Machine Learning: Homework #11

Due on January 22, 2018 at 09:59am

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Problem 1

Consider a mixture of K Gaussians

$$p(x) = \pi_k N(x|\mu_k, \Sigma_k).$$

Derive the expected value E[X] and the covariance Cov[x].
Hint: it is helpful to remember the identity $\mathrm{Cov}[x] = \mathrm{E}[xx^T]\mathrm{E}[x]\mathrm{E}[x]^T$.

Solution
Abusing the fact that expected values of probability distributions consisting of sums and factors of other probability distributions can be taken into the sum:

$$E_N[x] = \sum_k \pi_k E_{N_k}[N(x|\mu_k, \Sigma_k)] = \sum_k \pi_k \mu_k$$

$$\mathrm{Cov}[x] = \mathrm{E}[xx^T]\mathrm{E}[x]\mathrm{E}[x]^T$$

$$\mathrm{E}[xx^T] = \sum_k \pi_k E_N[xx^T] = \sum_k \pi_k(\mathrm{Cov}_{N,k}(x) + E_{N,k}[x]E_{N,k}[x]^T) = \sum_k \pi_k(\Sigma_k + \mu_k\mu_k^T I)$$

$$\mathrm{Cov}[x] = \sum_k \pi_k\Sigma_k + \sum_k \pi_k\mu_k\mu_k^T - [\sum_k \pi_k\mu_k][\sum_k \pi_k\mu_k]^T$$

The variance of the mixture is the mixture of variances plus a term that accounts for the weigthed dispersion of the means.

Problem 2

Consider a mixture of K isotropic Gaussians, all with the same known covariances $\Sigma_k = \sigma^2 I$. Derive the EM algorithm for the case when $\sigma^2 \to 0$, and show that it's equivalent to Lloyd's algorithm for K-means.

Solution

$$\gamma_k = \frac{\pi_k N(x|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j N(x|\mu_j, \Sigma_j)} = \frac{\pi_k exp(\frac{-||x-\mu_k||^2}{2\sigma^2})}{\sum_{j=1}^{K} \pi_j exp(\frac{-||x-\mu_j||^2}{2\sigma^2})} = \frac{1}{\sum_{j=1}^{K} \frac{\pi_j}{\pi_k} exp(\frac{-||x-\mu_j||^2+||x-\mu_j||^2}{2\sigma^2})}$$

When $\sigma^2 \to 0$ and k denotes the component that is closest to x, then the denomiator converges to 1.
When it is not the closest component, the denominator converges to ∞.
Thus, K-Means is a special case of the general gaussian EM algorithm.

Problem 3

Load the notebook 11_*homework_clustering.ipynb* from Piazza and the dataset *faithful.txt*. Fill in the missing code and run the notebook. Convert the evaluated notebook to pdf and add it to the printout of your homework.

Solution

Attached.

11_homework_clustering

January 21, 2018

1 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
```

1.1 Your task

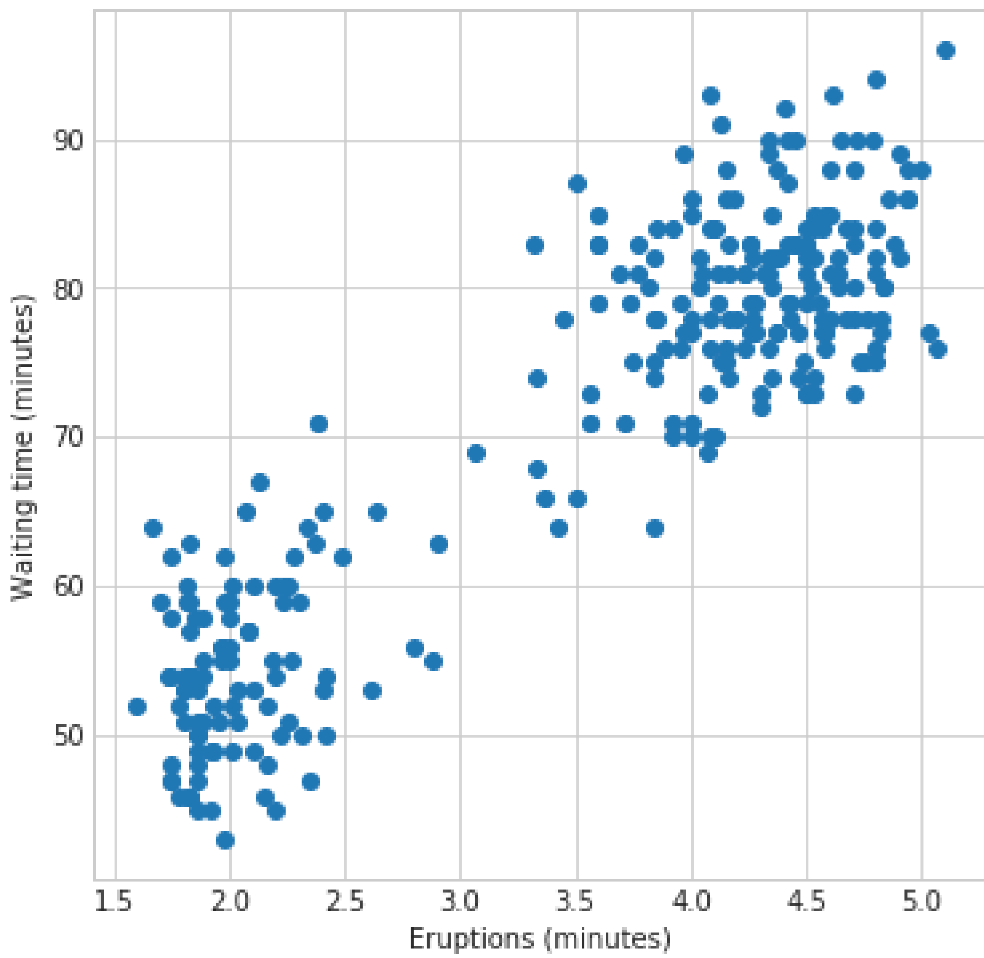
In this homework sheet we will implement Expectation-Maximization algorithm for learning & inference in a Gaussian mixture model.

We will use the dataset 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.

1.2 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()
```



1.3 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).

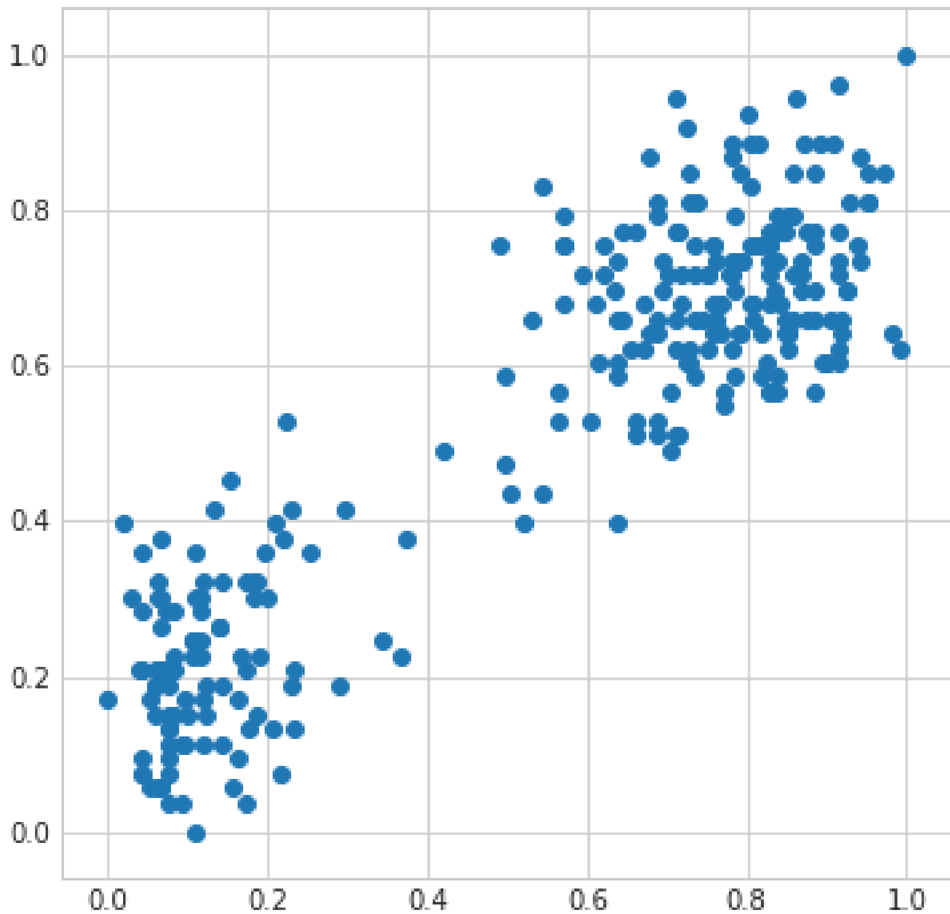
```
In [3]: def normalize_data(X):
            """Normalize data such that it lies in range [0, 1] along every dimension.

            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.
    """
    N = len(X[:,0])
    D = len(X[0,:])
    X_norm = (X-np.min(X,axis=0))/(np.max(X,axis=0) - np.min(X,axis=0))
    return X_norm
```

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



1.4 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 setting.
```

```
        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 given GMM.
        """

        log_likelihood = 0
        K = len(mixing_coefs)
        for i in range(np.size(X, 0)):
            log_likelihood += np.log(sum( \
                [mixing_coefs[k] * \
                 multivariate_normal.pdf(X[i, :], means[k, :], covs[k, :, :]) for k in range
        
        return log_likelihood
```

1.5 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([np.size(X, 0), len(mixing_coefs)])
    N = np.size(X, 0)
    K = len(mixing_coefs)

    for n in range(N):
        denominator = sum([mixing_coefs[k] * multivariate_normal.pdf( \
            X[n, :], means[k, :], covs[k, :, :]) \
                               for k in range(K)])

        responsibilities[n, :] = [mixing_coefs[k] * multivariate_normal.pdf( \
            X[n, :], means[k, :], covs[k, :, :]) \
                                      for k in range(K)] / denominator

    return responsibilities
```

1.6 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 | \theta)].

