Homework 11: Clustering

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Problem 1

In the first step we derive the expectation for a mixture of K gaussians.

$$
\begin{aligned}
p(x) &= \sum_k \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \\
\mathbb{E}(x) &= \int_{-\infty}^{\infty} x p(x) dx \\
&= \int_{-\infty}^{\infty} x \sum_k \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) dx \\
&= \sum_k \pi_k \int_{-\infty}^{\infty} x \mathcal{N}(x|\mu_k, \Sigma_k) dx
\end{aligned}
$$

We see that the integral itself fits the definition of an expectation, in this case the one of the respective gaussian. For $\mathcal{N}(x|\mu_k, \Sigma_k)$ this equals to μ_k. Therefor we get:

$$\mathbb{E}(x) = \sum_k \pi_k \mu_k$$

Now we will derive the covariance for the mixture of K gaussians.

$$
\begin{aligned}
cov(x) &= \mathbb{E}(xx^T) - \mathbb{E}(x)\mathbb{E}(x)^T \\
\mathbb{E}(xx^T) &= \int_{-\infty}^{\infty} xx^T \sum_k \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) dx \\
&= \sum_k \pi_k \int_{-\infty}^{\infty} xx^T \mathcal{N}(x|\mu_k, \Sigma_k) dx
\end{aligned}
$$

Again we see the integral itself is the expectation of one gaussian for xx^T. The matrix cookbook gives us the following equation for this (p.43 eq. 377)

$$\mathbb{E}(xx^T) = \Sigma + \mu\mu^T$$

Note that this only holds if the probability distribution has the form $\mathcal{N}(x|\mu_k, \Sigma_k)$.

We can now rewrite further:

$$\mathbb{E}(xx^T) = \sum_k \pi_k(\Sigma_k + \mu_k\mu_k^T)$$
$$\rightarrow cov(x) = \sum_k \pi_k(\Sigma_k + \mu_k\mu_k^T) - (\sum_k \pi_k\mu_k)(\sum_k \pi_k\mu_k)^T$$

0.1 Problem 2

To show that the EM-Algorithm is equal to Lloyds algorithm when using a mixture of K isotropic gaussians with the covariance $\Sigma_k = \sigma^2 I$ and $\sigma \rightarrow 0$ we first write down the responsibility $\gamma(z_{ik})$ used in the EM-algorithm:

$$\begin{aligned}\gamma(z_{ik}) &= \frac{\pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)}{\sum_{j=1}^K \mathcal{N}(x_i|\mu_j, \Sigma_j)} \\ &= \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{(x_i-\mu_k)^2}{2\sigma_i^2}}}{\sum_{j=1}^K \pi_j \frac{1}{\sqrt{(2\pi)}\sigma_j} e^{-\frac{(x_i-\mu_j)^2}{2\sigma_j^2}}}\end{aligned}$$

We see that both numerator and denominator will go to zero as $\sigma \rightarrow 0$. For the case $k = \underset{k}{argmin}\|x_i - \mu_j\|^2$ though numerator and denominator will be equal and therefor $\gamma(z_{ik})$ will be 1. This is because in this case the argument converges to zero slower. In the other cases $\gamma(z_{ik})$ will be 0. We see that for the given case $\sigma \rightarrow 0$ the following holds:

$$\gamma(z_{ik}) \begin{cases} 1 & if\ k = \underset{k}{argmin}\|x_i - \mu_j\|^2 \\ 0 & else \end{cases}$$

We see that this matches with the one-hot encoding in Lloyds algorithm and that therefor the update routine for μ will be the same

$$\mu_k^{new} = \frac{1}{N_k}\sum_i^N \gamma(z_{ik})x_i = \frac{1}{N_k}\sum_i^N z_{ik}x_i$$

Since for $\sigma \rightarrow 0$ all points will be assigned to the centroids the EM-update for σ_K will give 0 in everystep thus making both algorithms alike for the given case.

Programming assignment 11: Gaussian Mixture Model

In [1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.mlab as mlab
import seaborn as sns
sns.set_style('whitegrid')
%matplotlib inline

from scipy.stats import multivariate_normal
```

Your task

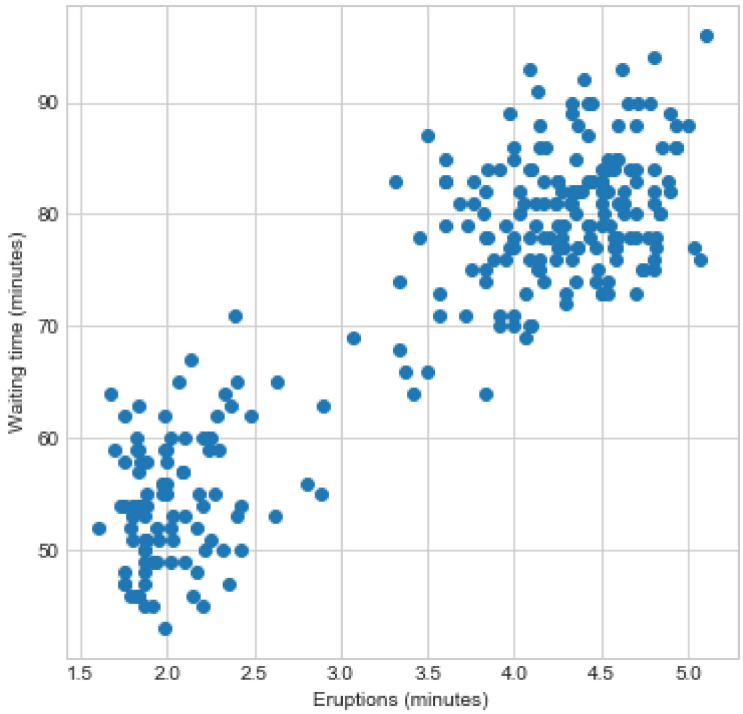
In this homework sheet we will implement Expectation-Maximization algorithm for learning & inference in a Gaussian mixture model.

We will use the dataset (http://www.stat.cmu.edu/~larry/all-of-statistics/=data/faithful.dat) containing information about eruptions of a geyser called "Old Faithful". The dataset in suitable format can be downloaded from Piazza.

As usual, your task is to fill out the missing code, run the notebook, convert it to PDF and attach it you your HW solution.

Generate and visualize the data

In [2]:
```
X = np.loadtxt('faithful.txt')
plt.figure(figsize=[6, 6])
plt.scatter(X[:, 0], X[:, 1])
plt.xlabel('Eruptions (minutes)')
plt.ylabel('Waiting time (minutes)')
plt.show()
```



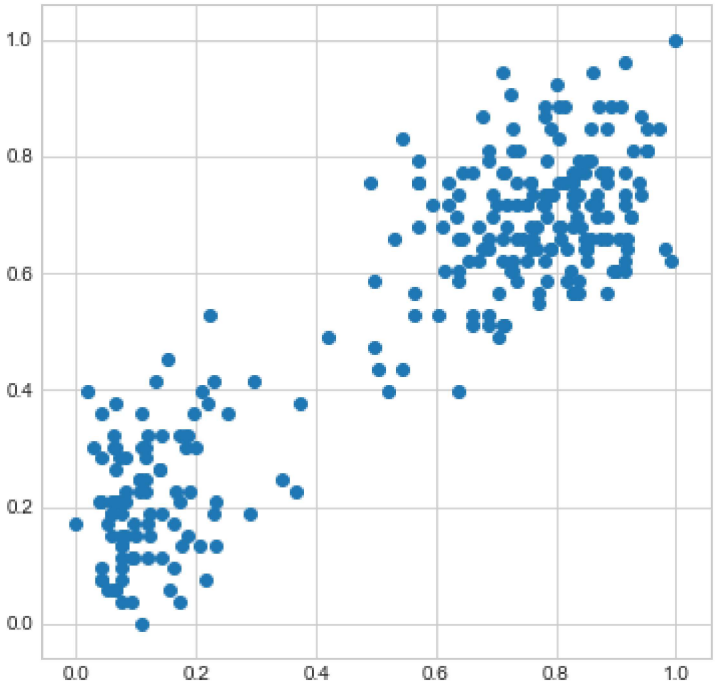
Task 1: Normalize the data

Notice, how the values on two axes are on very different scales. This might cause problems for our clustering algorithm.

Normalize the data, such that it lies in the range $[0, 1]$ along each dimension (each column of X).

In [3]:
```
def normalize_data(X):
    """Normalize data such that it lies in range [0, 1] along every dimension.

