

exercise3

January 14, 2021

1 EXERCISE 3 - ML - Grundverfahren

1.1 1.) Constrained Optimization (6 Points)

You are given the following Optimization problem:

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

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} independent 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.

The Lagrangian is

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

Thus, the dual optimization problem is

$$\max_{\lambda} \min_{\mathbf{x}} L(\mathbf{x}, \lambda)$$

We thus find \mathbf{x}^*

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

Observe that, since \mathbf{M} is symmetric

$$\mathbf{x}^{*T} = \frac{1}{2}(\lambda\mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1}$$

And

$$\begin{aligned} \mathbf{x}^T \mathbf{M} \mathbf{x} + \mathbf{x}^T \mathbf{h} - \lambda(\mathbf{x}^T \mathbf{b} - c) &= \mathbf{x}^T \mathbf{M} \mathbf{x} + \mathbf{x}^T (\mathbf{h} - \lambda\mathbf{b}) - \lambda c \\ &= \mathbf{x}^T \mathbf{M} \mathbf{x} + \mathbf{x}^T \mathbf{h} - \lambda(\mathbf{x}^T \mathbf{b} - c) \\ &= \mathbf{x}^T \mathbf{M} \mathbf{x} + \mathbf{x}^T (-1)(\lambda\mathbf{b} - \mathbf{h}) - \lambda c \end{aligned}$$

Thus,

$$\begin{aligned}
 L(\mathbf{x}^*, \lambda) &= \frac{1}{2}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1} \mathbf{M} \frac{1}{2} \mathbf{M}^{-1}(\lambda \mathbf{b} - \mathbf{h}) - \frac{1}{2}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1}(\lambda \mathbf{b} - \mathbf{h}) - \lambda c \\
 &= \frac{1}{4}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1}(\lambda \mathbf{b} - \mathbf{h}) - \frac{1}{2}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1}(\lambda \mathbf{b} - \mathbf{h}) - \lambda c \\
 &= -\frac{1}{4}(\lambda \mathbf{b} - \mathbf{h})^T \mathbf{M}^{-1}(\lambda \mathbf{b} - \mathbf{h}) - \lambda c
 \end{aligned}$$

We know find λ^* using the chain rule

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

It follows that

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

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.

```
[17]: %matplotlib inline

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

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.) Adjust centers by taking the average over all points assigned to it

Implementing them will be your task for this exercise

```

[18]: 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
    #####

    deltas = [p - centers for p in data_points]
    dist = lambda vs : [np.sqrt(np.sum(v ** 2)) for v in vs]
    distances = [dist(vs) for vs in deltas]
    onehot = lambda v : [1 if n == np.amin(v) else 0 for n in v]
    onehots = np.array([onehot(v) for v in distances])
    return onehots

```

```
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
    #####
    avgs = np.zeros((assignments_one_hot.shape[1], data_points.shape[1]))
    counts = np.sum(assignments_one_hot, axis=0)
    for idx in range(0, data_points.shape[0]):
        avgs[assignments_one_hot[idx].argmax()] += data_points[idx];
    avgs = avgs / counts[:,None]
    return avgs
```

```
[19]: data_points = np.array([[1,2],[3,4],[5,6],[7,8]])
      centers = np.array([[1,2],[3,4],[5,6]])
      print(assignment_step(data_points, centers))
```

```
[[1 0 0]
 [0 1 0]
 [0 0 1]
 [0 0 1]]
```

```
[20]: data_points = np.array([[1,2],[3,4],[5,6],[7,8]])
      centers = np.array([[1,2],[3,4],[5,6]])
      onehots = assignment_step(data_points, centers)
      print(adjustment_step(data_points, onehots))
```

```
[[1. 2.]
 [3. 4.]
 [6. 7.]]
```

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

