### Machine Learning Assignment

## Clustering

### Question 1 a

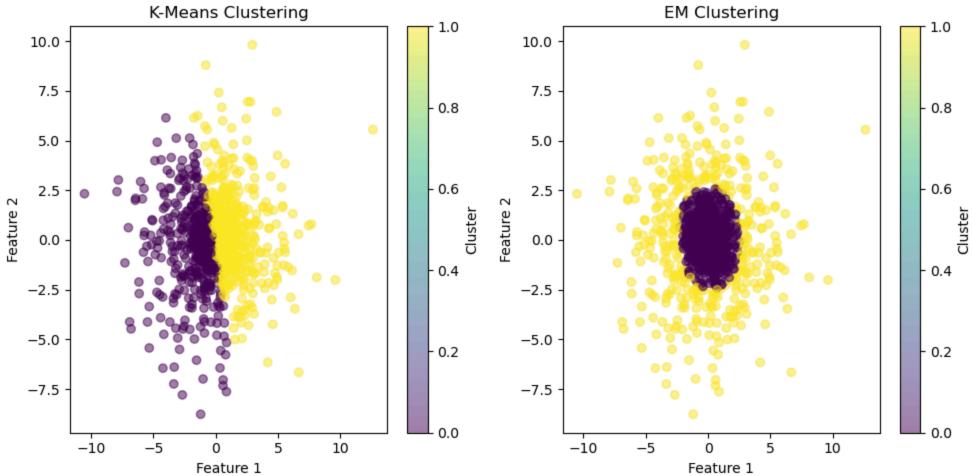
kmeans.fit(X dataset)

kmeans\_results[key].append(kmeans)

```
In [893... from sklearn.cluster import KMeans
         from sklearn.mixture import GaussianMixture
         import matplotlib.pyplot as plt
          import numpy as np
          from sklearn.metrics import accuracy_score, adjusted_rand_score
          from scipy.optimize import linear_sum_assignment
          import numpy as np
          from sklearn.datasets import make classification
          from sklearn.metrics.cluster import contingency_matrix
         from numpy import random
          import pandas as pd
         from scipy.stats import multivariate_normal
In [176... cov_matrix = 3**2 * np.eye(2)]
         X_Q = np.random.multivariate_normal(mean=[0, 0], cov=cov_matrix, size=500)
          y_Q = np.zeros(500, dtype=int)
In [177... def generate_Xa(a):
             Xa = np.random.multivariate_normal(mean=[a, 0], cov=np.eye(2), size=500)
              ya = np.ones(500, dtype=int)
              return Xa, ya
In [178... X_datasets = {}
         y labels = {}
         for a in range(5):
             Xa, ya = generate_Xa(a)
              X dataset combined = np.vstack((X Q, Xa))
             y_dataset_combined = np.concatenate((y_Q, ya))
             X_{datasets}[f'X_{a}] = X_{dataset\_combined}
             y_labels[f'y_{a}Q'] = y_dataset_combined
In [179... num_clusters = len(np.unique(y_labels['y_0Q'])) # since all lables have 0 and 1
          kmeans_results = {}
          em_results = {}
         for key, X_dataset in X_datasets.items():
              kmeans_results[key] = []
              for i in range(10):
                  kmeans = KMeans(n_clusters=num_clusters, init='random', n_init=1, random_state=i)
```

```
em_results[key] = []
for i in range(10):
    em = GaussianMixture(n_components=num_clusters, covariance_type='full', init_params='random', n_init=1, random_state=i)
    em.fit(X_dataset)
    em_results[key].append(em)
```

```
In [180... # we are choosing 5th Run
          kmeans_model_a_0 = kmeans_results['X_00'][5]
          em_model_a_0 = em_results['X_00'][5]
          kmeans_labels_a_0 = kmeans_model_a_0.predict(X_datasets['X_00'])
          em_labels_a_0 = em_model_a_0.predict(X_datasets['X_0Q'])