    Parameters
    ----------
    X : np.array, shape [N, D]
        Data matrix, each row represents a sample.

    Returns
    -------
    X_norm : np.array, shape [N, D]
        Normalized data matrix.
    """
    min_vector = np.amin(X,axis=0)
    max_vector = np.amax(X,axis=0)
    mean_vector = np.mean(X,axis = 0)
    var_vector = np.std(X,axis =0)
    X_new = (X - min_vector)/(max_vector - min_vector)

    return X_new
```

In [4]:
```
plt.figure(figsize=[6, 6])
X_norm = normalize_data(X)
plt.scatter(X_norm[:, 0], X_norm[:, 1]);
```



Task 2: Compute the log-likelihood of GMM

Here and in some other places, you might want to use the function `multivariate_normal.pdf` from the `scipy.stats` package.

In [5]:
```
def gmm_log_likelihood(X, means, covs, mixing_coefs):
    """Compute the log-likelihood of the data under current parameters settin
g.

    Parameters
    ----------
    X : np.array, shape [N, D]
        Data matrix with samples as rows.
    means : np.array, shape [K, D]
        Means of the GMM (\mu in lecture notes).
    covs : np.array, shape [K, D, D]
        Covariance matrices of the GMM (\Sigma in lecuture notes).
    mixing_coefs : np.array, shape [K]
        Mixing proportions of the GMM (\pi in lecture notes).

    Returns
    -------
    log_likelihood : float
        log p(X | \mu, \Sigma, \pi) - Log-likelihood of the data under the giv
en GMM.
    """
    mn = {}
    num = {}
    clus_sum = np.zeros(shape=(1,X.shape[0]))
    log_likelihood = 0
    for k in xrange(means.shape[0]):
        dist = multivariate_normal(mean = means[k], cov = covs[k])
        mn[k] = dist.pdf(X)
        num[k] = mixing_coefs[k] * mn[k]
        clus_sum = clus_sum + num[k]

    log_likelihood = np.sum(np.log(clus_sum))
    return log_likelihood
```

Task 3: E step

In [6]:
```
def e_step(X, means, covs, mixing_coefs):
    """Perform the E step.

    Compute the responsibilities.

    Parameters
    ----------
    X : np.array, shape [N, D]
        Data matrix with samples as rows.
    means : np.array, shape [K, D]
        Means of the GMM (\mu in lecture notes).
    covs : np.array, shape [K, D, D]
        Covariance matrices of the GMM (\Sigma in lecuture notes).
    mixing_coefs : np.array, shape [K]
        Mixing proportions of the GMM (\pi in lecture notes).

    Returns
    -------
    responsibilities : np.array, shape [N, K]
        Cluster responsibilities for the given data.
    """
    responsibilities = np.zeros(shape=(X.shape[0],means.shape[0]))
    mn = {}
    den = np.zeros(shape=(X.shape[0]))
    num = np.zeros(shape=(means.shape[0],X.shape[0]))
    for k in xrange(means.shape[0]):
        dist = multivariate_normal(mean = means[k], cov = covs[k])
        mn[k] = dist.pdf(X)
        num[k] = mixing_coefs[k] * mn[k]
        den = den + num[k]

    new_num = num.T
    new_den = den.T


    for i in xrange(X.shape[0]):
        for j in xrange(means.shape[0]):
            responsibilities[i,j] = new_num[i,j]/new_den[i]


    return responsibilities
```

Task 4: M step

In [7]:
```
def m_step(X, responsibilities):
    """Update the parameters \theta of the GMM to maximize E[log p(X, Z | \the
ta)].

    Parameters
    ----------
    X : np.array, shape [N, D]
        Data matrix with samples as rows.
    responsibilities : np.array, shape [N, K]
        Cluster responsibilities for the given data.

    Returns
    -------
    means : np.array, shape [K, D]
        Means of the GMM (\mu in lecture notes).
    covs : np.array, shape [K, D, D]
        Covariance matrices of the GMM (\Sigma in lecuture notes).
    mixing_coefs : np.array, shape [K]
        Mixing proportions of the GMM (\pi in lecture notes).

