Introduction to Probabilistic Graphical Models

Practical Session 2

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In [104]:
```
%matplotlib inline
import numpy as np
from scipy.linalg import norm
import matplotlib.pyplot as plt
import networkx as nx
import pyparsing
from IPython.display import Math
import copy
import math
from matplotlib.patches import Ellipse
## we first run the code with the warning enabled, if no error of relevant warning is to be found,
## we disable the warning then
# import warnings
# warnings.filterwarnings("ignore")
```

In [105]:
```
# choose a large font size by default and use tex for math
fontsize = 18
params = {'axes.labelsize': fontsize + 2,
      'font.size': fontsize + 2,
      'legend.fontsize': fontsize + 2,
      'xtick.labelsize': fontsize,
      'ytick.labelsize': fontsize,
      'text.usetex': True}
plt.rcParams.update(params)
```

In [106]:
```
math_pi = math.pi
```

Question 1

We need to compute

$$\gamma_i(x) = \frac{\pi_i \mathcal{N}(x; \mu_i, \Sigma_i)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x; \mu_j, \Sigma_j)}$$

We define $g_i(x) = \pi_i \mathcal{N}(x; \mu_i, \Sigma_i)$ and $lg_i = \log g_i(x)$, then the log of the nominator is equal to:

$$\begin{aligned}
\log g_i(x) &= \log(\pi_i \mathcal{N}(x; \mu_i, \Sigma_i)) \\
&= \log\left(\pi_i \frac{1}{(2\pi)^{K/2} |\Sigma_i|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i)\right)\right) \\
&= \log \pi_i - \frac{1}{2}(K \log(2\pi) + \log|\Sigma_i|) - \frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1}(x-\mu_i)
\end{aligned}$$

Then we could compute $gamma_i(x)$ as follows:

$$\begin{aligned}
\gamma_i(x) &= \frac{\pi_i \mathcal{N}(x; \mu_i, \Sigma_i)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x; \mu_j, \Sigma_j)} \\
&= \frac{g_i(x)}{\sum_{j=1}^{K} g_j(x)} = \frac{\exp(\log(g_i(x)))}{\sum_{j=1}^{K} \exp(\log(g_j(x)))} \\
&= \frac{\exp(lg_i - maxlg)\exp(maxlg)}{\sum_{j=1}^{K} \exp(lg_j - maxlg)\exp(maxlg)} \\
&= \frac{\exp(lg_i - maxlg)}{\sum_{j=1}^{K} \exp(lg_j - maxlg)}
\end{aligned}$$

where $maxlg = \max_j lg_j = \max_j \log g_j(x), j = 1, \ldots, K$

Question 2

From lecture notes, we have:

$$\mathcal{L}_t(\theta) = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma_k^{(t)}(x_n)\log\mathcal{N}(x_n;\mu_k,\Sigma_k) + \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma_k^{(t)}(x_n)\log\pi_k$$

$\mathcal{M}$-step

$$\theta^{(t+1)} = \arg\max_{\theta}\mathcal{L}_t(\theta)$$

where $\theta^{(t)} = (\mu_k^{(t)}, \Sigma_k^{(t)}, \pi_k^{(t)})$

For $\mu_k^{(t+1)}$:

$$\begin{aligned}
\frac{\partial\mathcal{L}_t(\theta)}{\partial\mu_k^*} \propto \sum_{n=1}^{N}\gamma_k^{(t)}(\Sigma_k)^{-1}(x_n-\mu_k^*) = 0 \;:\; & \sum_{n=1}^{N}\gamma_k^{(t)}(x_n)(\Sigma_k)^{-1}(x_n-\mu_k^*) = 0 \\
& \sum_{n=1}^{N}\gamma_k^{(t)}(x_n)(\Sigma_k)^{-1}x_n = \sum_{n=1}^{N}\gamma_k^{(t)}(\Sigma_k)^{-1}\mu_k^* \\
& \mu^*(:=\mu_k^{(t+1)}) = \frac{\sum_{n=1}^{N}\gamma_k^{(t)}(x_n).\,x_n}{\sum_{n=1}^{N}\gamma_k^{(t)}(x_n)}
\end{aligned}$$

