

## exercise3

January 12, 2021

### 1 EXERCISE 3 - ML - Grundverfahren

#### 1.1 1.) Constrained Optimization (6 Points)

You are given the following Optimization problem:

$$\begin{aligned} \min_{\mathbf{x}} \quad & \mathbf{x}^T \mathbf{M} \mathbf{x} + \mathbf{x}^T \mathbf{h} \\ \text{s.t.} \quad & \mathbf{x}^T \mathbf{b} \geq c, \end{aligned}$$

where  $\mathbf{M}$  is a positive definit, symmetric Matrix. Note that vectors and matrices are boldsymbol, where Matrices have capital letters. Derive the optimal solution for  $\mathbf{x}$  independant of the Lagrangian multiplier(s) (i.e. you have to solve for the dual). Make sure that you mark vectors and matrices as a boldsymbol and small letters and capital letters respectively. Symbols which are not marked as boldsymbols will count as scalar. Take care of vector/matrix multiplication and derivatives. And make use of the properties of  $\mathbf{M}$ . Don't forget to look up matrix-vector calculus in the matrix cookbook, if you don't remember the rules.

##### 1.1.1 Step 1: Setup the Lagrangian Function

$$L(x, \lambda) = \mathbf{x}^T \mathbf{M} \mathbf{x} + \mathbf{x}^T \mathbf{h} - \lambda \cdot (\mathbf{x}^T \mathbf{b} - c)$$

##### 1.1.2 Step 2: Find optimal $x^*$ with respect to $\lambda$

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{x}} &= 2\mathbf{M}\mathbf{x} + \mathbf{h} - \lambda\mathbf{b} \stackrel{!}{=} 0 && \text{Reformulate} \\ 2\mathbf{M}\mathbf{x} &= \lambda\mathbf{b} - \mathbf{h} && \text{Inverse multiplication} \\ \mathbf{x}^* &= \frac{1}{2}\mathbf{M}^{-1}(\lambda\mathbf{b} - \mathbf{h}) \end{aligned}$$

##### 1.1.3 Step 3: Create Dual Function $g(\lambda)$

$$g(\lambda) = \left(\frac{1}{2}\mathbf{M}^{-1}(\lambda\mathbf{b} - \mathbf{h})\right)^T \mathbf{M} \left(\frac{1}{2}\mathbf{M}^{-1}(\lambda\mathbf{b} - \mathbf{h})\right) + \left(\frac{1}{2}\mathbf{M}^{-1}(\lambda\mathbf{b} - \mathbf{h})\right)^T \mathbf{h} - \lambda \cdot \left(\left(\frac{1}{2}\mathbf{M}^{-1}(\lambda\mathbf{b} - \mathbf{h})\right)^T \mathbf{b} - c\right)$$

#### 1.1.4 Step 4: Find $\lambda^* = \operatorname{argmin}[g(\lambda)]$

$$\begin{aligned}
 \frac{\partial g}{\partial \lambda} &= \frac{1}{2}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1} \mathbf{b} && \text{This line} \\
 &+ \frac{1}{2} \mathbf{h}^T \mathbf{M}^{-1} \mathbf{b} \\
 &- \frac{1}{2}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1} \mathbf{b} && \text{and this, cancel out.} \\
 &+ c \\
 &- \frac{1}{2} \lambda \mathbf{b}^T \mathbf{M}^{-1} \mathbf{b} \stackrel{!}{=} 0 \\
 0 &= \frac{1}{2} \mathbf{h}^T \mathbf{M}^{-1} \mathbf{b} + c - \frac{1}{2} \lambda \mathbf{b}^T \mathbf{M}^{-1} \mathbf{b} \\
 \frac{1}{2} \lambda \mathbf{b}^T \mathbf{M}^{-1} \mathbf{b} &= \frac{1}{2} \mathbf{h}^T \mathbf{M}^{-1} \mathbf{b} + c \\
 \lambda^* &= \frac{\mathbf{h}^T \mathbf{M}^{-1} \mathbf{b} + c}{\mathbf{b}^T \mathbf{M}^{-1} \mathbf{b}}
 \end{aligned}$$

#### 1.1.5 Step 5: Profit

$$\begin{aligned}
 \mathbf{x}^* &= \frac{1}{2} \mathbf{M}^{-1}(\lambda \mathbf{b} - \mathbf{h}) && \text{insert } \lambda^* \text{ here} \\
 \mathbf{x}^* &= \frac{1}{2} \mathbf{M}^{-1} \left( \frac{\mathbf{h}^T \mathbf{M}^{-1} \mathbf{b} + c}{\mathbf{b}^T \mathbf{M}^{-1} \mathbf{b}} \mathbf{b} - \mathbf{h} \right)
 \end{aligned}$$

## 1.2 2.) k-Means (7 Points)

Here we will implement one of the most basic approaches to clustering - the k-Means algorithm. Let us start with some basic imports and implementing functionality to visualize our results.

```
[1]: %matplotlib inline

import numpy as np
import matplotlib.pyplot as plt
from typing import Tuple, Optional
from scipy.spatial import distance
from scipy.stats import multivariate_normal as mvn

def visualize_2d_clustering(data_points: np.ndarray, assignments_one_hot: np.
    ↳ ndarray, centers: np.ndarray, k: int,
                                centers_history: Optional[np.ndarray] = None, title:
    ↳ Optional[str] = None):
    """Visualizes clusters, centers and path of centers"""
    plt.figure(figsize=(6, 6), dpi=100)
    assignments = np.argmax(assignments_one_hot, axis=1)

    for i in range(k):
        # get next color
```

```

        c = next(plt.gca()._get_lines.prop_cycler)['color']
        # get cluster
        cur_assignments = assignments == i
        # plot clusters
        plt.scatter(data_points[cur_assignments, 0],
↪data_points[cur_assignments, 1], c=c,
                    label="Cluster {:02d}".format(i))

        #plot history of centers if it is given
        if centers_history is not None:
            plt.scatter(centers_history[:, i, 0], centers_history[:, i, 1],
↪marker="x", c=c)
            plt.plot(centers_history[:, i, 0], centers_history[:, i, 1], c=c)

        plt.scatter(centers[:, 0], centers[:, 1], label="Centers", color="black",
↪marker="X")

        if title is not None:
            plt.title(title)

    plt.legend()

```

Next we going to implement the actual algorithm. As a quick reminder, K-Means works by iterating the following steps:

Start with k randomly picked centers

- 1.) Assign each point to the closest center
- 2.) Addjust centers by taking the average over all points assigned to it

Implementing them will be your task for this exerisce

```

[2]: def assignment_step(data_points: np.ndarray, centers: np.ndarray) -> np.ndarray:
    """
    Assignment Step: Computes assignments to nearest cluster
    :param data_points: Data points to cluster (shape: [N x data_dim])
    :param centers: current cluster centers (shape: [k, data_dim])
    :return Assignments (as one hot) (shape: [N, k])
    """
    #####
    # TODO Implement the assignment step of the k-Means algorithm
    # DONE
    one_hot = []

    for data_point in data_points:
        index_of_closest = distance.cdist([data_point], centers).argmin()
        k_one_hot = np.zeros(centers.shape[0])
        k_one_hot[index_of_closest] = 1
        one_hot.append(k_one_hot)

```

```

return np.asarray(one_hot)
#####

def adjustment_step(data_points: np.ndarray, assignments_one_hot: np.ndarray) → np.ndarray:
    """
    Adjustment Step: Adjust centers given assignment
    :param data_points: Data points to cluster (shape: [N x data_dim])
    :param assignments_one_hot: assignment to adjust to (one-hot representation) (shape: [N, k])
    :return Adjusted Centers (shape: [k, data_dim])
    """
    #####
    # TODO Implement the adjustment step of the k-Means algorithm
    # DONE
    N = data_points.shape[0]          # amount of data points
    C = assignments_one_hot.shape[1]   # amount of Centers k

    patches = np.empty((C,0)).tolist() # get empty array of length C

    ind = np.nonzero(assignments_one_hot) # get tuple of indices
    for i,j in zip(ind[0], ind[1]):
        patches[j].append(data_points[i])

    new_centers = []
    for patch in patches:
        patch_size = len(patch)
        new_centers.append(np.sum(np.array(patch), axis=0) / patch_size)

    return np.array(new_centers)
#####

```

Now to the final algorithm, as said we initialize the centers with random data points and iterate the assignment and adjustment step

```

[3]: def k_means(data_points: np.ndarray, k: int, max_iter: int = 100, vis_interval: int = 3) → Tuple[np.ndarray, np.ndarray, np.ndarray, np.ndarray]:
    """
    Simple K Means Implementation
    :param data_points: Data points to cluster (shape: [N x data_dim])
    :param k: number of clusters

```

```

        :param max_iter: Maximum number of iterations to run if convergence is not
        ↪reached
        :param vis_interval: After how many iterations to generate the next plot
        :return: - cluster labels (shape: [N])
                 - means of clusters (shape: [k, data_dim])
                 - SSD over time (shape: [2 * num_iters])
                 - History of means over iterations (shape: [num_iters, k,
        ↪data_dim])
    """
    # Bookkeeping
    i = 0
    means_history = []
    ssd_history = []
    assignments_one_hot = np.zeros(shape=[data_points.shape[0], k])
    old_assignments = np.ones(shape=[data_points.shape[0], k])

    # Initialize with k random data points
    initial_idx = np.random.choice(len(data_points), k, replace=False)
    centers = data_points[initial_idx]
    means_history.append(centers.copy())

    # Iterate while not converged and max number iterations not reached
    while np.any(old_assignments != assignments_one_hot) and i < max_iter:
        old_assignments = assignments_one_hot

        # assignment
        assignments_one_hot = assignment_step(data_points, centers)

        # compute SSD
        diffs = np.sum(np.square(data_points[:, None, :] - centers[None, :, :
        ↪]), axis=-1)
        ssd_history.append(np.sum(assignments_one_hot * diffs))

        # adjustment
        centers = adjustment_step(data_points, assignments_one_hot)

        # compute SSD
        diffs = np.sum(np.square(data_points[:, None, :] - centers[None, :, :
        ↪]), axis=-1)
        ssd_history.append(np.sum(assignments_one_hot * diffs))

    # Plotting
    if i % vis_interval == 0:
        visualize_2d_clustering(data_points, assignments_one_hot, centers,
        ↪k, title="Iteration {:02d}".format(i))

