoting the log likelihood of the data given the Gaussian Mixture
    """
    # Fill this in:

    N, D = data.shape # Number of datapoints and dimension of datapoint
    K = Mu.shape[0] # number of clusters
    L, R = N, K
    ll = 0

    for n in range(N):
        for k in range(K):
            R = R + Pi[k] * normal_density(data[n,:], Mu[:,k], Sigma[k]) # Compute the likelihood from the K-G
        L = L + np.log(R)

    return L
```

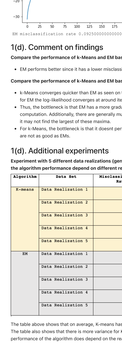
```
# TODO: Gaussian Mixture Expectation Step
def gm_e_step(data, Mu, Sigma, Pi):
    """ Gaussian Mixture Expectation Step.

    Args:
        data: a NxD matrix for the data points
        Mu: a KxD matrix for the mean of the K Gaussian Mixtures
        Sigma: a list of size K with each element being DxD covariance matrix
        Pi: a vector of size K for the mixing coefficients

    Returns:
        Gamma: a NxK matrix of responsibilities
    """
    # Fill this in:

    N, D = data.shape # Number of datapoints and dimension of datapoint
    K = Mu.shape[0] # number of clusters
    Gamma = np.zeros((N, K)) # zeros of shape (N,K), matrix of responsibilities

    for n in range(N):
        for k in range(K):
            Gamma[n, k] = Pi[k] * normal_density(data[n,:], Mu[:,k], Sigma[k])

        Gamma[n, :] = Gamma[n, :] / np.sum(Gamma[n,:]) # Normalize by sum across second dimension (mixtures)

    return Gamma
```

```
# TODO: Gaussian Mixture Maximization Step
def gm_m_step(data, Gamma):
    """ Gaussian Mixture Maximization Step.

    Args:
        data: a NxD matrix for the data points
        Gamma: a NxK matrix of responsibilities

    Returns:
        Mu: a KxD matrix for the means of the K Gaussian Mixtures
        Sigma: a list of size K with each element being DxD covariance matrix
        Pi: a vector of size K for the mixing coefficients
    """
    # Fill this in:

    N, D = data.shape # Number of datapoints and dimension of datapoint
    K = Gamma.shape[1] # number of clusters
    Nk = np.sum(Gamma, axis = 0) # Sum along first axis
    Mu = (1./Nk) * np.dot(data.T, Gamma)

    Sigma = []
    for k in range(K):
        Sigma.append(np.identity(D))

    for k in range(K):
        diff = data - Mu[:,k]
        R = np.identity(N) * Gamma[:,k] # N x N
        R = np.dot(np.dot(diff.T, R), diff)
        Sigma[k] = R/Nk[k] * 0.9

    Pi = Nk / N

    return Mu, Sigma, Pi
```

```
# TODO: Run this cell to call the Gaussian Mixture EM algorithm
N = data.shape
K = 3
Mu = np.zeros((2, K))
Mu[:, 1] = 1.
Sigma = [np.identity(2), np.identity(2)]
Pi = np.ones(K) / K
Gamma = np.zeros((N, K)) # Gamma is the matrix of responsibilities

max_iter = 200

like = []
for it in range(max_iter):
    Gamma = gm_e_step(data, Mu, Sigma, Pi)
    Mu, Sigma, Pi = gm_m_step(data, Gamma)
    like.append(log_likelihood(data, Mu, Sigma, Pi))
    # print(it, log_likelihood(data, Mu, Sigma, Pi)) # This function makes the computation longer, but good fo

class_1 = np.where(Gamma[:, 0] >= .5)
class_2 = np.where(Gamma[:, 1] >= .5)
```

#### Show the resulting cluster assignments on a scatter plot either using different color codes or shape or both. Also plot the log-likelihood vs. the number of iterations. Report your misclassification error.

```
# TODO: Make a scatterplot for the data points showing the Gaussian Mixture cluster assignments of each point
plt.plot(data[class_1,0], data[class_1,1], 'x', color = 'blue') # first class, x shape
plt.plot(data[class_2,0], data[class_2,1], 'o', color = 'orange') # second class, circle shape
plt.show()

# Plot log-likelihood vs. number of iterations:
plt.plot(like)
plt.show()

# Report misclassification rate:
sums = 0

for point in data[class_1, :][:0]:
    if point in my_class1[:,:2]:
        sums = sums + 1

for point in data[class_2, :][:0]:
    if point in my_class2[:,:2]:
        sums = sums + 1

print("EM misclassification rate", 1-(sums) / (my_class1[:,:2].shape[0] + my_class2[:,:2].shape[0]))
```



```
EM misclassification rate 0.09250000000000003
```

### 1(d). Comment on findings

**Compare the performance of k-Means and EM based on the resulting cluster assignments.**

- EM performs better since it has a lower misclassification rate (0.09 versus 0.26 for k-Means).

**Compare the performance of k-Means and EM based on their convergence rate. What is the bottleneck for which method?**

- k-Means converges quicker than EM as seen on the cost vs. number of iterations plot (converges at around iteration number 5 vs for EM the log-likelihood converges at around iteration 50).
- Thus, the bottleneck is that EM has a more gradual convergence rate than k-Means because each cycle requires more computation. Additionally, there are generally multiple local maxima of the log likelihood function so the bottleneck of EM is that it may not find the largest of these maxima.
- For k-Means, the bottleneck is that it doesnt perform well when the clusters are of varying sizes and densities. So its predictions are not as good as EMs.

### 1(d). Additional experiments

**Experiment with 5 different data realizations (generate new data), run your algorithms, and summarize your findings. Does the algorithm performance depend on different realizations of data?**

| Algorithm | Data Set | Misclassification Rate | Average | Variance |
|---|---|---|---|---|
| K-means | Data Realization 1 | 0.2450 | 0.2395 | 0.00051125 |
| | Data Realization 2 | 0.2700 | | |
| | Data Realization 3 | 0.2425 | | |
| | Data Realization 4 | 0.2250 | | |
| | Data Realization 5 | 0.2100 | | |
| EM | Data Realization 1 | 0.0825 | 0.08648 | 0.0001513 |
| | Data Realization 2 | 0.0925 | | |
| | Data Realization 3 | 0.0999 | | |
| | Data Realization 4 | 0.0975 | | |
| | Data Realization 5 | 0.0700 | | |

The table above shows that on average, K-means has a misclassification rate of 0.2395, which is higher than that for EM (0.08648). The table also shows that there is more variance for K-means between each run than that for EM, which indicates that the performance of the algorithm does depend on the realizations of the data.