For $\pi_k^{(t+1)}$

We rewirte the formula for

$$\mathcal{L}_t(\theta) = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_k^{(t)}(x_n) \log(\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k))$$

$$= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_k^{(t)}(x_n) l_k(x_n)$$

$$= \sum_{n=1}^{N}$$

$$\sum_{k=1}^{K} \gamma_k^{(t)}(x_n) \left(\log \pi_k - \frac{1}{2}(K \log(2\pi) + \log|\Sigma_k|) - \frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_i)) \right)$$

$$\frac{\partial \mathcal{L}_t(\theta)}{\partial \pi_k^*} = 0 \ : \ \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_k^{(t)}(x_n) \frac{1}{\pi_k^*} = 0$$

Together With $\sum_{k=1}^{K} \pi_k^* = 1$, we get:

$$\pi_k^*(: \pi_k^{(t+1)}) = \frac{1}{N} \sum_{n=1}^{N} \gamma_k^{(t)}(x_n)$$

For $\Sigma_k^{(t+1)}$:

$$\frac{\partial \mathcal{L}_t(\theta)}{\partial \Sigma_k^*} = 0 \ : \ \propto \ \sum_{n=1}^{N} \gamma_k^{(t)}(x_n)\left(-(\Sigma_k^*) + (x-\mu_k)(x-\mu_k)^T\right) = 0$$

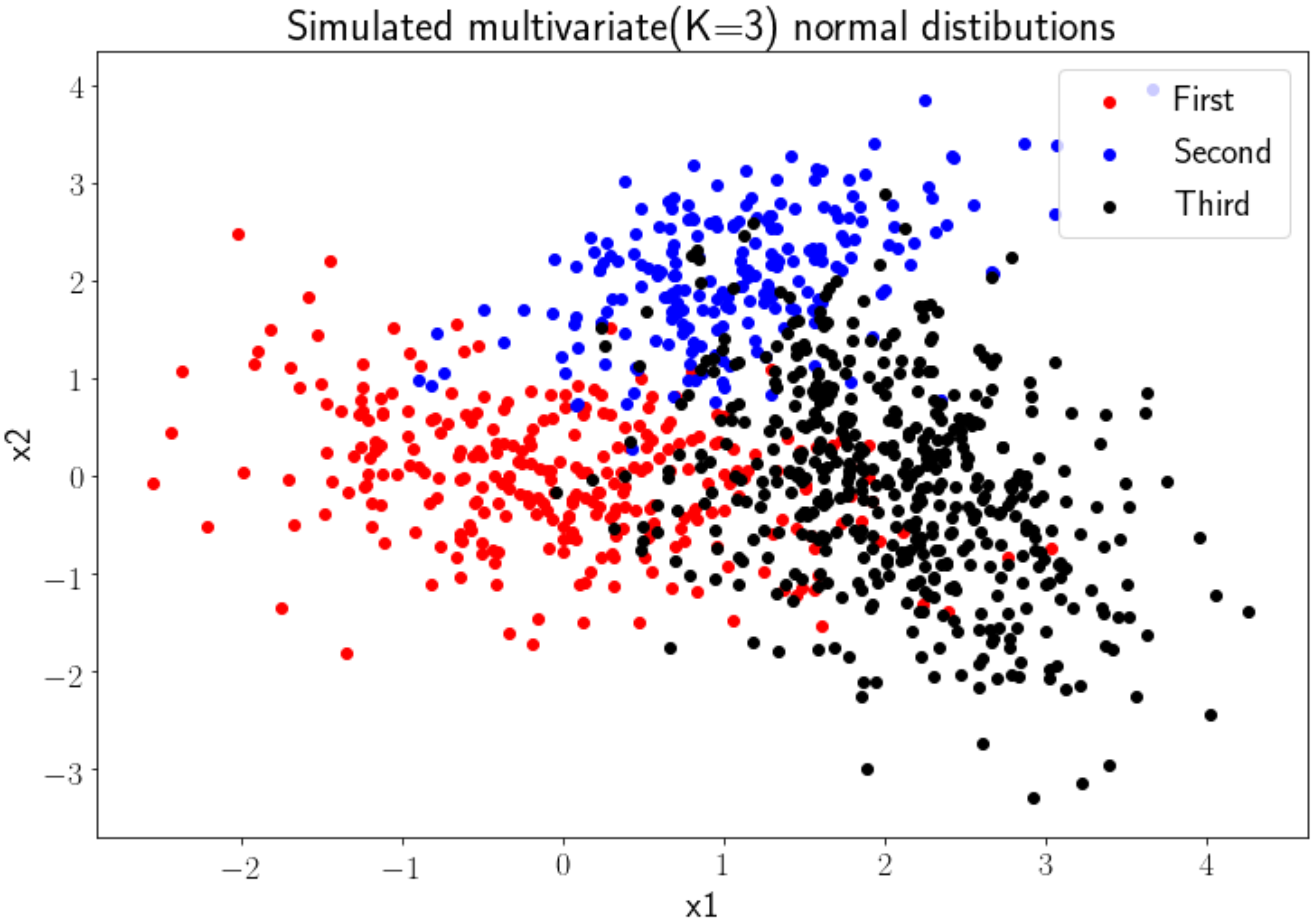
$$\sum_{n=1}^{N} \gamma_k^{(t)}(x_n)\Sigma_k^* = \sum_{n=1}^{N} \gamma_k^{(t)}(x_n)\left((x-\mu_k)(x-\mu_k)^T\right)$$