```

```

    # Bookkeeping
    means_history.append(centers.copy())
    i += 1

    print("Took", i, "iterations to converge")
    return assignments_one_hot, centers, np.array(ssd_history), np.
    ↳stack(means_history, 0)

```

Finally we run the dataset and visualize the results. Here we provide 4 random datasets, each containing 500 2 samples and you can play around with the number of clusters,  $k$ , as well as the seed of the random number generator. Based on this seed the initial centers, and thus the final outcome, will vary.

```

[4]: np.random.seed(42)

data = np.load("samples_3.npy")
k = 8

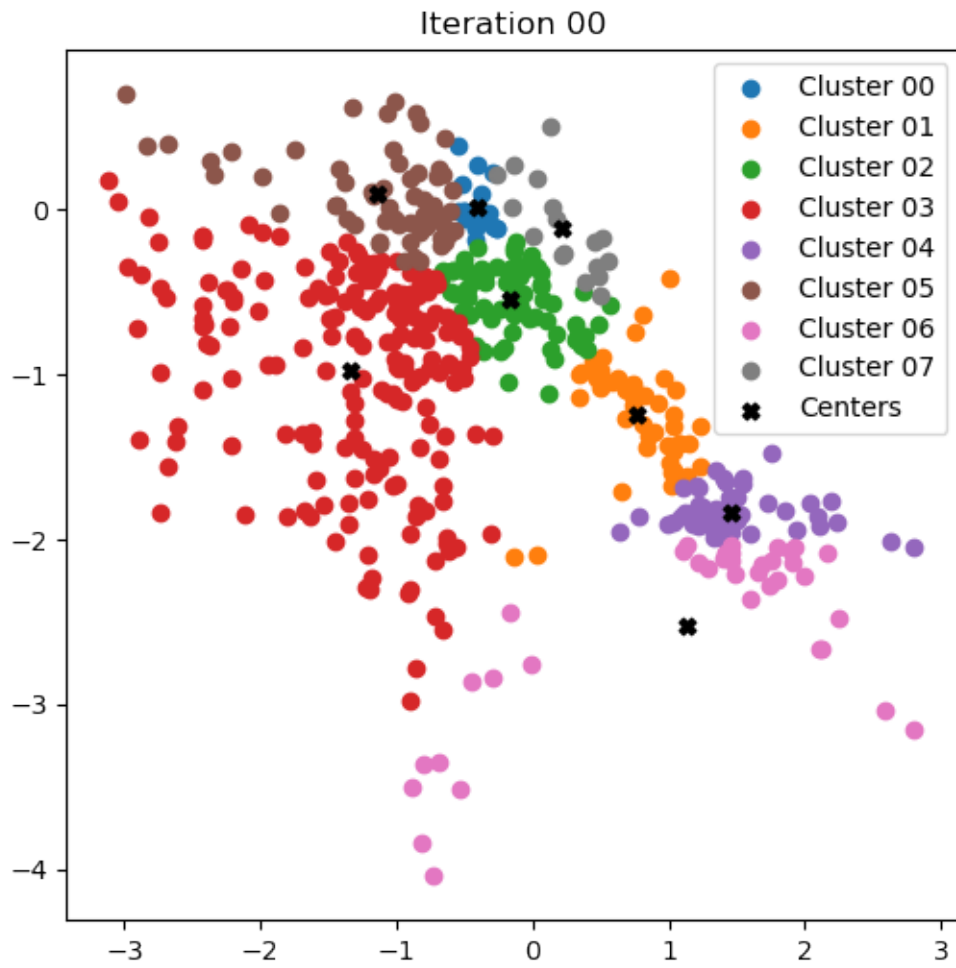
cluster_labels, centers, ssd_history, centers_history = k_means(data, k)

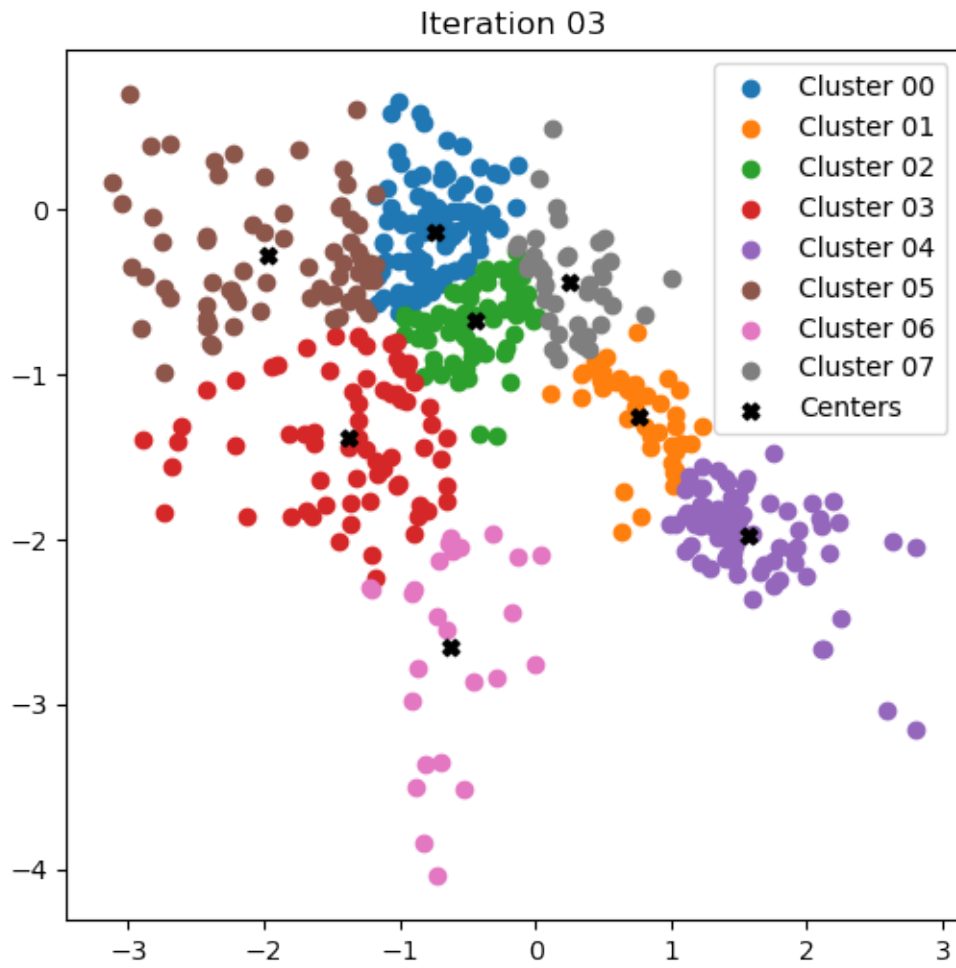
# plot final clustering with history of centers over iterations
visualize_2d_clustering(data, cluster_labels, centers, k=k,
    ↳centers_history=centers_history, title="Final Clustering")

# plot SSD
plt.figure("SSD")
plt.semilogy(np.arange(start=0, stop=len(ssd_history) / 2, step=0.5),
    ↳ssd_history)
plt.xlabel("Iteration")
plt.ylabel("SSD")
plt.show()

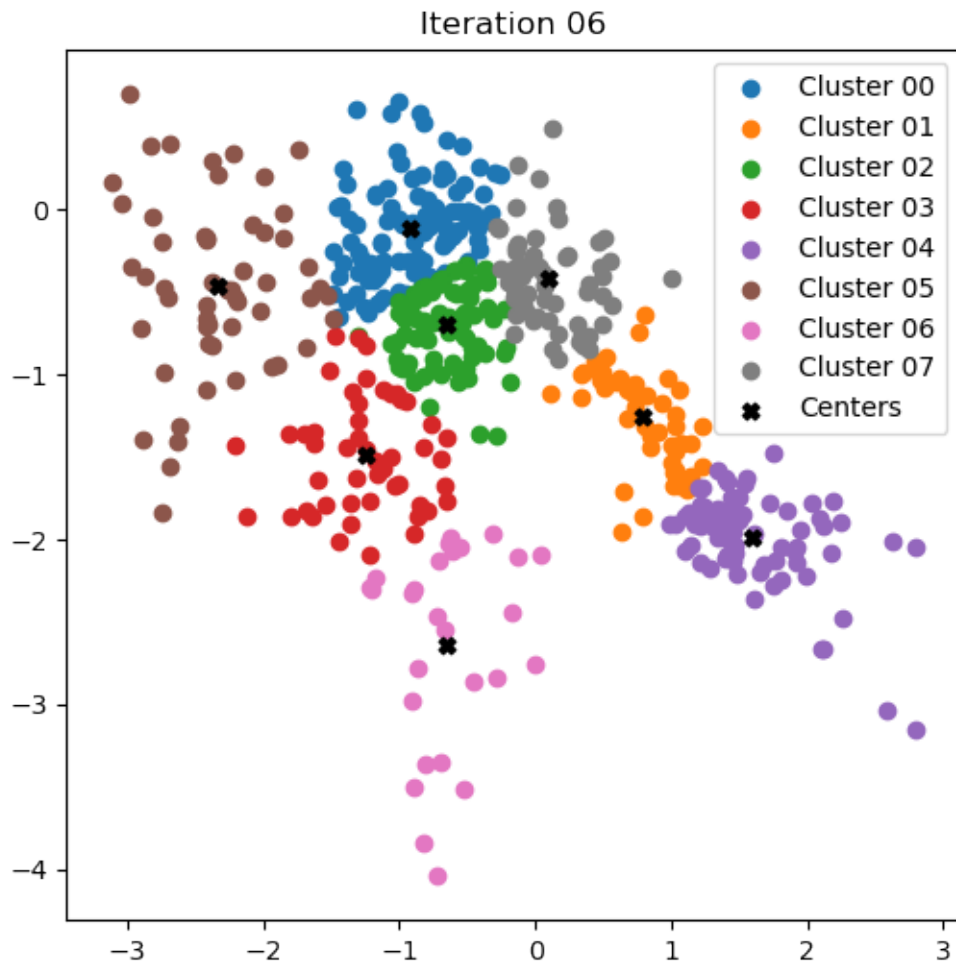
```

