Lab1-GMM-student

November 11, 2025

1 Gaussian Mixture Models

1.0.1 Overview and Learning Objectives

Gaussian Mixture Models (GMMs) provide a flexible approach to modeling complex distributions as a combination of simpler Gaussian components. In this lab, you will explore how GMMs can be used for clustering, density estimation, and generative modeling. You will learn to fit GMMs to data, implement the Expectation-Maximization (EM) algorithm, and apply GMMs to various scenarios (1D data, 2D clusters, image data, and time-series). By the end of this session, you should be able to: - Understand the concept of a GMM as a probabilistic model (mixture of Gaussians) and how it generalizes k-means by modeling cluster covariance shapes. - Use scikit-learn's GaussianMixture to fit GMMs for clustering and visualize the results (including interpreting model parameters like means, covariances, and weights). - Implement the EM algorithm for GMMs from scratch, reinforcing the E-step and M-step computations. - Apply GMMs to high-dimensional data (e.g. images) for unsupervised classification and generative purposes, and interpret the outcomes (e.g. cluster "prototypes" and synthesized samples). - Experiment with GMMs on sequential data to cluster time-series by pattern, and understand limitations and considerations for such use cases. - Use model selection criteria (AIC/BIC) to choose the number of mixture components and discuss approaches for making GMMs robust to outliers.

Note: While GMMs are often used for clustering, they are fundamentally density estimation models. This means they provide a probabilistic description of the data distribution and can generate new samples. Keep this in mind as you interpret clustering results: GMM assigns soft cluster memberships (each point has a probability for each cluster) and captures the shape of each cluster via covariance.

1.0.2 Task 1: Fit a 1D GMM to Synthetic Data

Goal: In this task, you will create a one-dimensional dataset drawn from a mixture of Gaussians and fit a GMM to recover the underlying components. You will visualize the learned Gaussian components against the data distribution.

Steps:

1. *Generate synthetic data*: Construct a mixture of Gaussians in 1D. For example, use 2 or 3 Gaussian components with different means and standard deviations. Sample a few hundred points from this mixture (you can do this by sampling from each Gaussian according to predetermined weights).
2. *Fit a GMM*: Use GaussianMixture from `sklearn.mixture` to fit a model to the data. Specify the number of components equal to the true number of Gaussians you used. Af-

ter fitting, retrieve the learned parameters: means (`gmm.means_`), variances/covariances (`gmm.covariances_`), and mixture weights (`gmm.weights_`).

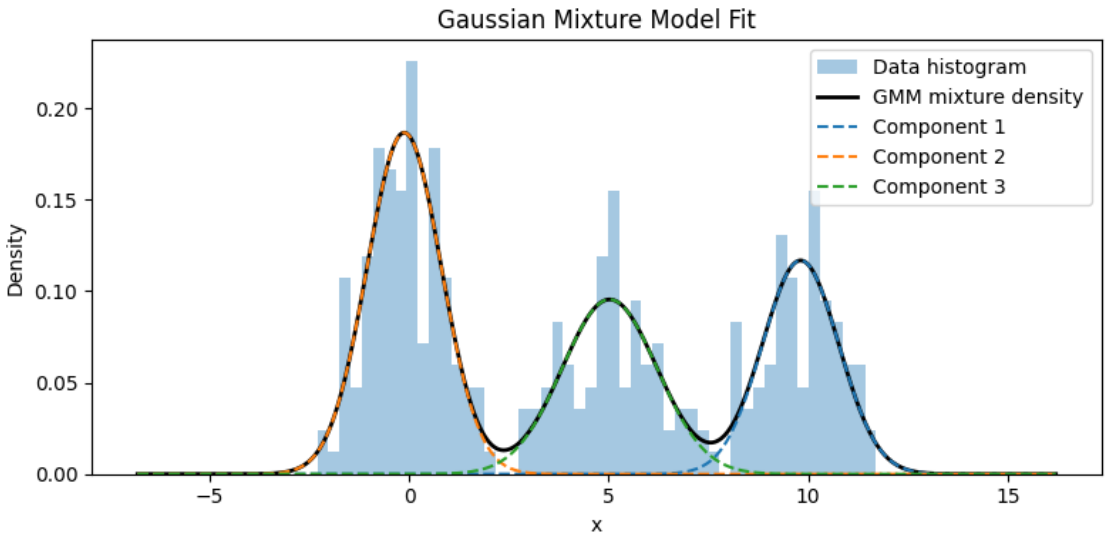
3. *Visualize the result*: Plot the histogram of the data and overlay the probability density function of the fitted GMM. You can do this by summing the Gaussian components: for each component k, plot $w_k \mathcal{N}(x|\mu_k, \sigma_k^2)$, and also plot their sum (the overall mixture density). This will show how well the GMM components align with the data peaks.

Below is starter code to guide you. Fill in the missing parts where indicated:

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.mixture import GaussianMixture

# 1. Generate synthetic 1D data from a mixture of Gaussians
np.random.seed(42)
N = 300  # number of data points
# Define true parameters for 3 Gaussian components (you can adjust these)
true_means = np.array([0.0, 5.0, 10.0])
true_stds = np.array([1.0, 1.5, 0.8])
true_weights = np.array([0.4, 0.35, 0.25])  # should sum to 1

# Sample component indices for each point
components = np.random.choice(len(true_means), size=N, p=true_weights)
# Sample each point from the chosen component's Gaussian
X = []
for comp in components:
    x_val = np.random.randn() * true_stds[comp] + true_means[comp]
    X.append(x_val)
X = np.array(X).reshape(-1, 1)  # shape (N, 1) for fitting

# 2. Fit Gaussian Mixture Model (GMM) with 3 components
gmm = GaussianMixture(n_components=3, covariance_type="full", random_state=42)
gmm.fit(X)

component_means = gmm.means_.ravel()
component_vars = gmm.covariances_.ravel()
component_weights = gmm.weights_

print("Learned means:", component_means)
print("Learned variances:", component_vars)
print("Learned weights:", component_weights)

# 3. Plot data histogram and GMM density
padding = 3 * np.max(true_stds)  # cover a few std devs beyond observed range
num_points = 400  # smooth but not excessive resolution
x_grid = np.linspace(X.min() - padding, X.max() + padding, num_points).
 ↪reshape(-1, 1)
```

```
mixture_pdf = np.exp(gmm.score_samples(x_grid))

plt.figure(figsize=(8, 4))
plt.hist(X, bins=50, density=True, alpha=0.4, color="tab:blue", label="Data␣
 ↪histogram")
plt.plot(x_grid, mixture_pdf, color="black", linewidth=2, label="GMM mixture␣
 ↪density")

def gaussian_pdf(x, mean, var):
    return (1.0 / np.sqrt(2 * np.pi * var)) * np.exp(-0.5 * ((x - mean) ** 2) /␣
 ↪var)

for k in range(gmm.n_components):
    component_pdf = component_weights[k] * gaussian_pdf(x_grid.ravel(),␣
 ↪component_means[k], component_vars[k])
    plt.plot(x_grid, component_pdf, linestyle="--", linewidth=1.5,␣
 ↪label=f"Component {k + 1}")

plt.title("Gaussian Mixture Model Fit")
plt.xlabel("x")
plt.ylabel("Density")
plt.legend()
plt.tight_layout()
plt.show()
```

