Statistical and Machine Learning (01.113) - HW4 Question 4

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In this problem, we will implement the EM algorithm for clustering. Start by importing the required packages and preparing the dataset.

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt

from numpy import linalg as LA
from matplotlib.patches import Ellipse
from sklearn.datasets.samples_generator import make_blobs
```

In [2]:

```
def load_data():
    K = 3
    NUM_DATAPTS = 150

    X,y = make_blobs(n_samples=NUM_DATAPTS,
                     centers=K,shuffle=False,
                     random_state=0,
                     cluster_std=0.6)

    g1 = np.asarray([[2.0,0],[-0.9,1]])
    g2 = np.asarray([[1.4,0],[0.5,0.7]])

    mean1 = np.mean(X[:int(NUM_DATAPTS/K)])
    mean2 = np.mean(X[int(NUM_DATAPTS/K):2*int(NUM_DATAPTS/K)])

    X[:int(NUM_DATAPTS/K)] = np.einsum('nj, ij -> ni',
                                       X[:int(NUM_DATAPTS/K)] - mean1, g1) + mean1
    X[int(NUM_DATAPTS/K):2*int(NUM_DATAPTS/K)] = np.einsum('nj, ij -> ni',
                                                           X[int(NUM_DATAPTS/K):2*int(NUM_DATAPTS/K)] - mean2
,
                                                            g2) + mean2
    X[:,1] -= 4
    return X
```

a) Initialize μ_k, Σ_k, π_k

- Randomly initialize a numpy array MEANS of shape (K, 2) to represent the mean of the clusters,
- initialize an array COVARIANCES of shape (K, 2, 2) such that cov[k] is the identity matrix for each k. COVARIANCES will be used to represent the covariance matrices of the clusters.
- Finally, set pi CLUSTERING_COEFFICIENTS to be the uniform distribution at the start of the program.

In [3]:

```
def init_centroids(X, n_cluster):
    N, d = X.shape
    mean_indices = [np.random.randint(N)]
    for j in range(n_cluster-1):
        furthest_distance = 0
        furthest_point_index = None
        for i in range(N):
            if i in mean_indices:
                continue

            current_point = X[i]
            current_distance = sum([sum((current_point - X[index])**2) for index in mean_indices])

            if current_distance > furthest_distance:
                furthest_distance = current_distance
                furthest_point_index = i

        mean_indices.append(furthest_point_index)
    return X[mean_indices]

def initialize(X):
    N, d = X.shape
    MEANS = init_centroids(X, n_cluster=3)
    COVARIANCES = np.array([np.eye(N=d) for _ in range(K)])
    CLUSTER_COEFFICIENTS = np.random.uniform(size=(K))
    return MEANS, COVARIANCES, CLUSTER_COEFFICIENTS

K = 3
NUM_DATAPTS = 150
X = load_data()
MEANS, COVARIANCES, CLUSTER_COEFFICIENTS = initialize(X)

print(f"Means: \n{MEANS}\n")
print(f"Covariance Matrix: \n{COVARIANCES}\n")
print(f"Cluster Coefficient (pi): \n{CLUSTER_COEFFICIENTS}")
```

```
Means:
[[ 2.40911555 -2.33141878]
 [-3.75534522  3.57579775]
 [ 4.27095142 -1.53650922]]

Covariance Matrix:
[[[1. 0.]
  [0. 1.]]

 [[1. 0.]
  [0. 1.]]

 [[1. 0.]
  [0. 1.]]]

Cluster Coefficient (pi):
[0.57416043 0.43546833 0.82046407]
```

E-step:

Evaluate the responsibilities using the current parameter values:

$$\gamma\left(z_{nk}\right) = \frac{\pi_k \quad \left(\mathbf{x}_n \,|\, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_{j=1}^{K} \pi_j \quad \left(\mathbf{x}_n \,|\, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)}$$

where

$$(\mathbf{x} \,|\, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{ -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) \right\}$$

In [4]:

```
def multivariate_gaussian_pdf(x, mu, sigma):
    D = x.shape[0]
    exp_term = np.exp(-0.5*(x - mu).T@np.linalg.inv(sigma)@(x - mu))
    a = 1/ (np.sqrt(2*np.pi)**D)
    b = 1/np.sqrt(LA.det(sigma))
    return a*b*exp_term

def calc_gamma(x, cluster_idx):
    mu = MEANS[cluster_idx]
    sigma = COVARIANCES[cluster_idx]
    pi_k = CLUSTER_COEFFICIENTS[cluster_idx]
    gamma =  pi_k*multivariate_gaussian_pdf(x, mu, sigma) / sum([CLUSTER_COEFFICIENTS[cluster_j]*multivariat
e_gaussian_pdf(x, MEANS[cluster_j], COVARIANCES[cluster_j])
     for cluster_j in range(K)])
    return gamma

def E_step():
    gamma = np.zeros((NUM_DATAPTS, K))
    for i in range(NUM_DATAPTS):
        x = X[i]
        for cluster_idx in range(K):
            current_gamma = calc_gamma(x, cluster_idx)
            gamma[i, cluster_idx] = current_gamma
    return gamma
```

M-step

Re-estimate the parameters using the current responsibilities $\gamma\left(z_{nk}\right)$

- $\mu_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma\left(z_{nk}\right)\mathbf{x}_n$
- $\Sigma_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma\left(z_{nk}\right)\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}}$
- $\pi_k^{\text{new}} = \frac{N_k}{N}$

where $N_k = \sum_{n=1}^{N}\gamma\left(z_{nk}\right)$, in the code below, we call this `N_effect` where it is the effective number of points in a cluster.

$\sum_{j=1}^{K}N_j$ = NUM_DATAPTS

In [5]:

```
def M_step(gamma):
    N_effect = np.sum(gamma, axis=0)
    MEANS = np.array([
        (1/N_effect[cluster_idx]) * sum([gamma[i, cluster_idx]*X[i] for i in range(NUM_DATAPTS)])
              for cluster_idx in range(K)])

    COVARIANCES = np.zeros((3,2,2))
    for cluster_idx in range(K):
        mean = MEANS[cluster_idx]
        sigma_k = 0
        for i in range(NUM_DATAPTS):
            x = X[i]
            x_minus_mu = (x - mean).reshape(-1,1)
            sigma_k += gamma[i, cluster_idx]*x_minus_mu@(x_minus_mu.T)
        COVARIANCES[cluster_idx] = (1/N_effect[cluster_idx] * sigma_k)

    CLUSTER_COEFFICIENTS = [N_k/NUM_DATAPTS for N_k in N_effect]

    return MEANS, COVARIANCES, CLUSTER_COEFFICIENTS
```

Now write a loop that iterates through the E and M steps

That Terminates after the change in log-likelihood is below some threshold (In our case we set this to be 0.01)

The log-likelihood formula is as follows:

$$\ln p(\mathbf{X} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \quad \left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \right\}$$

In [6]:

```
def log_likelihood(X, mu, sigma, cluster_coef):
    ll = 0
    for i in range(NUM_DATAPTS):
        x = X[i]
        ll_i = 0
        for cluster_idx in range(K):
            ll_i += cluster_coef[cluster_idx]*multivariate_gaussian_pdf(x, mu[cluster_idx], sigma[cluster_id
x])
        ll += np.log(ll_i)
    return ll

def plot_result(gamma=None):
    ax = plt.subplot(111, aspect='equal')
    ax.set_xlim([-5,5])
    ax.set_ylim([-5,5])
    ax.scatter(X[:, 0], X[:, 1], c=gamma, s=50, cmap=None)

    for k in range(K):
        l, v = LA.eig(COVARIANCES[k])
        theta = np.arctan(v[1,0]/v[0,0])
        e = Ellipse((MEANS[k,0],MEANS[k,1]),6*l[0],6*l[1],
                    theta*180/np.pi)
        e.set_alpha(0.5)
        ax.add_artist(e)
    plt.show()
```

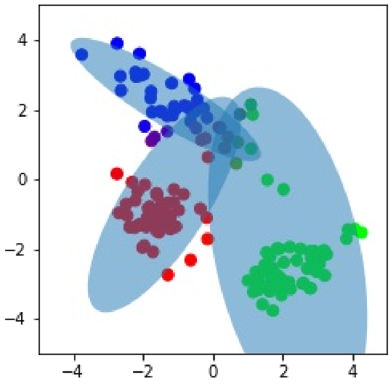
At each iteration,

- E_step to calculate gamma
- M_step using this gamma to calculate the new MEANS, COVARIANCES and CLUSTER_COEFFICIENTS
- print out the log-likelihood, and use
- the following function (plot_result) to plot the progress of the algorithm:

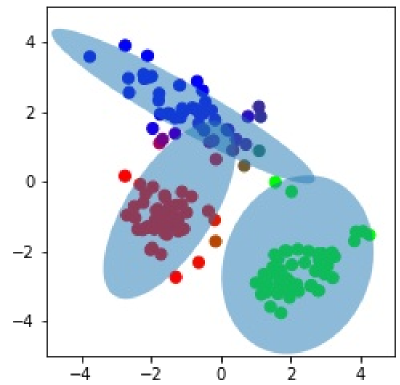
In [7]:

```
K = 3
NUM_DATAPTS = 150
X = load_data()
MEANS, COVARIANCES, CLUSTER_COEFFICIENTS = initialize(X)

max_iter = 50;

prev_ll = -np.inf
for _ in range(max_iter):
    gamma = E_step()
    MEANS, COVARIANCES, CLUSTER_COEFFICIENTS = M_step(gamma)
    ll = log_likelihood(X, MEANS, COVARIANCES, CLUSTER_COEFFICIENTS)
    improvement = ll - prev_ll
    prev_ll = ll

    # stopping condition: if converge
    if improvement < 0.01:
        print(f"Algorithm converges within {_} iterations")
        break

    print(f"Log Likelihood: {ll}")
    print(f"Improvement: {improvement}")
    plot_result(gamma)
```

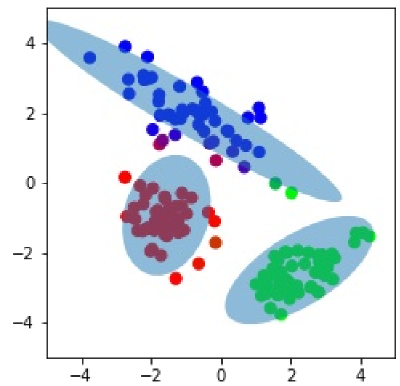
```
Log Likelihood: -521.5012320104992
Improvement: inf
```



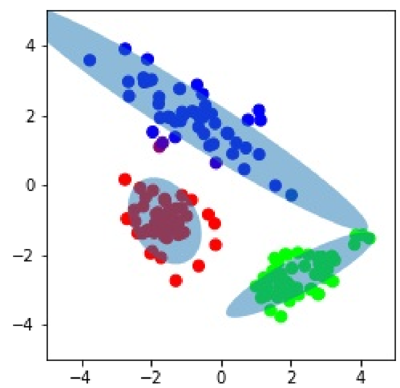
```
Log Likelihood: -500.3143700440223
Improvement: 21.18686196647684
```



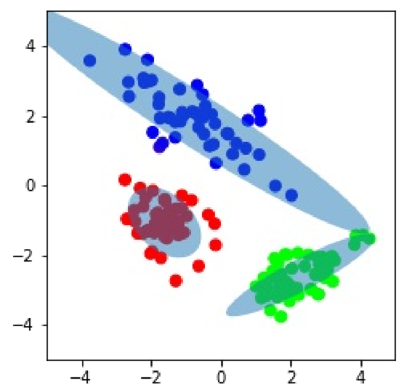

```
Log Likelihood: -478.4039374950258
Improvement: 21.91043254899654
```



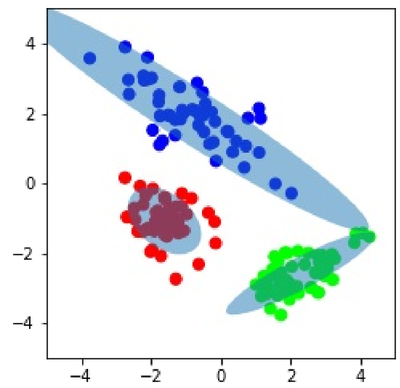

```
Log Likelihood: -464.7653943810236
Improvement: 13.638543114002175
```




```
Log Likelihood: -463.3989974270026
Improvement: 1.3663969540210132
```




```
Log Likelihood: -463.34233970853563
Improvement: 0.056657718466965434
```



Algorithm converges within 6 iterations