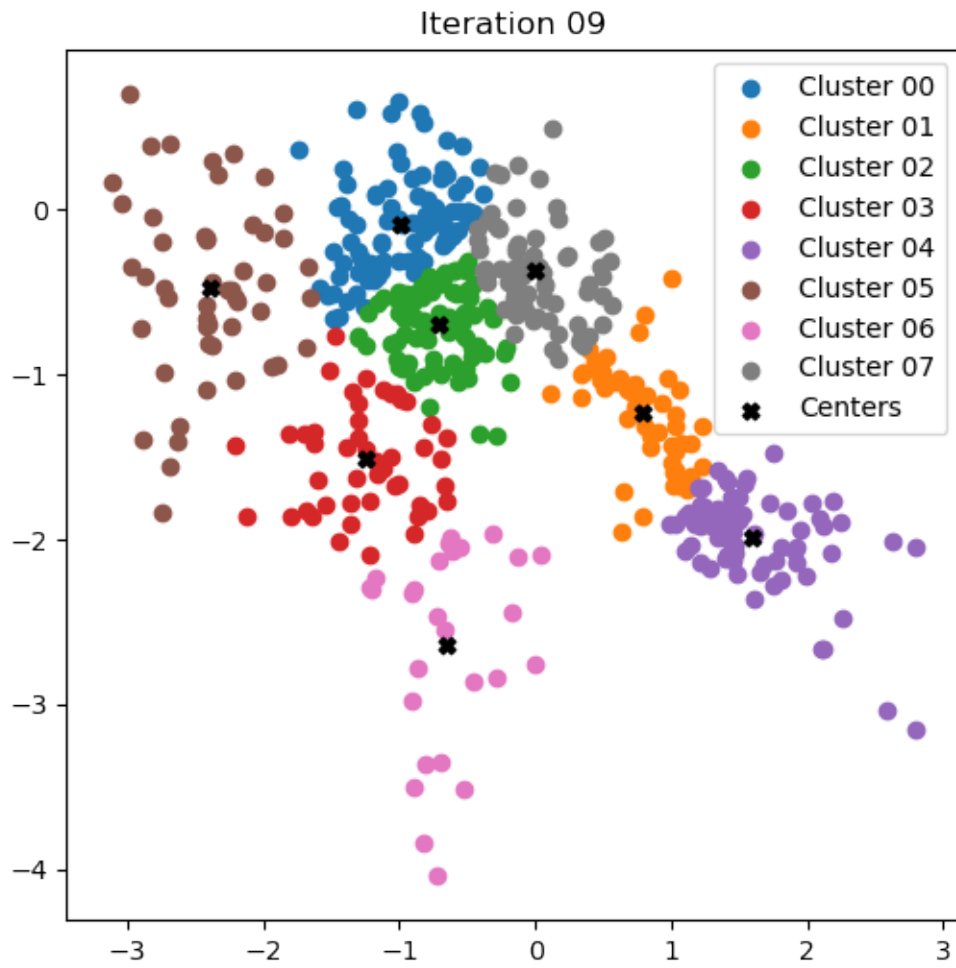
Took 17 iterations to converge

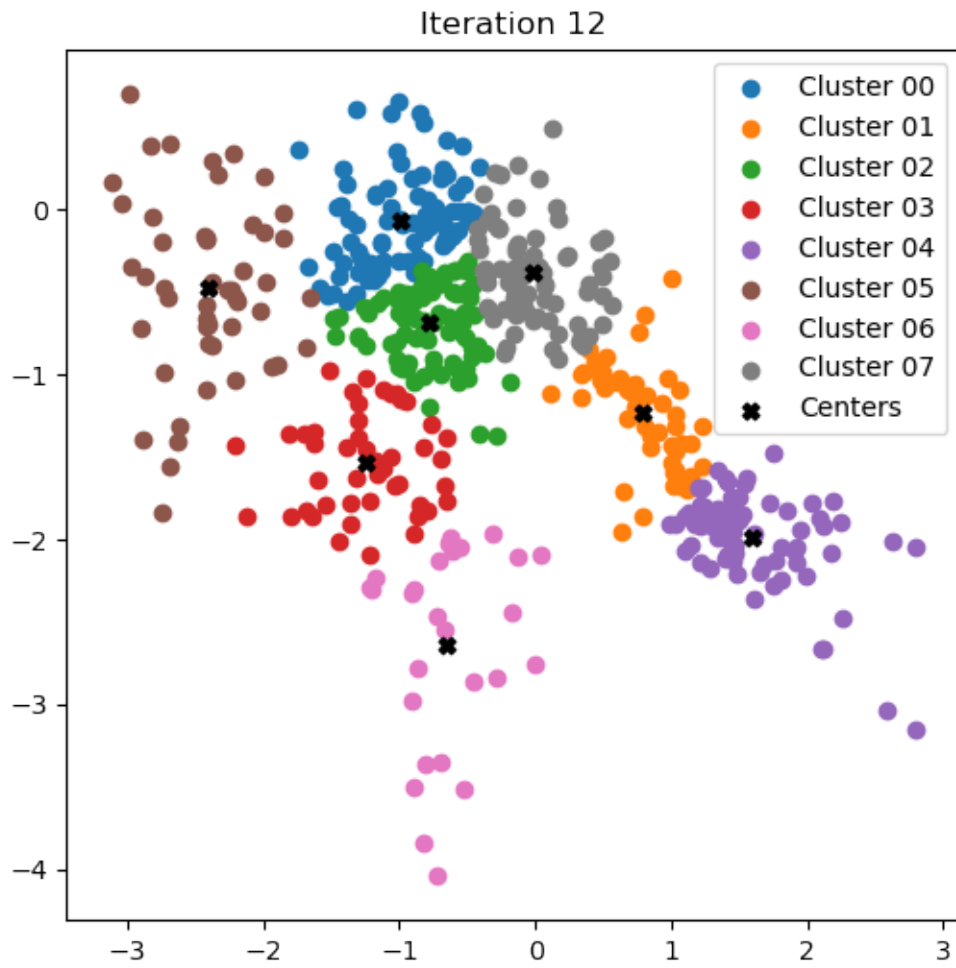


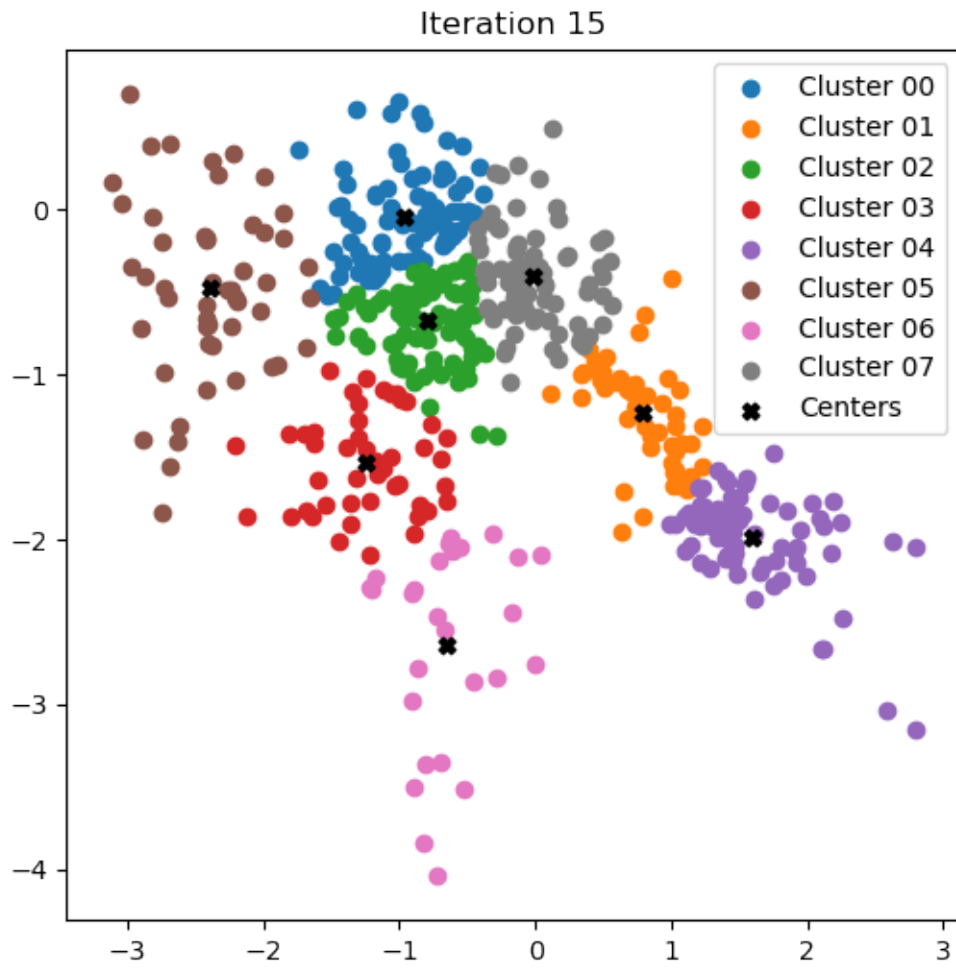


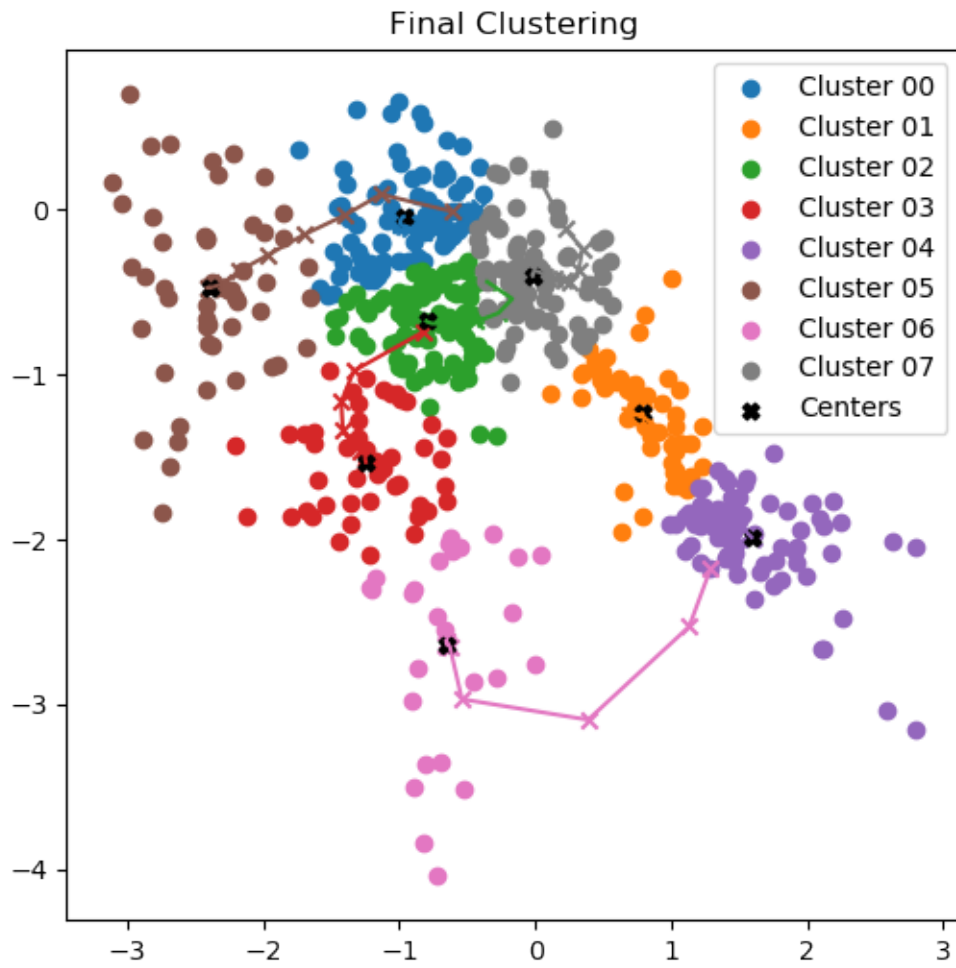


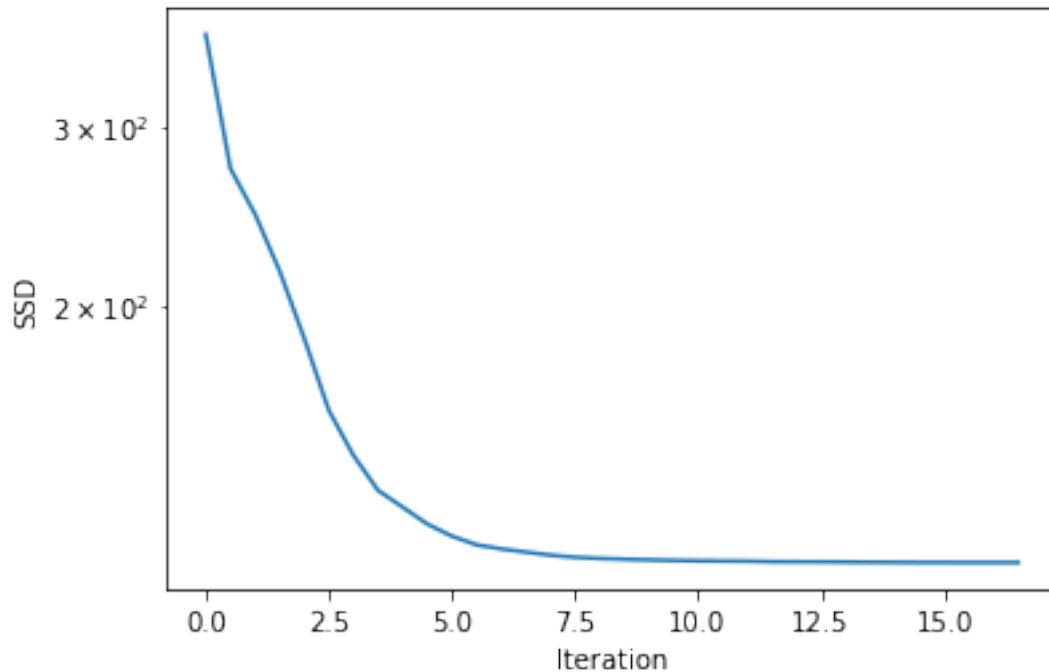












### 1.3 3.) Expectation Maximization for Gaussian Mixture Models (7 Points)

In the following we implement the Expectation Maximization (EM) Algorithm to fit a Gaussian Mixture Model (GMM) to data. We start with an implementation for the log density of a single Gaussian (take some time to compare this implementation with the one used in the first exercises)...

```
[5]: %matplotlib inline

import numpy as np
import matplotlib.pyplot as plt
from typing import Tuple

def gaussian_log_density(samples: np.ndarray, mean: np.ndarray, covariance: np.
    ↳ ndarray) -> np.ndarray:
    """
    Computes Log Density of samples under a Gaussian Distribution.
    We already saw an implementation of this in the first exercise and noted_
    ↳ there that this was not the "proper"
    way of doing it. Compare the two implementations.
    :param samples: samples to evaluate (shape: [N x dim])
    :param mean: Mean of the distribution (shape: [dim])
    :param covariance: Covariance of the distribution (shape: [dim x dim])
    :return: log N(x|mean, covariance) (shape: [N])
    """
    dim = mean.shape[0]
```

```

chol_covariance = np.linalg.cholesky(covariance)
# Efficient and stable way to compute the log determinant and squared term
→efficiently using the cholesky
logdet = 2 * np.sum(np.log(np.diagonal(chol_covariance) + 1e-25))
# (Actually, you would use scipy.linalg.solve_triangular but I wanted to
→spare you the hustle of setting
