Assignment 3: Clustering Models

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Part 1: Implement the K-means algorithm

In [1]:
```python
# Import libraries
import numpy as np
import matplotlib.pyplot as plt
from PIL import Image
import os
from math import log2
```

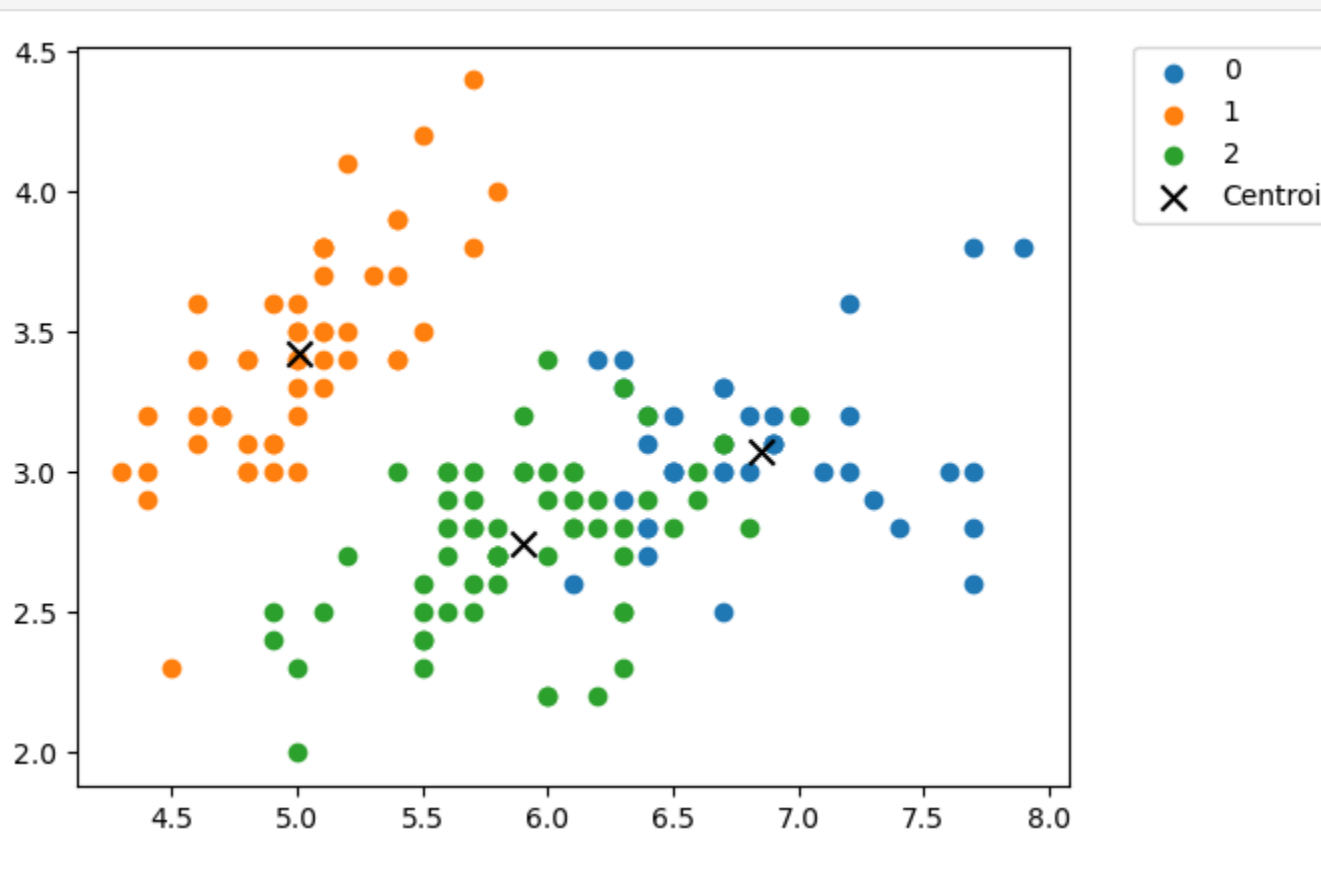
In [2]:
```python
# Import iris dataset
from sklearn.datasets import load_iris
iris = load_iris()
X = iris.data
```