```
[21]: 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.

```

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

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

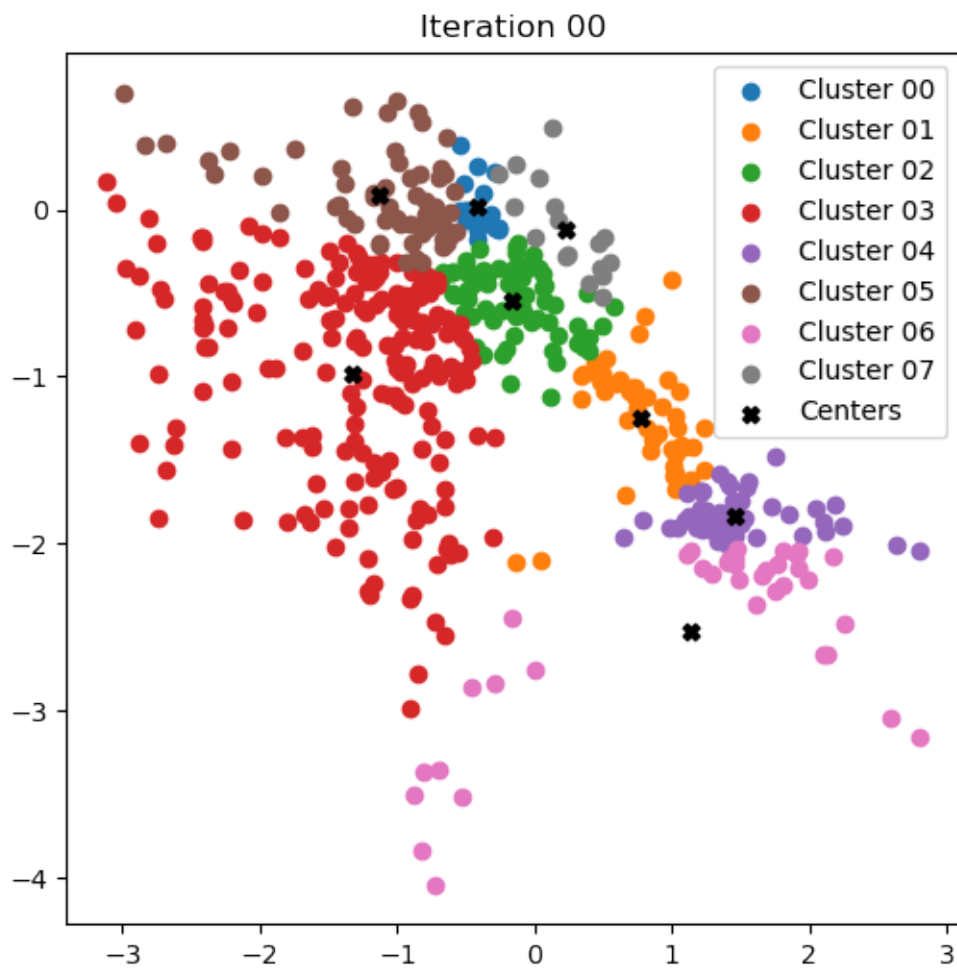