    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 = np.size(responsibilities, 0)
    K = np.size(responsibilities, 1)
    D = np.size(X, 1)

    covs = np.zeros([K, D, D])

    N_k = np.array([sum(responsibilities[:, k]) for k in range(K)])
    mixing_coefs = N_k[:] / N
    # assign \mu_k
```

```
        means = np.array([1 / N_k[k] * sum([responsibilities[n, k] * X[n, :] for \
                      n in range(N)]) for k in range(K)])
        # assign covs_k
        for k in range(K):
            covs[k, :, :] = 1 / N_k[k] * np.sum([responsibilities[n, k] * \
                    np.outer((X[n, :] - means[k, :]), (X[n, :] - means[k, :])) for \
                    n in range(N)], axis=0)

        return means, covs, mixing_coefs
```

1.7 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()
```

1.8 Run the EM algorithm

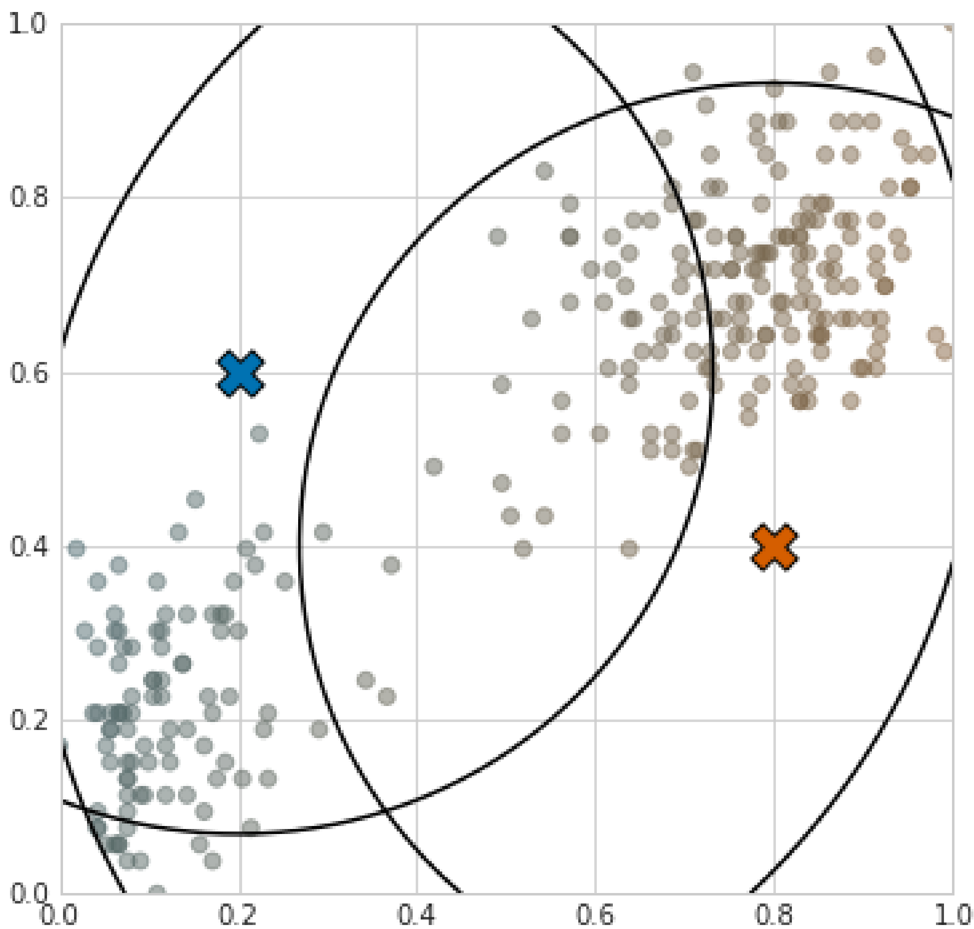
```
In [9]: X_norm = normalize_data(X)
        max_iters = 20

        # 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])
```

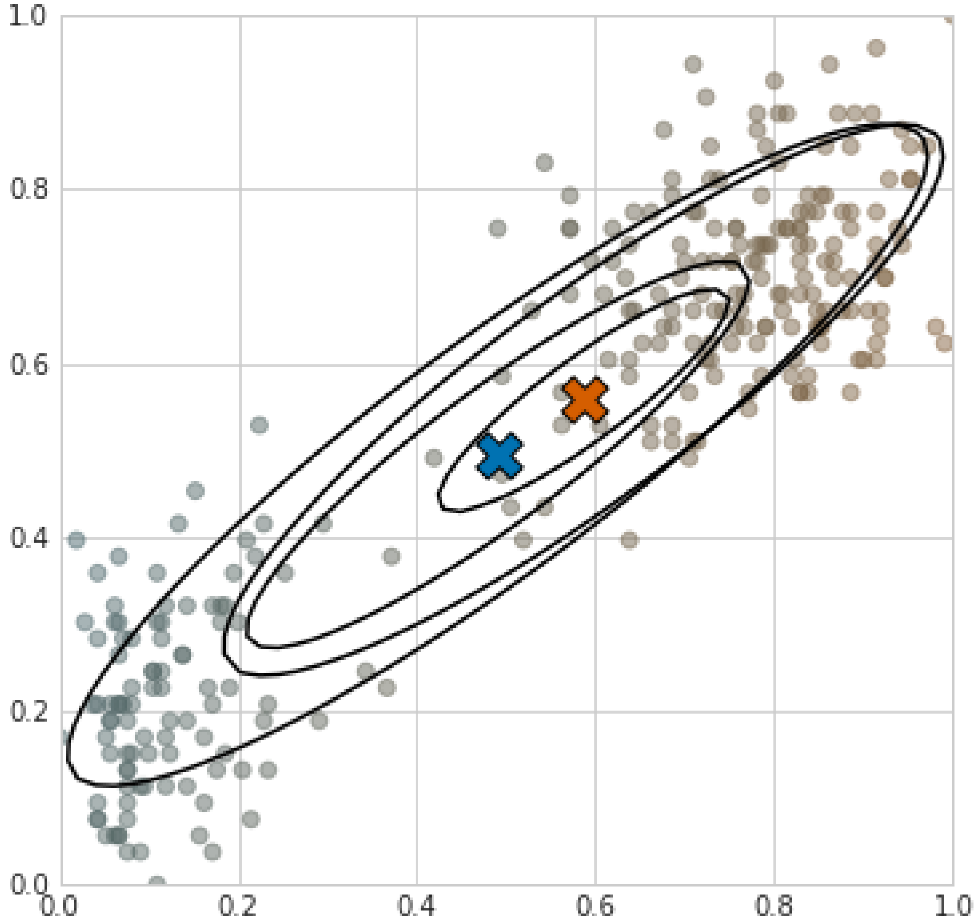
```
old_log_likelihood = gmm_log_likelihood(X_norm, means, covs, mixing_coefs)
responsibilities = e_step(X_norm, means, covs, mixing_coefs)
print('At initialization: log-likelihood = {0}'
      .format(old_log_likelihood))
plot_gmm_2d(X_norm, responsibilities, means, covs, mixing_coefs)

# 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_likelihood))
    old_log_likelihood = new_log_likelihood
    plot_gmm_2d(X_norm, responsibilities, means, covs, mixing_coefs)
```