In [3]:
```python
def kmeans(x, K, n_init):
    """
    Implementation of the K-means clustering algorithm.
    """
    # Initialize centroids randomly
    centroids = x[np.random.choice(len(x), K, replace=False)]
    labels = np.zeros(len(x))

    # Run until convergence
    while True:
        prev_labels = labels.copy()

        # Assign data points to the nearest centroid
        distances = np.linalg.norm(x[:, np.newaxis] - centroids, axis=2)
        labels = np.argmin(distances, axis=1)

        # Update centroids
        centroids = np.array([np.mean(x[labels == k], axis=0) if np.sum(labels == k) > 0 else np.random.rand(x.shape[1]) for k in range(K)])

        # Check for convergence
        if np.array_equal(prev_labels, labels):
            break

    return centroids, labels
```

In [4]:
```python
centroids, labels = kmeans(X, 3, 1000)

print("Centroids:")
print(centroids)
print()
print("Labels:")
print(labels)
```

```
Centroids:
[[6.85       3.07368421 5.74210526 2.07105263]
 [5.006      3.428      1.462      0.246     ]
 [5.9016129  2.7483871  4.39354839 1.43387097]]

Labels:
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 0 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 0 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 0 2 0 0 0 0 2 0 0 0 0
 0 0 2 2 0 0 0 0 2 0 2 0 2 0 0 2 2 0 0 0 0 0 2 0 0 0 0 2 0 0 0 2 0 0 0 2 0
 0 2]
```

In [5]:
```python
# Visualize the results
u_labels = np.unique(labels)

for i in u_labels:
    plt.scatter(X[labels == i, 0], X[labels == i, 1], label=i)
plt.scatter(centroids[:, 0], centroids[:, 1], s=80, color="black", label="Centroids", marker="x")
plt.legend(bbox_to_anchor=(1.3, 1), borderaxespad=0)
plt.show()
```



If you run this algorithm multiple times, do you get the same result every time? If so, why; if not, how do you determine which result is the best one?

If we run this algorithm multiple times, we will not get the same result every time. This is because the sensitivity to the initial centroids, so the algorithm will converge to different local minima, that is, different initilizations of the centroids will lead to a different local minima. To determine which result is the best one, we can use the elbow method to determine the optimal number of clusters. The elbow method involves plotting the sum of squared errors (SSE) for different values of K. The elbow in the curve indicates the optimal value of K.

How do you choose what K value to use?

The Elbow Method involves plotting the sum of squared errors (SSE) for different values of K. The elbow in the curve indicates the optimal value of K. The optimal K value is the value that is at the inflection point on the curve where the SSE begins to decrease in a linear way. It consists of the following steps:

1. Run the K-means clustering algorithm for a range of K values (e.g. K=1 to 10)
2. For each value of K, calculate the sum of squared errors (SSE)
3. Plot SSE vs K (number of clusters)
4. Identify the elbow in the plot (the point where the SSE curve starts to bend) and select this as the best K value for the data.

Another method is the Silhouette method. The silhouette value measures how similar a point is to its own cluster (cohesion) compared to other clusters (separation). The range of the Silhouette value is between +1 and -1. A high value is desirable and indicates that the point is placed in the correct cluster. If many points have a negative Silhouette value, it may indicate that we have created too many or too few clusters.