$$\Sigma_k^*(:= \Sigma_k^{t+1}) = \frac{\sum_{n=1}^{N} \gamma_k^{(t)}(x_n)(x-\mu_k)(x-\mu_k)^T}{\sum_{n=1}^{N} \gamma_k^{(t)}(x_n)}$$

Question 3

In [107]:

```
# hyper-parameters

K = 3
pi = np.array([0.3, 0.2, 0.5])
us = np.array([[0, 0], [1, 2], [2,0]])

# sg1 = np.array([[1, -0.25], [-0.25, 0.5]])
# sg2 = np.array([[0.5, 0.25],[0.25, 0.5]])
# sg3 = np.array([[0.5, -0.25],[-0.25, 1]])
# sigmas = [sg1, sg2, sg3]
sgs = np.array([[[1, -0.25], [-0.25, 0.5]], [[0.5, 0.25],[0.25, 0.5]], [[0.5, -0.25],[-0.25, 1]]])

def sample_loc (prob, pi_distrbution):
    # return the idx loction of prob in the prob_distrbution
    nr_loc = len(pi_distrbution)
    cum_sum = np.cumsum(pi_distrbution)
    idx = np.where(prob < cum_sum)[0]
    return idx[0]


N = 1000  # number of samples

xs = np.zeros((N, 3))
# simulator the trajectory
for i in np.arange(0,N):

    si_pi = np.random.uniform(0,1)
    gs_id = sample_loc(si_pi, pi)
    ui = us[gs_id]
    sgi = sgs[gs_id]
    xs[i,[0,1]] = np.random.multivariate_normal(ui, sgi)
    xs[i,2] = gs_id


x_g1 = xs[xs[:,2] == 0][:,[0,1]]
x_g2 = xs[xs[:,2] == 1][:,[0,1]]
```


Simulated multivariate(K=3) normal distibutions
First
Second
Third
x1
x2
−2
−1
0
1
2
3
4
−3