cluster_labels, centers, ssd_history, centers_history = k_means(data, k)

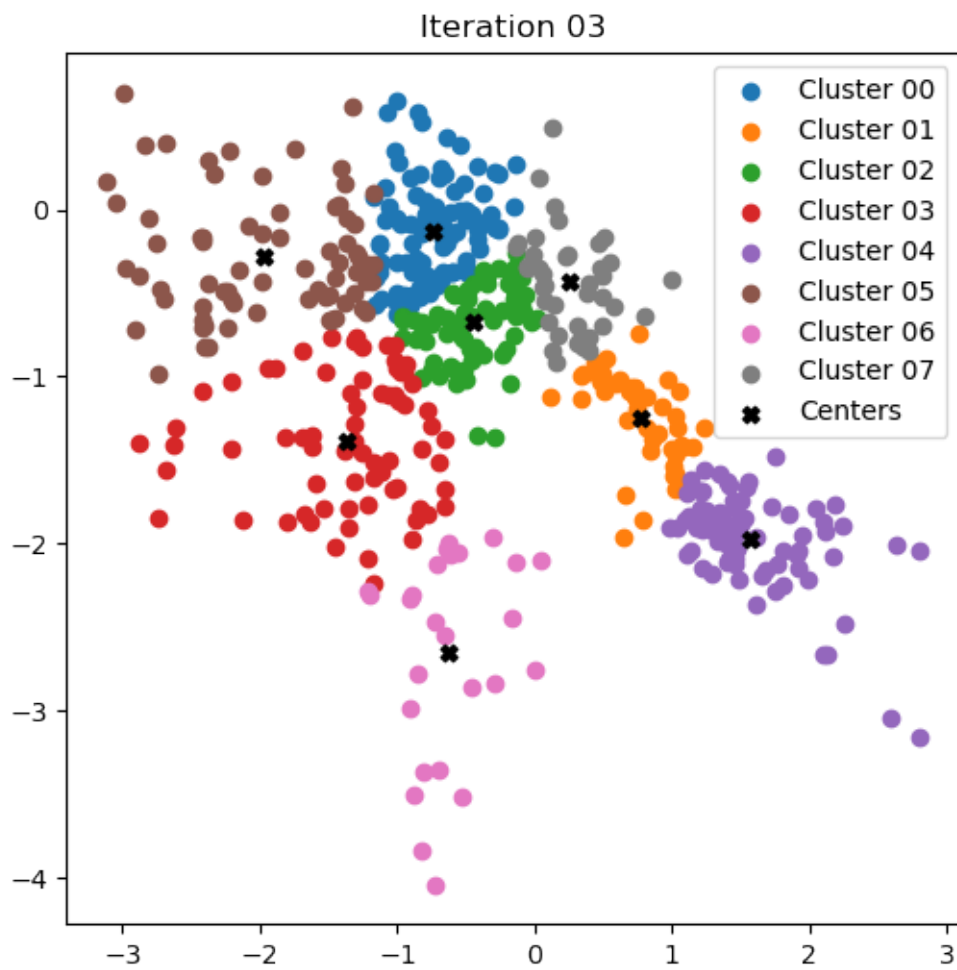
# plot final clustering with history of centers over iterations
visualize_2d_clustering(data, cluster_labels, centers, k=k,
→centers_history=centers_history, title="Final Clustering")

