PRINCIPLES OF MACHINE LEARNING

Exercise sheet 4 - fun with Frank-Wolfe

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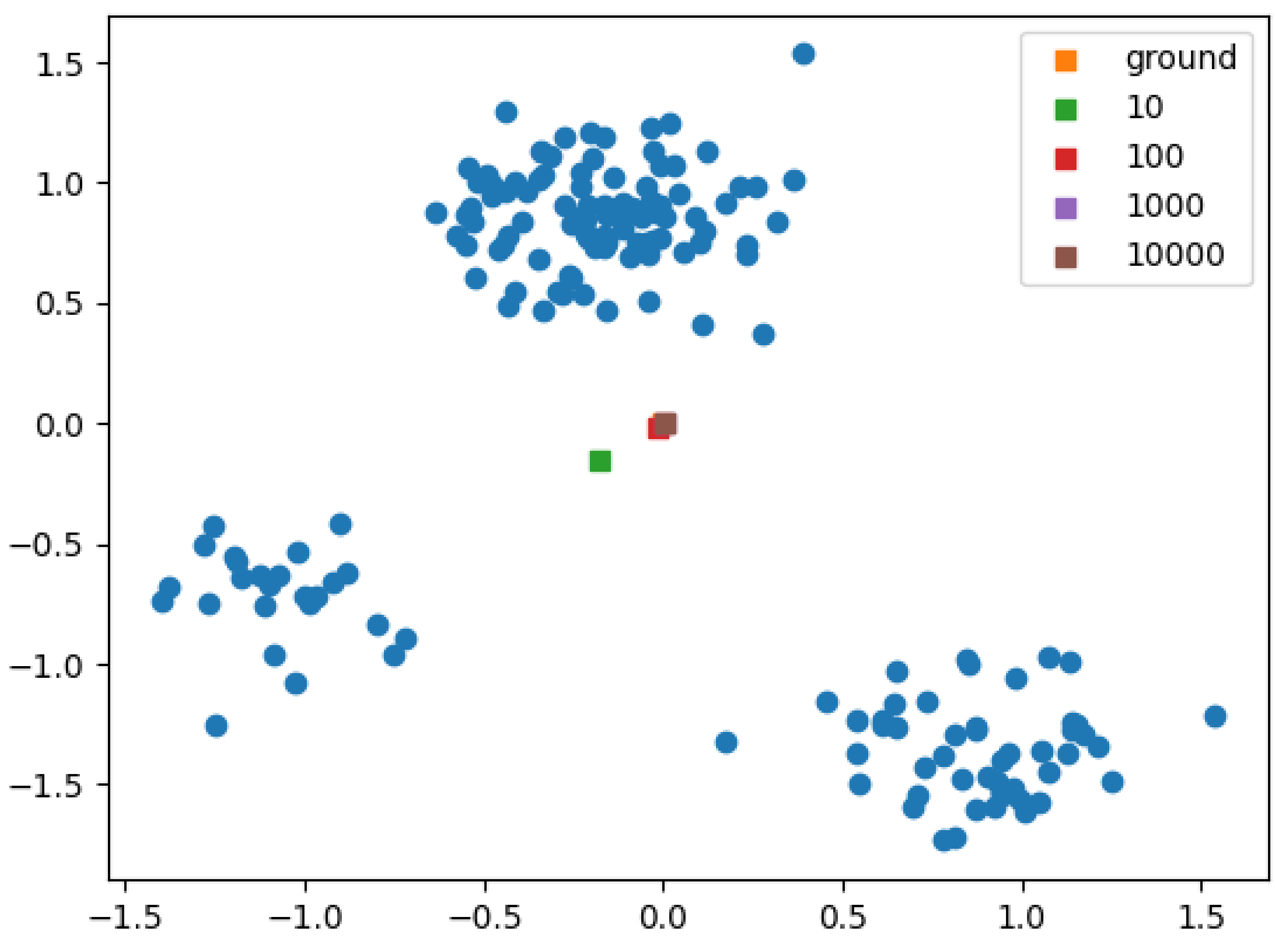
4.1: sample means (part 1)

Increase in the number of iterations results in increase of proximity/correctness of the estimated mean.

```
def gradientF(vector: np.ndarray, n: int, data: np.ndarray) -> np.ndarray:
    return 2 * data.transpose() @ data @ (vector - np.ones(n) / n)
def frank_wolfe(T:int, n: int, data: np.ndarray) -> np.ndarray:
    vecW = np.ones(n) / n  # center of the standard simplex
    for t in tqdm(range(T)):
        beta = 2 / (t + 2)
        vecG = gradientF(vecW, n, data) imin = np.argmin(vecG)
        vecW *= (1 - beta)
        vecW[imin] += beta
    return data @ vecW
```