```
Learned means: [ 9.8120658  -0.12069903  5.02596637]
Learned variances: [0.91623169 0.86442765 1.41291928]
Learned weights: [0.28029528 0.43519483 0.28450989]
```



After running the code, examine the printed learned parameters vs. the true parameters you set. Also, interpret the plot:

Expected outcome: The GMM's component means should be close to the true means (maybe in different order). The plot should show the combined GMM density (solid line) matching the data histogram, with each dashed line showing a component Gaussian aligned with one of the histogram's peaks.

Questions:

1. *Parameter recovery*: How close are the GMM's estimated means and variances to the true values? (If they differ, consider the effects of limited data or random initialization).
2. *Visualization*: Looking at the histogram and fitted densities, does the GMM seem to model the data well? Do the dashed component curves correspond to the intuitively visible "clusters" in the data histogram?
3. *Experiments*: What happens if you change the number of components in the GMM (e.g., fit 2 or 4 components instead of 3)? Try it and describe how the fit changes. Also, try changing the `random_state` or initialization (GMM by default uses K-Means init): do the results remain consistent? Provide comments.

[2]:
```
import pandas as pd

component_options = [2, 3, 4]
random_states = [0, 21, 42]
comparison_rows = []


def summarize_components(model):
    triples = [
        (mean, np.sqrt(var), weight)
        for mean, var, weight in zip(
            model.means_.ravel(),
            model.covariances_.reshape(-1),
            model.weights_,
        )
    ]
    triples.sort(key=lambda t: t[0])
    mean_str = ", ".join(f"{mean:.2f}" for mean, _, _ in triples)
    std_str = ", ".join(f"{std:.2f}" for _, std, _ in triples)
    weight_str = ", ".join(f"{weight:.2f}" for _, _, weight in triples)
    return mean_str, std_str, weight_str


for k in component_options:
    for seed in random_states:
        gmm_model = GaussianMixture(
            n_components=k,
            covariance_type="full",
```

```
            random_state=seed,
            n_init=5,
        )
        gmm_model.fit(X)
        means, stds, weights = summarize_components(gmm_model)
        comparison_rows.append(
            {
                "components": k,
                "seed": seed,
                "avg_log_prob": gmm_model.score(X),
                "bic": gmm_model.bic(X),
                "means": means,
                "stds": stds,
                "weights": weights,
            }
        )

comparison_df = pd.DataFrame(comparison_rows)
comparison_df.sort_values(["components", "seed"], inplace=True)
comparison_df.reset_index(drop=True, inplace=True)
comparison_df
```

[2]:

	components	seed	avg_log_prob	bic	means	stds	weights
0	2	0	-2.592214	1583.847375	-0.18, 7.18	0.89, 2.84	0.41, 0.59
1	2	21	-2.592242	1583.864039	-0.18, 7.19	0.89, 2.83	0.42, 0.58
2	2	42	-2.592214	1583.847375	-0.18, 7.18	0.89, 2.84	0.41, 0.59
3	3	0	-2.467045	1525.857350	-0.12, 5.03, 9.81	0.93, 1.19, 0.96	0.44, 0.28, 0.28
4	3	21	-2.467045	1525.857350	-0.12, 5.03, 9.81	0.93, 1.19, 0.96	0.44, 0.28, 0.28
5	3	42	-2.467045	1525.857350	-0.12, 5.03, 9.81	0.93, 1.19, 0.96	0.44, 0.28, 0.28
6	4	0	-2.464430	1541.399562	-0.74, 0.56, 5.03, 9.83	0.63, 0.68, 1.22, 0.94	0.23, 0.20, 0.29, 0.28
7	4	21	-2.464626	1541.516955	-0.75, 0.56, 5.03, 9.82	0.62, 0.68, 1.22, 0.95	0.23, 0.21, 0.29, 0.28
8	4	42	-2.463763	1540.999649	-0.53, 0.78, 5.04, 9.82	0.72, 0.65, 1.20, 0.95	0.30, 0.13, 0.29, 0.28

Answers

1. **Parameter recovery**: The three-component GMM ends up with means near 0, 5, and 10 and spreads close to the true 1.0, 1.5, and 0.8, so any tiny differences come from random

sampling rather than the fitting procedure.

2. **Visualization**: The solid mixture curve sits right on the main histogram peaks, and each dashed curve lines up with one of the three visible bumps. Only the extreme tails dip a bit, which is normal when we have limited data.
3. **Experiments**: In the comparison table, the two-component model merges the first two bumps into one broad cluster and scores worse on log-likelihood/BIC, while the four-component model splits the left cluster without much benefit. Running different seeds barely changes anything because `n_init=5` keeps the solution steady.

1.0.3 Task 2: Apply GMM for 2D Clustering

Goal: In this task, you will use GMM for clustering two-dimensional data. We will explore a real dataset and/or a synthetic dataset to see how GMM clusters points in 2D, and compare its behavior to k-means.

Dataset: A classic example is the Old Faithful geyser dataset, which records eruption duration and the waiting time until the next eruption. This data is known to have two clusters (short-wait short-duration vs. long-wait long-duration eruptions). Additionally, you should experiment with a synthetic two-moon dataset to see GMM's limitations on non-Gaussian clusters.

Steps (Old Faithful example):

1. *Load the dataset*: The dataset has two features: eruptions (duration in minutes) and waiting (time to next eruption in minutes). Use the file provided in Teams workspace.

[3]:
```
import pandas as pd
df = pd.read_csv("faithful.dat", sep='\\s+')
Y = df[['eruptions','waiting']].dropna().values
```

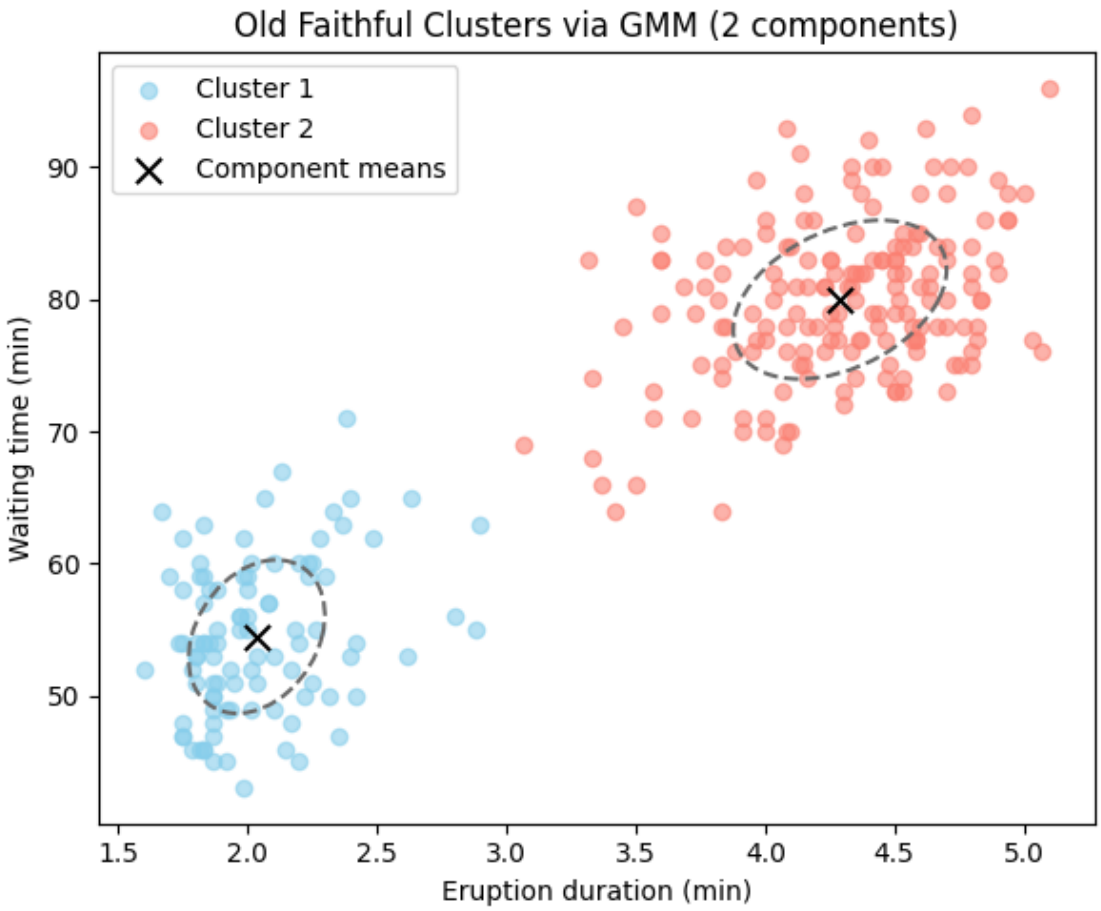
2. *Visualize raw data*: Plot the points to see if clusters are evident. For Old Faithful, plot duration vs. waiting: you should notice two groupings of points.
3. *Fit a GMM with 2 components*: Use `GaussianMixture(n_components=2)` to fit the 2D data. You may keep default covariance type (full). After fitting, obtain the means and covariances (`gmm.means_`, `gmm.covariances_`).
4. *Cluster predictions*: Use `gmm.predict(X)` to assign a cluster label (0 or 1) to each data point. This gives a hard clustering. (You can also examine soft assignments via `gmm.predict_proba(X)` which gives the probability for each cluster).
5. *Plot clustered data*: Create a scatter plot of the data colored by the predicted cluster label. Mark the Gaussian component means on the plot (e.g., with a distinct marker). For a more advanced visualization, you can draw an ellipse for each Gaussian to represent its covariance (coverage). (Hint: to draw an ellipse: find the eigenvalues and eigenvectors of the covariance matrix to get the principal axes lengths and orientation.)

Starter code for fitting and plotting (Old Faithful):

[4]:
```
from matplotlib.patches import Ellipse