# up scipy)
chol_inv = np.linalg.inv(chol_covariance)
exp_term = np.sum(np.square((samples - mean) @ chol_inv.T), axis=-1)
return -0.5 * (dim * np.log(2 * np.pi) + logdet + exp_term)

```

... and some plotting functionality for 2D GMMs:

```

[6]: def visualize_2d_gmm(samples, weights, means, covs, title):
    """Visualizes the model and the samples"""
    plt.figure(figsize=[7,7])
    plt.title(title)
    plt.scatter(samples[:, 0], samples[:, 1], label="Samples", c=next(plt.gca().
→_get_lines.prop_cycler)['color'])

    for i in range(means.shape[0]):
        c = next(plt.gca().get_lines.prop_cycler)['color']

        (largest_eigval, smallest_eigval), eigvec = np.linalg.eig(covs[i])
        phi = -np.arctan2(eigvec[0, 1], eigvec[0, 0])

        plt.scatter(means[i, 0:1], means[i, 1:2], marker="x", c=c)

        a = 2.0 * np.sqrt(largest_eigval)
        b = 2.0 * np.sqrt(smallest_eigval)

        ellipse_x_r = a * np.cos(np.linspace(0, 2 * np.pi, num=200))
        ellipse_y_r = b * np.sin(np.linspace(0, 2 * np.pi, num=200))

        R = np.array([[np.cos(phi), np.sin(phi)], [-np.sin(phi), np.cos(phi)]])
        r_ellipse = np.array([ellipse_x_r, ellipse_y_r]).T @ R
        plt.plot(means[i, 0] + r_ellipse[:, 0], means[i, 1] + r_ellipse[:, 1],
→c=c,
                    label = ("Component %02d, Weight: %0.4f" % (i, weights[i])))
    plt.legend()

```

Now to the actual task: You need to implement 3 functions: - the log likelihood of a GMM for evaluation - the E-Step of the EM algorithm for GMMs - the M-Step of the EM algorithm for GMMs (for this one now for loops are allowed. Using them here will lead to point deduction)