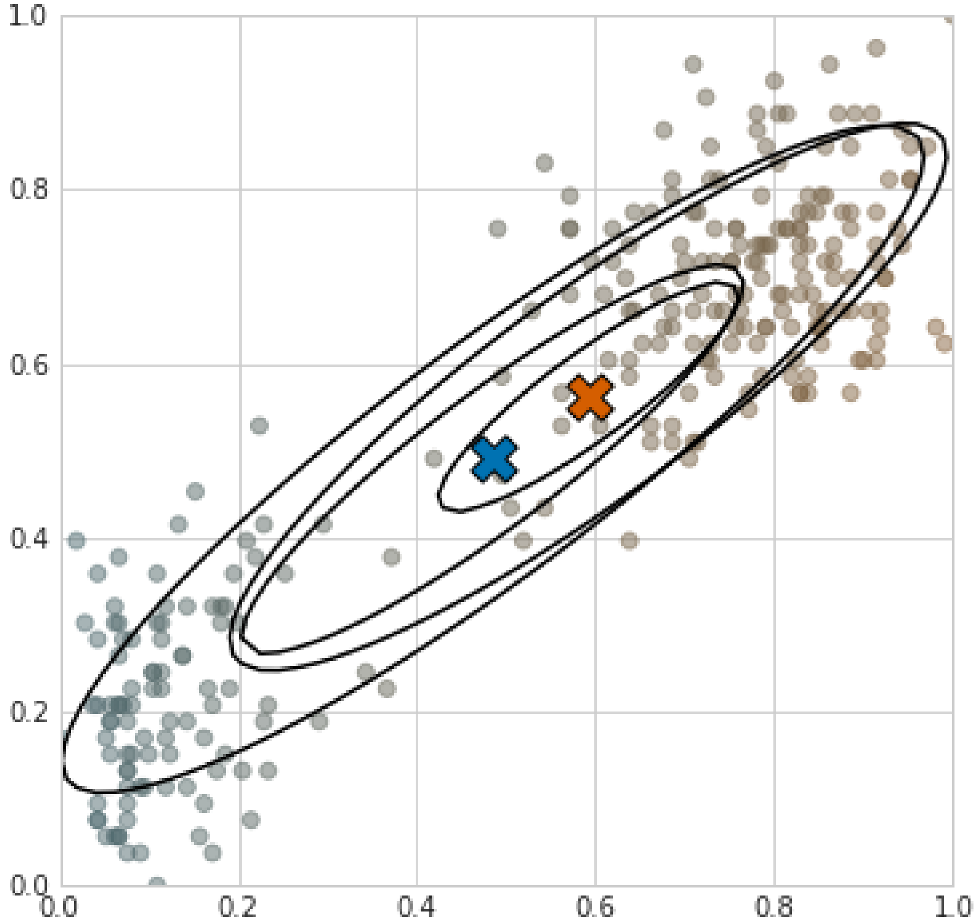
```
At initialization: log-likelihood = -382.70551524206564
```



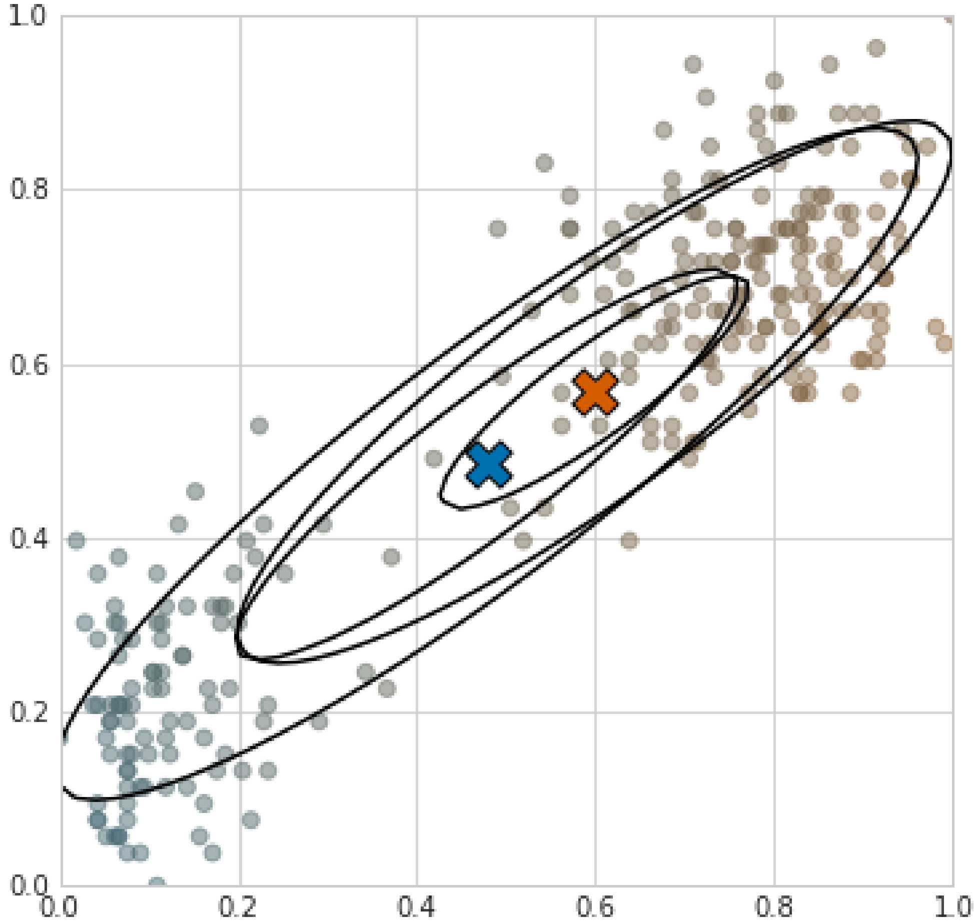
```
Iteration 0: log-likelihood = 131.29, improvement = 513.99
```



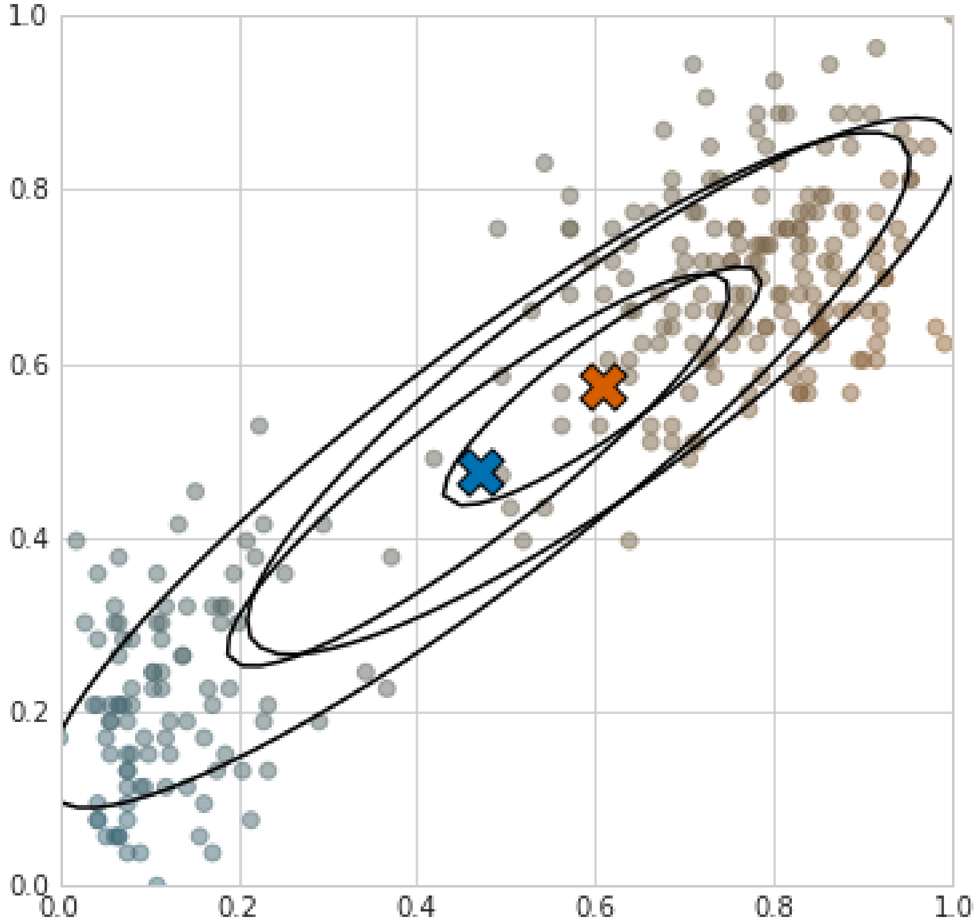

```
Iteration 1: log-likelihood = 131.48, improvement = 0.19
```