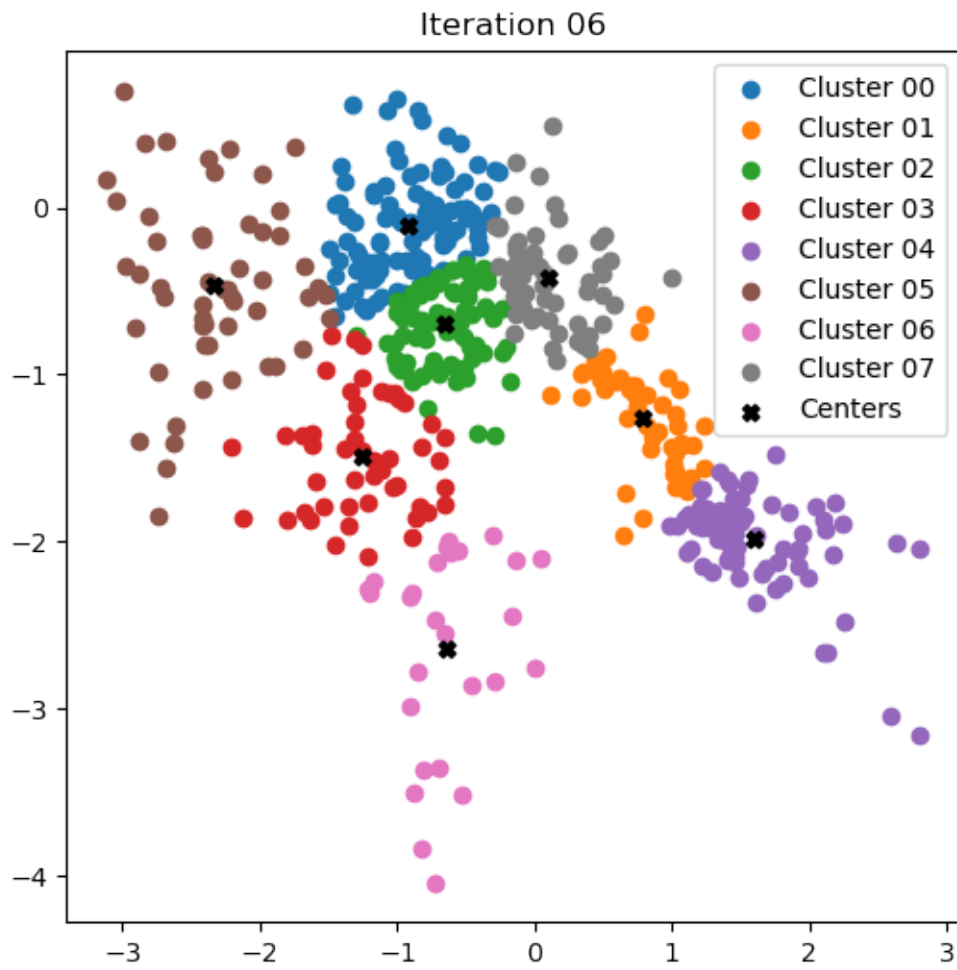
# plot SSD
plt.figure("SSD")
plt.semilogy(np.arange(start=0, stop=len(ssd_history) / 2, step=0.5),
→ssd_history)
plt.xlabel("Iteration")
plt.ylabel("SSD")
plt.show()

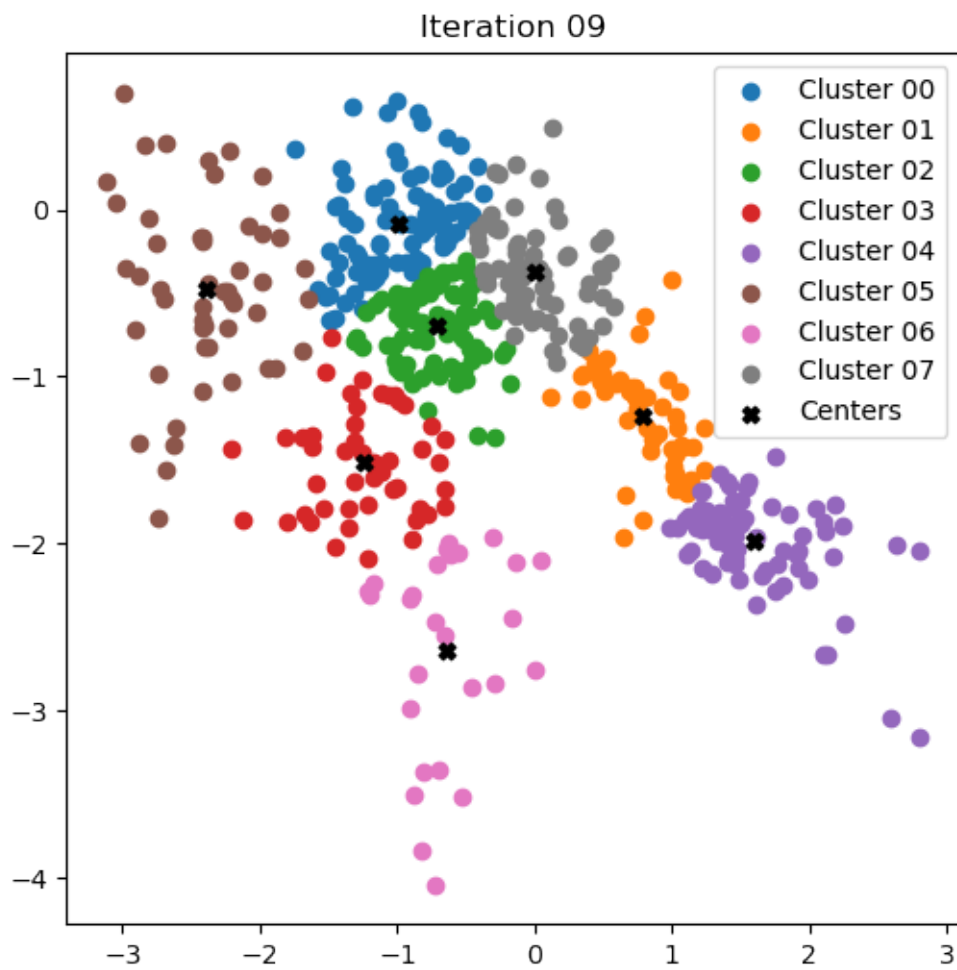
```