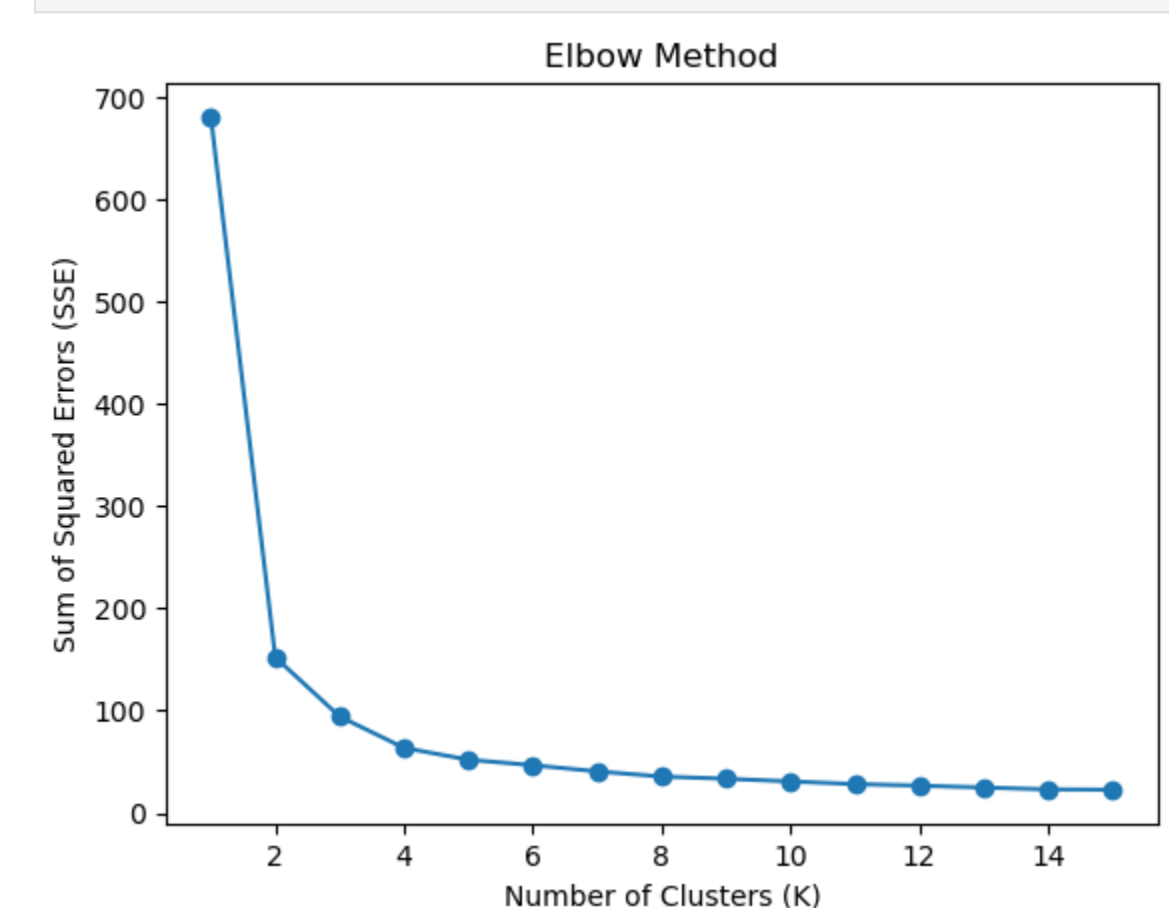
Implement both SSE and the Silhouette score; use them to address these questions.

In [20]:
```python
# Implementing SSE
def calculate_sse(x, centroids, labels):
    """
    Calculate the sum of squared errors (SSE) for a given clustering.
    """
    sse = np.sum((x - centroids[labels])**2)
    return sse

# Calculate SSE
sse = calculate_sse(X, centroids, labels)
print(f'SSE: {sse}')
```

```
SSE: 78.85144142614601
```

In [7]:
```python
# Elbow Method
def plot_elbow_method(data, max_k, n_init=10):
    """
    Plot the sum of squared errors (SSE) for different values of K.
    """
    sse_values = []

    for k in range(1, max_k + 1):
        sse = 0

        for _ in range(n_init):
            centroids, labels = kmeans(data, k, n_init=10)
            sse += calculate_sse(data, centroids, labels)

        sse_values.append(sse / n_init)

    # Plot
    plt.plot(range(1, max_k + 1), sse_values, marker='o')
    plt.xlabel('Number of Clusters (K)')
    plt.ylabel('Sum of Squared Errors (SSE)')
    plt.title('Elbow Method')
    plt.show()
```

In [8]:
```python
plot_elbow_method(X, 15, n_init=50)
```



On the x-axis, we have the number of clusters (k). On the y-axis, there's the sum of squared errors (SSE), which tells us how far away the points in a cluster are from the cluster center. A high SSE means the points are spread out and not very close to the center. To find the "elbow" in the graph, we refer to the point where the SSE curve starts to bend. After this points, more clusters don't make a big difference. If we look at the graph, we see a big drop from 1 to 2 clusters, and then from 2 to 3 clusters. After 3 clusters, the SSE drops slower. So, the 'elbow' is around 3 clusters. This means that 3 is a good number of clusters to use for our dataset, which in fact is correct, because we know that the iris dataset have 3 labels "setosa", "versicolor" and "virginica" . With 3 clusters, each one is different enough from the others, but we also don't have too many clusters to manage.