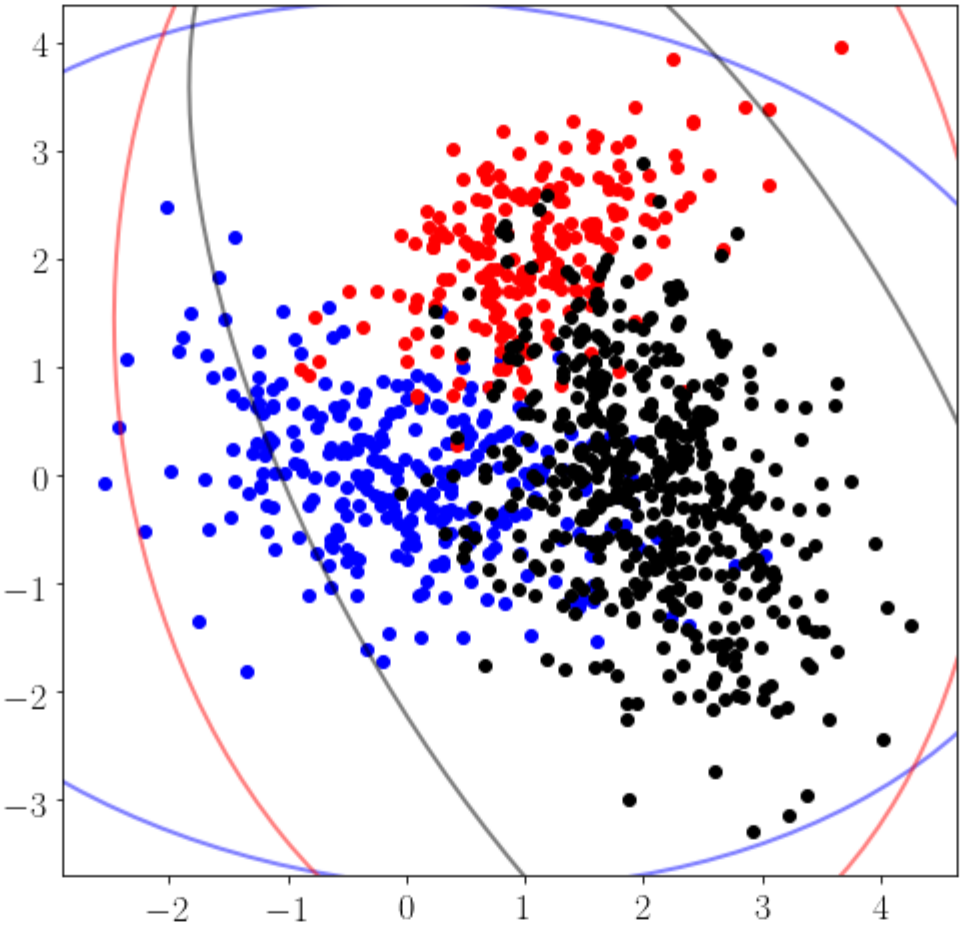
In [108]:
```
def cal_loggi(pi, ui, sigi, x, nr_x):

    sigi_inv = np.linalg.inv(sigi)
    log2pi = np.log(2* math_pi)
    log_sigi_det = np.log(np.linalg.det(sigi))

    diff = x - ui
    exp_part = [- diff[j,:].dot(sigi_inv).dot(diff[j,:]) / 2 for j in np.arange(nr_x)]
    loggi = np.log(pi) - (K * log2pi + log_sigi_det) / 2 + exp_part

    return loggi


def cal_gammas(K, ps, us, sigs, xs):
    gamma_KNs = np.zeros((K,N))

    nr_x = N
    logg_KN = np.zeros((K, N))
    for j in np.arange(K):
        logg_KN[j,:] = cal_loggi(ps[j], us[j], sigs[j], xs, nr_x)

    max_lgs = np.max(logg_KN, axis=0)
    lg_diff = logg_KN - max_lgs
    sum_exp = np.sum(np.exp(lg_diff), axis=0)

    for j in np.arange(K):
        gamma_KNs[j,:] = np.divide(np.exp(logg_KN[j,:] - max_lgs), sum_exp)

    return gamma_KNs
```