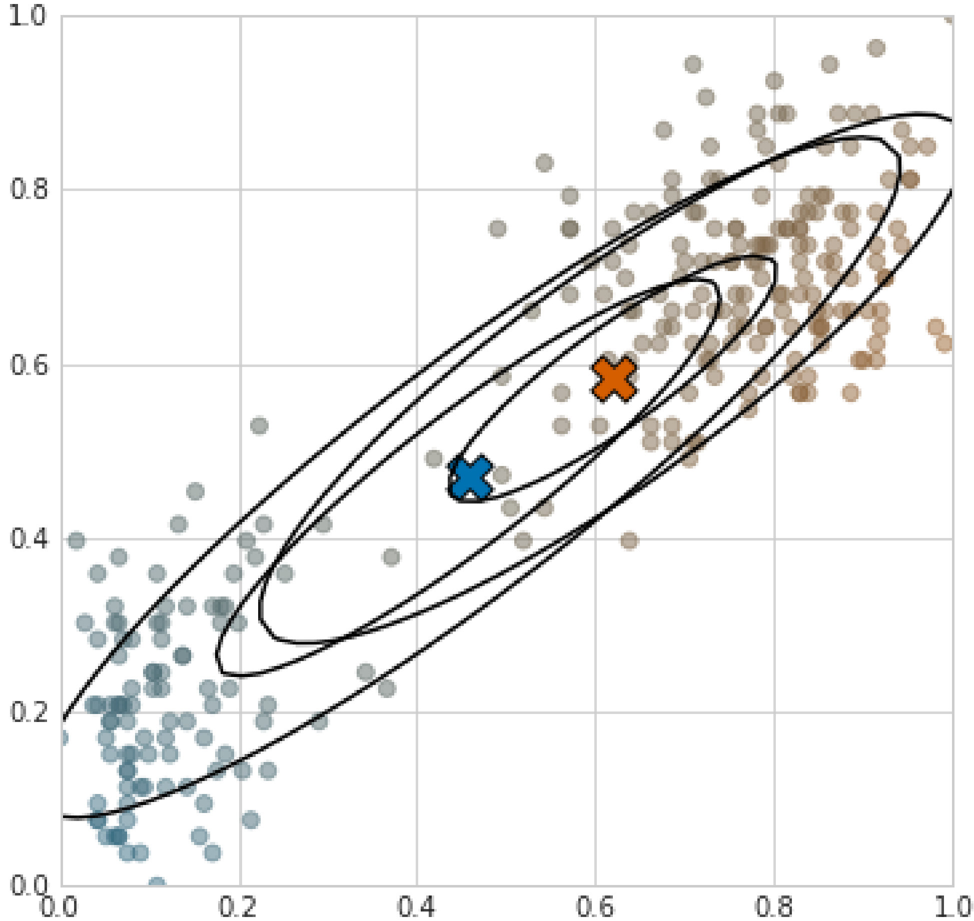

```
Iteration 2: log-likelihood = 131.75, improvement = 0.27
```



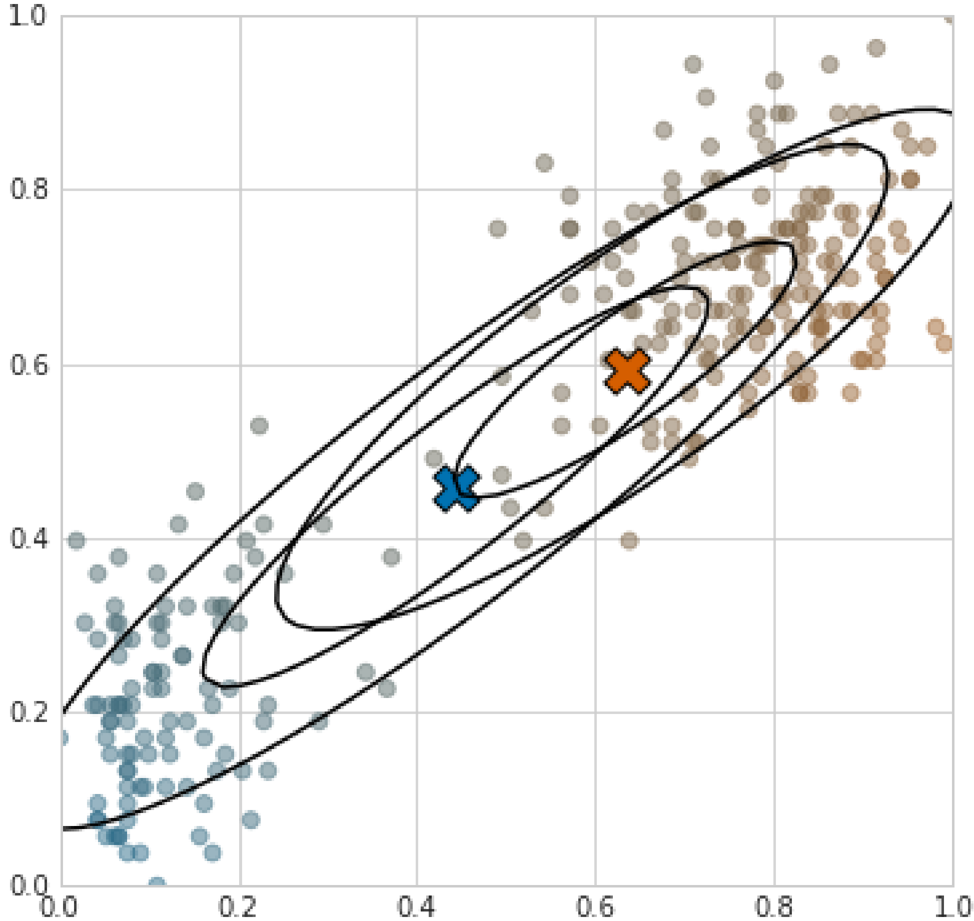

```
Iteration 3: log-likelihood = 132.15, improvement = 0.40
```



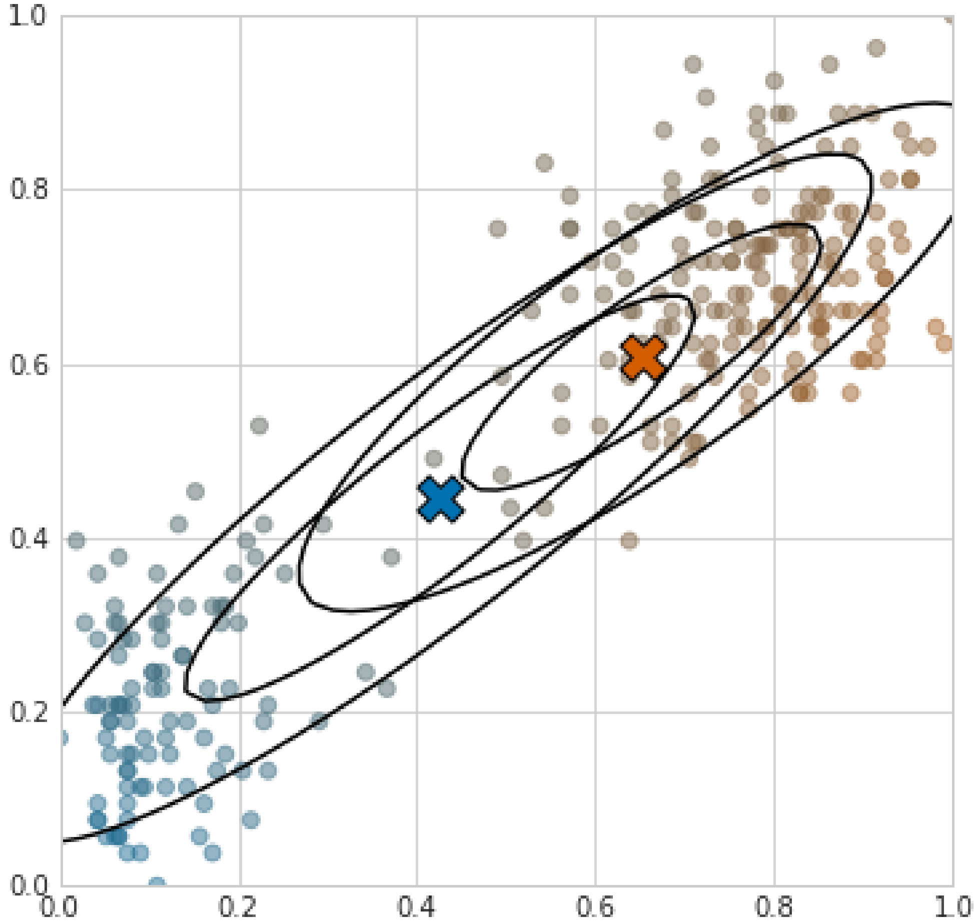

```
Iteration 4: log-likelihood = 132.77, improvement = 0.62
```



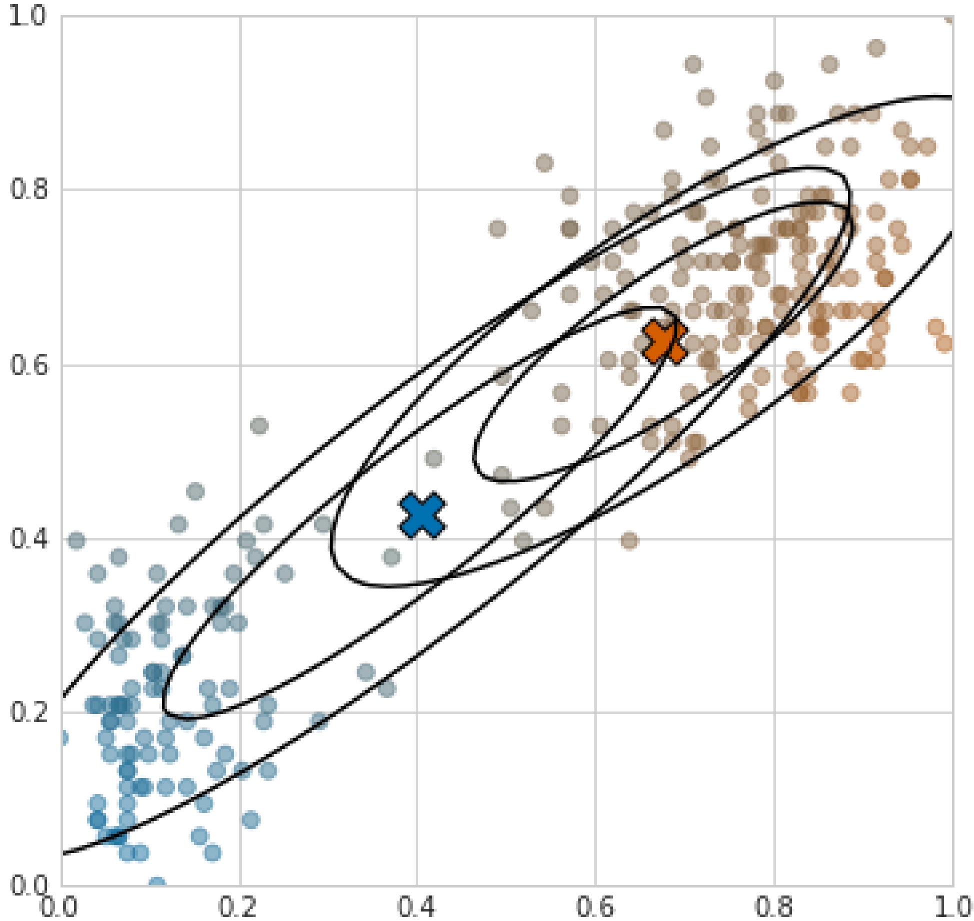

```
Iteration 5: log-likelihood = 133.81, improvement = 1.04
```