    """
    N = X.shape[0]
    N_k = np.sum(responsibilities,axis=0)

    means = np.zeros(shape=(responsibilities.shape[1],X.shape[1]))
    covs = np.array([np.eye(2),np.eye(2)])
    mixing_coefs = np.zeros(shape=(responsibilities.shape[1]))

    for k in xrange(X.shape[1]):
        temp = 0
        for i in xrange(responsibilities.shape[0]):
            temp += responsibilities[i,k]*X[i]
        mean = temp/N_k[k]
        means[k] = mean

        cov_i = np.zeros(shape=(X.shape[1],X.shape[1]))

        for i in xrange(X.shape[0]):
            temp2 = np.zeros(shape=(X.shape[1],X.shape[1]))
            t = np.matrix(X[i] - means[k])
            temp2 = responsibilities[i,k]*(t.T*t)
            cov_i += temp2
        covs[k] = cov_i/N_k[k]
        mixing_coefs[k] = N_k[k]/N



    #means, covs, mixing_coefs = None, None, None
    return means, covs, mixing_coefs
```

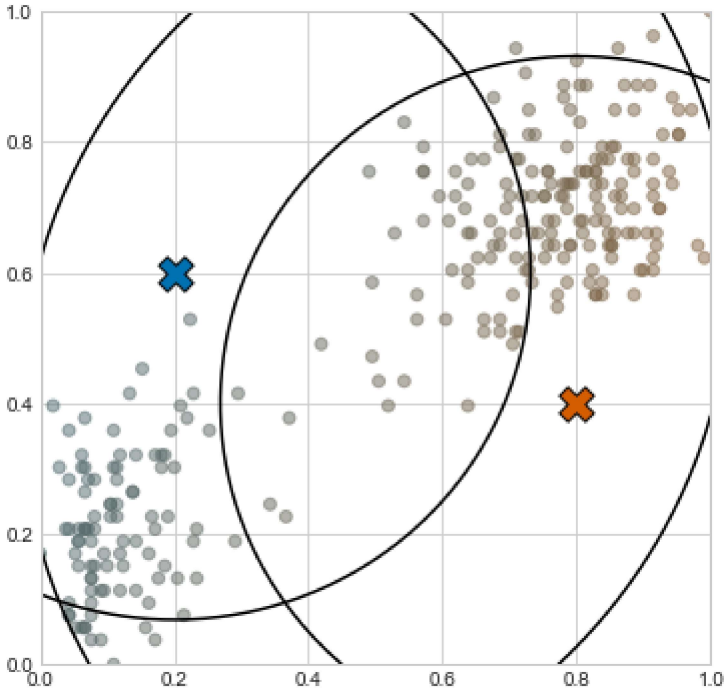
Visualize the result (nothing to do here)

In [8]:
```
def plot_gmm_2d(X, responsibilities, means, covs, mixing_coefs):
    """Visualize a mixture of 2 bivariate Gaussians.

    This is badly written code. Please don't write code like this.
    """
    plt.figure(figsize=[6, 6])
    palette = np.array(sns.color_palette('colorblind', n_colors=3))[[0, 2]]
    colors = responsibilities.dot(palette)
    # Plot the samples colored according to p(z|x)
    plt.scatter(X[:, 0], X[:, 1], c=colors, alpha=0.5)
    # Plot locations of the means
    for ix, m in enumerate(means):
        plt.scatter(m[0], m[1], s=300, marker='X', c=palette[ix],
                    edgecolors='k', linewidths=1,)
    # Plot contours of the Gaussian
    x = np.linspace(0, 1, 50)
    y = np.linspace(0, 1, 50)
    xx, yy = np.meshgrid(x, y)
    for k in range(len(mixing_coefs)):
        zz = mlab.bivariate_normal(xx, yy, np.sqrt(covs[k][0, 0]),
                                   np.sqrt(covs[k][1, 1]),
                                   means[k][0], means[k][1], covs[k][0, 1])
        plt.contour(xx, yy, zz, 2, colors='k')
    plt.xlim(0, 1)
    plt.ylim(0, 1)
    plt.show()
```

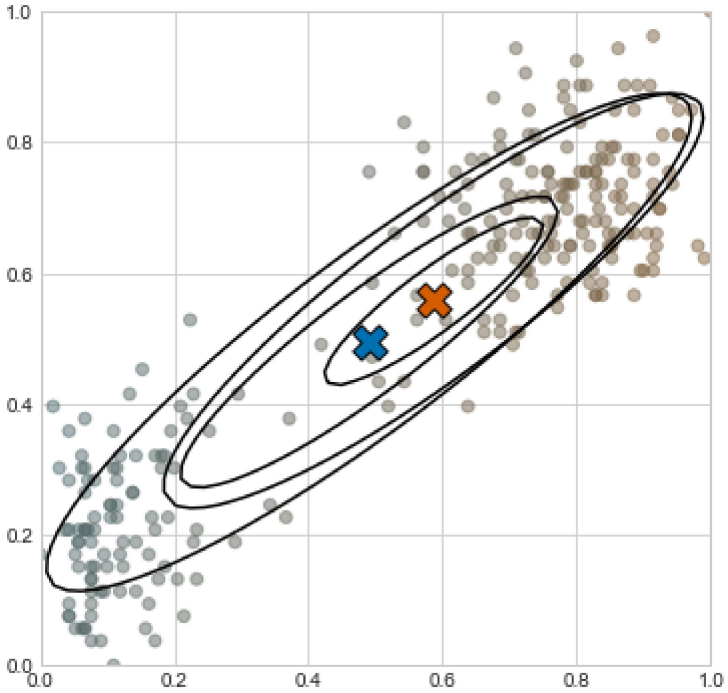
Run the EM algorithm

In [9]:
```
X_norm = normalize_data(X)
max_iters = 20

# Initialize the parameters
means = np.array([[0.2, 0.6], [0.8, 0.4]])
covs = np.array([0.5 * np.eye(2), 0.5 * np.eye(2)])
mixing_coefs = np.array([0.5, 0.5])

old_log_likelihood = gmm_log_likelihood(X_norm, means, covs, mixing_coefs)
responsibilities = e_step(X_norm, means, covs, mixing_coefs)
print('At initialization: log-likelihood = {0}'
      .format(old_log_likelihood))
plot_gmm_2d(X_norm, responsibilities, means, covs, mixing_coefs)