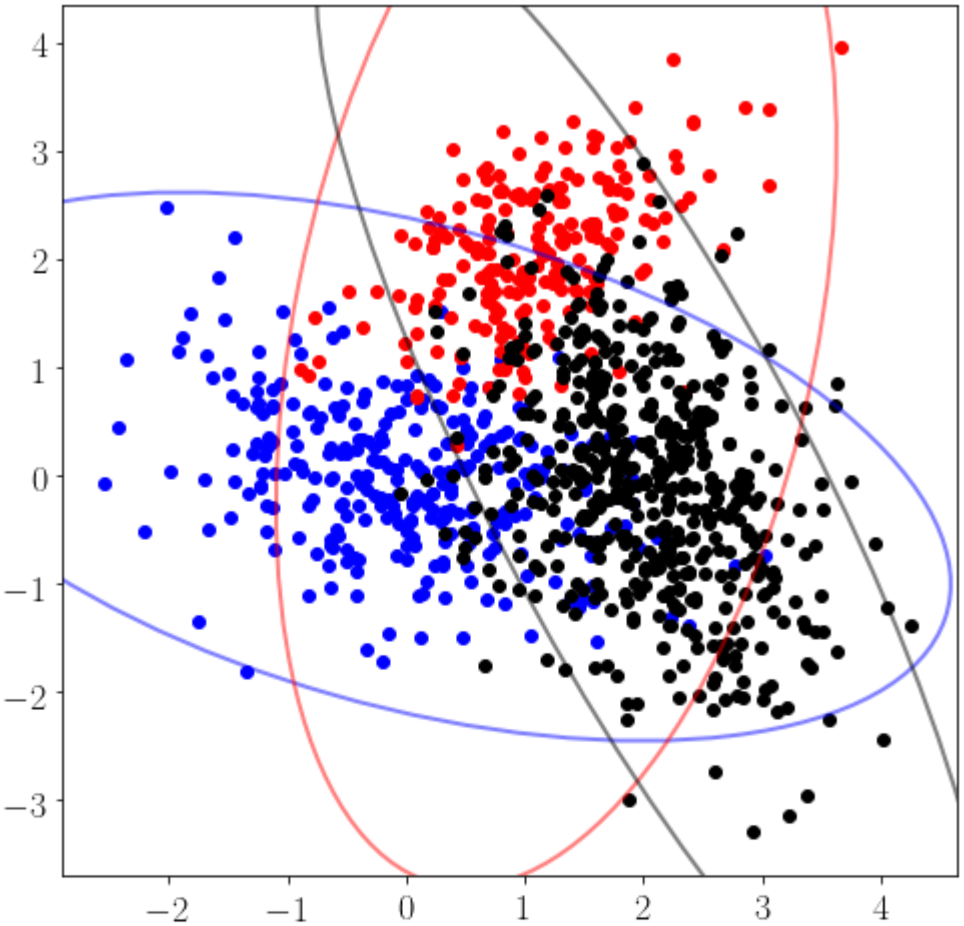
In [109]:
```
def update_para(gammas, K, ps, us, sigs, xs):

    ps_new = ps.copy()
    us_new = us.copy()
    sigs_new = sigs.copy()

    for j in np.arange(K):

        sum_gamma = np.sum(gammas[j,:])
        us_new[j,:] = np.sum(xs.T * gammas[j,:], axis=1) / sum_gamma
        ps_new[j] = sum_gamma / N
        diff = xs - us_new[j,:]
        sig_nom = [gammas[j,i] * np.outer(diff[i,:], diff[i,:]) for i in np.arange(N)]
        sigs_new[j,:] = np.sum(sig_nom, axis=0) / sum_gamma

    return us_new, ps_new, sigs_new
```