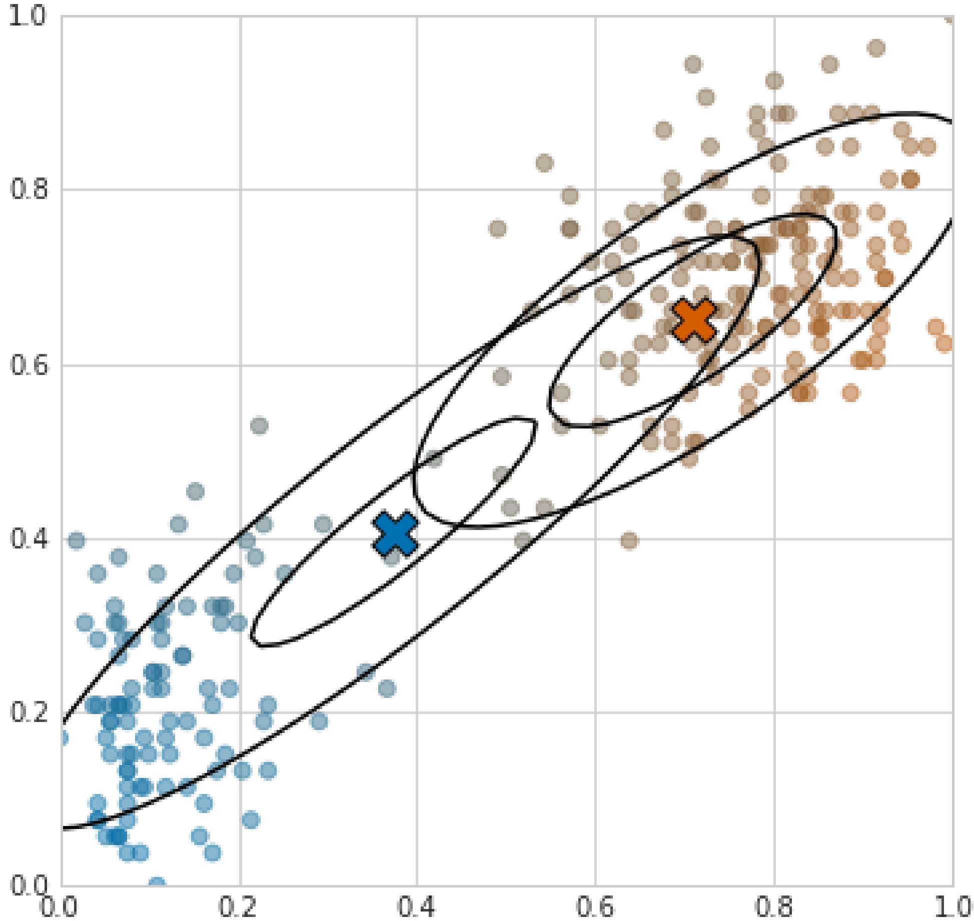

```
Iteration 6: log-likelihood = 135.74, improvement = 1.93
```



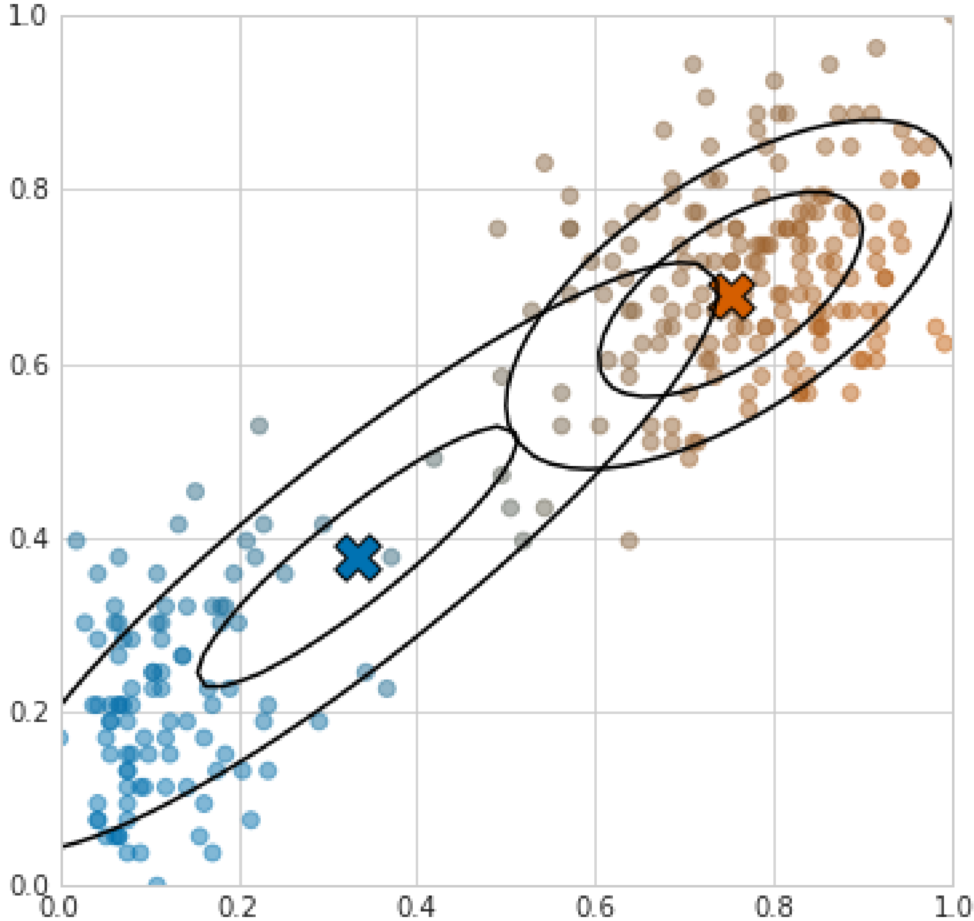

```
Iteration 7: log-likelihood = 139.88, improvement = 4.14
```



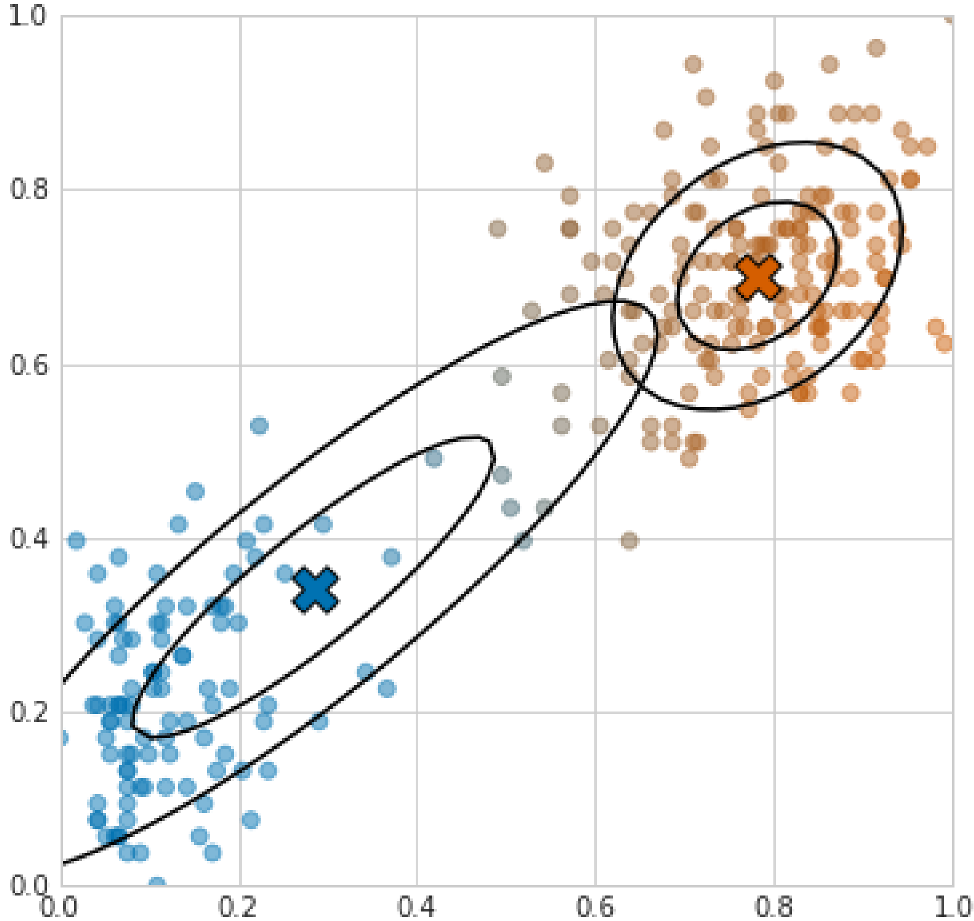

```
Iteration 8: log-likelihood = 150.67, improvement = 10.79
```