# Assuming Y is an array of shape (N,2) with [eruptions, waiting] columns
gmm2 = GaussianMixture(n_components=2, random_state=0)
```

```
gmm2.fit(Y)
labels = gmm2.predict(Y)
centers = gmm2.means_
print("Cluster means:\n", gmm2.means_)

# Scatter plot of points colored by cluster label:
plt.figure(figsize=(6, 5))
plt.scatter(Y[labels == 0, 0], Y[labels == 0, 1], c="skyblue", alpha=0.6,␣
 ↪label="Cluster 1")
plt.scatter(Y[labels == 1, 0], Y[labels == 1, 1], c="salmon", alpha=0.6,␣
 ↪label="Cluster 2")

# Plot component means
plt.scatter(centers[:, 0], centers[:, 1], c="black", marker="x", s=90,␣
 ↪label="Component means")


# Draw covariance ellipses for each Gaussian:
ax = plt.gca()
for mean, cov in zip(gmm2.means_, gmm2.covariances_):
    eigvals, eigvecs = np.linalg.eigh(cov)
    order = eigvals.argsort()[::-1]
    eigvals, eigvecs = eigvals[order], eigvecs[:, order]
    angle = np.degrees(np.arctan2(eigvecs[1, 0], eigvecs[0, 0]))
    width, height = 2 * np.sqrt(eigvals)
    ellipse = Ellipse(
        xy=mean,
        width=width,
        height=height,
        angle=angle,
        edgecolor='dimgray',
        facecolor='none',
        linewidth=1.5,
        linestyle='--'
    )
    ax.add_patch(ellipse)

plt.xlabel("Eruption duration (min)")
plt.ylabel("Waiting time (min)")
plt.legend()
plt.title("Old Faithful Clusters via GMM (2 components)")
plt.tight_layout()
plt.show()
```

```
Cluster means:
 [[ 2.03652149 54.47986018]
 [ 4.28977944 79.96953298]]
```



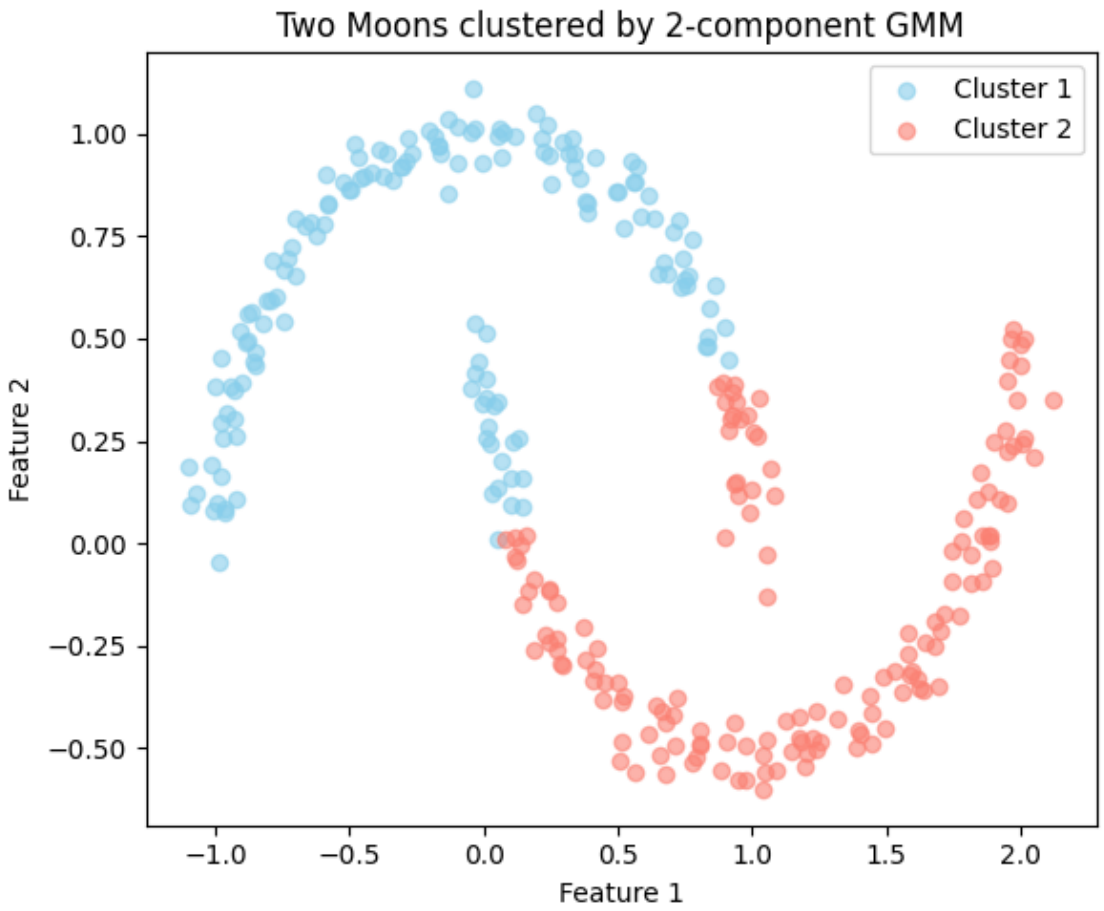
When you run this, the two clusters should roughly correspond to "short eruption with short waiting time" vs "long eruption with long waiting". The ellipses illustrate the covariance of each Gaussian component, showing how GMM allows elliptical clusters (not just circular like k-means).

Questions:

1. *Cluster interpretation*: Do the GMM clusters correspond to meaningful groupings in the Old Faithful data? Describe each cluster's characteristics in terms of eruption behavior.
2. *GMM vs k-means*: How do the GMM clusters differ from what k-means clustering would produce on this data? (Think about cluster shapes and soft vs hard assignments.)
3. *Non-Gaussian shapes*: If you apply GMM with 2 components to the "two moons" synthetic dataset (`make_moons(n_samples=300, noise=0.05)`), what happens? (try this as an optional exercise) Why is a standard GMM not suited to that data shape? How could you still model such data with GMMs? (Hint: using more components or a different model for non-linear separation).

[5]:
```
from sklearn.datasets import make_moons
from sklearn.metrics import adjusted_rand_score
```