# Perform the EM iteration
for i in range(max_iters):
    responsibilities = e_step(X_norm, means, covs, mixing_coefs)
    means, covs, mixing_coefs = m_step(X_norm, responsibilities)
    new_log_likelihood = gmm_log_likelihood(X_norm, means, covs, mixing_coefs)
    # Report & visualize the optimization progress
    print('Iteration {0}: log-likelihood = {1:.2f}, improvement = {2:.2f}'
          .format(i, new_log_likelihood, new_log_likelihood - old_log_likeliho
od))
    old_log_likelihood = new_log_likelihood
    plot_gmm_2d(X_norm, responsibilities, means, covs, mixing_coefs)
```

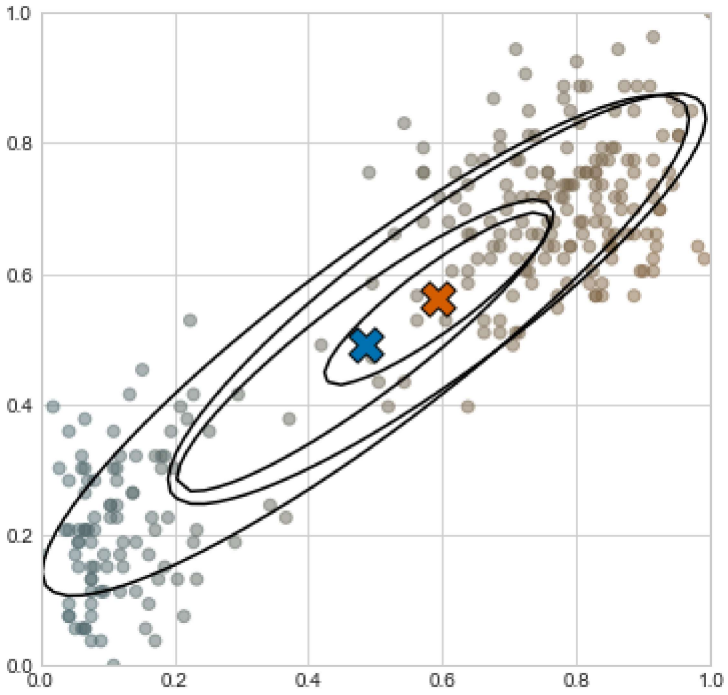
```
At initialization: log-likelihood = -382.705515242
```



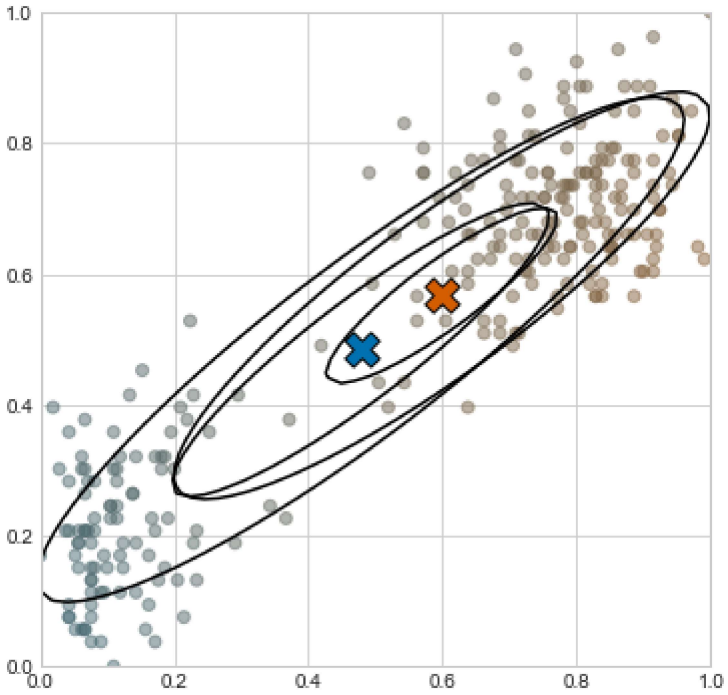

```
Iteration 0: log-likelihood = 131.29, improvement = 513.99
```



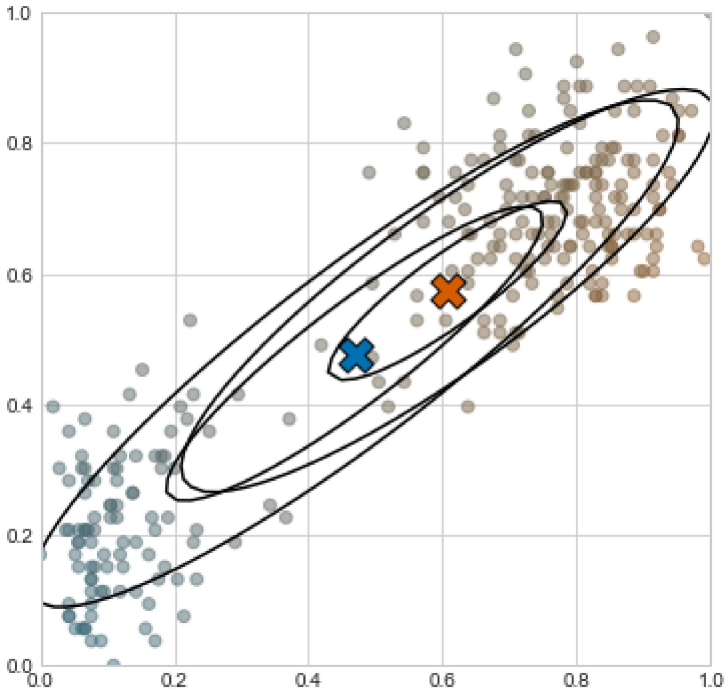

```
Iteration 1: log-likelihood = 131.48, improvement = 0.19
```



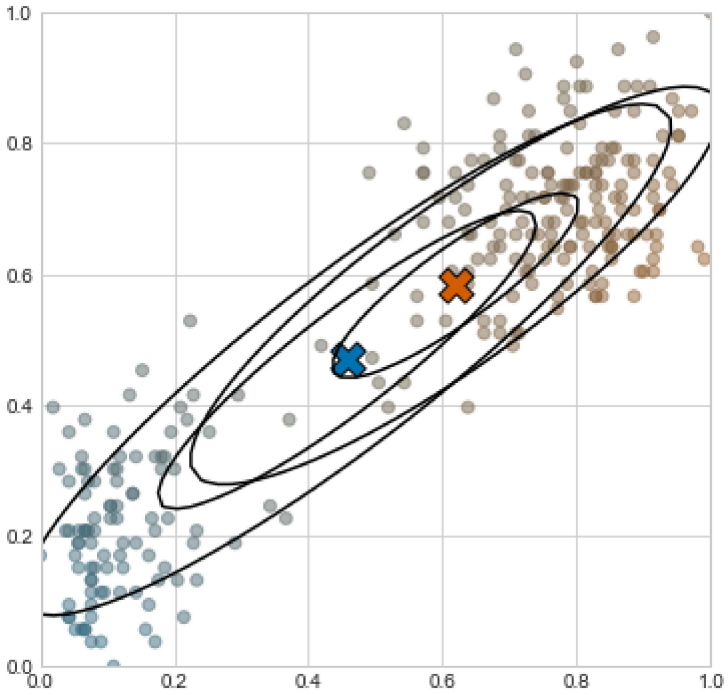