All needed equations are in the slides

```

[7]: def gmm_log_likelihood(samples: np.ndarray, weights: np.ndarray, means: np.
    → ndarray, covariances: np.ndarray) -> float:
        """ Computes the Log Likelihood of samples given parameters of a GMM.
        :param samples: samples "x" to compute ess for (shape: [N, dim])
        :param weights: weights (i.e.,  $p(z)$ ) of old model (shape: [num_components])
        :param means: means of old components  $p(x/z)$  (shape: [num_components, dim])
        :param covariances: covariances of old components  $p(x/z)$  (shape:
    → [num_components, dim, dim])
        :return: log likelihood
        """
        #####
        # TODO Implement the log-likelihood for Gaussian Mixtures
        # DONE
        C = np.arange(weights.shape[0]) # number of Clusters -> array serving as
    → time saver
        N = samples.shape[0] # number of samples

        results = np.array([np.sum(gaussian_log_density(samples, means[c],
    → covariances[c]) + np.log(weights[c])) for c in C])

        return np.sum(results)
        #####

def e_step(samples: np.ndarray, weights: np.ndarray, means: np.ndarray,
    → covariances: np.ndarray) -> np.ndarray:
        """ E-Step of EM for fitting GMMs. Computes estimated sufficient statistics
    → (ess),  $p(z/x)$ , using the old model from
        the previous iteration. In the GMM case they are often referred to as
    → "responsibilities".
        :param samples: samples "x" to compute ess for (shape: [N, dim])
        :param weights: weights (i.e.,  $p(z)$ ) of old model (shape: [num_components])
        :param means: means of old components  $p(x/z)$  (shape: [num_components, dim])
        :param covariances: covariances of old components  $p(x/z)$  (shape:
    → [num_components, dim, dim])
        :return: Responsibilities  $p(z/x)$  (Shape: [N x num_components])
        """
        #####
        # TODO Implement the E-Step for EM for Gaussian Mixtrue Models.
        # DONE
        C = np.arange(means.shape[0]) # number of Clusters -> array serving as time
    → saver
        N = samples.shape[0] # number of samples

        # for loop for checking on positive definiteness of covariance matrices
        # can be deleted later

```



```

# for c in C:
#     print(covariances[c])
#     mvn(means[c], covariances[c])

# use scipy's "multivariate normal" to define Clusters
# may also use scipy's "norm"
clusters = np.array([mvn(means[c], covariances[c]) for c in C])
→ # len C

# implement "mixture component" and "mixture distribution" from lecture 6,
→ slide 41
# using mvn's "pdf" for probability density (function)
mix_comp = np.array([weights[c] * clusters[c].pdf(samples) for c in C])
→ # shape CxN
mix_distr = np.sum(mix_comp, axis=0)
→ # len C

# compute "responsibilities" as in lecture 6, slide 41
responsibilities = (mix_comp / mix_distr).T
→ # shape N x C

return responsibilities
#####

def m_step(samples: np.ndarray, responsibilities: np.ndarray) -> Tuple[np.
→ ndarray, np.ndarray, np.ndarray]:
    """ M-Step of EM for fitting GMMs. Computes new parameters given samples
    → and responsibilities p(z|x)
        :param samples: samples "x" to fit model to (shape: [N, dim])
        :param responsibilities: p(z|x) (Shape: [N x num_components]), as computed
    → by E-step
        :return: - new weights p(z) (shape [num_components])
                - new means of components p(x/z) (shape: [num_components, dim])
                - new covariances of components p(x/z) (shape: [num_components,
    → dim, dim]
        """
    #####
    # TODO: Implement the M-Step for EM for Gaussian Mixture models. You are
    → not allowed to use any for loops!
    # Hint: Writing it directly without for loops is hard, especially if you
    → are not experienced with broadcasting.
    # It's maybe easier to first implement it using for loops and then try
    → getting rid of them, one after another.
    # DONE
    C = responsibilities.shape[1]                # number of Clusters

```

```

N = samples.shape[0]                # number of samples
dim = samples.shape[1]              # dimension of Data Points

# print("Number of Clusters:", C, ", Number of Samples:", N)

# get summed "responsibility" for each cluster
# nominator of equation pi_k lecture 6, slide 43
m_c = np.sum(responsibilities, axis=0)
# print("Shape of m_c:", m_c.shape)          # len C

# calculate new weights / responsibility fraction that a data point
→ promotes to Cluster c
# final implementation of equation pi_k lecture 6, slide 43
pi_c = (m_c / np.sum(m_c)).reshape(C,1)
# print("Shape of pi_c:", pi_c.shape)        # len C

# calculate the new mean for each cluster as in lecture 6, slide 43
# considering all data points and their "responsibility" w.r.t. the cluster
→ respectively
X = samples.reshape(N,1,dim)          # reshaped samples
p = responsibilities.reshape(N,C,1)    # reshaped responsibilities
mu_c = np.sum(X*p, axis=0) / m_c.reshape(C,1)
# print("Shape of mu_c", mu_c.shape)

# calculate covariance without for loop
# calculate the new covariances for each cluster as in lecture 6, slide 43

# for c in range(C):
#     r = responsibilities[:,c].reshape(N,1)          # Nx1
#     diff = (samples.reshape(N,dim) - mu_c[c]).T    # N x dim - 1 x dim →
→ dim x N
#     cov_c[c] = np.dot(r.T*diff, diff.T) / m_c[c]    # 1 x N * dim x N . N x
→ dim → dim x dim

diff = samples*np.ones((C,N,dim)) - mu_c.reshape(C,1,dim)*np.ones((C,N,dim))
p    = responsibilities.T.reshape(C,N,1)*np.ones((C,N,dim))
dot  = np.tensordot(p*diff, diff, axes=([1],[1]))
ind  = np.arange(C)
cov_c = dot[ind, :, ind, :] / m_c.reshape(C,1,1)*np.ones((C,dim,dim))
# print("Shape of covariance:", cov_c.shape)

return pi_c, mu_c, cov_c
#####

```

We wrap out functions with the actual algorithm, iterating E and M step

```
[8]: def fit_gaussian_mixture(samples: np.ndarray, num_components: int, num_iters:
    ↪int = 30, vis_interval: int = 5):
    """Fits a Gaussian Mixture Model using the Expectation Maximization
    ↪Algorithm
    :param samples: Samples to fit the model to (shape: [N, dim]
    :param num_components: number of components of the GMM
    :param num_iters: number of iterations
    :param vis_interval: After how many iterations to generate the next plot
    :return: - final weights  $p(z)$  (shape [num_components])
             - final means of components  $p(x/z)$  (shape: [num_components, dim])
             - final covariances of components  $p(x/z)$  (shape: [num_components,
    ↪dim, dim]
             - log_likelihoods: log-likelihood of data under model after each
    ↪iteration (shape: [num_iters])
    """
    # Initialize Model: We initialize with means randomly picked from the data,
    ↪unit covariances and uniform
    # component weights. This works here but in general smarter initialization
    ↪techniques might be necessary, e.g.,
    # k-means
    initial_idx = np.random.choice(len(samples), num_components, replace=False)
    means = samples[initial_idx]
    covs = np.tile(np.eye(data.shape[-1])[None, ...], [num_components, 1, 1])
    weights = np.ones(num_components) / num_components

    # bookkeeping:
    log_likelihoods = np.zeros(num_iters)

    # iterate E and M Steps
    for i in range(num_iters):
        responsibilities = e_step(samples, weights, means, covs)
        weights, means, covs = m_step(samples, responsibilities)

        # Plotting
        if i % vis_interval == 0:
            visualize_2d_gmm(data, weights, means, covs, title="After Iteration
    ↪{:02d}".format(i))

        log_likelihoods[i] = gmm_log_likelihood(samples, weights, means, covs)
    ↪return weights, means, covs, log_likelihoods
```