          plt.figure(figsize=(10, 5))
         plt.subplot(1, 2, 1)
         plt.scatter(X_datasets['X_00'][:, 0], X_datasets['X_00'][:, 1], c=kmeans_labels_a_0, cmap='viridis', alpha=0.5)
         plt.title('K-Means Clustering')
         plt.xlabel('Feature 1')
         plt.ylabel('Feature 2')
         plt.colorbar(label='Cluster')
         plt.subplot(1, 2, 2)
         plt.scatter(X_datasets['X_0Q'][:, 0], X_datasets['X_0Q'][:, 1], c=em_labels_a_0, cmap='viridis', alpha=0.5)
         plt.title('EM Clustering')
         plt.xlabel('Feature 1')
         plt.ylabel('Feature 2')
         plt.colorbar(label='Cluster')
         plt.tight_layout()
         plt.show()
```



```
row_ind, col_ind = linear_sum_assignment(-cont_matrix)
             accuracy = np.sum(cont_matrix[row_ind, col_ind]) / len(y_true)
             ari = adjusted_rand_score(y_true, y_pred)
             return accuracy, ari
In [182... kmeans metrics all = {}
         em_metrics_all = {}
         for a in range(5):
             dataset_key = f"X_{a}Q"
             label key = f''y \{a\}Q''
             kmeans metrics = []
             em_metrics = []
             true_labels = y_labels[label_key]
             for run_index in range(10):
                  kmeans_accuracy, kmeans_ari = compute_metrics(true_labels, kmeans_results[dataset_key][run_index].labels_)
                 kmeans metrics.append((kmeans accuracy, kmeans ari))
                 em accuracy, em ari = compute metrics(true labels, em results[dataset key][run index].predict(X datasets[dataset key]))
                 em_metrics.append((em_accuracy, em_ari))
              kmeans_metrics_all[dataset_key] = kmeans_metrics
              em_metrics_all[dataset_key] = em_metrics
         for dataset_key in kmeans_metrics_all.keys():
             print()
             print(f"Dataset: {dataset_key}")
             print("Accuracy and ARI for k-means clustering:")
             for i, (accuracy, ari) in enumerate(kmeans_metrics_all[dataset_key]):
                 print(f"Run {i + 1}: Accuracy = {accuracy:.4f}, ARI = {ari:.4f}")
             print("\nAccuracy and ARI for EM clustering:")
             for i, (accuracy, ari) in enumerate(em_metrics_all[dataset_key]):
                 print(f"Run {i + 1}: Accuracy = {accuracy:.4f}, ARI = {ari:.4f}")
```