```
Iteration 2: log-likelihood = 131.75, improvement = 0.27
```



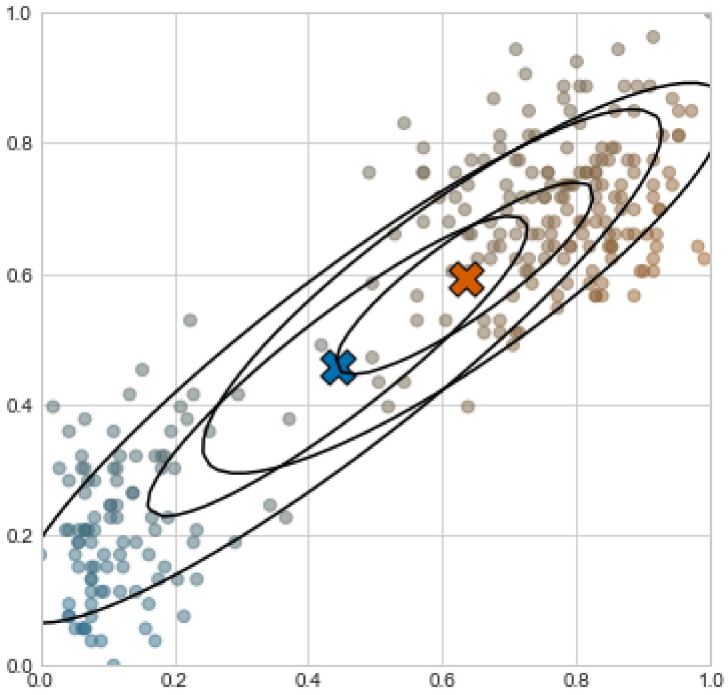

```
Iteration 3: log-likelihood = 132.15, improvement = 0.40
```



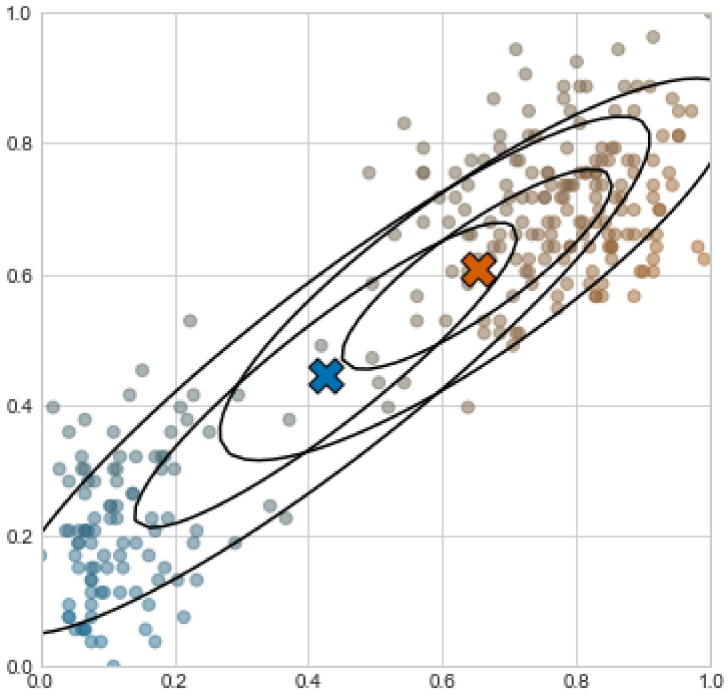

```
Iteration 4: log-likelihood = 132.77, improvement = 0.62
```



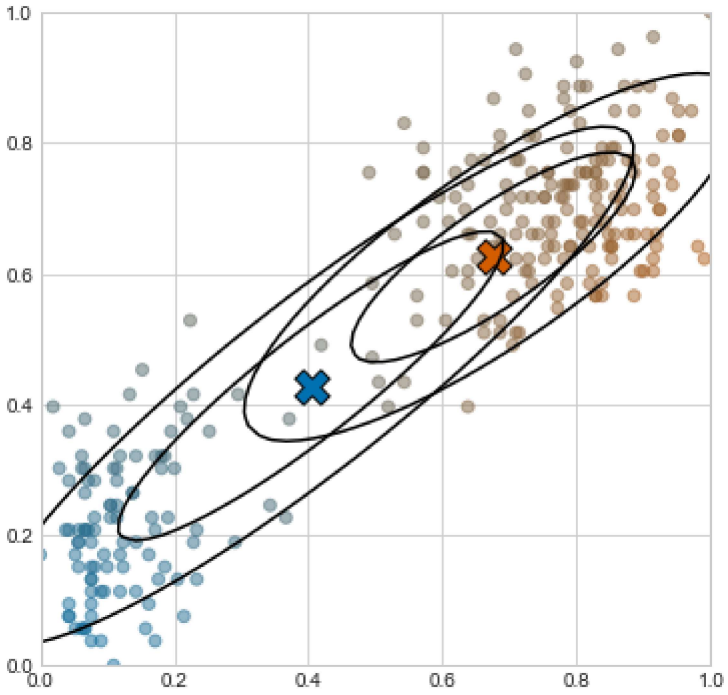

```
Iteration 5: log-likelihood = 133.81, improvement = 1.04
```



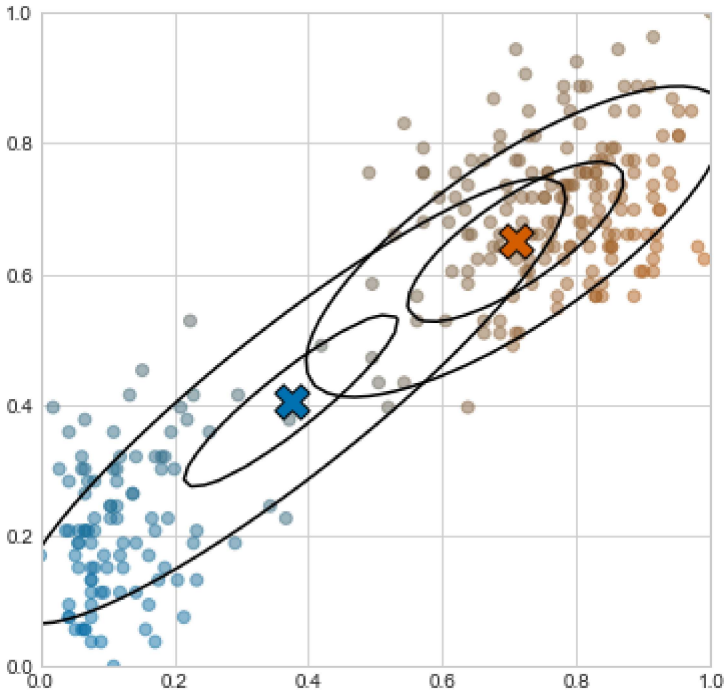