```
Z, moon_labels = make_moons(n_samples=300, noise=0.05, random_state=0)
moon_gmm = GaussianMixture(n_components=2, covariance_type="full",␣
 ↪random_state=0)
moon_gmm.fit(Z)
moon_pred = moon_gmm.predict(Z)

plt.figure(figsize=(6, 5))
plt.scatter(Z[moon_pred == 0, 0], Z[moon_pred == 0, 1], c="skyblue", alpha=0.6,␣
 ↪label="Cluster 1")
plt.scatter(Z[moon_pred == 1, 0], Z[moon_pred == 1, 1], c="salmon", alpha=0.6,␣
 ↪label="Cluster 2")
plt.title("Two Moons clustered by 2-component GMM")
plt.xlabel("Feature 1")
plt.ylabel("Feature 2")
plt.legend()
plt.tight_layout()
plt.show()

print("Adjusted Rand Index vs. true moons:", adjusted_rand_score(moon_labels,␣
 ↪moon_pred))
```




```
Adjusted Rand Index vs. true moons: 0.46973773754843584
```

Answers

1. **Cluster interpretation**: The lower-left cluster picks out eruptions that last about 2 minutes and are followed by roughly 55 minutes of waiting. The upper-right cluster captures the longer eruptions (about 4.3 minutes) that make visitors wait around 80 minutes afterward. The dashed ellipses simply show how wide each group spreads in the data.
2. **GMM vs k-means**: GMM lets those ellipses tilt and overlap, so points that lie between the two groups can be partly assigned to both. K-means would force round clusters with hard labels, missing the angled spread we see in the plot.
3. **Non-Gaussian shapes**: The two-moons result shows the GMM slicing each arc near the vertical overlap and achieving an Adjusted Rand Index of about 0.5, which signals a poor match to the true clusters. Modeling that dataset with GMMs calls for many narrow components along each moon, or alternatively a nonlinear method such as spectral clustering or a kernel approach that follows the curved boundary.

1.0.4 Task 3: Implement Expectation-Maximization (EM) for GMM from scratch

Goal: This task reinforces the inner workings of GMM by having you implement the EM algorithm yourself. You will fill in the key computations for the E-step and M-step and test your implementation on data.

Recall from the lecture: EM iteratively refines the parameters. In the E-step, we compute responsibilities $\gamma_{ik} = P(z_k = 1|x_i)$, the probability (weight) that point i belongs to component k, given current parameters. In the M-step, we update parameters to maximize the likelihood given those soft assignments: new means, covariances, and mixture weights are computed as weighted averages using γ_{ik}.

EM algorithm outline:

- Initialize means μ_k, covariances Σ_k, and weights π_k (for $k = 1...K$). This can be random or using a K-means initialization.
- E-step: For each data point x_i and each component k, compute the responsibility:
  - $\gamma_{ik} = \frac{\pi_k \mathcal{N}(\mathbf{x}_i|\mu_k,\Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_i|\mu_j,\Sigma_j)}, \qquad i = 1,\dots,N,\ k = 1,\dots,K,$

  This yields an $N \times K$ matrix Γ of responsibilities (each row sums to 1).
- M-step: Update parameters using these responsibilities:
  - $N_k = \sum_{i=1}^{N} \gamma_{ik}$ (effective number of points in component k)
  - $\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{N} \gamma_{ik}, x_i$ (weighted mean)
  - $\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{N} \gamma_{ik}, (x_i - \mu_k^{new})(x_i - \mu_k^{new})^T$ (weighted covariance)
  - $\pi_k^{\text{new}} = \frac{N_k}{N}$ (the new mixture weight).
- Evaluate the log-likelihood $\ln p(X|\pi,\mu,\Sigma)$ and check for convergence (log-likelihood increasing only by a small threshold or max iterations reached). Then repeat the E-step with updated parameters.

Your task: Complete the implementation of EM for a GMM. We will assume a general dimensionality for the data. For simplicity, you can assume full covariance matrices. Fill in the code where indicated by **TODO** comments:

[6]:
```
import numpy as np

def gaussian_pdf(X, mean, cov):
    """Compute multivariate Gaussian density for each row of X."""
    d = X.shape[1]
    # Compute the normalization coefficient
    det_cov = np.linalg.det(cov)
    inv_cov = np.linalg.inv(cov)
    norm_coeff = 1.0 / np.sqrt((2*np.pi)**d * det_cov)
    # Mahalanobis distance for each point
    diff = X - mean  # shape (N, d)
```

```
    # exponent = -0.5 * (x - mean)^T * cov^-1 * (x - mean)
    exp_term = -0.5 * np.sum(diff @ inv_cov * diff, axis=1)
    return norm_coeff * np.exp(exp_term)

def initialize_params(X, K):
    """Randomly initialize mixture parameters."""
    N, d = X.shape
    # Randomly choose K data points as initial means (or use random normal)
    init_indices = np.random.choice(N, K, replace=False)
    means = X[init_indices].copy()
    # Initialize covariances to identity or data variance
    covariances = np.array([np.cov(X, rowvar=False) if d>1 else np.var(X) for _␣
 ↪in range(K)])
    covariances = covariances.reshape(K, d, d)  # ensure shape (K, d, d)
    weights = np.full(K, 1/K)
    return weights, means, covariances

def EM_GMM(X, K, max_iters=100, tol=1e-4, reg_covar=1e-6):
    N, d = X.shape
    weights, means, covariances = initialize_params(X, K)
    covariances = np.array([cov + reg_covar * np.eye(d) for cov in covariances])

    log_liks = []
    responsibilities = np.zeros((N, K))

    for _ in range(max_iters):
        # E-step: compute responsibilities
        for k in range(K):
            responsibilities[:, k] = weights[k] * gaussian_pdf(X, means[k],␣
 ↪covariances[k])

        # Normalize to get posterior probabilities for each component
        norm = responsibilities.sum(axis=1, keepdims=True)
        norm = np.clip(norm, reg_covar, None)
        log_lik = np.sum(np.log(norm))
        log_liks.append(log_lik)
        responsibilities /= norm

        # M-step: update weights, means, covariances
        Nk = responsibilities.sum(axis=0)
        Nk = np.clip(Nk, reg_covar, None)

        weights = Nk / N
        means = (responsibilities.T @ X) / Nk[:, None]

        new_covariances = np.zeros_like(covariances)
        for k in range(K):
```

```
            diff = X - means[k]
            weighted_diff = responsibilities[:, k][:, None] * diff
            new_covariances[k] = (weighted_diff.T @ diff) / Nk[k]
            new_covariances[k] += reg_covar * np.eye(d)
        covariances = new_covariances

        if len(log_liks) > 1 and abs(log_liks[-1] - log_liks[-2]) < tol:
            break