In [9]:
```python
# Implementing the Silhouette Score
def calculate_silhouette_score(x, labels):
    """
    Calculate the silhouette score for a given clustering.
    """
    num_samples = len(x)
    silhouette_values = np.zeros(num_samples)

    for i in range(num_samples):
        # Calculate the average distance from each sample to all other samples in the same cluster
        intra_cluster_dist = np.mean(np.linalg.norm(x[labels == labels[i]] - x[i], axis=1))

        # Calculate the average distance from each sample to all samples in the nearest other cluster
        other_clusters_dist = np.min([np.mean(np.linalg.norm(x[labels == k] - x[i], axis=1)) for k in set(labels) if k != labels[i]])

        # Calculate the silhouette score for each sample
        silhouette_values[i] = (other_clusters_dist - intra_cluster_dist) / max(other_clusters_dist, intra_cluster_dist)

    # Calculate the overall silhouette score
    silhouette = np.mean(silhouette_values)

    return silhouette
```

In [10]:
```python
silhouette = calculate_silhouette_score(X, labels)
print(f'Silhouette Score: {silhouette}')
```

```
Silhouette Score: 0.5617085758870528
```

A Silhouette Score of 0.56 is slightly closer to 1. This suggest that the clusters we got by using k=3 has done a good job in groupoing the data points. Most of the data in each cluster is of the same type.

Discuss the similarities and differences between 1) K-means, 2) Gaussian Mixture Models (GMM) and 3) the Gaussian naive Bayes classifier in terms of their assumptions and parameter estimation methods. In particular, write down the implications of each assumption (e.g., x and y are assumed to be independent, and therefore we have ....). You can choose to write your answers as Python code, pseudo code or mathematical equations.

K-means

Assumptions and Implications:

- K-means assumes that clusters are spherical and equally sized with the centroid being the center of the sphere. This implies that clusters with non-spherical shapes can be poorly represented by centroids, also, if clusters have different sizes, K-means might not represent them accurately, preferring clusters with more points.
- Assumes that all clusters have equal variance (homodedasticity). If the scales of the variables are different, then variables with larger scales may dominate the clustering process, making the algorithm biased towards those features. This is why it's often recommended to standardize variables before applying K-means.
- Assigns each data point exclusively to one cluster (hard clustering), which can lead to misclassifications if the true underlying structure involves overlapping clusters.
- The number of clusters is assumed to be known in advance. In real world scenarios, the number of cluster is not known in advance. There is no one defined true number of cluster, it has to be determined from methods, data-based criteria and knowledge of the domain.
- The K-means algorithm implicitly assumes that the features within each cluster are independent. This assumption is reflected in the way the algorithm calculates distances between data points and cluster centroids. However, this assumption of feature independence is not always realistic in real-world data. Many datasets contain features that are correlated with each other.

Parameter Estimation:

- Centroids: They are estimated by iteratively updating the mean of the data points assigned to each cluster. The algorithm starts with a random initialization of these centroids. Then it alternates between assigning data points to the nearest centroid and updating the centroids based on the current assignment of data points. Because the initial selection of centroids is random (it is sensitive to the initial selection of centroids), different runs of the K-means algorithm on the same data may produce different results. This is known as the problem of local optima. In other words, the K-means algorithm may converge to different solutions depending on the initial selection of centroids.
- K-means uses distance-based metrics to identify similar points for clustering. This becomes a problem when we have numerous dimensions (curse of dimensionality). As the number of dimensions increases, the distances between different data points tend to be closer together.
- Labels: Assign each data point to the cluster with the nearest centroid, this process helps in forming the different clusters. Each cluster is a group of data points that are closer to one centroid than to any other.