In [12]: def compute\_metrics(y\_true, y\_pred):

cont\_matrix = contingency\_matrix(y\_true, y\_pred)

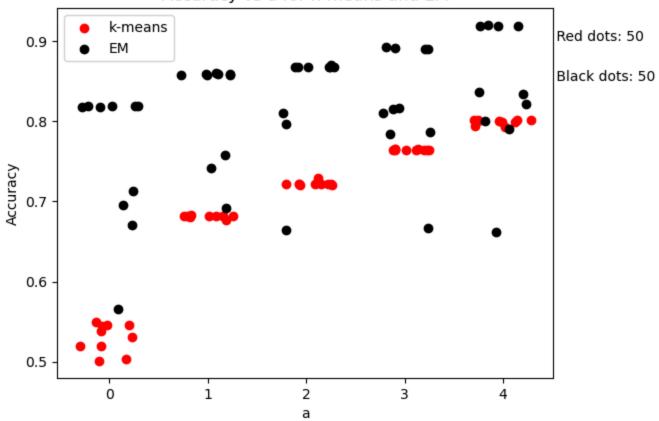
#### Dataset: X\_0Q Accuracy and ARI for k-means clustering: Run 1: Accuracy = 0.5780, ARI = 0.0234Run 2: Accuracy = 0.5160, ARI = 0.0000 Run 3: Accuracy = 0.5080, ARI = -0.0007Run 4: Accuracy = 0.5480, ARI = 0.0082Run 5: Accuracy = 0.5700, ARI = 0.0187Run 6: Accuracy = 0.5520, ARI = 0.0098Run 7: Accuracy = 0.5710, ARI = 0.0192Run 8: Accuracy = 0.5850, ARI = 0.0280Run 9: Accuracy = 0.5740, ARI = 0.0210Run 10: Accuracy = 0.5160, ARI = 0.0000Accuracy and ARI for EM clustering: Run 1: Accuracy = 0.8300, ARI = 0.4351Run 2: Accuracy = 0.8320, ARI = 0.4404Run 3: Accuracy = 0.6750, ARI = 0.1219Run 4: Accuracy = 0.5550, ARI = 0.0112Run 5: Accuracy = 0.8340, ARI = 0.4457Run 6: Accuracy = 0.8350, ARI = 0.4484Run 7: Accuracy = 0.5410, ARI = 0.0058Run 8: Accuracy = 0.8320, ARI = 0.4404Run 9: Accuracy = 0.7050, ARI = 0.1675Run 10: Accuracy = 0.8330, ARI = 0.4430Dataset: X 10 Accuracy and ARI for k-means clustering: Run 1: Accuracy = 0.6900, ARI = 0.1437Run 2: Accuracy = 0.6850, ARI = 0.1362Run 3: Accuracy = 0.6860, ARI = 0.1377Run 4: Accuracy = 0.6890, ARI = 0.1422Run 5: Accuracy = 0.6890, ARI = 0.1422Run 6: Accuracy = 0.6890, ARI = 0.1422Run 7: Accuracy = 0.6890, ARI = 0.1422Run 8: Accuracy = 0.6890, ARI = 0.1422Run 9: Accuracy = 0.6860, ARI = 0.1377Run 10: Accuracy = 0.6910, ARI = 0.1452Accuracy and ARI for EM clustering: Run 1: Accuracy = 0.8300, ARI = 0.4351Run 2: Accuracy = 0.8330, ARI = 0.4430Run 3: Accuracy = 0.6870, ARI = 0.1393Run 4: Accuracy = 0.8010, ARI = 0.3618Run 5: Accuracy = 0.8350, ARI = 0.4484Run 6: Accuracy = 0.8330, ARI = 0.4430Run 7: Accuracy = 0.6890, ARI = 0.1422Run 8: Accuracy = 0.8320, ARI = 0.4404Run 9: Accuracy = 0.7310, ARI = 0.2129Run 10: Accuracy = 0.8330, ARI = 0.4430Dataset: X\_2Q Accuracy and ARI for k-means clustering: Run 1: Accuracy = 0.7420, ARI = 0.2337Run 2: Accuracy = 0.7420, ARI = 0.2337Run 3: Accuracy = 0.7420, ARI = 0.2337Run 4: Accuracy = 0.7420, ARI = 0.2337Run 5: Accuracy = 0.7420, ARI = 0.2337Run 6: Accuracy = 0.7420, ARI = 0.2337Run 7: Accuracy = 0.7420, ARI = 0.2337Run 8: Accuracy = 0.7420, ARI = 0.2337Run 9: Accuracy = 0.7420, ARI = 0.2337Run 10: Accuracy = 0.7420, ARI = 0.2337