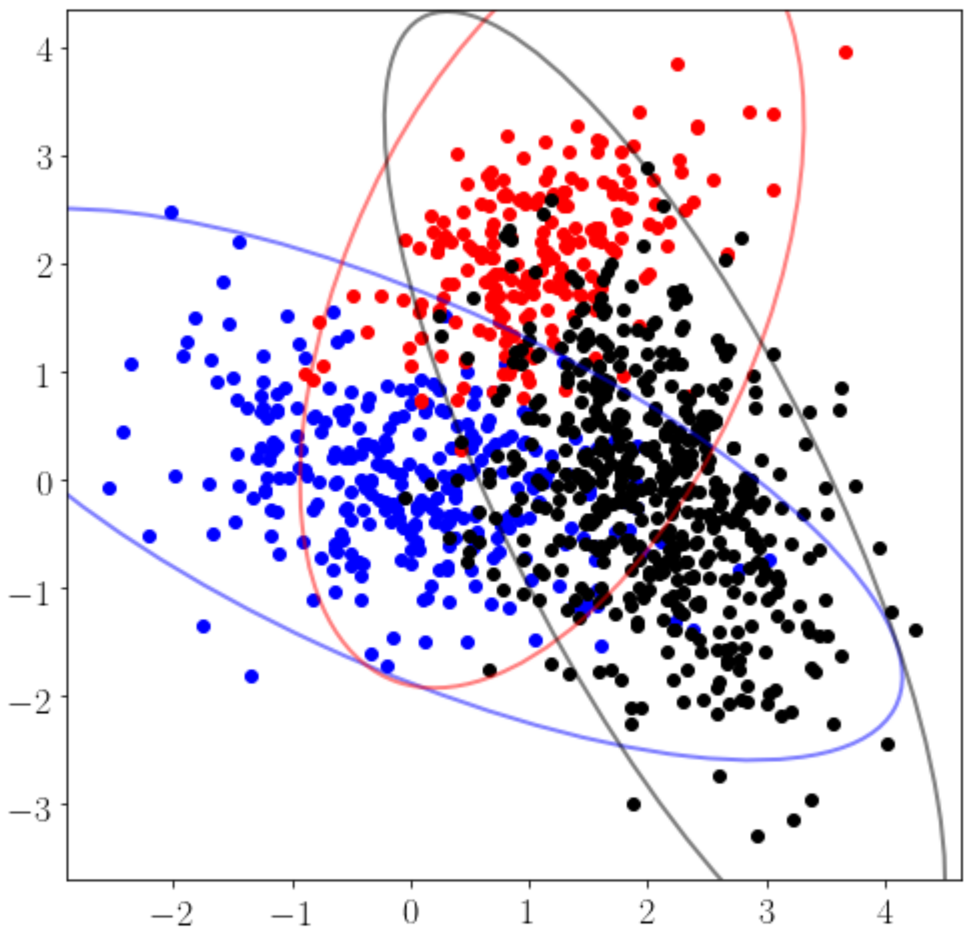
In [ ]:
```
def cal_loglik(K, ps, us, sigs, xs, gammas):


    for k in range(K):
        for j in range(N):

            sigi_inv = np.linalg.inv(sigi)
            log2pi = np.log(2* math_pi)
            log_sigi_det = np.log(np.linalg.det(sigi))

            diff = x - ui
            exp_part = [- diff[j,:].dot(sigi_inv).dot(diff[j,:]) / 2 for j in np.arange(nr_x)]

            ll += gammas[j,k] * ( - (K * log2pi + log_sigi_det) / 2 + exp_part)
    return ll
```