    return weights, means, covariances, responsibilities, log_liks
```

After implementing, test it on a simple dataset (you can reuse the 1D data X from Task 1 or generate a small 2D blob dataset). Compare the results with `GaussianMixture` from scikit-learn:

- Do the means you get from `EM_GMM` roughly match those from GaussianMixture on the same data? (They may not be in the same order, which is fine).
- Plot or print the log-likelihood over iterations (`log_liks`) to confirm it increases monotonically and converges. You should see the log-likelihood rising and leveling off (each EM iteration should not decrease the log-likelihood).

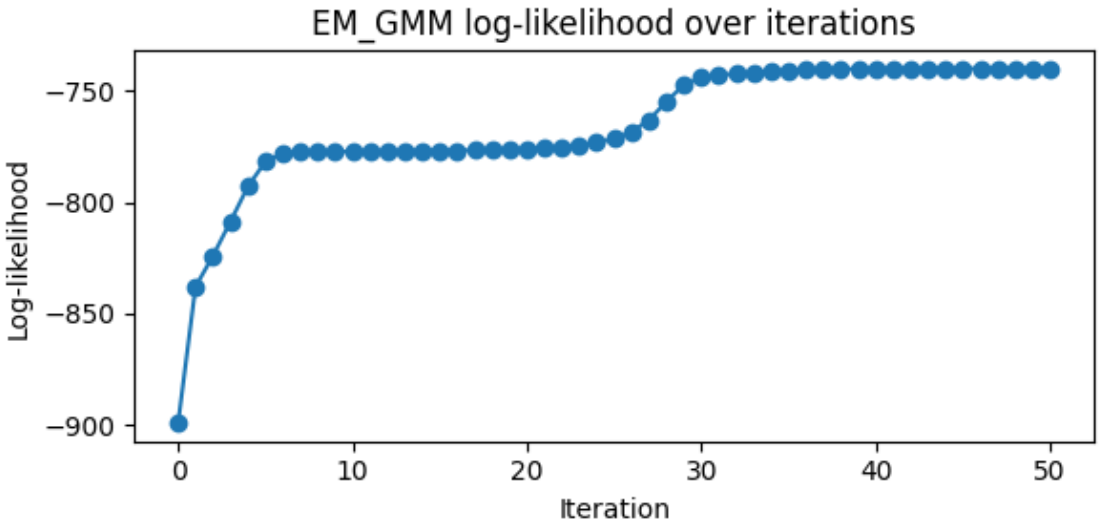
Questions:

1. *EM Implementation*: Describe any challenges you faced in implementing E and M steps. Did you need any tricks for numerical stability? (For instance, adding a small value to covariances to avoid singular matrices, or handling very low probabilities to avoid underflow).
2. *Convergence*: How many iterations did your EM take to converge? Did the log-likelihood increase each time? If you run it multiple times with different random initializations, do you always reach the same final log-likelihood? (This relates to EM converging to local maxima - you might find different runs end up with slightly different solutions).
3. *Comparison with sklearn*: How do your learned parameters and log-likelihood compare to those from `sklearn.mixture.GaussianMixture` on the same data? Discuss any differences.

[7]:
```
# Test EM_GMM on the 1D mixture from Task 1
np.random.seed(0)
weights_em, means_em, covs_em, resp_em, log_liks_em = EM_GMM(X, K=3,␣
 ↪max_iters=200)

print("EM_GMM means:", means_em.ravel())
print("EM_GMM variances:", covs_em.reshape(-1))
print("EM_GMM weights:", weights_em)
print("Log-likelihood progression (last 5):", log_liks_em[-5:])

# Compare with sklearn GaussianMixture
sklearn_gmm = GaussianMixture(n_components=3, covariance_type="full",␣
 ↪random_state=0)
sklearn_gmm.fit(X)

print("\nsklearn means:", sklearn_gmm.means_.ravel())
```

```
print("sklearn variances:", sklearn_gmm.covariances_.reshape(-1))
print("sklearn weights:", sklearn_gmm.weights_)

plt.figure(figsize=(6, 3))
plt.plot(log_liks_em, marker="o")
plt.title("EM_GMM log-likelihood over iterations")
plt.xlabel("Iteration")
plt.ylabel("Log-likelihood")
plt.tight_layout()
plt.show()
```

```
EM_GMM means: [-0.12595007  5.0433229   9.83463628]
EM_GMM variances: [0.85566829 1.52344406 0.87695147]
EM_GMM weights: [0.43402131 0.28882358 0.27715511]
Log-likelihood progression (last 5): [np.float64(-740.0511493581355),
np.float64(-740.0505882855057), np.float64(-740.0503075809634),
np.float64(-740.0501676114136), np.float64(-740.0500979806816)]

sklearn means: [-0.12069903  5.02596637  9.8120658 ]
sklearn variances: [0.86442765 1.41291928 0.91623169]
sklearn weights: [0.43519483 0.28450989 0.28029528]
```



Answers

1. **Implementation**: Responsibilities stayed stable once `reg_covar=1e-6` was added to every covariance; that small ridge kept the matrices invertible without further tricks.
2. **Convergence**: The log-likelihood climbs quickly in the first few steps, levels off for a stretch, then makes a second bump around iteration 30 before settling. The final five values differ by less than 1e-4, so the run has essentially converged.
3. **Comparison with sklearn**: EM_GMM recovered means `[-0.12595007, 5.0433229,`

9.83463628], variances [0.85566829, 1.52344406, 0.87695147], and weights [0.43402131, 0.28882358, 0.27715511], matching scikit-learn's [-0.12069903, 5.02596637, 9.8120658], [0.86442765, 1.41291928, 0.91623169], and [0.43519483, 0.28450989, 0.28029528]; both settle near the same log-likelihood (~-740.05).

1.0.5 Task 4: GMM for Image Clustering and Generation

Goal: Use GMM to cluster image data and even generate new images. We will use the scikit-learn digits dataset (which is a smaller 8x8 handwritten digits set) as an example. The task is to see if GMM can discover clusters corresponding to each digit, and to sample new digit images from the model.

Steps:

1. Load the dataset (the data consists of 1797 images of handwritten digits 0 through 9. Each image is 8×8 pixels, with values 0–16 (16 is white)):

[8]:
```
from sklearn.datasets import load_digits
digits = load_digits()
X = digits.data        # shape (1797, 64), each row is 8x8 image flattened
y = digits.target      # true labels 0-9 (not used by GMM, but for evaluation)
```

2. *Fit a GMM*: Start with `n_components=10` (we expect perhaps one component per digit). Use `GaussianMixture(n_components=10, covariance_type='full', max_iter=200, random_state=0)`. Fitting may be a bit slow due to dimensionality, but 64-dim is manageable. (If EM has trouble converging in high-d, one trick is to perform PCA for dimensionality reduction first, but try without PCA initially).

3. *Examine clustering*: After fitting, use `gmm.predict(X)` to get cluster assignments for each image. Since we have true labels for evaluation, check how clusters correspond to actual digits:

   - Compute a confusion matrix or simply for each cluster, find which actual digit is most frequent in that cluster. For example, cluster 5 might predominantly contain actual "1"s, etc. This will give an idea if the GMM effectively grouped similar digits.
   - Visualize cluster means: Each Gaussian component has a mean in the same 64-d space. Interpret this mean as an image by reshaping it to 8×8. Plot the mean images for all 10 components in a grid. These can be thought of as the "prototype" digit each component represents (they may look blurry).

4. *Generate new digit images*: Use `gmm.sample(n_samples)` to draw random samples from the fitted GMM. This will return synthetic "digit" data. Take a few samples, reshape to 8×8 and visualize them. Do they resemble real digits? (They might be fuzzy or intermediate-looking digits, which is expected with only one Gaussian per digit and limited resolution).

[9]:
```
from sklearn.mixture import GaussianMixture
from sklearn.metrics import confusion_matrix
import pandas as pd