```
Iteration 6: log-likelihood = 135.74, improvement = 1.93
```



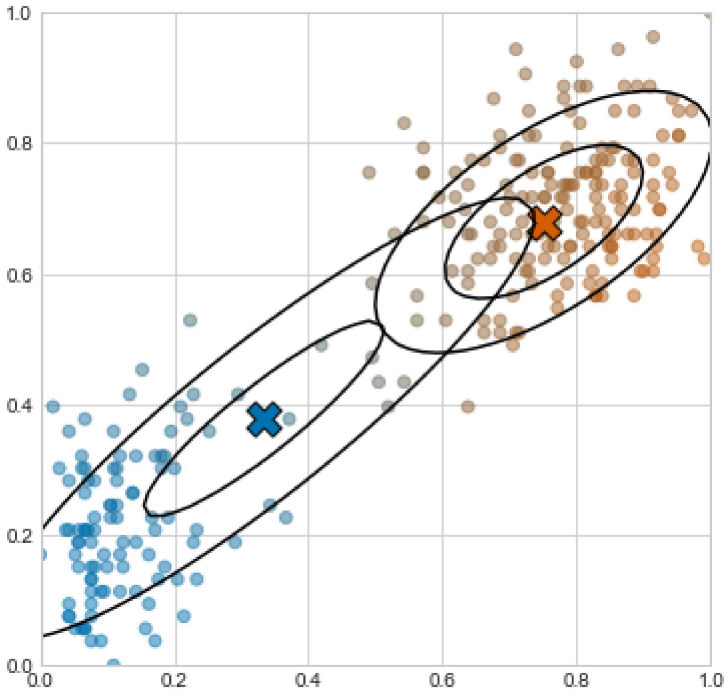

```
Iteration 7: log-likelihood = 139.88, improvement = 4.14
```



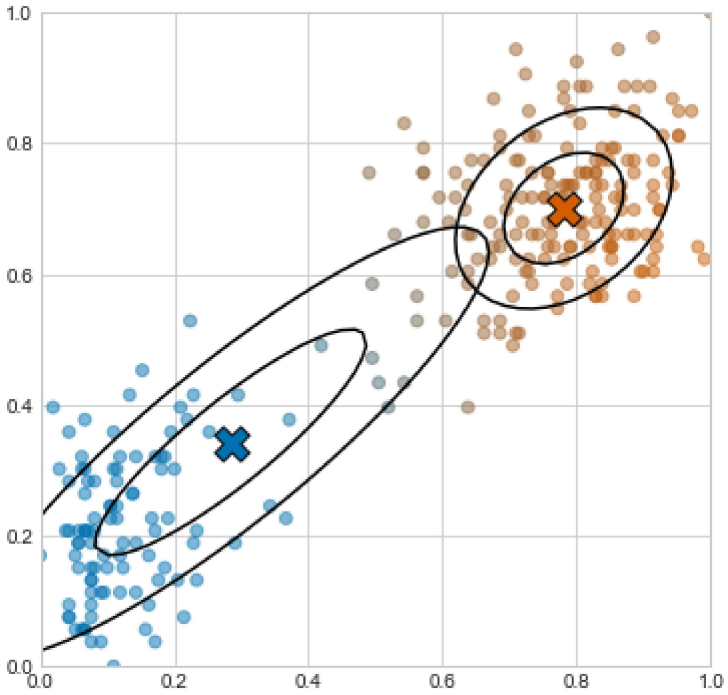

```
Iteration 8: log-likelihood = 150.67, improvement = 10.79
```



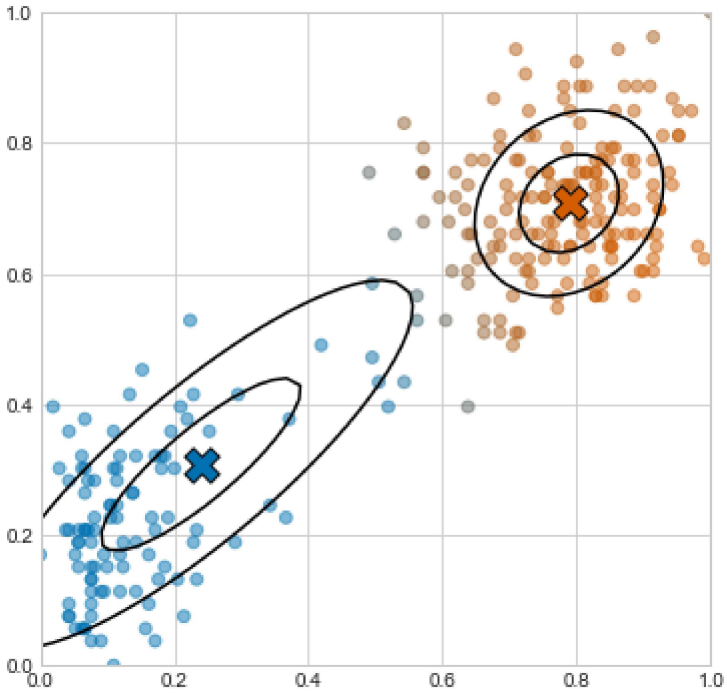