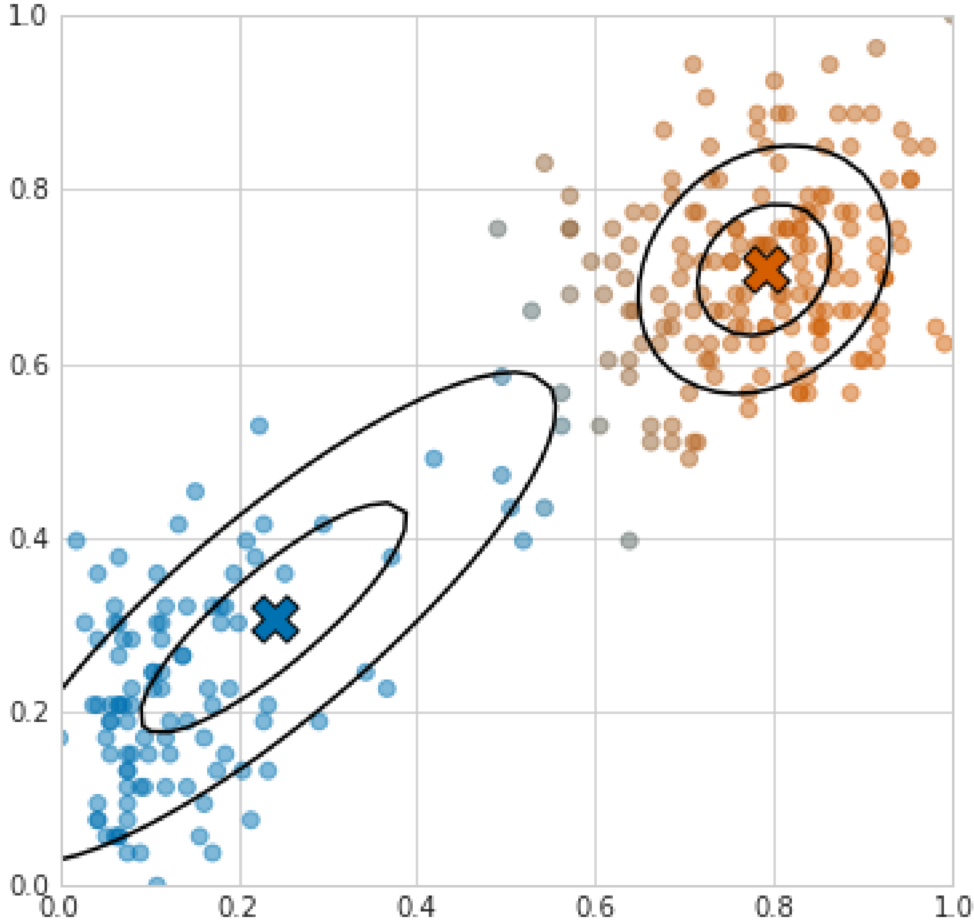

```
Iteration 9: log-likelihood = 181.12, improvement = 30.45
```



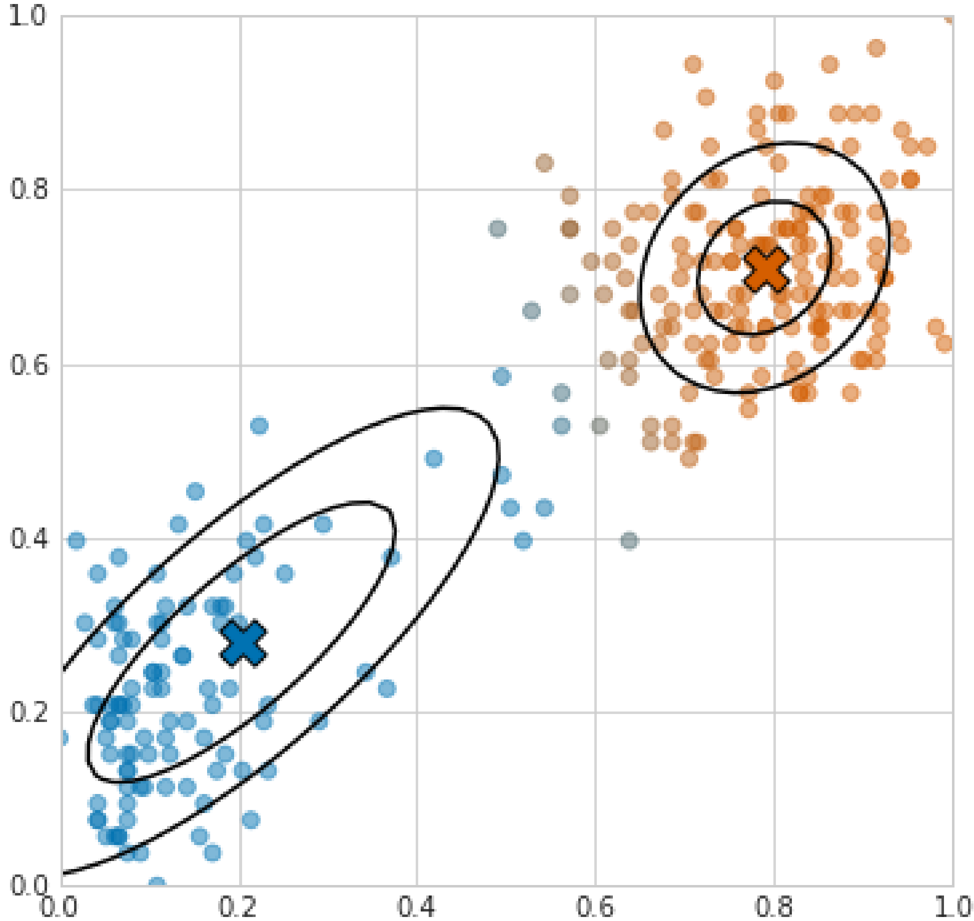

```
Iteration 10: log-likelihood = 220.93, improvement = 39.81
```



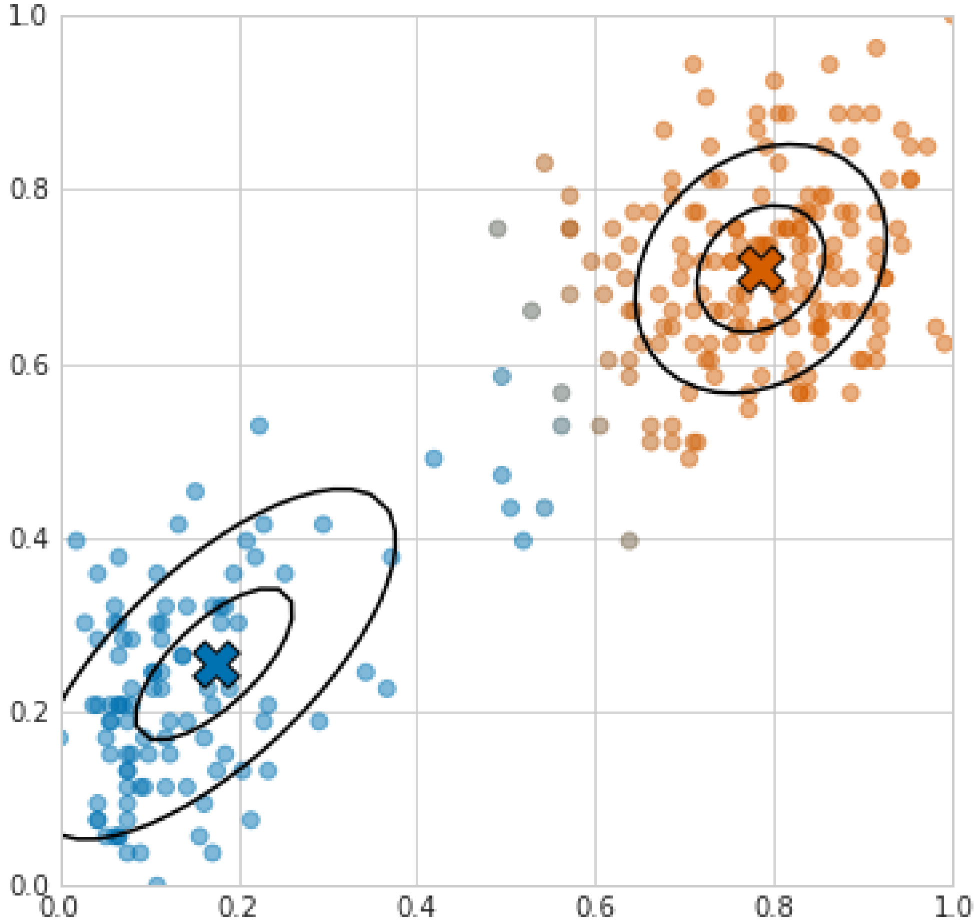

```
Iteration 11: log-likelihood = 234.06, improvement = 13.14
```