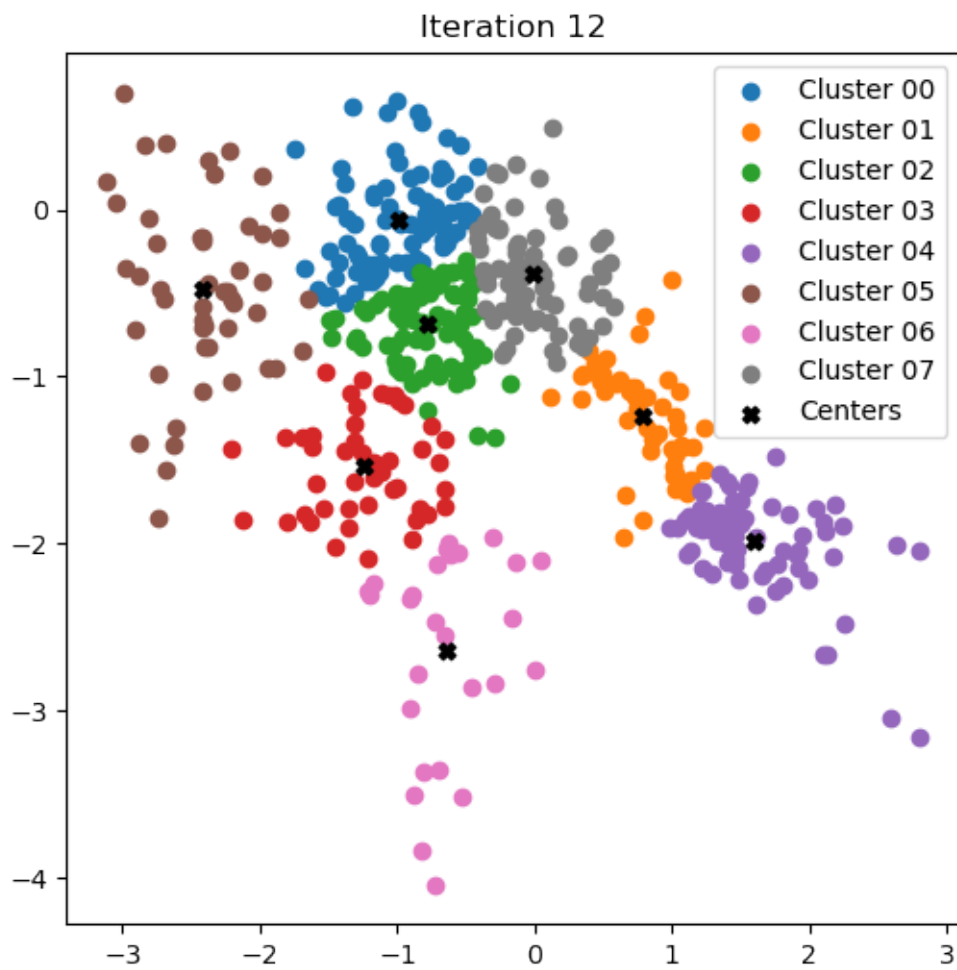
Took 17 iterations to converge

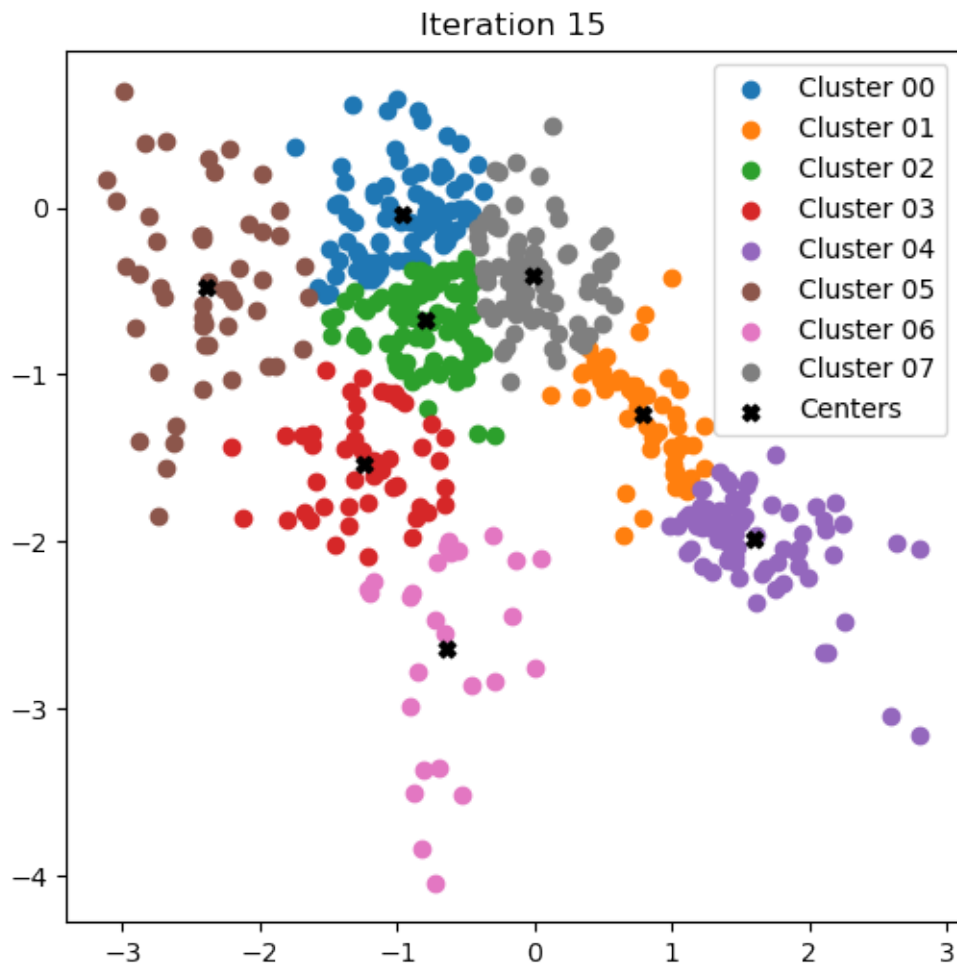


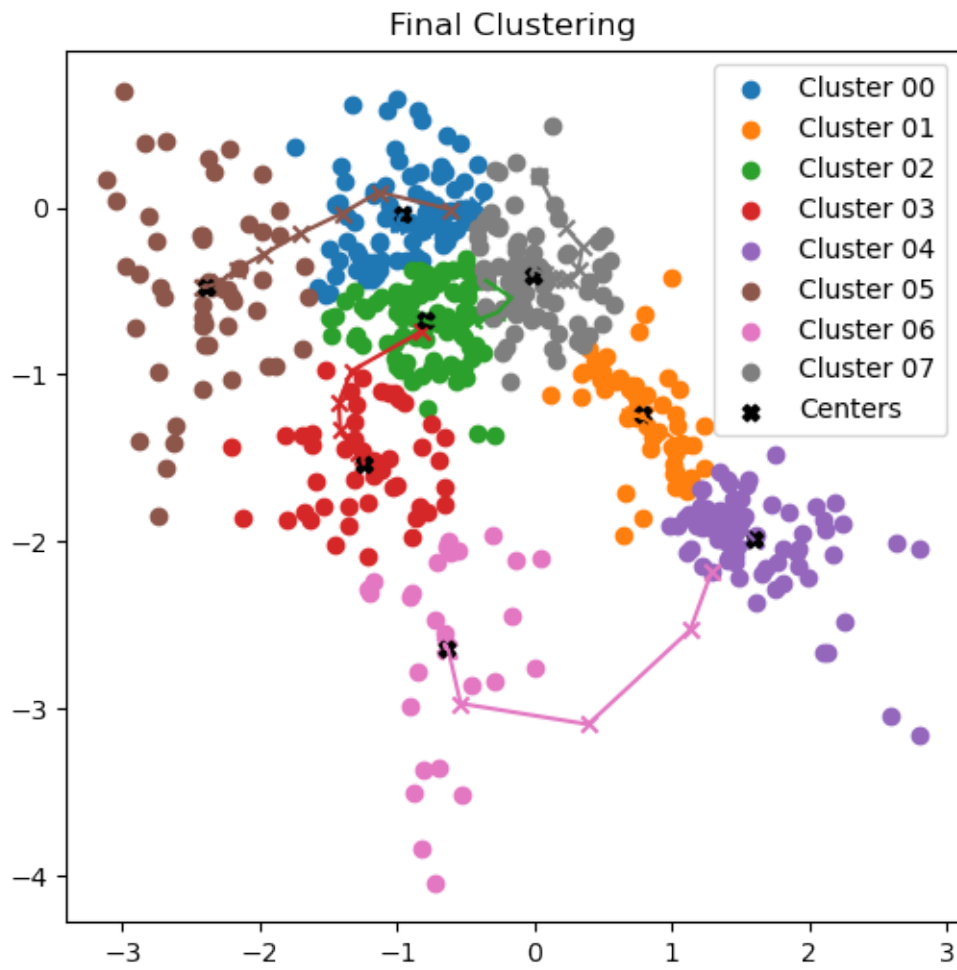


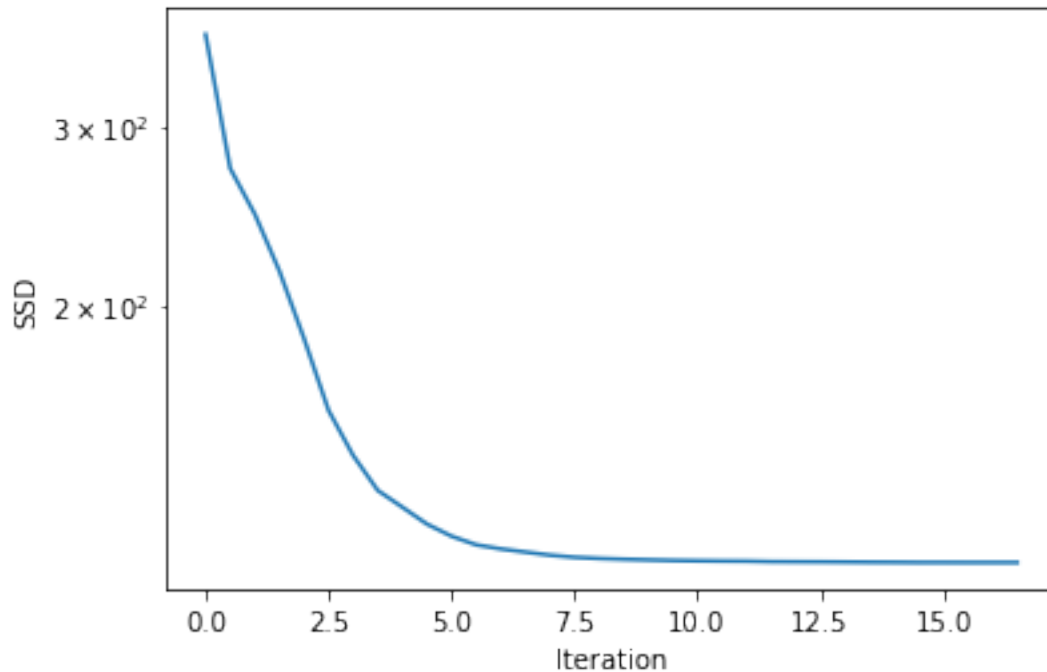












1.3 3.) Expectation Maximization for Gaussian Mixture Models (7 Points)

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)...

```
[23]: %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:

```

[24]: 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 {0:02d}, Weight: {0.4f}".format(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

```
[25]: 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
    #####
    N = samples.shape[0]
    num_components = weights.shape[0]
    probs = np.zeros((N, num_components))
    for idx in range(0, num_components):