Gaussian Mixture Models (GMM):

Assumptions and Implications:

- Data points are generated from a mixture of of several Gaussian distributions with unknown parameters. This means each cluster is modeled as a Gaussian distribution, allowing for more flexibility compared to K-means.
- GMM assumes that clusters can be elliptical and can have different sizes. This implies that GMM can capture more complex cluster structures and sizes, also overlapping clusters.
- GMM model different covariance structures for each cluster, which is a key feature allowing GMM to adapt to various cluster shapes and orientations.
- In GMM, a point can belong to different clusters with different levels of membership (probabilities). This probabilistic approach provides a nuanced view of the data structure, accommodating uncertainty in cluster membership.

Parameter Estimation:

- Means, covariances, weights are estimated through the Expectation-Maximization (EM) algorithm. The algorithm iteratively updates the mean, covariance, and weight parameters to maximize the likelihood of the data. This iterative process involves alternating between assigning data points to clusters (expectation step) and updating the parameters based on these assignments (maximization step). This implies that GMM is generally more computationally expensive than K-means

Gaussian Naive Bayes Classifier:

Assumptions and Implications:

- Features are assumed to be conditionally independent given the class label, which means that knowing the value of one feature doesn't change our belief about any other feature given the class. The independence assumption simplifies the computation and ignores potential interactions between features. However is often violated in real world scenarios.
- Features are assumed to be normally distributed (Gaussian), which is a strong assumption about the data structure. Gaussian distribution assumption may not hold for all features, which can negatively affect the model's performance if features have different distributions.
- The prior probabilities of classes are either uniform (assumed to be equal) or can be estimated from the training dataset.
- The model tends to perform well even when this assumption is violated if the dataset is large enough or if the dependencies between features do not discriminate between classes.

Parameter Estimation:

- Mean and variance for each feature in each class are estimated Maximum Likelihood Estimation.

Part 2: Apply the K-means algorithm to compress images

In [11]:
```python
# Load multiple images
def load_images(image_path):
    """
    Load multiple images from a list of file paths.
    """
    for path in image_path:
        with Image.open(path) as image:
            yield np.asarray(image)

def save_images(images, titles, base_folder="images", sub_folder="compressed"):
    """
    Save images to a folder.
    """
    folder_path = os.path.join(base_folder, sub_folder)
    os.makedirs(folder_path, exist_ok=True)
    for i, image in enumerate(images):
        path = os.path.join(folder_path, f'{titles[i]}.png')
        Image.fromarray(image).save(path)
```

In [12]:
```python
# Compress images utilizing our K-means implementation
def compress_images(images, K):
    """
    Compress images using K-means clustering.
    """
    # Initialize compressed images
    compressed_images = []

    for image in images:
        # Reshape the image to a 2D array
        pixels = image.reshape(-1, 3)

        # Run K-means clustering
        centroids, labels = kmeans(pixels, K, n_init=10)

        # Replace each pixel value with its corresponding centroid
        compressed_image = centroids[labels].reshape(image.shape).astype(np.uint8)
        compressed_images.append(compressed_image)
    return compressed_images
```

In [13]:
```python
# Plot original and compressed images side by side
def plot_images(original_images, compressed_images, titles, K):
    """
    Plot original and compressed images side by side.
    """
    plt.figure(figsize=(15, 5 * len(original_images)))
    for i, (original, compressed) in enumerate(zip(original_images, compressed_images)):
        # Plotting original image
        plt.subplot(len(original_images), 2, 2*i + 1)
        plt.imshow(original)
        plt.title(f'Original Image: {titles[i]}')
        plt.axis('off')

        # Plotting compressed image
        plt.subplot(len(original_images), 2, 2*i + 2)
        plt.imshow(compressed)
        plt.title(f'Compressed Image (K={K}): {titles[i]}')
        plt.axis('off')

    plt.tight_layout()
    plt.show()
```

In [14]:
```python
def compute_compression_ratio(original_images, compressed_images, K):
    """Compute the compression ratio for each image"""
    ratios = []
    for original, compressed in zip(original_images, compressed_images):
        # Calculate the number of unique colors in the original image.
        original_unique_colors = len(np.unique(original.reshape(-1, original.shape[2]), axis=0))

        # Calculate the total number of pixels in the image
        number_of_pixels = original.shape[0] * original.shape[1]

        # Estimate the compressed image size
        compressed_size = K * 24 + number_of_pixels * log2(K)

        # Estimate the original image size
        original_size = original_unique_colors * 24

        # Calculate the compression ratio
        ratio = original_size / compressed_size
        ratios.append(ratio)
    return ratios
```