```
Iteration 9: log-likelihood = 181.12, improvement = 30.45
```



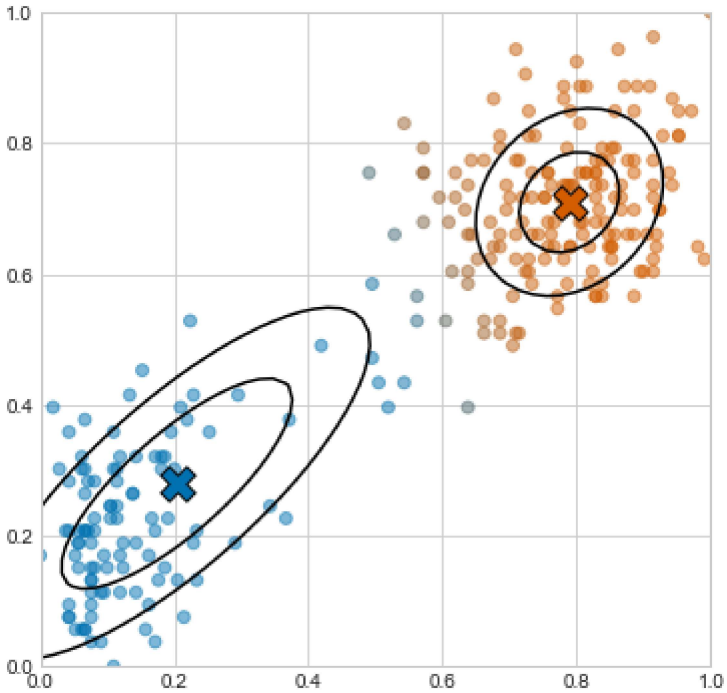

```
Iteration 10: log-likelihood = 220.93, improvement = 39.81
```



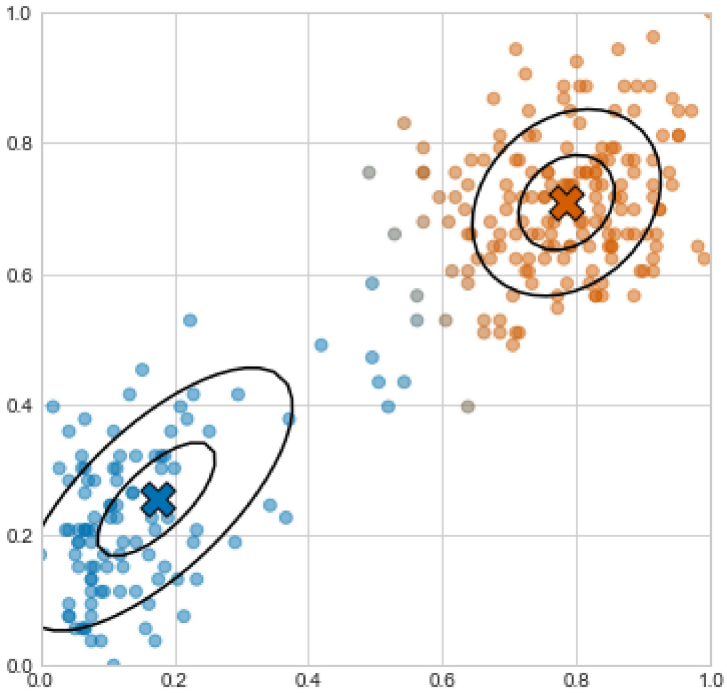

```
Iteration 11: log-likelihood = 234.06, improvement = 13.14
```



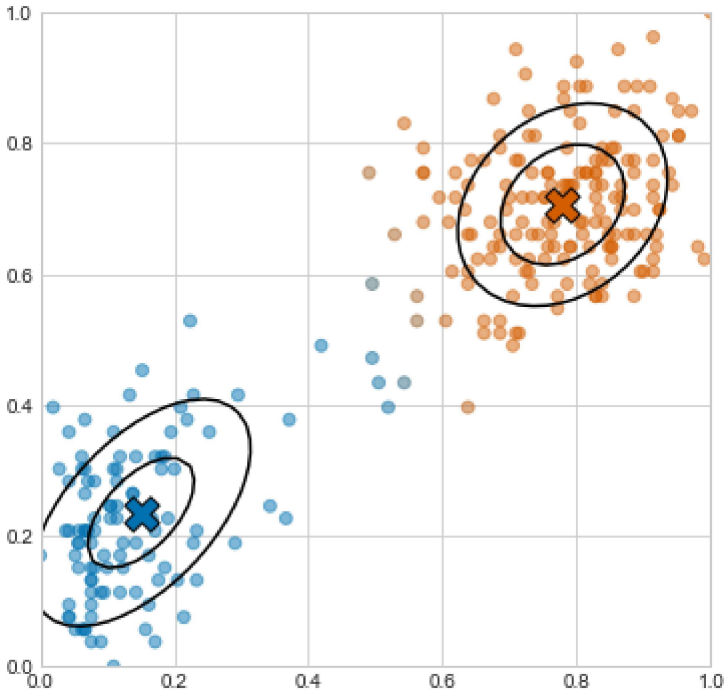

```
Iteration 12: log-likelihood = 244.83, improvement = 10.77
```



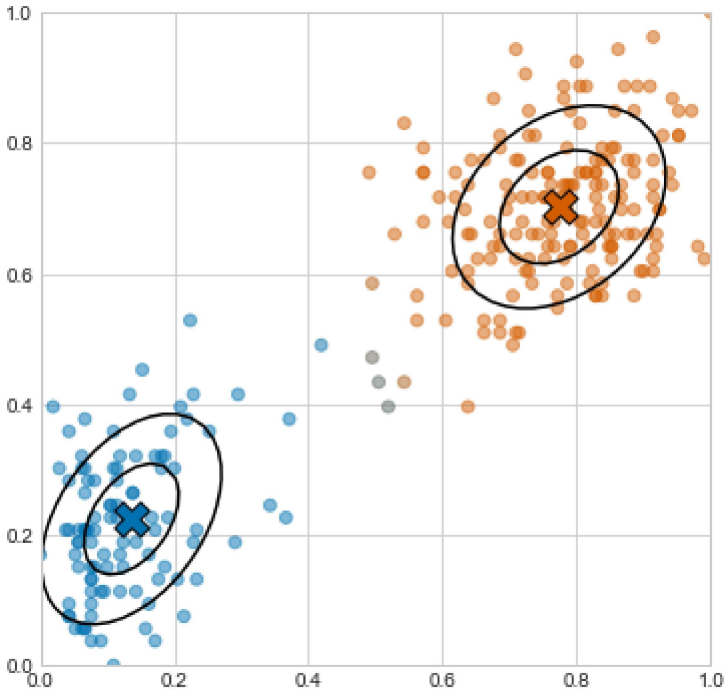