Accuracy and ARI for EM clustering:

```
Run 1: Accuracy = 0.8630, ARI = 0.5266
Run 2: Accuracy = 0.8640, ARI = 0.5295
Run 3: Accuracy = 0.7230, ARI = 0.1984
Run 4: Accuracy = 0.8210, ARI = 0.4116
Run 5: Accuracy = 0.8670, ARI = 0.5383
Run 6: Accuracy = 0.8630, ARI = 0.5266
Run 7: Accuracy = 0.7330, ARI = 0.2165
Run 8: Accuracy = 0.8660, ARI = 0.5354
Run 9: Accuracy = 0.7560, ARI = 0.2616
Run 10: Accuracy = 0.8630, ARI = 0.5266
Dataset: X 30
Accuracy and ARI for k-means clustering:
Run 1: Accuracy = 0.7820, ARI = 0.3175
Run 2: Accuracy = 0.7790, ARI = 0.3108
Run 3: Accuracy = 0.7820, ARI = 0.3175
Run 4: Accuracy = 0.7830, ARI = 0.3198
Run 5: Accuracy = 0.7830, ARI = 0.3198
Run 6: Accuracy = 0.7790, ARI = 0.3108
Run 7: Accuracy = 0.7760, ARI = 0.3041
Run 8: Accuracy = 0.7700, ARI = 0.2910
Run 9: Accuracy = 0.7790, ARI = 0.3108
Run 10: Accuracy = 0.7760, ARI = 0.3041
Accuracy and ARI for EM clustering:
Run 1: Accuracy = 0.7610, ARI = 0.2719
Run 2: Accuracy = 0.8690, ARI = 0.5442
Run 3: Accuracy = 0.6930, ARI = 0.1484
Run 4: Accuracy = 0.8360, ARI = 0.4511
Run 5: Accuracy = 0.8700, ARI = 0.5472
Run 6: Accuracy = 0.8690, ARI = 0.5442
Run 7: Accuracy = 0.7020, ARI = 0.1625
Run 8: Accuracy = 0.8700, ARI = 0.5472
Run 9: Accuracy = 0.7240, ARI = 0.2001
Run 10: Accuracy = 0.8700, ARI = 0.5472
Dataset: X_4Q
Accuracy and ARI for k-means clustering:
Run 1: Accuracy = 0.8310, ARI = 0.4377
Run 2: Accuracy = 0.8310, ARI = 0.4377
Run 3: Accuracy = 0.8310, ARI = 0.4377
Run 4: Accuracy = 0.8310, ARI = 0.4377
Run 5: Accuracy = 0.8310, ARI = 0.4377
Run 6: Accuracy = 0.8310, ARI = 0.4377
Run 7: Accuracy = 0.8310, ARI = 0.4377
Run 8: Accuracy = 0.8300, ARI = 0.4351
Run 9: Accuracy = 0.8310, ARI = 0.4377
Run 10: Accuracy = 0.8310, ARI = 0.4377
Accuracy and ARI for EM clustering:
Run 1: Accuracy = 0.7740, ARI = 0.2997
Run 2: Accuracy = 0.9120, ARI = 0.6787
Run 3: Accuracy = 0.6970, ARI = 0.1547
Run 4: Accuracy = 0.8890, ARI = 0.6049
Run 5: Accuracy = 0.9120, ARI = 0.6787
Run 6: Accuracy = 0.9130, ARI = 0.6820
Run 7: Accuracy = 0.6200, ARI = 0.0569
Run 8: Accuracy = 0.9130, ARI = 0.6820
Run 9: Accuracy = 0.6760, ARI = 0.1234
Run 10: Accuracy = 0.9120, ARI = 0.6787
```

```
for dataset_key in kmeans_metrics_all.keys():
    a = int(dataset_key.split('_')[1][:-1])
    kmeans_metrics = kmeans_metrics_all[dataset_key]
    em_metrics = em_metrics_all[dataset_key]
    for i in range(10):
        kmeans_accuracies.append((a, kmeans_metrics[i][0]))
        em_accuracies.append((a, em_metrics[i][0]))
a_kmeans, acc_kmeans = zip(*kmeans_accuracies)
a_em, acc_em = zip(*em_accuracies)
jitter_amount = 0.3
a_kmeans_jitter = np.array(a_kmeans) + np.random.uniform(-jitter_amount, jitter_amount, size=len(a_kmeans))
a_em_jitter = np.array(a_em) + np.random.uniform(-jitter_amount, jitter_amount, size=len(a_em))
plt.scatter(a_kmeans_jitter, acc_kmeans, color='red', label='k-means')
plt.scatter(a_em_jitter, acc_em, color='black', label='EM')
plt.xlabel('a')
plt.ylabel('Accuracy')
plt.xticks(range(5))
plt.title('Accuracy vs a for k-means and EM')
plt.legend()
plt.text(4.5, 0.9, f' Red dots: {len(acc_kmeans)}')
plt.text(4.5, 0.85, f' Black dots: {len(acc_em)}')
plt.show()
# added jitter for interpretability of scatter plots (to deal with overlapping data points)
```