In [15]:
```python
# Load images
image_paths = ['images/original/img1.png', 'images/original/img2.png', 'images/original/img3.png']
original_images = list(load_images(image_paths))
compressed_images = compress_images(original_images, K=12)

# Plot images
plot_images(original_images, compressed_images, ['Image 1', 'Image 2', 'Image 3'], K=12)

# Save images
save_images(compressed_images, ['Image1', 'Image2', 'Image3'])
```

In [16]:
```python
# Calculate compression ratio
ratios = compute_compression_ratio(original_images, compressed_images, K=12)
print(f'Compression Ratios: {ratios}')

# Calculate original image sizes
original_image_sizes = [os.path.getsize(path) for path in image_paths]
compressed_image_sizes = [os.path.getsize(f'images/compressed/{title}.png') for title in ['Image1', 'Image2', 'Image3']]

# Convert to Megabytes
original_image_sizes_mb = [size / (1024 * 1024) for size in original_image_sizes]
compressed_image_sizes_mb = [size / (1024 * 1024) for size in compressed_image_sizes]
print(f'Sorted Original Image Sizes: {[f"{size:.2f} MB" for size in original_image_sizes_mb]}')
print(f'Sorted Compressed Image Sizes: {[f"{size:.2f} MB" for size in compressed_image_sizes_mb]}')
```

```
Compression Ratios: [0.4926535405512305, 0.27171666869431893, 0.5363781428581245]
Sorted Original Image Sizes: ['2.65 MB', '1.68 MB', '2.45 MB']
Sorted Compressed Image Sizes: ['0.60 MB', '0.47 MB', '0.50 MB']
```

Image Compression Results

For the chosen value of K=12, the following observations were made:

- **Compression Ratios**: The calculated compression ratios for the images were [0.49, 0.27, 0.54]. These ratios indicate the proportion of the original image size to the compressed image size meaning a significant reduction in size.
- **File Sizes**: The sizes of the original images were 2.65 MB, 1.68 MB, and 2.45 MB. After compression and saving as PNG files, the sizes were reduced to 0.60 MB, 0.47 MB, and 0.50 MB.