        probs[:, idx] = weights[idx] * np.exp(gaussian_log_density(samples,
→ means[idx, :], covariances[idx, :, :]))

    return np.log(np.sum(probs))

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.
    #####
    # for each sample, how much does each component contribute

    num_components = weights.shape[0]
    R = np.array([np.exp(gaussian_log_density(samples, means[idx, :],
→ covariances[idx, :, :])) for idx in range(0, num_components)])
    R = np.multiply(R, weights[:, None]).T
    divisor = np.sum(R, axis=1)
```



```

return np.divide(R,divisor[:,None])

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.
        #####

        N = samples.shape[0]
        norm = N
        num_components = responsibilities.shape[1]
        dim = samples.shape[1]

        sum_qi= np.sum(responsibilities,axis=0)
        weights = sum_qi/norm
        means = np.divide((responsibilities.T@samples), sum_qi[:,None])

        vecs = samples[:,None,:] - means

        covs = np.einsum('...j,...k->...jk',vecs,vecs)
        covs = (covs.reshape(N,num_components,dim ** 2) * responsibilities[:,
→ None]).reshape(N,num_components,dim,dim)
        cov_sums = np.sum(covs, axis=0)
        cov_sums = cov_sums.reshape(num_components, dim ** 2) / sum_qi[:,None]
        cov_sums = cov_sums.reshape(num_components, dim, dim)
        return weights,means,cov_sums

```

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

```
[27]: 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.

```
[28]: ## 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()

```