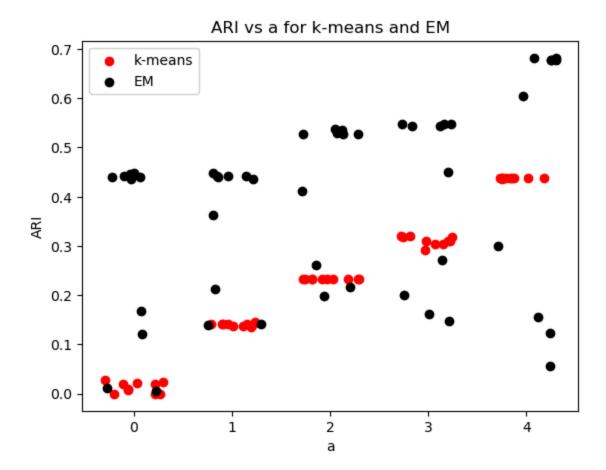
#### Accuracy vs a for k-means and EM



```
In [183... kmeans_ari_values = []
em ari values = []
```

```
for dataset_key in kmeans_metrics_all.keys():
    a = int(dataset_key.split('_')[1][:-1])
    kmeans_metrics = kmeans_metrics_all[dataset_key]
    em_metrics = em_metrics_all[dataset_key]
   for i in range(10):
        kmeans_ari_values.append((a, kmeans_metrics[i][1]))
        em_ari_values.append((a, em_metrics[i][1]))
a_kmeans_ari, ari_kmeans = zip(*kmeans_ari_values)
a_em_ari, ari_em = zip(*em_ari_values)
jitter_amount = 0.3
a_kmeans_ari_jitter = np.array(a_kmeans_ari) + np.random.uniform(-jitter_amount, jitter_amount, size=len(a_kmeans_ari))
a_em_ari_jitter = np.array(a_em_ari) + np.random.uniform(-jitter_amount, jitter_amount, size=len(a_em_ari))
plt.scatter(a_kmeans_ari_jitter, ari_kmeans, color='red', label='k-means')
plt.scatter(a_em_ari_jitter, ari_em, color='black', label='EM')
plt.xlabel('a')
plt.ylabel('ARI')
plt.xticks(range(5))
plt.title('ARI vs a for k-means and EM')
plt.legend()
plt.text(4.5, 0.9, f' Red dots: {len(ari_kmeans)}')
plt.text(4.5, 0.85, f' Black dots: {len(ari_em)}')
plt.show()
# added jitter for interpretability of scatter plots (to deal with overlapping data points)
```

Red dots: 50 Black dots: 50



# Question 1 b

```
distances = np.zeros((n_samples, n_clusters))
             for _ in range(max_iters):
                 for i, center in enumerate(cluster_centers):
                     distances[:, i] = np.linalg.norm(X - center, axis=1)
                 new_labels = np.argmin(distances, axis=1)
                 if np.all(new_labels == labels):
                     break
                 labels = new_labels
                 for i in range(n_clusters):
                     cluster_centers[i] = np.mean(X[labels == i], axis=0)
             return cluster centers, labels
In [110... def kmeans_with_full_covariance(X, n_clusters, max_iters=300, tol=1e-4):
             n_samples, n_features = X.shape
             cluster_centers = X[np.random.choice(n_samples, n_clusters, replace=False)]
             labels = np.zeros(n samples)
             distances = np.zeros((n_samples, n_clusters))
             for _ in range(max_iters):
                 for i, center in enumerate(cluster_centers):
                     diff = X - center
                     distances[:, i] = np.sqrt(np.sum(np.dot(diff, np.linalg.inv(np.cov(X.T))) * diff, axis=1))
                 new_labels = np.argmin(distances, axis=1)
                 if np.all(new_labels == labels):
                     break
                 labels = new_labels
                 for i in range(n clusters):
                     cluster_centers[i] = np.mean(X[labels == i], axis=0)
                 cov matrices = []
                 for i in range(n_clusters):
                     indices = np.where(labels == i)[0]
                     if len(indices) > 1:
                         diff = X[indices] - cluster_centers[i]
                         cov_matrix = np.dot(diff.T, diff) / (len(indices) - 1)
                         cov_matrices.append(cov_matrix)
                     else:
                         cov_matrices.append(np.zeros((n_features, n_features)))
             return cluster_centers, labels
In [112... def fit_gaussian_mixture(X, n_components, max_iters=300, tol=1e-4, random_state=None):
             np.random.seed(random_state)
```

labels = np.zeros(n\_samples)