4.1: result



4.2: sample means (part 2)

Given that: $\boldsymbol{X} \in \mathbb{R}^{m\times n}, \boldsymbol{X^T} \in \mathbb{R}^{n\times m}, z \in \mathbb{R}^{n\times 1}, z^T \in \mathbb{R}^{1\times n}, \omega \in \mathbb{R}^{n\times 1}, \omega^T \in \mathbb{R}^{1\times n}$

$\boldsymbol{Inferring}$: $\boldsymbol{X}\omega \in \mathbb{R}^{n\times 1}, z\omega^T \in \mathbb{R}^{n\times n}, z\omega^T\boldsymbol{X^T}\boldsymbol{X}\omega \in \mathbb{R}^{n\times 1}, \boldsymbol{X}\omega z^T \in \mathbb{R}^{n\times n}, \mathrm{tr}[\boldsymbol{X^T}\boldsymbol{X}\omega z^T] \in \mathbb{R}^1, z^T\boldsymbol{X^T}\boldsymbol{X}\omega \in \mathbb{R}^1$

Proof: Let $v_1 = \boldsymbol{X^T}\boldsymbol{X}\omega$ and $v_2 = z^T$ in case 1 and $v_1 = z\omega^T\boldsymbol{X^T}\boldsymbol{X}\omega$ and $v_2 = z^T$ in case 2. Therefore:

The trace of the product $\mathbf{v}_2\mathbf{v}_1$ is given by:

$$\mathrm{Tr}(\mathbf{v}_2\mathbf{v}_1)$$

The product $\mathbf{v}_2\mathbf{v}_1$ results in an $n \times n$ matrix. Let's compute the product:

$$\mathbf{v}_2\mathbf{v}_1 = \begin{bmatrix} v_{21} \\ v_{22} \\ \vdots \\ v_{2n} \end{bmatrix} \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1n} \end{bmatrix}$$

The resulting matrix $\mathbf{v}_2\mathbf{v}_1$ is:

$$\begin{bmatrix} v_{21}v_{11} & v_{21}v_{12} & \cdots & v_{21}v_{1n} \\ v_{22}v_{11} & v_{22}v_{12} & \cdots & v_{22}v_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ v_{2n}v_{11} & v_{2n}v_{12} & \cdots & v_{2n}v_{1n} \end{bmatrix}$$

4.2: sample means (part 2)

Now, the trace is the sum of the diagonal elements:

$$\mathrm{Tr}(\mathbf{v}_2\mathbf{v}_1) = v_{21}v_{11} + v_{22}v_{12} + \cdots + v_{2n}v_{1n}$$

Now, let's consider the product $\mathbf{v}_1\mathbf{v}_2$, which is a 1×1 matrix (a scalar):

$$\mathbf{v}_1\mathbf{v}_2 = \begin{bmatrix} v_{11} \\ v_{12} \\ \vdots \\ v_{1n} \end{bmatrix} \begin{bmatrix} v_{21} & v_{22} & \cdots & v_{2n} \end{bmatrix}$$

The result is:

$$\mathbf{v}_1\mathbf{v}_2 = v_{11}v_{21} + v_{12}v_{22} + \cdots + v_{1n}v_{2n}$$

Now, observe that these two expressions are the same:

$$\mathrm{Tr}(\mathbf{v}_2\mathbf{v}_1) = \mathbf{v}_1\mathbf{v}_2$$

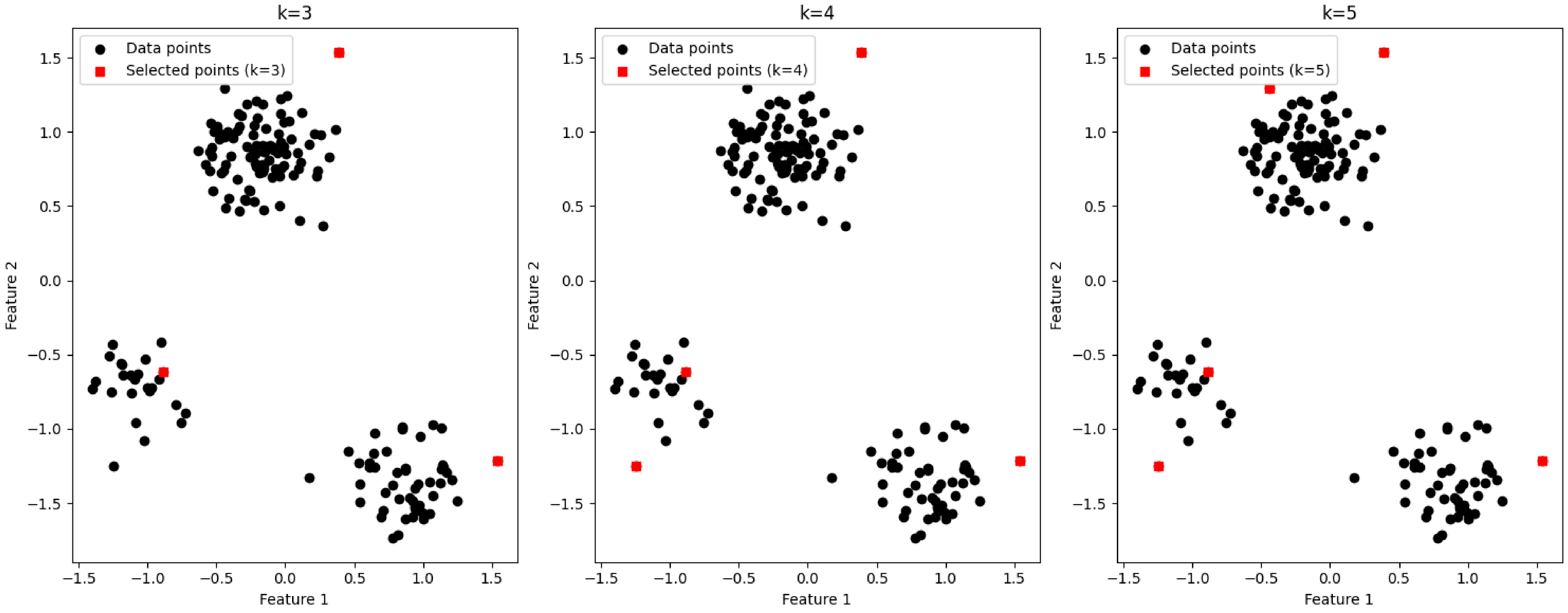
Therefore, we have shown that the trace of the product $\mathbf{v}_2\mathbf{v}_1$ is equal to the trace of the product $\mathbf{v}_1\mathbf{v}_2$.

4.3: finding maximally different data points

```
def select_diverse_points(X, k):
    if k >= X.shape[0]:
        raise ValueError("k must be smaller than the number of data
points")
    selected_indices = []
    for _ in range(k):
        max_dist = 0
        max_idx = -1
        for i in range(X.shape[0]):
            if i not in selected_indices:
                dist_sum = sum(np.linalg.norm(X[i] - X[j]) for j in
selected_indices)
                if dist_sum > max_dist:
                    max_dist = dist_sum
                    max_idx = i
        selected_indices.append(max_idx)

    return selected_indices
```

4.3: finding maximally different data points



4.3: finding maximally different data points (4,9,16,25)

4.3: finding maximally different data points (k=49)

4.3: finding maximally different data points (k=100)

4.4.1: unconventional k-means clustering (part 1)

```
def FW_update_Z(X, M, tmax=1):
    n = X.shape[1]  # Number of data points
    k = M.shape[1]  # Number of clusters
    Z = np.zeros((k, n))  # Initialize Z matrix

    for t in range(tmax):
        GZ = 2 * np.dot(np.dot(M.T, M), Z) - 2 * np.dot(M.T, X)
        row_indices = np.argmin(GZ, axis=0)
        Z = np.zeros_like(Z)  # Reset Z
        Z[row_indices, np.arange(n)] = 1  # Assign each data
point to the closest centroid

    return Z
```

4.4.1: unconventional k-means clustering (part 1)

```
def FW_kMeans_Version1(X, k, Tmax=100):
    m, n = X.shape
    # Randomly initialize centroids by selecting k data points
    indices = np.random.choice(n, k, replace=False)
    M = X[:, indices]

    for T in range(Tmax):
        Z = FW_update_Z(X, M)
        M = np.dot(X, Z.T) @ np.linalg.pinv(Z @ Z.T)  # Update centroids

    return M, Z
```