Finally we load some data and run the algorithm. Feel free to play around with the parameters a bit.

```
[9]: ## ADAPTABLE PARAMETERS:

np.random.seed(0)
```

```

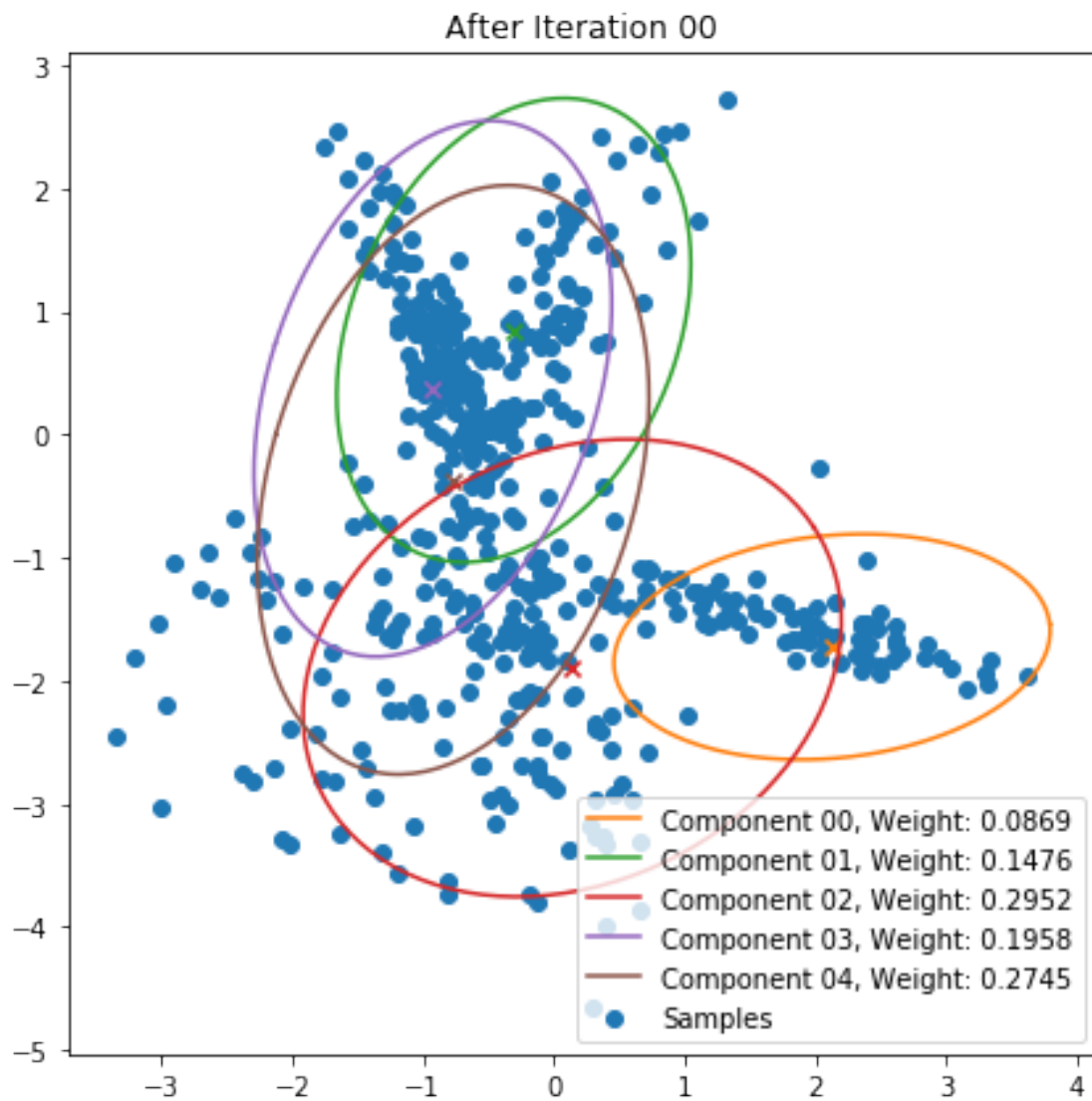
num_components = 5
num_iters = 30
vis_interval = 5

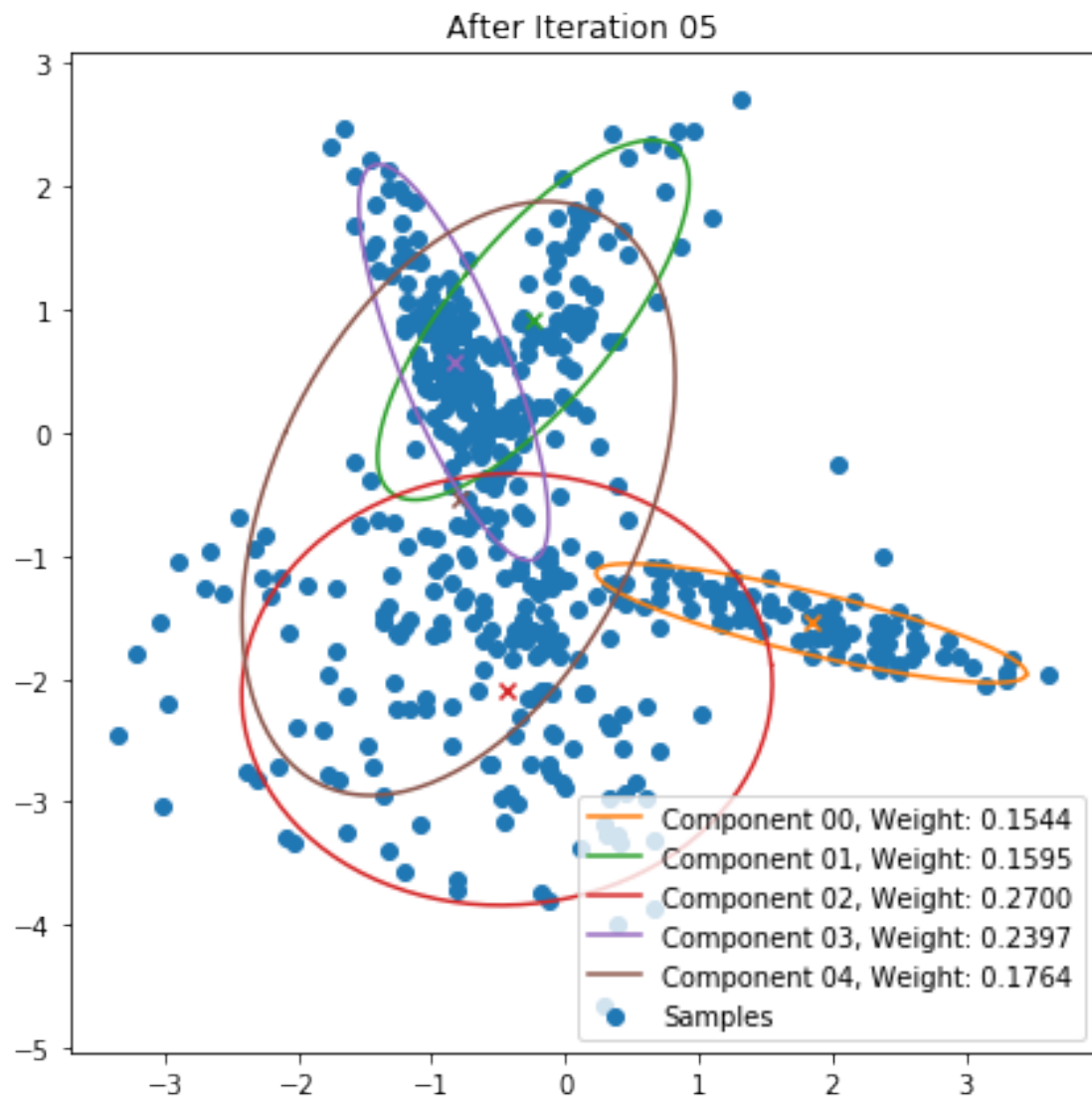
# CHOOSE A DATASET
# data = np.load("samples_1.npy")
data = np.load("samples_2.npy")
# data = np.load("samples_3.npy")
# data = np.load("samples_u.npy")

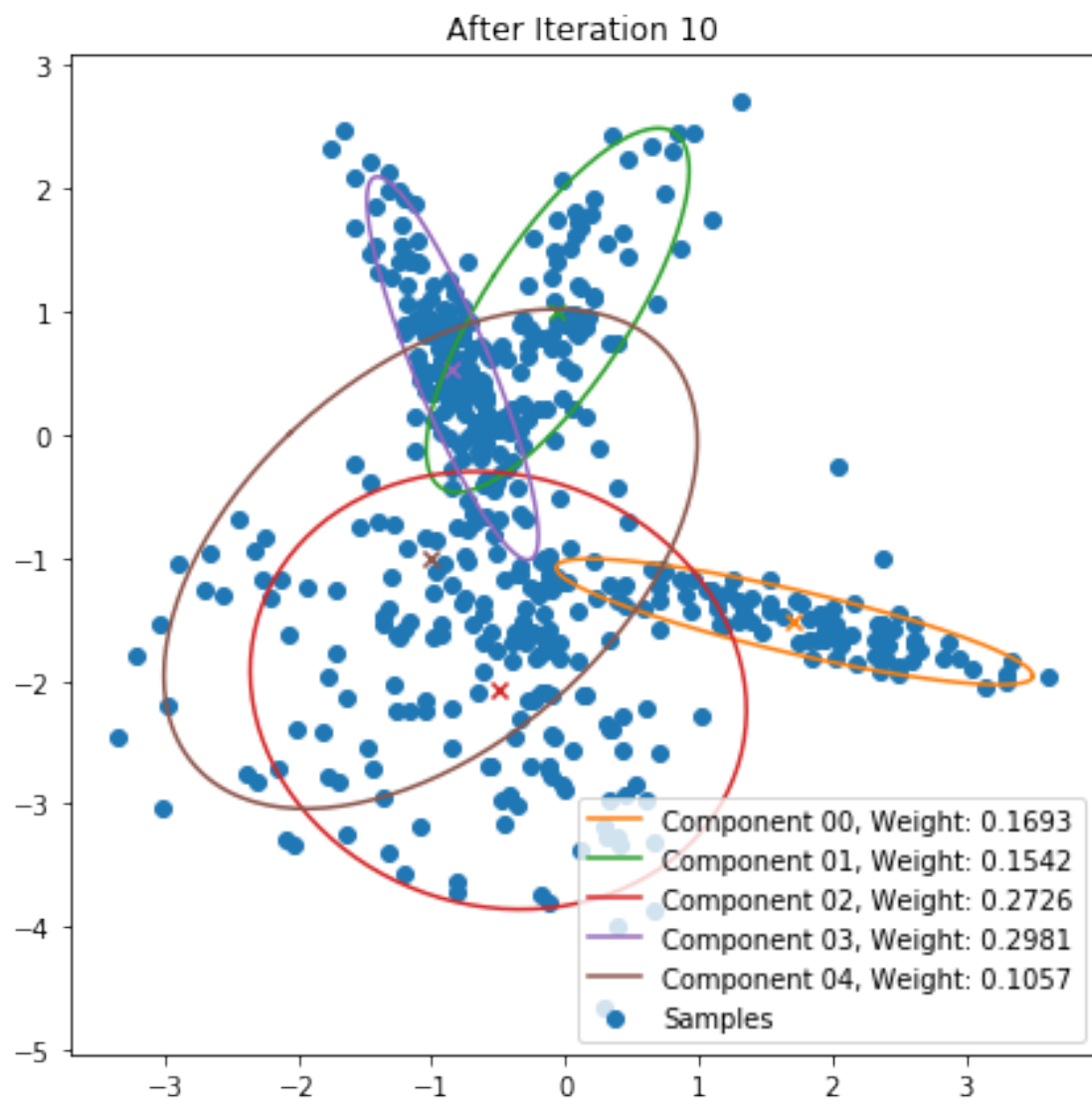