Image Compression Discussion

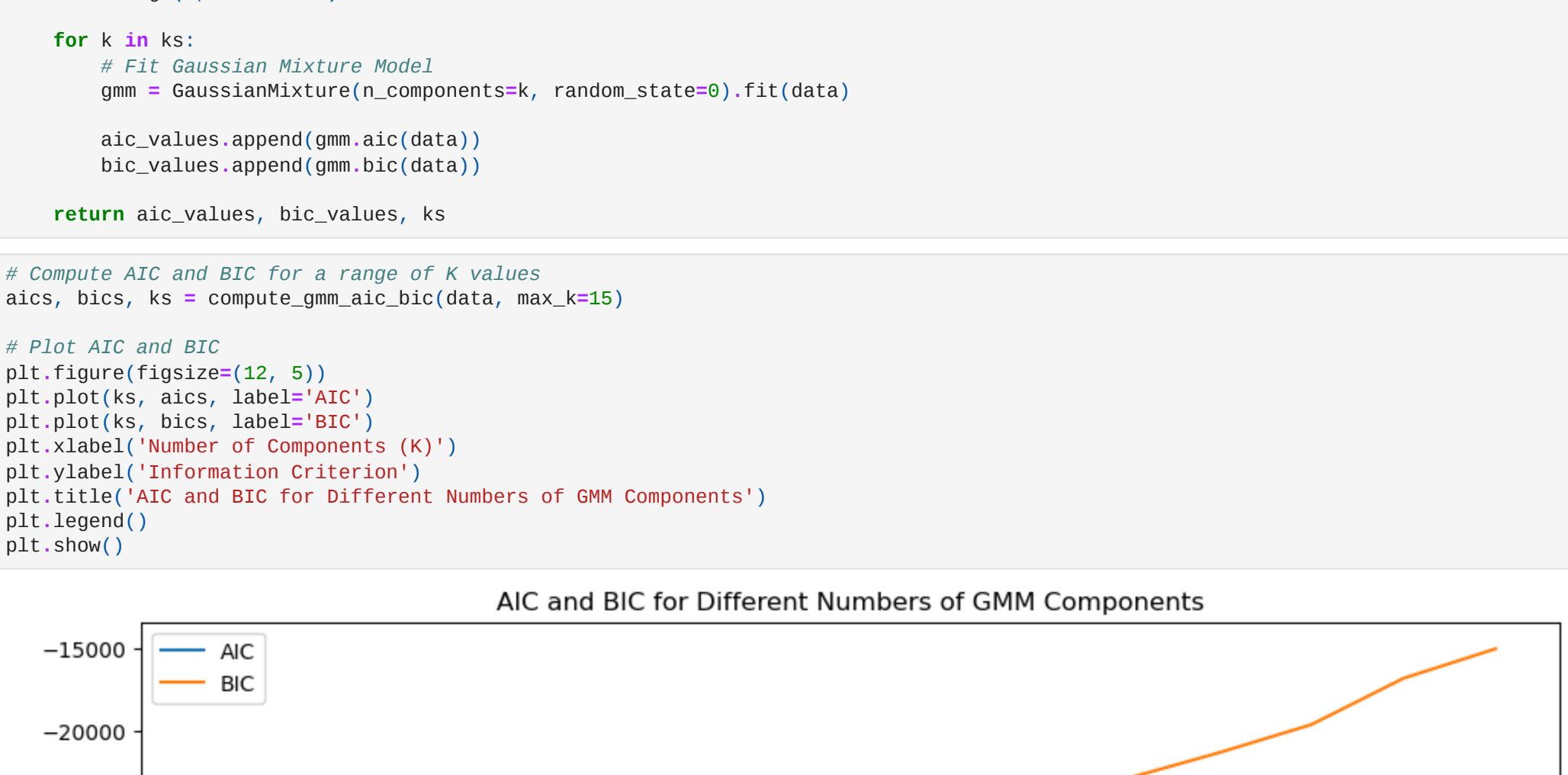
- The compressed images are considerably smaller in size compared to the original images, which confirms the effectiveness of the K-means compression technique.
- The observed file size reduction is consistent with the calculated compression ratios, indicating a successful application of the algorithm.
- The choice of K=12 appears to be effective for this dataset, as it significantly reduces file size while presumably maintaining a reasonable level of detail in the images.
- Saving the compressed images as PNGs provided an accurate representation of the compression's impact on file size without additional file size that might have been introduced by a JPEG.
- This experiment demonstrates the potential of K-means for practical image compression and especially in scenarios where reducing storage space is crucial.

Part 3 Use AIC and BIC to choose K for Gaussian Mixture Models

In [17]:
```python
# Import libraries
from sklearn.mixture import GaussianMixture
from sklearn.datasets import load_breast_cancer

# Load dataset
data = load_breast_cancer().data
```

In [18]:
```python
def compute_gmm_aic_bic(data, max_k):
    """
    Compute the AIC and BIC for a range of K values.
    """
    aic_values = []
    bic_values = []
    ks = range(1, max_k + 1)

    for k in ks:
        # Fit Gaussian Mixture Model
        gmm = GaussianMixture(n_components=k, random_state=0).fit(data)

        aic_values.append(gmm.aic(data))
        bic_values.append(gmm.bic(data))

    return aic_values, bic_values, ks
```

In [19]:
```python
# Compute AIC and BIC for a range of K values
aics, bics, ks = compute_gmm_aic_bic(data, max_k=15)

# Plot AIC and BIC
plt.figure(figsize=(12, 5))
plt.plot(ks, aics, label='AIC')
plt.plot(ks, bics, label='BIC')
plt.xlabel('Number of Components (K)')
plt.ylabel('Information Criterion')
plt.title('AIC and BIC for Different Numbers of GMM Components')
plt.legend()
plt.show()
```



Choose the best K on the breast_cancer data set using AIC and BIC and discuss your observations

The optimal number of components for the breast cancer dataset appears to be K=2, as indicated by the lowest AIC and BIC values at this point. This suggests that a model with two Gaussian components best captures the data's structure without unnecessary complexity. Beyond K=2, the increasing AIC and BIC values imply that additional components are not justified, favoring a simpler model that sufficiently explains the data.

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