```
Iteration 13: log-likelihood = 258.67, improvement = 13.84
```



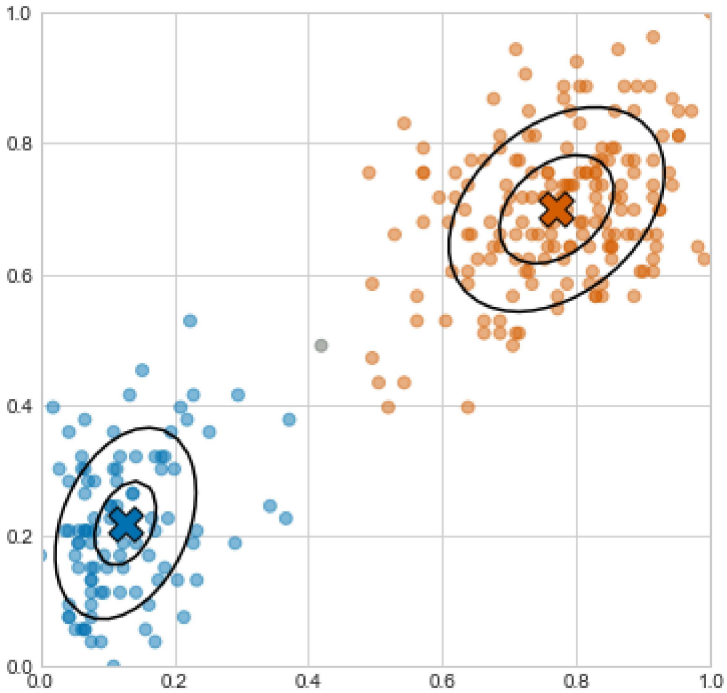

```
Iteration 14: log-likelihood = 272.91, improvement = 14.23
```



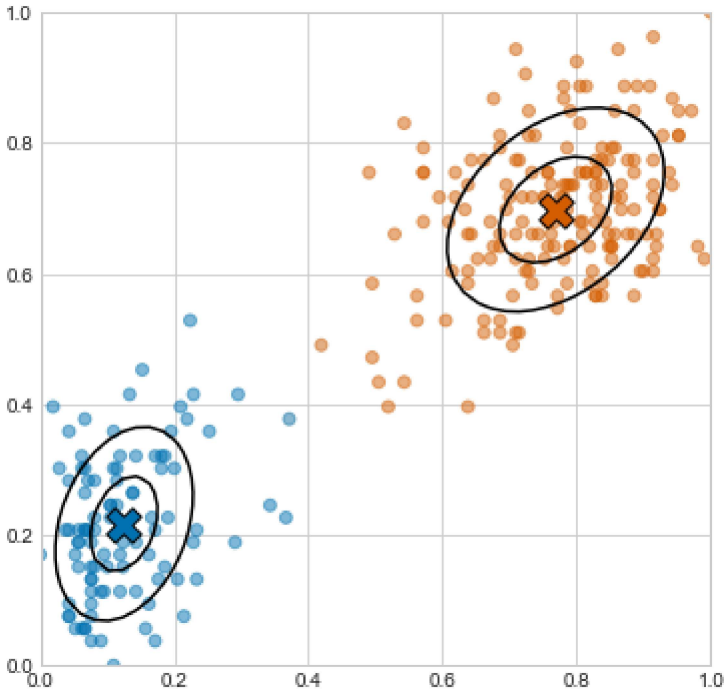

```
Iteration 15: log-likelihood = 284.29, improvement = 11.38
```



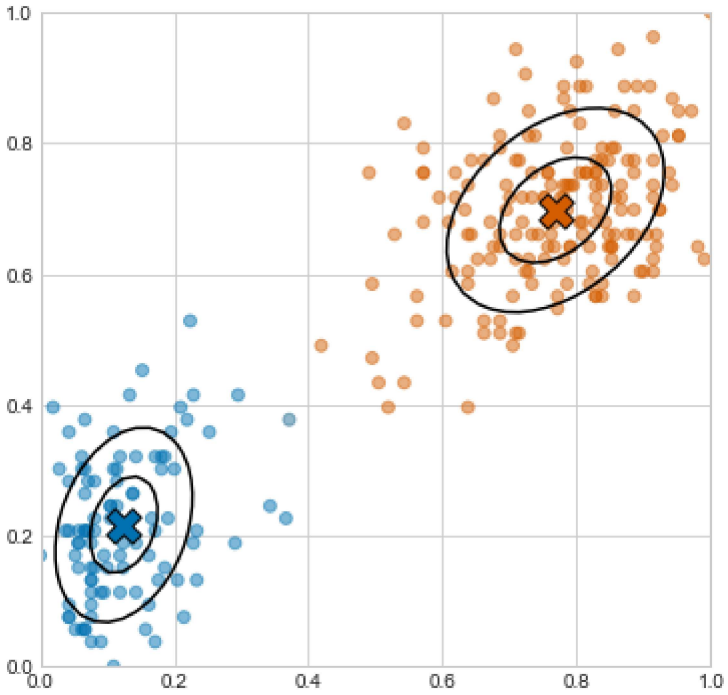

```
Iteration 16: log-likelihood = 289.94, improvement = 5.65
```



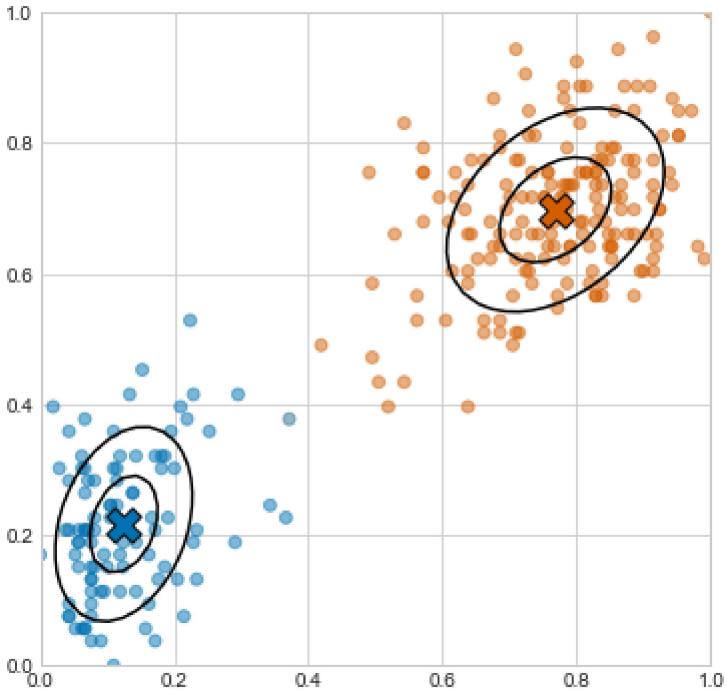

```
Iteration 17: log-likelihood = 290.39, improvement = 0.45
```




```
Iteration 18: log-likelihood = 290.41, improvement = 0.01
```




```
Iteration 19: log-likelihood = 290.41, improvement = 0.00
```


1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0