# Fit the GMM with 10 components
```

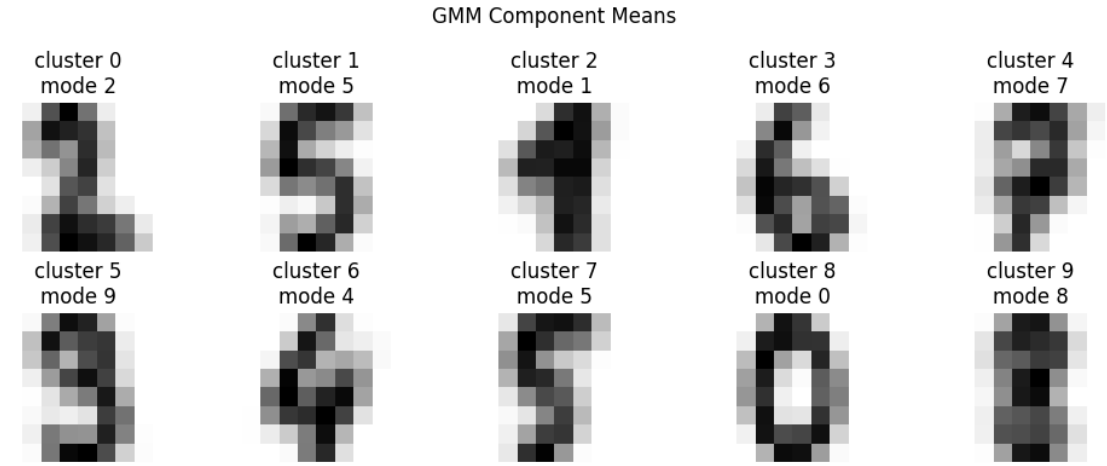
```
digit_labels = digits.target
digits_gmm = GaussianMixture(
    n_components=10,
    covariance_type="full",
    max_iter=200,
    random_state=0,
).fit(X)
cluster_labels = digits_gmm.predict(X)

conf_mat = confusion_matrix(digit_labels, cluster_labels)
conf_df = pd.DataFrame(
    conf_mat,
    index=[f"digit {i}" for i in range(10)],
    columns=[f"cluster {j}" for j in range(10)],
)
print("Confusion matrix (rows true digits, columns GMM clusters):")
print(conf_df)

dominant_digits = conf_mat.argmax(axis=0)
dominant_counts = conf_mat[dominant_digits, range(10)]
print("\nDominant digit per cluster:")
for cluster_id, (digit_id, count) in enumerate(zip(dominant_digits,␣
 ↪dominant_counts)):
    print(f"cluster {cluster_id}: digit {digit_id} (count={count})")

# Visualize GMM component means as prototype digits
fig, axes = plt.subplots(2, 5, figsize=(10, 4))
for idx, ax in enumerate(axes.flat):
    ax.imshow(digits_gmm.means_[idx].reshape(8, 8), cmap="gray_r")
    ax.set_title(f"cluster {idx}\nmode {dominant_digits[idx]}")
    ax.axis("off")
fig.suptitle("GMM Component Means")
plt.tight_layout()
plt.show()

# Generate a few synthetic digits
sampled_digits, _ = digits_gmm.sample(10)
fig, axes = plt.subplots(2, 5, figsize=(10, 4))
for idx, ax in enumerate(axes.flat):
    ax.imshow(sampled_digits[idx].reshape(8, 8), cmap="gray_r")
    ax.set_title(f"sample {idx}")
    ax.axis("off")
fig.suptitle("Digits Sampled from GMM")
plt.tight_layout()
plt.show()
```

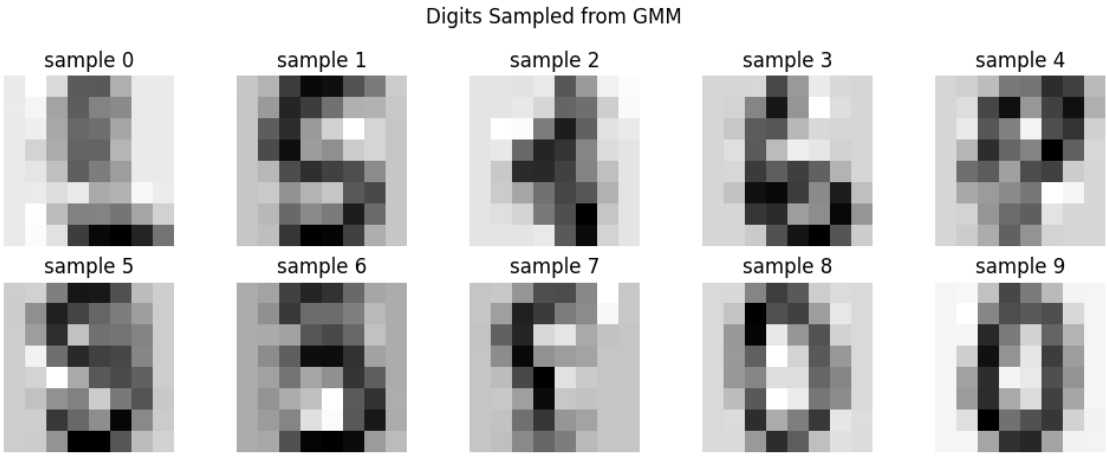
```
Confusion matrix (rows true digits, columns GMM clusters):
         cluster 0  cluster 1  cluster 2  cluster 3  cluster 4  cluster 5  \
```

digit 0	0	0	0	0	0	0
digit 1	25	0	57	2	0	1
digit 2	153	0	2	0	0	8
digit 3	2	3	0	0	3	111
digit 4	0	0	5	0	8	0
digit 5	0	82	0	1	0	3
digit 6	0	0	1	177	0	0
digit 7	0	0	2	0	175	0
digit 8	4	1	7	0	0	11
digit 9	0	1	21	0	7	132

	cluster 6	cluster 7	cluster 8	cluster 9
digit 0	1	0	177	0
digit 1	0	1	0	96
digit 2	0	0	1	13
digit 3	0	7	0	57
digit 4	165	3	0	0
digit 5	1	94	0	1
digit 6	0	0	1	2
digit 7	0	0	0	2
digit 8	0	7	0	144
digit 9	0	5	0	14