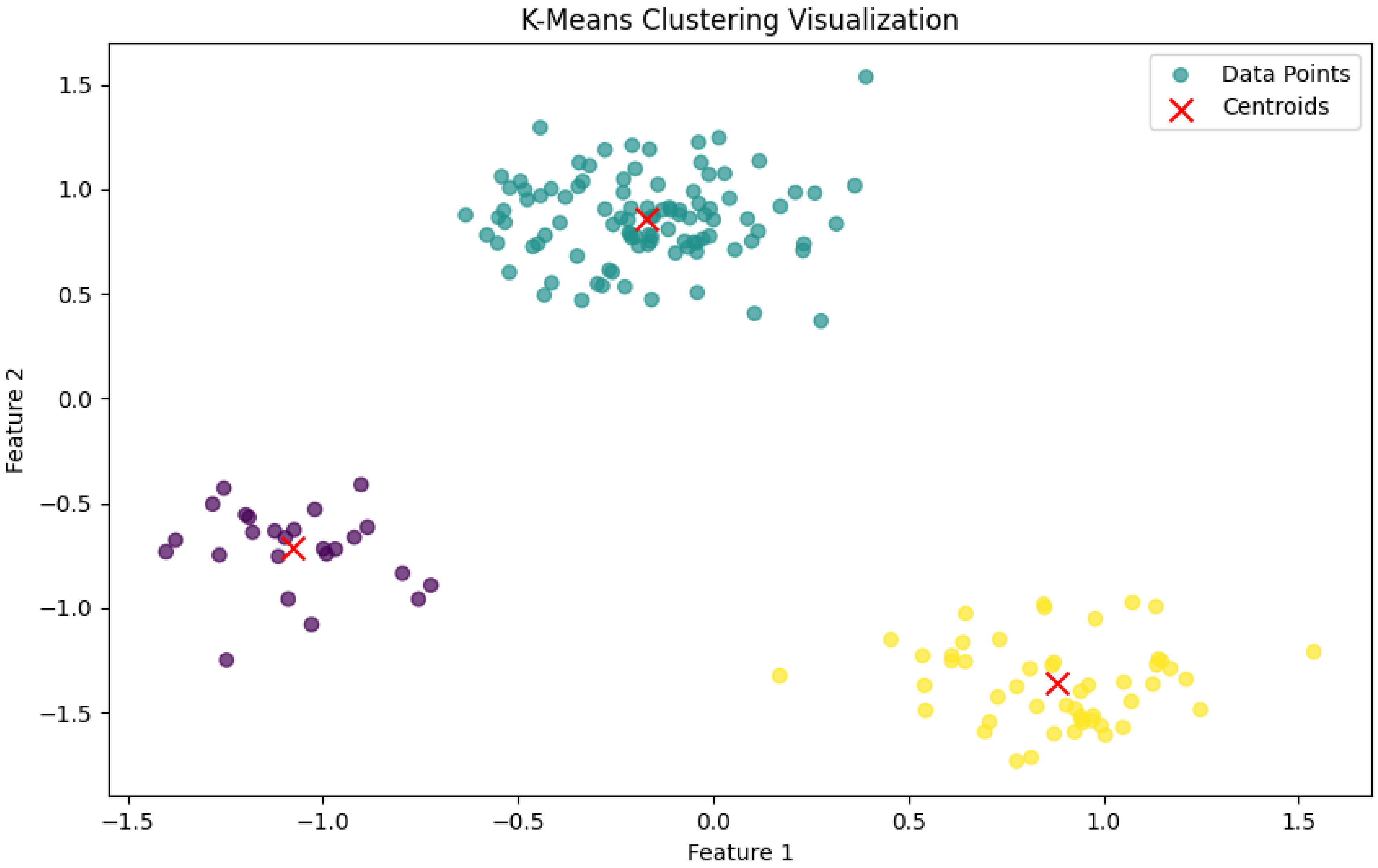
4.4.1: unconventional k-means clustering (part 1)

```
def FW_kMeans_Version1(X, k, Tmax=100):
    m, n = X.shape
    # Randomly initialize centroids by selecting k data points
    indices = np.random.choice(n, k, replace=False)
    M = X[:, indices]

    for T in range(Tmax):
        Z = FW_update_Z(X, M)
        M = np.dot(X, Z.T) @ np.linalg.pinv(Z @ Z.T)  # Update centroids

    return M, Z
```

4.4.1: unconventional k-means clustering (part 1)