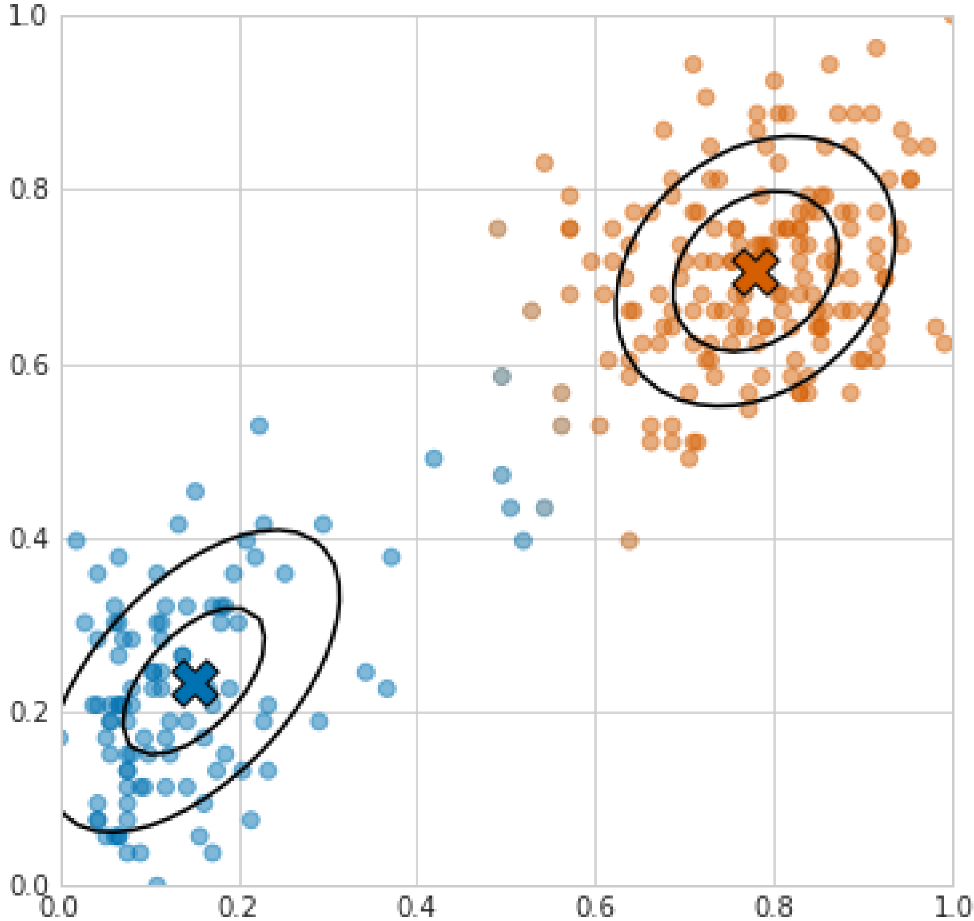

```
Iteration 12: log-likelihood = 244.83, improvement = 10.77
```



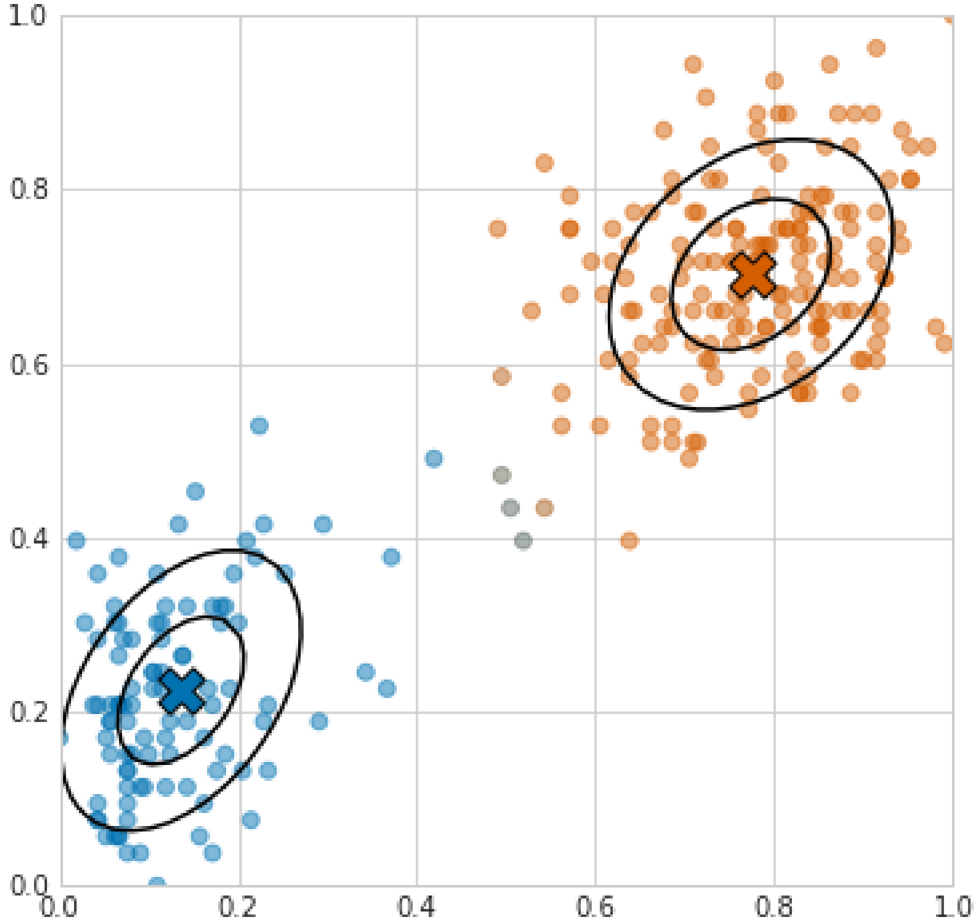

```
Iteration 13: log-likelihood = 258.67, improvement = 13.84
```



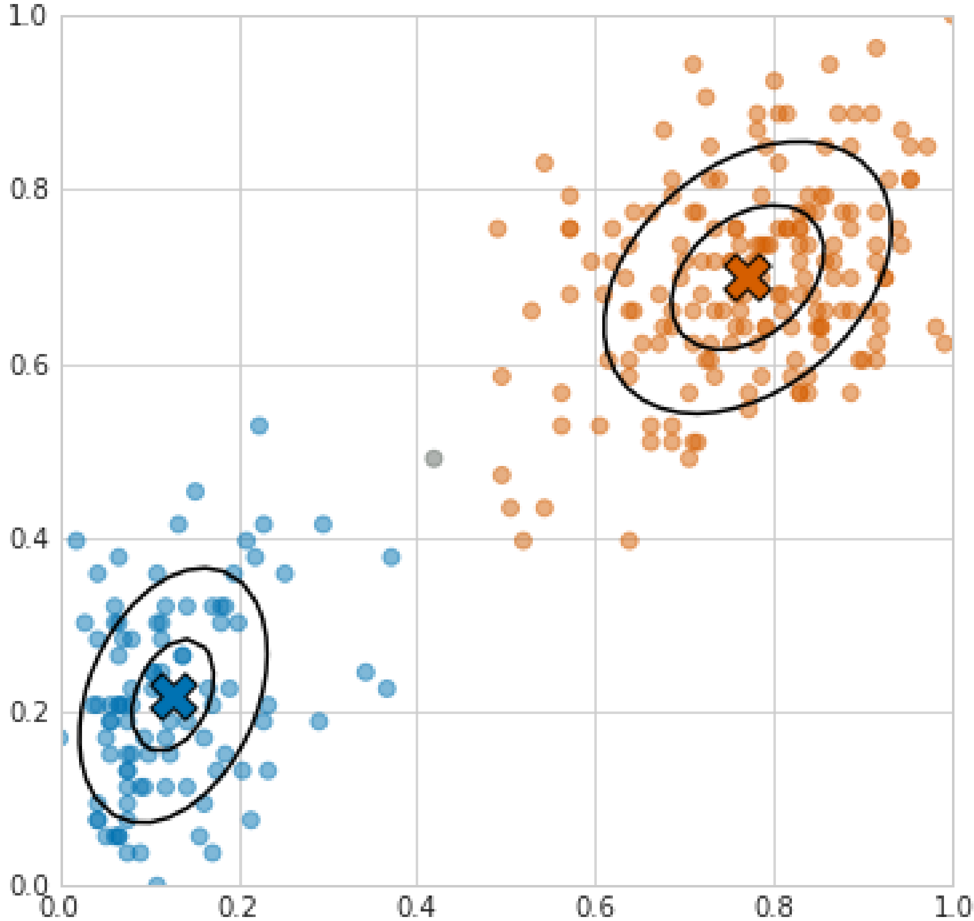

```
Iteration 14: log-likelihood = 272.91, improvement = 14.23
```