# running and plotting
final_weights, final_means, final_covariances, log_likelihoods = \
    fit_gaussian_mixture(data, num_components, num_iters, vis_interval)
visualize_2d_gmm(data, final_weights, final_means, final_covariances,
    ↪title="Final Model")

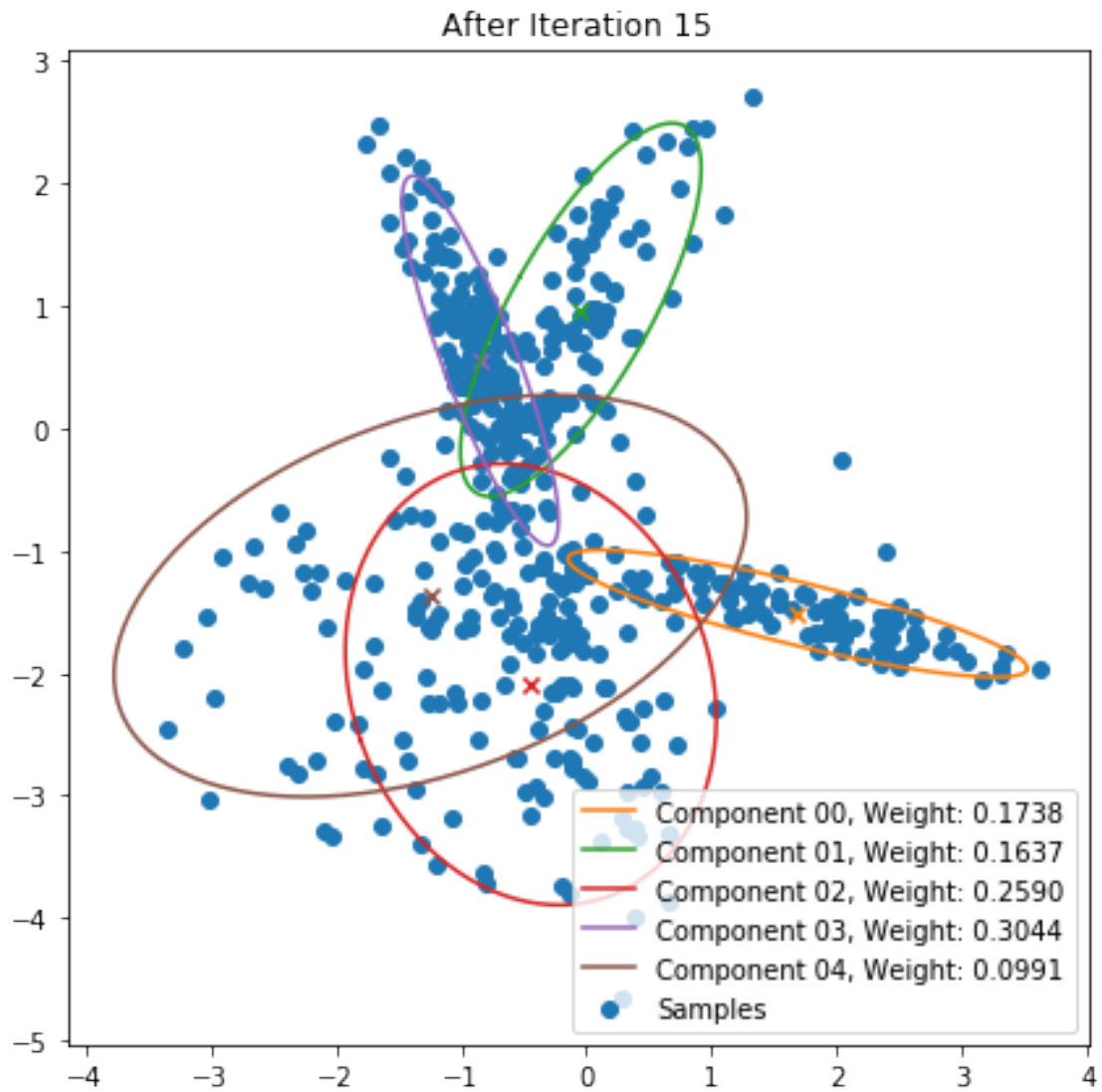
plt.figure()
plt.title("Log-Likelihoods over time")
plt.plot(log_likelihoods)
plt.xlabel("iteration")
plt.ylabel("log-likelihood")
plt.show()