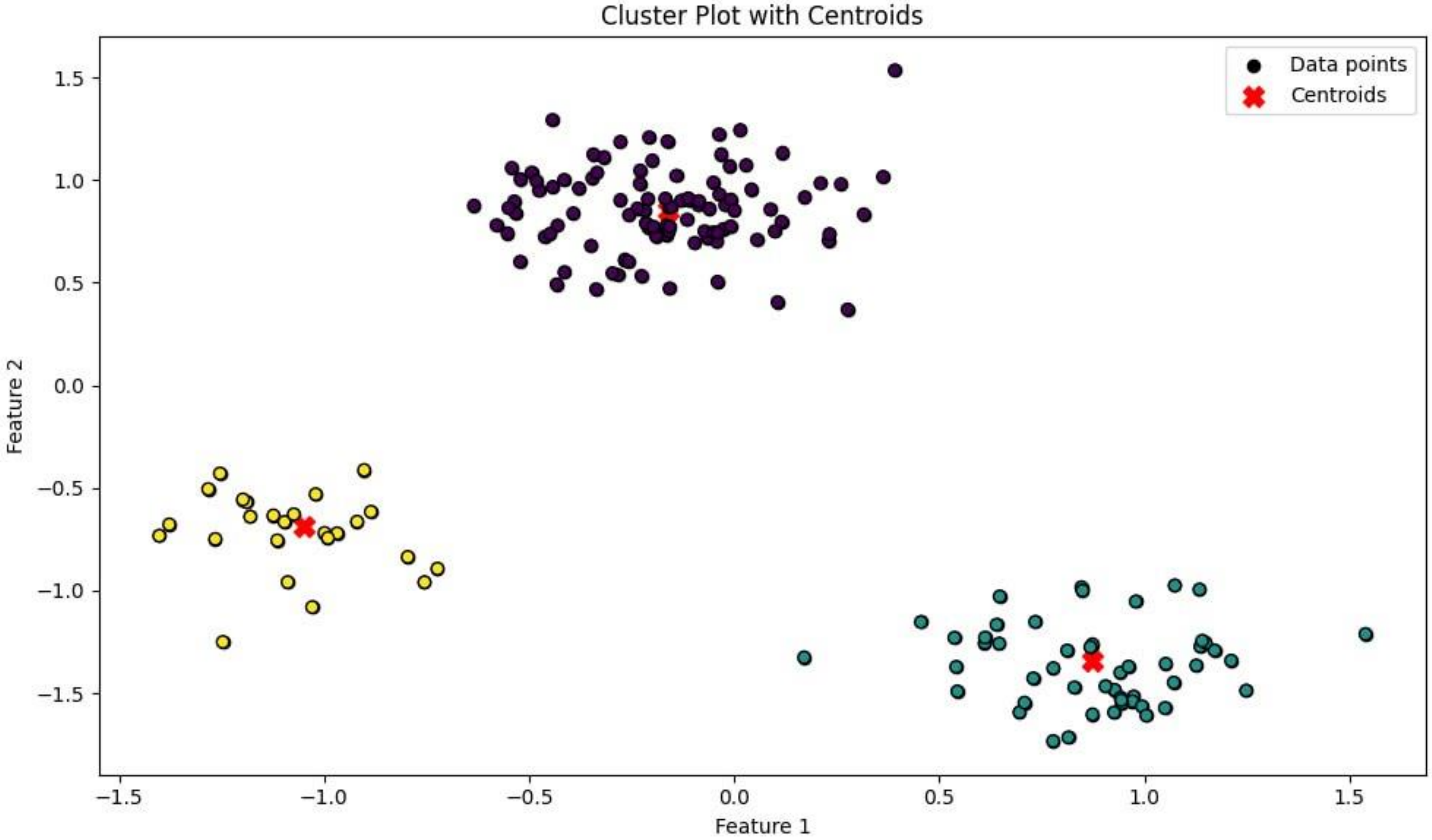
4.4.2: unconventional k-means clustering (part 1)

4.5: unconventional k-means clustering (part 2)

```
def FW_update_Y(X, Y, Z, t_max):
  for t in range(t_max):
    G_y = 2 * (X @ X.T @ Y @ Z @ Z.T - X @ X.T @ Z.T)
    for i in range(Y.shape[1]):
      o = np.argmin(G_y[:, i])
      Y[:, i] = Y[:, i] + (2 / (t + 2)) * (np.eye(Y.shape[0])[o] - Y[:, i])
  return Y

def FW_kMeans_Version2 (X, k, t_max):
  n, m = X.shape
  M = np.random.rand(m, k)
  for _ in range(t_max):
    Z = np.ones((k, n)) / k
    Z = FW_UPDATE_Z(X, M, Z, t_max=1)
    Y = np.ones((n, k)) / n
    Y = FW_UPDATE_Y(X, Y, Z, t_max=100)
    M = np.dot(X.T, Y)
  return M, Y, Z
```

4.5: unconventional k-means clustering (part 2)



4.5: unconventional k-means clustering (part 2)

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4.6: archetypal analysis

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