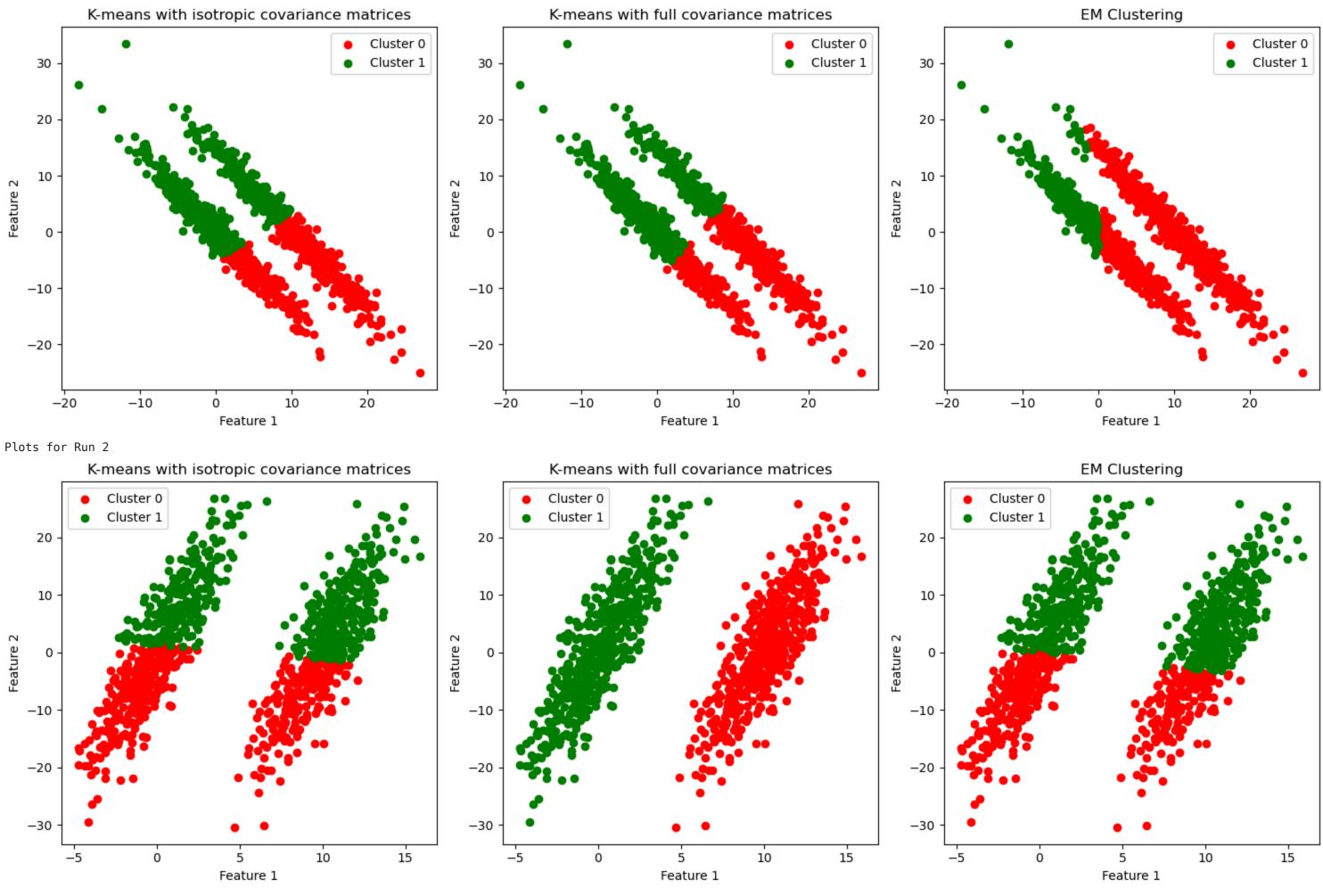
n\_samples, n\_features = X.shape

```
covariances = [np.cov(X.T) for _ in range(n_components)]
              weights = np.ones(n_components) / n_components
              log_likelihood_prev = -np.inf
              for _ in range(max_iters):
                  # E-step
                  responsibilities = np.zeros((n_samples, n_components))
                  for k in range(n components):
                      responsibilities[:, k] = weights[k] * multivariate_normal.pdf(X, mean=means[k], cov=covariances[k])
                  responsibilities /= responsibilities.sum(axis=1, keepdims=True)
                  # M-step
                  means = np.dot(responsibilities.T, X) / responsibilities.sum(axis=0)[:, np.newaxis]
                  covariances = [np.dot(responsibilities[:, k] * (X - means[k]).T, X - means[k]) / responsibilities[:, k].sum()
                                 for k in range(n_components)]
                  weights = responsibilities.mean(axis=0)
                  log_likelihood = np.log(np.sum([weights[k] * multivariate_normal.pdf(X, mean=means[k], cov=covariances[k])
                                                    for k in range(n_components)]))
                  if np.abs(log likelihood - log likelihood prev) < tol:</pre>
                      break