```

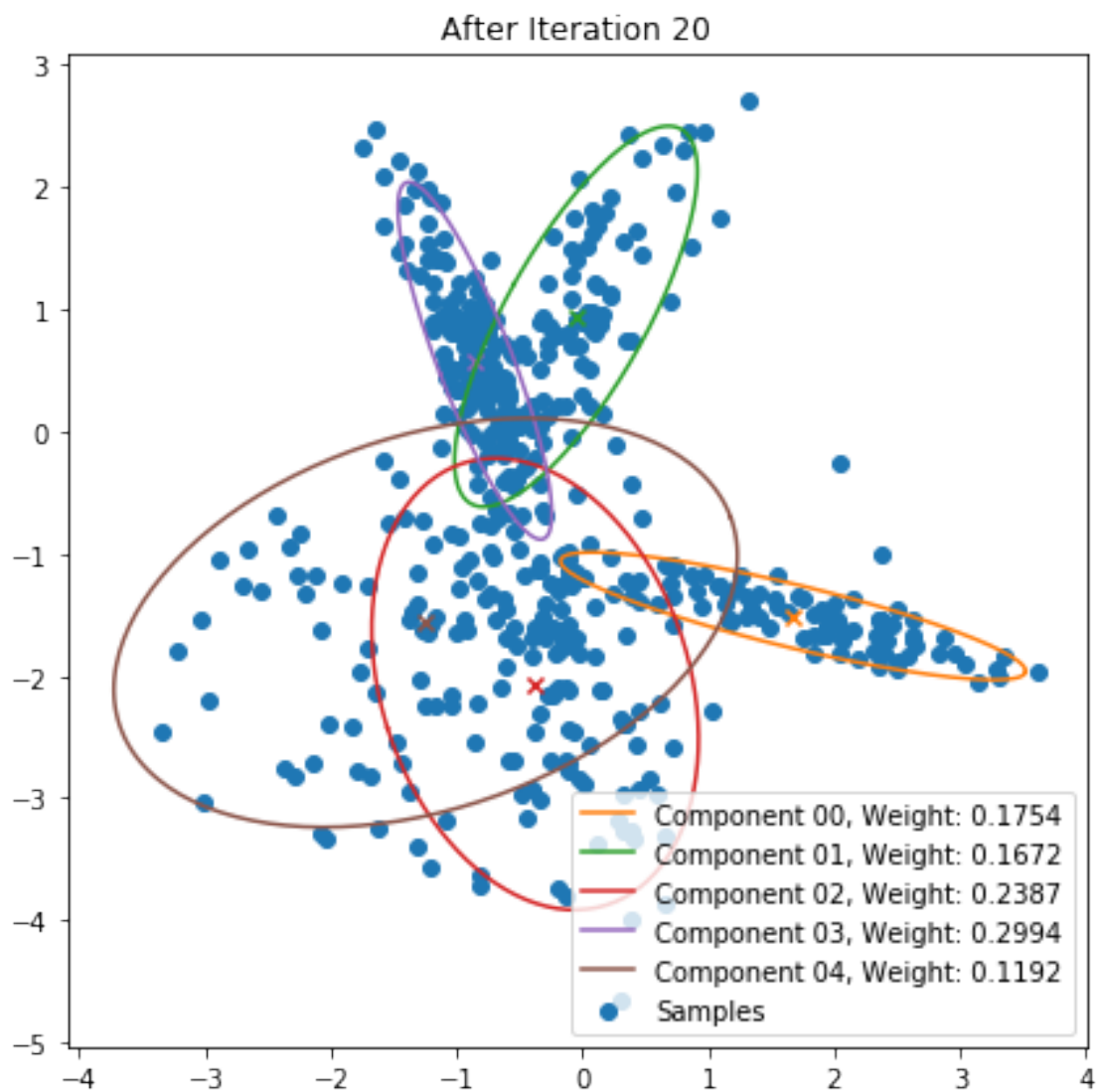


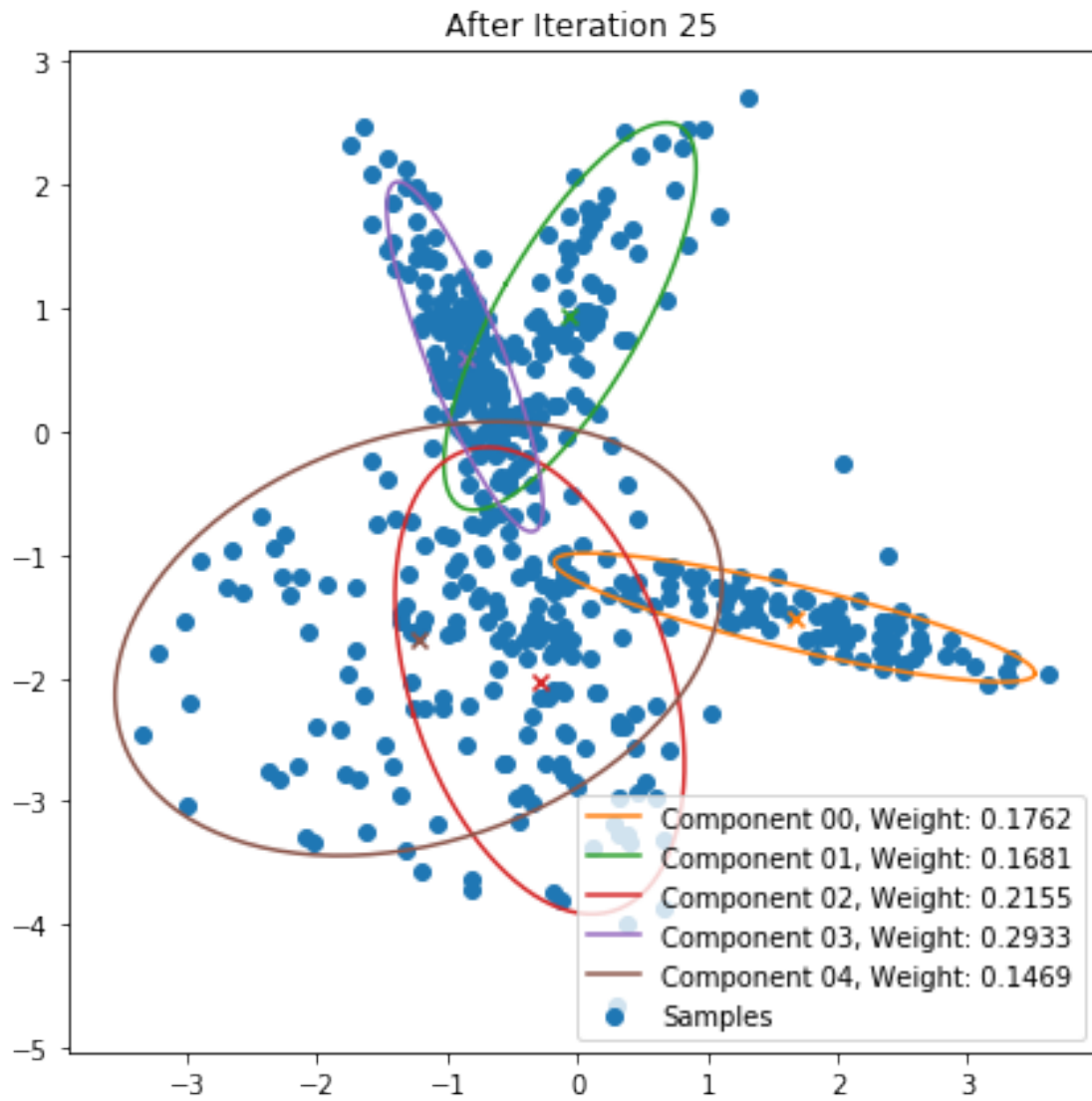


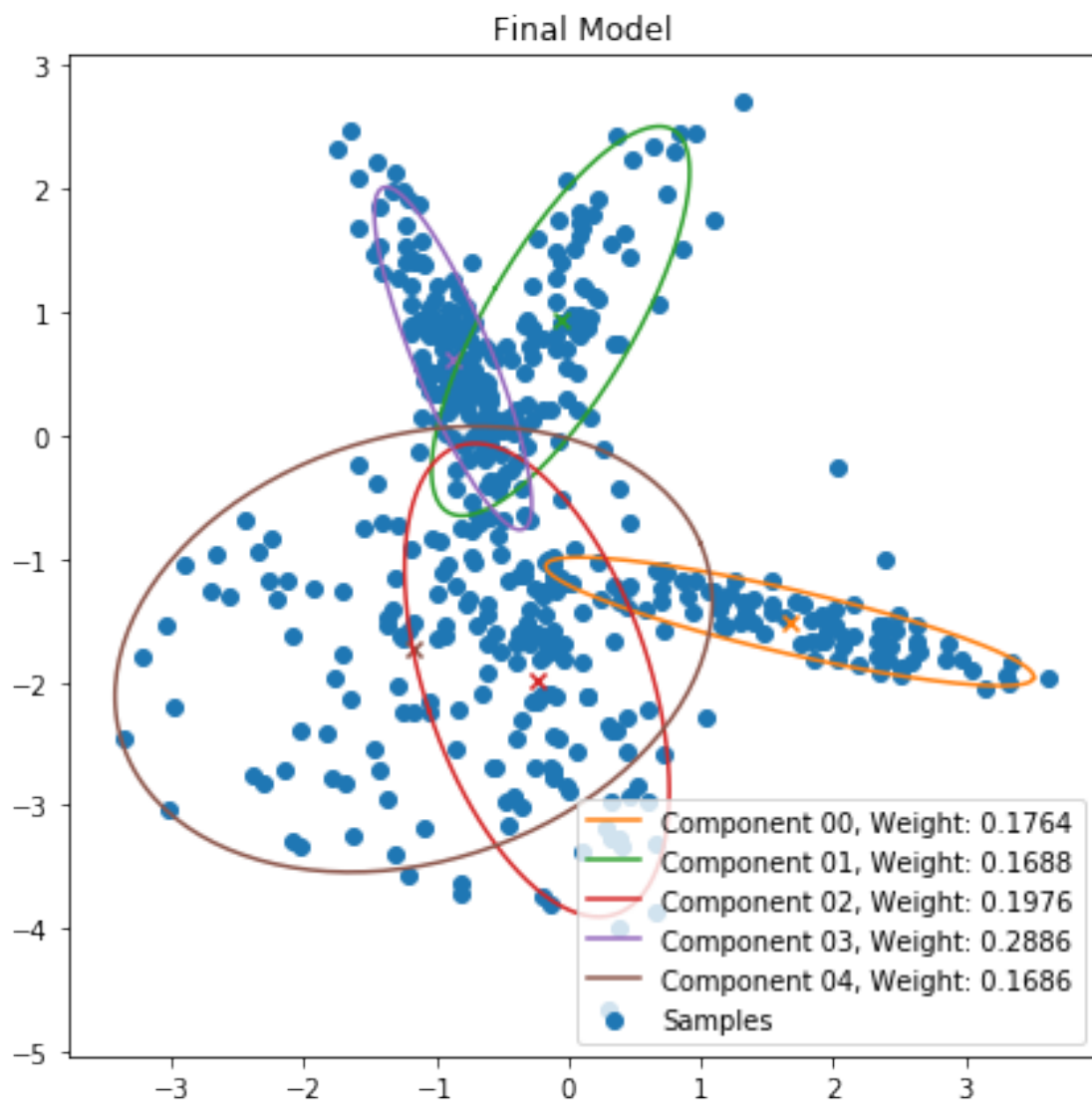


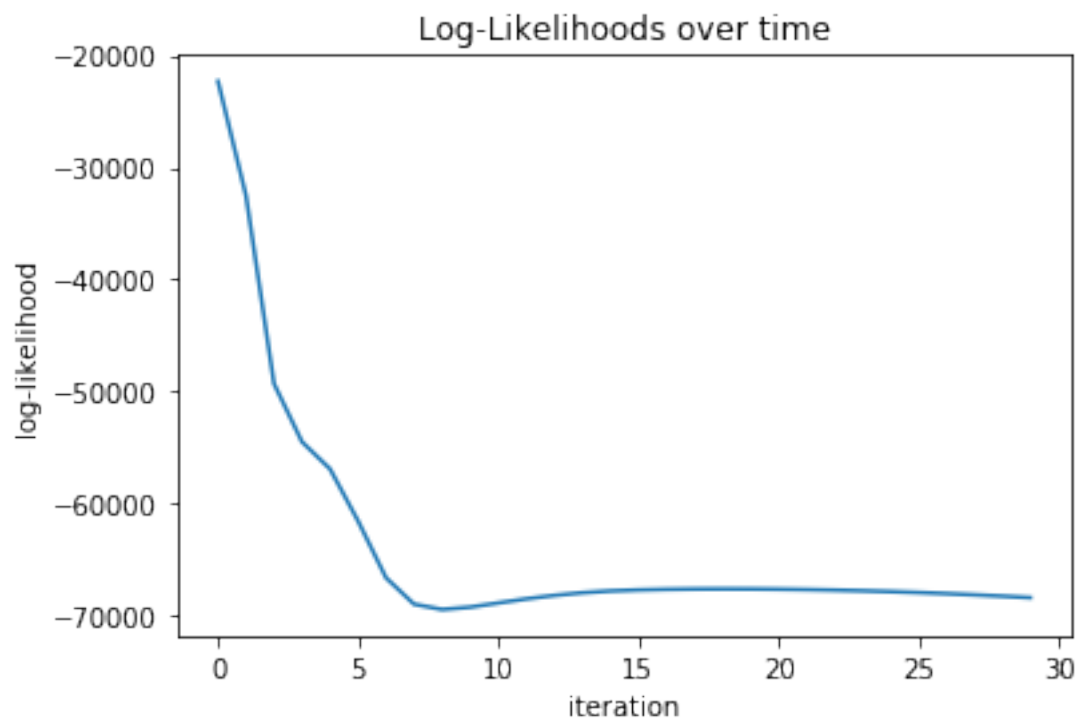












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