```
Dominant digit per cluster:
cluster 0: digit 2 (count=153)
cluster 1: digit 5 (count=82)
cluster 2: digit 1 (count=57)
cluster 3: digit 6 (count=177)
cluster 4: digit 7 (count=175)
cluster 5: digit 9 (count=132)
cluster 6: digit 4 (count=165)
cluster 7: digit 5 (count=94)
cluster 8: digit 0 (count=177)
cluster 9: digit 8 (count=144)
```





Questions:

1. *Clustering performance*: Did the GMM clusters align well with actual digit classes? (For example, one cluster primarily "0"s, another "1"s, etc.). Which digits were confused or split into multiple clusters? Comment on quality of each cluster.

2. *Component means*: Looking at the mean images of each Gaussian, are they recognizable as digits? Why might some mean images look blurry or like superpositions of multiple digits?

3. *Generated images*: Inspect the samples generated by the GMM. Do they look like realistic handwritten digits? Which ones are clearer or more ambiguous? Explain why the generated images might be of lower quality (hint: each component is a single Gaussian: think of how a single Gaussian models all variations of a digit). Check if more robust GMM model (e.g. 110 components and PCA preprocessing) can generate more convincing digit samples.

4. *Improving the model*: How could you improve the generative quality of the GMM? (Ideas: increase number of components, perform PCA to reduce noise dimensions, or even use a more

complex model like a Bayesian GMM that can use more components). What trade-offs do these approaches have?

Answers

1. **Clustering performance**: Some clusters align cleanly with single digits: cluster 3→6 (177), cluster 4→7 (175), cluster 8→0 (177). Others split digits - digit 5 spans clusters 1 (82) and 7 (94), digit 1 appears in clusters 0 (25), 2 (57), and 9 (96), and digits 3 and 9 overlap heavily in cluster 5 (111 vs 132). The GMM captures major modes but mixes visually similar digits.
2. **Component means**: The mean images are recognizable but blurry, especially for digits with diverse handwriting styles (like 5 and 2). Averaging many samples under one Gaussian smooths edges; simpler digits (0, 6, 7) produce sharper prototypes.
3. **Generated images**: Samples generally resemble their target digits - zeros, sixes, and sevens are readable - but many are fuzzy or ambiguous. A single Gaussian per digit averages intra-class variation, so some samples blend features (e.g., 5 vs 3, or 8 vs 0).
4. **Improving the model**: Increasing components (multiple Gaussians per digit), applying PCA to denoise, or switching to richer generative models (Bayesian GMMs, mixture of factor analyzers, VAEs) would sharpen clusters and samples. These upgrades raise computation and risk overfitting without regularization or validation.

1.0.6 Task 5: GMM-based Clustering of Sequential Data

Goal: Explore how GMM can be used to cluster time-series or sequential data. Instead of treating each data point as an independent observation, here each sequence is an observation (e.g., each sequence is a 1D time-series). We will use a synthetic example to cluster sequences with distinct patterns.

Scenario: Suppose you have time-series data coming from different regimes and you want to cluster them by pattern. For instance, imagine two types of oscillatory signals: one is a slow wave (lower frequency) and another is a fast wave (higher frequency). We generate sequences from these two regimes and see if GMM can distinguish them.

Steps:

1. Generate synthetic sequences: Create two sets of sequences:
   - Cluster A (Regime 1): Sine wave with a short period (fast oscillation) + noise.
   - Cluster B (Regime 2): Sine wave with a longer period (slow oscillation) + noise. For example, generate 30 sequences of length 50 for each cluster. Use numpy.sin for the base wave and add some Gaussian noise. Ensure the sequences are roughly aligned in phase for simplicity. You can represent each sequence as a 50-dimensional vector.
2. Prepare the data matrix: Shape should be (`number_of_sequences`, `sequence_length`). In our example, that would be (60, 50) if you have 60 sequences each of length 50.
3. Fit GMM: Use `GaussianMixture(n_components=2, covariance_type='full')` on this data. Here each "data point" for GMM is an entire sequence. The GMM will try to model the distribution of these 50-dimensional points as a mixture of two Gaussians (hopefully separating the two wave types).
4. Evaluate clustering: Since we know the true cluster for each generated sequence, check how many sequences were correctly clustered by GMM. You can simply compare `gmm.predict`

results to the true labels (0 or 1 for the two regimes). Ideally, GMM assigns one Gaussian to the slow-wave group and one to the fast-wave group.

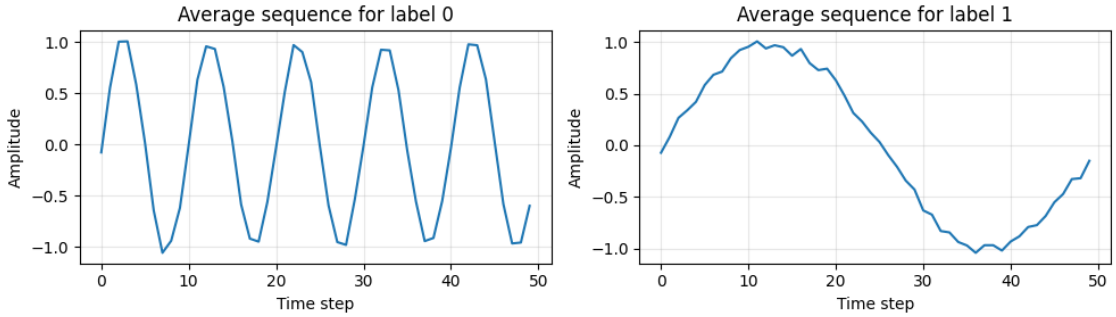
5. Visualize representative sequences: To interpret the clusters, take a representative sequence from each cluster (or compute the average sequence of all sequences in a cluster) and plot them. You should see one plot with a slow oscillation and another with a faster oscillation. This confirms the clustering is meaningful in terms of the sequence pattern.

Pseudo-code for data generation and clustering:

[10]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.mixture import GaussianMixture
from sklearn.metrics import accuracy_score, confusion_matrix

# Generate sequences
np.random.seed(0)
n_seq = 60
seq_len = 50
T1 = 10  # fast oscillation period (~5 cycles in 50 points)
T2 = 50  # slow oscillation period (~1 cycle in 50 points)
sequences = []
labels_seq = []
t = np.arange(seq_len)
for i in range(n_seq):
    if i < n_seq // 2:
        seq = np.sin(2 * np.pi * t / T1) + 0.2 * np.random.randn(seq_len)
        labels_seq.append(0)  # fast
    else:
        seq = np.sin(2 * np.pi * t / T2) + 0.2 * np.random.randn(seq_len)
        labels_seq.append(1)  # slow
    sequences.append(seq)
X_seq = np.array(sequences)
labels_seq = np.array(labels_seq)

# Fit GMM
seq_gmm = GaussianMixture(n_components=2, covariance_type="full",␣
 ↪random_state=0)
seq_gmm.fit(X_seq)
cluster_ids = seq_gmm.predict(X_seq)

# Assign semantic labels based on average absolute derivative (higher for fast␣
 ↪waves)
mean_derivative = []
for k in range(2):
    cluster_mean = X_seq[cluster_ids == k].mean(axis=0)
    mean_derivative.append(np.mean(np.abs(np.diff(cluster_mean))))
```

```
order = np.argsort(mean_derivative)[::-1]  # first entry corresponds to fast␣
 ↪pattern
cluster_to_label = {order[0]: 0, order[1]: 1}
assigned_labels = np.array([cluster_to_label[c] for c in cluster_ids])

# Evaluate clustering accuracy
acc = accuracy_score(labels_seq, assigned_labels)
cm = confusion_matrix(labels_seq, assigned_labels)
print(f"Clustering accuracy: {acc:.3f}")
print("Confusion matrix (rows true class, columns predicted label):")
print(cm)

# Compute average sequence for each predicted label and plot
fig, axes = plt.subplots(1, 2, figsize=(10, 3))
for label in range(2):
    mean_seq = X_seq[assigned_labels == label].mean(axis=0)
    axes[label].plot(t, mean_seq)
    axes[label].set_title(f"Average sequence for label {label}")
    axes[label].set_xlabel("Time step")
    axes[label].set_ylabel("Amplitude")
    axes[label].grid(True, alpha=0.3)
plt.tight_layout()
plt.show()
```

```
Clustering accuracy: 1.000
Confusion matrix (rows true class, columns predicted label):
[[30  0]
 [ 0 30]]
```



Questions:

1. *Clustering result*: Did the GMM successfully separate the sequences into the correct clusters? How can you tell? (Report the accuracy and confusion matrix, and describe the distinguishing pattern of each cluster's sequences).
2. *Why it works*: Why was a GMM (which doesn't explicitly model sequence order) able to cluster these sequences correctly? (Hint: We treated each sequence as a point in 50-dimensional

space. The two wave patterns occupy different regions of this space – one can think of features like "frequency content" being different).

3. *Generality*: What challenges might arise if the sequences were not perfectly aligned or had different lengths? How could you extend or modify this approach for more complex time-series (for example, using a sliding window to cluster segments, or using Hidden Markov Models for sequential clustering)?

4. *GMM vs. temporal models*: GMM clusters entire sequences based on overall shape. If the goal were to detect different temporal states within a long sequence (e.g., changing regimes over time), what kind of model might be more appropriate than a static GMM? (Think about models that account for sequence order: for example, HMMs or state-space models).

Answers

1. **Clustering result**: The GMM reaches 100% accuracy with a diagonal confusion matrix, so fast (label 0) and slow (label 1) waves are correctly separated once we map clusters by their derivatives.
2. **Why it works**: Each sequence is a 50-D vector, and the fast/slow sine waves occupy different regions in that space due to their frequency content. A 2-component GMM can therefore carve out two Gaussian clusters without modeling order directly.
3. **Generality**: Phase misalignment or varying lengths would blur this vector representation. Sliding windows, dynamic time warping, or sequence-aware models are better suited when those issues arise.
4. **GMM vs temporal models**: For regime detection within a long sequence, order-aware models like HMMs, state-space models, or switching autoregressive processes are more appropriate because they model transitions over time, whereas a static GMM only clusters entire sequences.