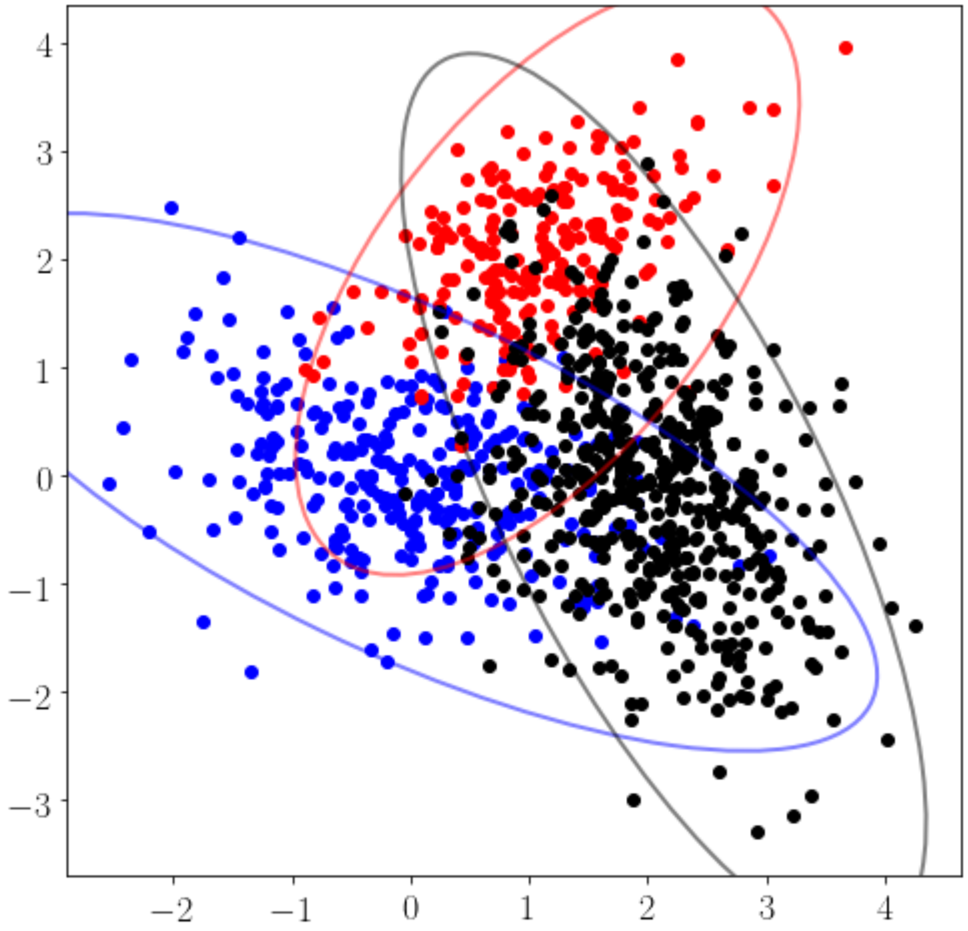
In [110]:
```
def plot_contour(ax, us, sigs, lcolors):
    '''
    This function plot on the axe ax ellipses (mu, sigma): reference to Henri Hours code for this
plot
    '''
    for k in range(K):
        v, w = np.linalg.eigh(sigs[k])
        u = w[0] / np.linalg.norm(w[0])
        angle = np.arctan2(u[1], u[0])
        angle = 180 * angle / np.pi  # convert to degrees
        v *= 8
        ellipse = Ellipse(us[k], v[0], v[1], 180 + angle, lw=2, ec=lcolors[k], fc='none')
        ellipse.set_clip_box(ax.bbox)
        ellipse.set_alpha(0.5)
        ax.add_artist(ellipse)
```

In [112]:
```
#### 2. Implement the EM algorithm for GMMs

xs_nl = xs[:,:2]  # not labeled data
xs_mean = np.mean(xs_nl, axis=0)
xs_cov = np.cov(xs_nl.T)

colors = ['b', 'r', 'k']

# initilize the parameters: set them to be equal
xs = xs_nl.copy()
ps = np.ones((3,1)) / K

us = np.array([[0, 0.5], [1, 1.2], [2,0.1]])
#us = np.array([xs_mean, xs_mean, xs_mean])
sigs = np.array([xs_cov, xs_cov, xs_cov])

# fig, ax = plt.subplots(figsize=(8,8))
# ax.scatter(X[:,0],X[:,1], marker='+', c = ycolors)
# ax.scatter(mu[:, 0], mu[:, 1], marker = 'o', c='black', alpha=0.5)
# ax.scatter(gmm2.list_mu[i][:, 0], gmm2.list_mu[i][:, 1], marker = 'o', c='r')

# fig, ax = plt.figure(figsize=(12, 8))
# fig, ax = plt.subplots(figsize=(8,8))
# plt.scatter(x_g1[:,0], x_g1[:,1], c='r', label='First')
# plt.scatter(x_g2[:,0], x_g2[:,1], c='b', label='Second')
# plt.scatter(x_g3[:,0], x_g3[:,1], c='k', label='Third')


Nr_iter = 20
for it in np.arange(Nr_iter):

    gammas = cal_gammas(K, ps, us, sigs, xs)
    us_new, ps_new, sigs_new = update_para(gammas, K, ps, us, sigs, xs)

    if it % 5 == 0:
        fig, ax = plt.subplots(figsize=(8,8))
```


4
3
2
1
0
−1
−2
−3
−2
−1
0
1
2
3
4


4
3
2
1
0
−1
−2
−3
−2 −1 0 1 2 3 4


4
3
2
1
0
−1
−2
−3
−2 −1 0 1 2 3 4


4
3
2
1
0
−1
−2
−3
−2
−1
0
1
2
3
4