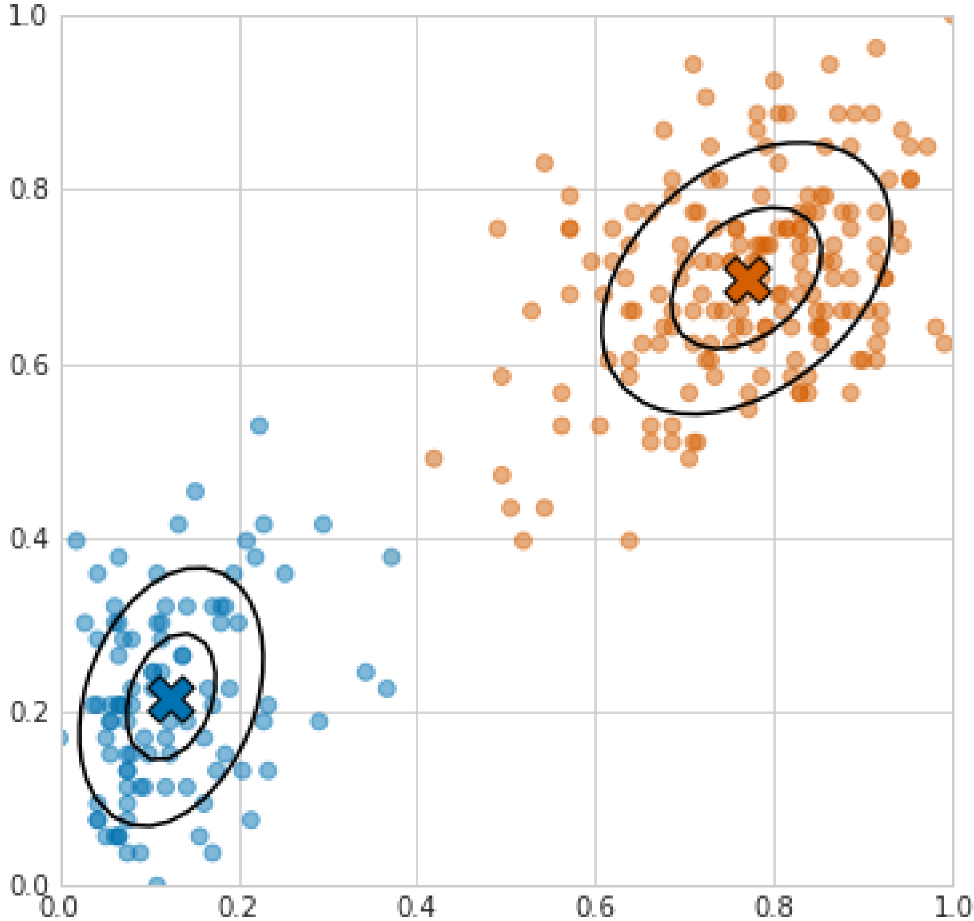

```
Iteration 15: log-likelihood = 284.29, improvement = 11.38
```



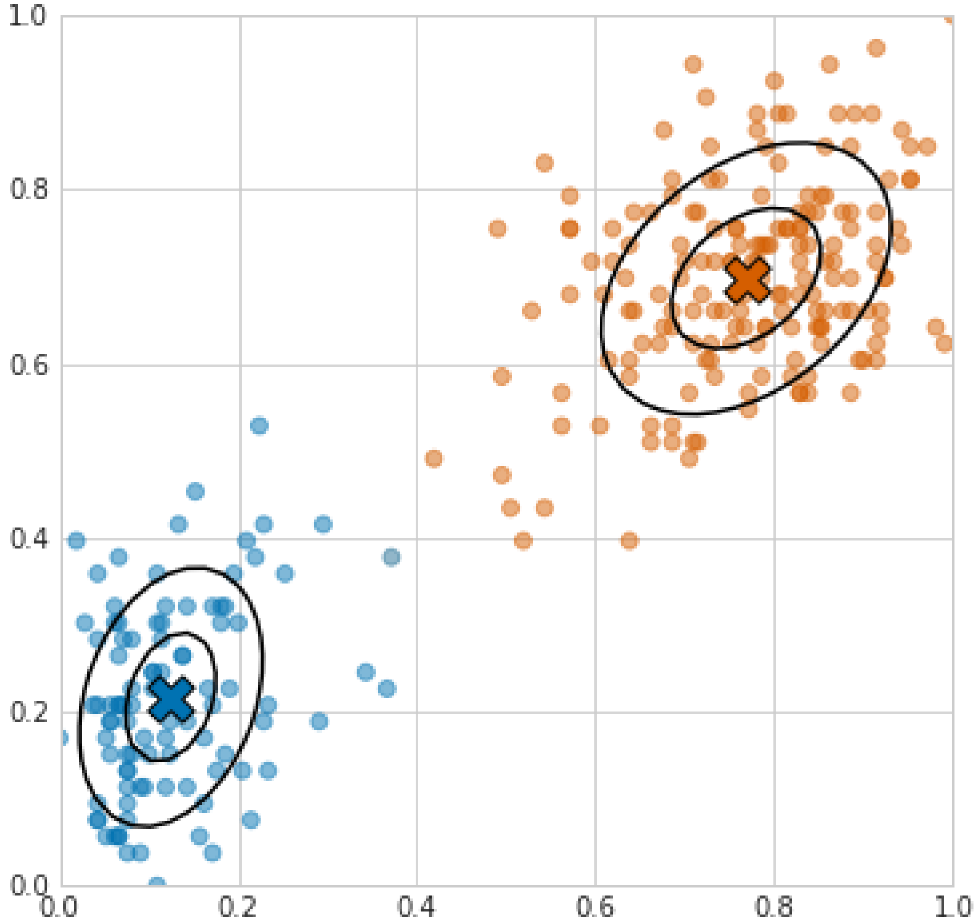

```
Iteration 16: log-likelihood = 289.94, improvement = 5.65
```



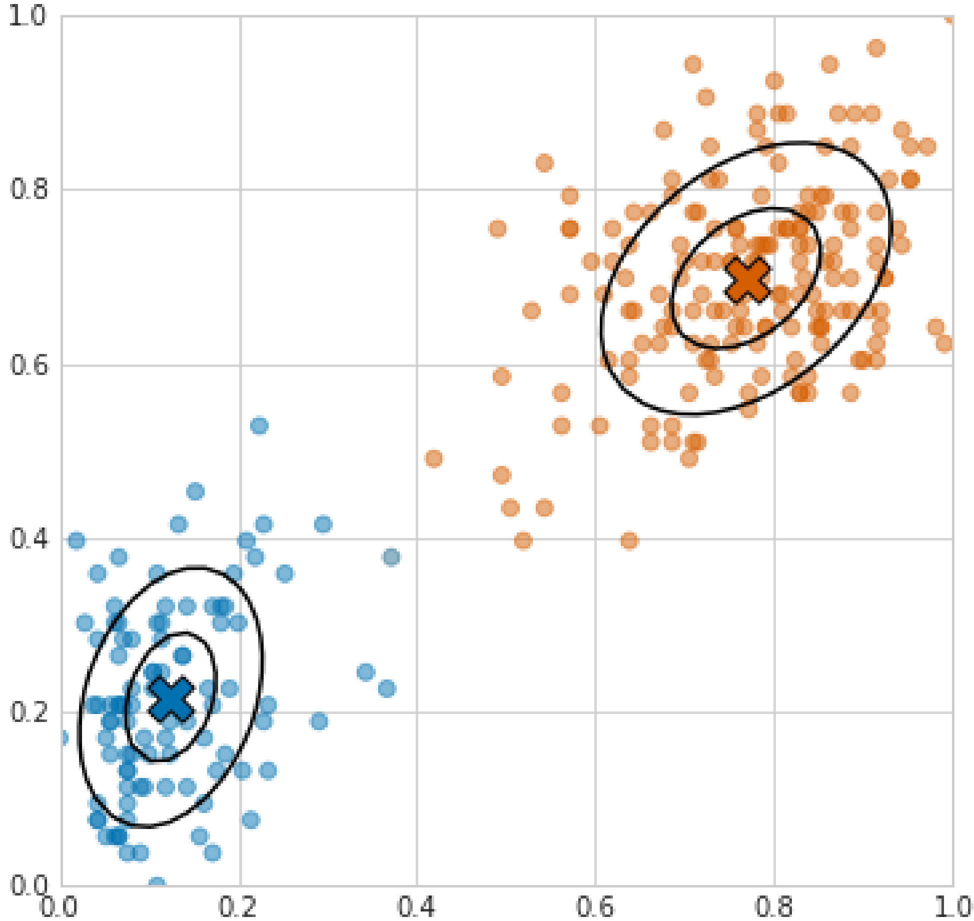

```
Iteration 17: log-likelihood = 290.39, improvement = 0.45
```




```
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