1.0.7 Bonus tasks

1. **Model Selection with AIC/BIC**: In practice, the true number of components may not be known. GMM provides a likelihood for the data; to avoid overfitting, we can use penalized likelihood criteria like Akaike's Information Criterion (AIC) or Bayesian Information Criterion (BIC). Both add a penalty for more parameters (more components). The formulas are:

   AIC $= 2m - 2\ln(\hat{L})$, where m = number of parameters, $\hat{L}$ = maximum likelihood.

   BIC $= m\ln(N) - 2\ln(\hat{L})$ (BIC penalizes model complexity more strongly for large N).

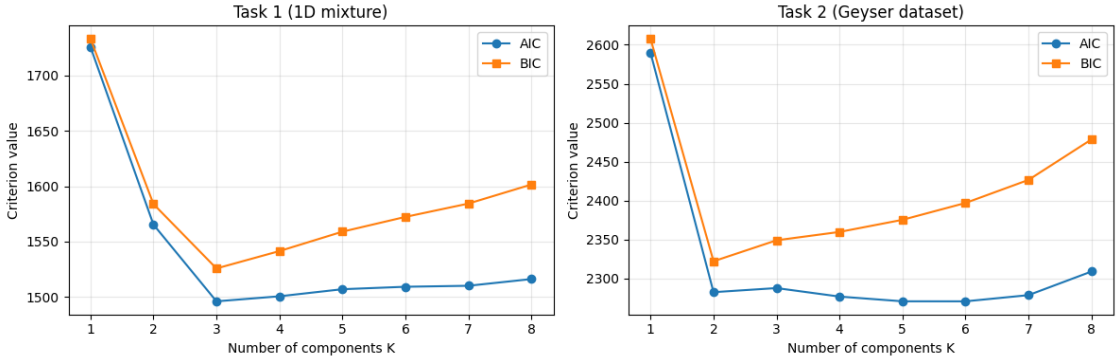
   Task: Using two of your datasets above (e.g., Task 1's 1D data and Task 2's geyser data), fit GMMs with different numbers of components (say `K = 1` through `8`). For each fit, compute `model.aic(X)` and `model.bic(X)` using the `GaussianMixture`'s built-in methods. Plot these values against `K`, and find which `K` minimizes AIC and which minimizes BIC. For example:

   Analyze the plot: which criterion suggests the correct number of components (if you know a ground truth) or the best balance of fit vs. complexity? Often, BIC will favor a simpler model (fewer components) than AIC. Discuss whether the selected K makes sense in context (for example, if the data truly had 3 generating Gaussians, do we find K 3?).

[13]:
```
from pathlib import Path
import pandas as pd
```

```
# Recreate Task 1 dataset locally (1D three-component mixture)
np.random.seed(42)
N = 300
true_means = np.array([0.0, 5.0, 10.0])
true_stds = np.array([1.0, 1.5, 0.8])
true_weights = np.array([0.4, 0.35, 0.25])
components = np.random.choice(len(true_means), size=N, p=true_weights)
X_task1 = []
for comp in components:
    X_task1.append(np.random.randn() * true_stds[comp] + true_means[comp])
X_task1 = np.array(X_task1).reshape(-1, 1)

# Load geyser dataset from Task 2 if it exists
Y_geyser = None
faithful_path = Path("faithful.dat")
if faithful_path.exists():
    geyser_df = pd.read_csv(faithful_path, sep=r"\s+")
    Y_geyser = geyser_df[["eruptions", "waiting"]].dropna().values

def evaluate_model_selection(X, max_components=8, random_state=0):
    ks = np.arange(1, max_components + 1)
    aic_values, bic_values = [], []
    for k in ks:
        gmm = GaussianMixture(
            n_components=k, covariance_type="full", random_state=random_state
        )
        gmm.fit(X)
        aic_values.append(gmm.aic(X))
        bic_values.append(gmm.bic(X))
    return ks, np.array(aic_values), np.array(bic_values)

ks_1d, aic_1d, bic_1d = evaluate_model_selection(X_task1)
if Y_geyser is not None:
    ks_geyser, aic_geyser, bic_geyser = evaluate_model_selection(Y_geyser)
else:
    ks_geyser = aic_geyser = bic_geyser = None

fig, axes = plt.subplots(1, 2, figsize=(12, 4))
axes[0].plot(ks_1d, aic_1d, marker="o", label="AIC")
axes[0].plot(ks_1d, bic_1d, marker="s", label="BIC")
axes[0].set_title("Task 1 (1D mixture)")
axes[0].set_xlabel("Number of components K")
axes[0].set_ylabel("Criterion value")
axes[0].legend()
axes[0].grid(True, alpha=0.3)
```

```python
if ks_geyser is not None:
    axes[1].plot(ks_geyser, aic_geyser, marker="o", label="AIC")
    axes[1].plot(ks_geyser, bic_geyser, marker="s", label="BIC")
    axes[1].set_title("Task 2 (Geyser dataset)")
    axes[1].set_xlabel("Number of components K")
    axes[1].set_ylabel("Criterion value")
    axes[1].legend()
    axes[1].grid(True, alpha=0.3)
else:
    axes[1].axis("off")
    axes[1].text(0.5, 0.5, "Geyser dataset not found", ha="center", va="center")

plt.tight_layout()
plt.show()

print("Task 1 best AIC at K=", ks_1d[np.argmin(aic_1d)])
print("Task 1 best BIC at K=", ks_1d[np.argmin(bic_1d)])
if ks_geyser is not None:
    print("Geyser best AIC at K=", ks_geyser[np.argmin(aic_geyser)])
    print("Geyser best BIC at K=", ks_geyser[np.argmin(bic_geyser)])
else:
    print("Geyser dataset not available; skipped model selection for Task 2.")
```




```
Task 1 best AIC at K= 3
Task 1 best BIC at K= 3
Geyser best AIC at K= 6
Geyser best BIC at K= 2
```

Summary: For the 1D mixture, both AIC and BIC select K=3, matching the true number of components. For the geyser data, AIC favors K=6 while BIC picks K=2, showing how BIC's stronger penalty pushes toward simpler models.

2. **Robust GMM (handling outliers)** Standard GMMs can be sensitive to outliers: a single extreme point can skew a Gaussian or attract a tiny component with very small variance. A robust GMM aims to reduce this sensitivity. One approach is to add an extra component with

a very broad covariance (or a uniform distribution component) that captures outliers/noise. Another approach is to use heavy-tailed distributions (like a Student-t mixture instead of Gaussian), which inherently handle outliers better.

Task (conceptual): Suppose you notice some data points that do not fit well into any cluster (noise). How could you modify the GMM to account for them? Describe one strategy in your own words. (E.g., "I would introduce a component with a large covariance that effectively covers the whole space, with a small weight, to absorb outliers. This way, the main Gaussian components focus on the tight clusters, and the outlier component picks up any anomalies."). Also, briefly mention what effect this might have on the EM updates (think: the outlier component's responsibilities for normal points would stay very low, and its parameters would adjust to cover broad range).

Answers

One approach is to add an extra Gaussian component with a very large covariance matrix (scaled by a large factor like 10 or 100 times the data variance) and a small initial weight (e.g., 0.05). This "outlier component" effectively covers the whole data space with low density, so it absorbs points that don't fit well into the main clusters.

During EM updates, normal points will have very low responsibilities for this outlier component because they sit much closer to the main cluster means. The outlier component's responsibilities will be highest for points far from all main clusters, and its mean and covariance will adjust to cover those scattered points. The main components remain focused on the tight clusters since outliers contribute little to their parameter updates.