                  log_likelihood_prev = log_likelihood
              return means, covariances, weights
In [113... | results = {
              "kmeans_with_isotropic": [],
              "kmeans_full": [],
              "em clustering": [],
              "KL divergence": []
         for run number in range(10):
             M_{\text{matrix}} = \text{np.random.normal}(0, 1, (2, 2))
              U, D, Vt = np.linalg.svd(M_matrix)
              U matrix = U
              Cov_matrix = np.dot(U_matrix, np.dot(np.diag([100, 1]), U_matrix.T))
              Q = np.random.multivariate_normal(mean=[0, 0], cov=Cov_matrix, size=500)
              Q labels = np.zeros(500)
              P = np.random.multivariate_normal(mean=[10, 0], cov=Cov_matrix, size=500)
              P_{\text{labels}} = np.ones(500)
              #KL divergence = calculate KL divergence(P, Q, Cov matrix)
              KL_divergence = calculate_KL_divergence(Cov_matrix)
              QP_dataset = np.vstack((Q, P))
              true_labels = np.concatenate((Q_labels, P_labels))
              _, kmeans_iso_labels = kmeans_with_isotropic(QP_dataset, n_clusters=2)
              _, kmeans_full_labels = kmeans_with_full_covariance(QP_dataset, n_clusters=2)
              means, covariances, weights = fit_gaussian_mixture(QP_dataset, n_components=2)
```

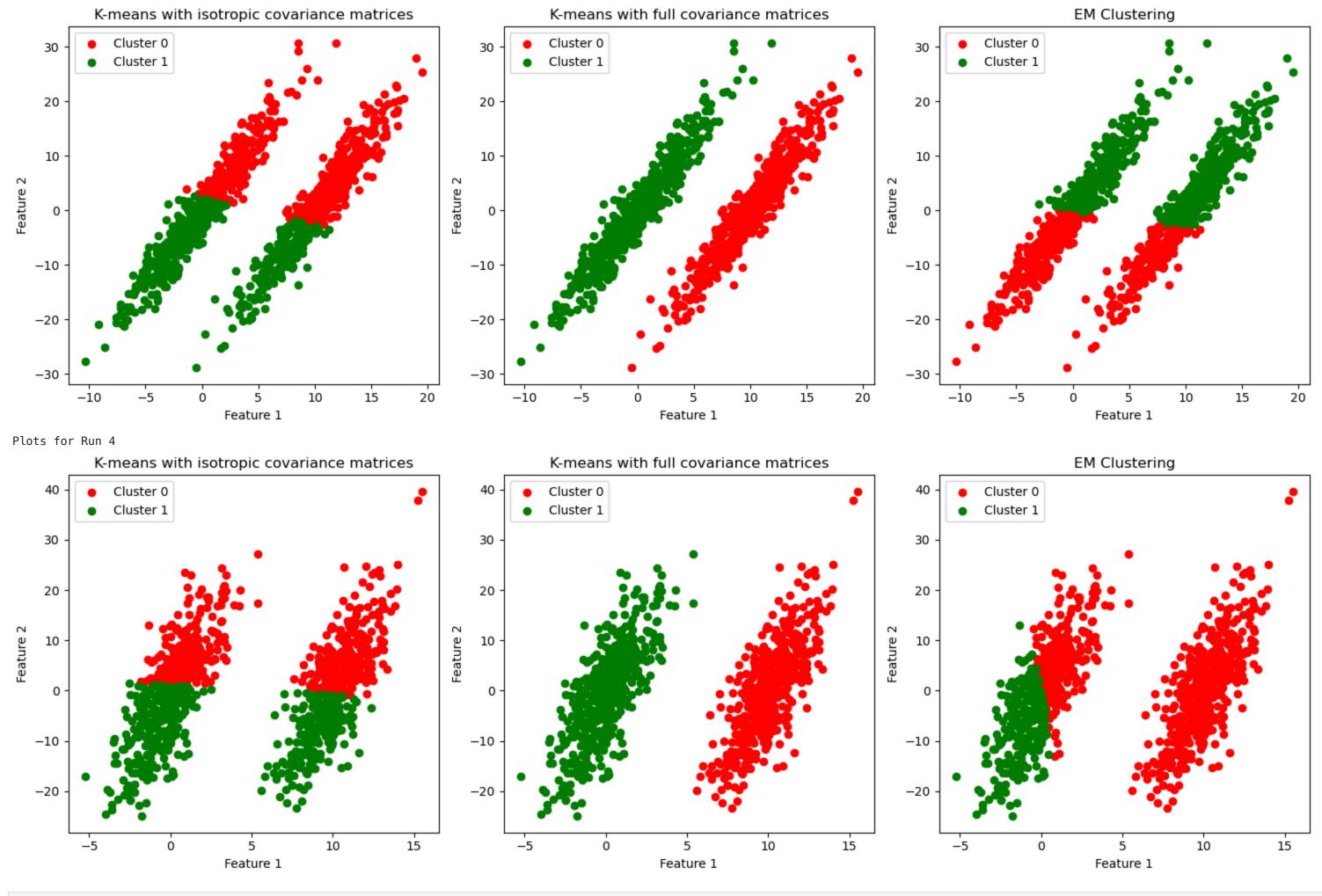
means = X[np.random.choice(n\_samples, n\_components, replace=False)]

```
em_labels = np.argmax(np.dot(QP_dataset, means.T) + np.log(weights), axis=1)
accuracy_iso, ari_iso = compute_metrics(true_labels, kmeans_iso_labels)
accuracy_full, ari_full = compute_metrics(true_labels, kmeans_full_labels)
accuracy_em, ari_em = compute_metrics(true_labels, em_labels)
results["kmeans_with_isotropic"].append({"run_number": run_number + 1, "accuracy": accuracy_iso, "ari": ari_iso})
results["kmeans full"].append({"run number": run number + 1, "accuracy": accuracy full, "ari": ari full})
results["em_clustering"].append({"run_number": run_number + 1, "accuracy": accuracy_em, "ari": ari_em})
results["KL divergence"].append(KL divergence)
colors = ['r', 'g', 'b', 'c', 'm', 'y', 'k']
if run_number < 4:</pre>
    print(f"Plots for Run {run number + 1}")
    plt.figure(figsize=(15, 5))
    plt.subplot(1, 3, 1)
    for label in np.unique(kmeans_iso_labels):
        plt.scatter(QP_dataset[kmeans_iso_labels == label][:, 0], QP_dataset[kmeans_iso_labels == label][:, 1], color=colors[label], label=f'Cluster {label}')
    plt.title('K-means with isotropic covariance matrices')
    plt.xlabel('Feature 1')
    plt.ylabel('Feature 2')
    plt.legend()
    plt.subplot(1, 3, 2)
    for label in np.unique(kmeans full labels):
        plt.scatter(QP_dataset[kmeans_full_labels == label][:, 0], QP_dataset[kmeans_full_labels == label][:, 1], color=colors[label], label=f'Cluster {label}')
    plt.title('K-means with full covariance matrices')
    plt.xlabel('Feature 1')
   plt.ylabel('Feature 2')
    plt.legend()
    plt.subplot(1, 3, 3)
    for label in np.unique(em_labels):
        plt.scatter(QP dataset[em labels == label][:, 0], QP dataset[em labels == label][:, 1], color=colors[label], label=f'Cluster {label}')
    plt.title('EM Clustering')
    plt.xlabel('Feature 1')
    plt.ylabel('Feature 2')
    plt.legend()
    plt.tight_layout()
    plt.show()
```

Plots for Run 1

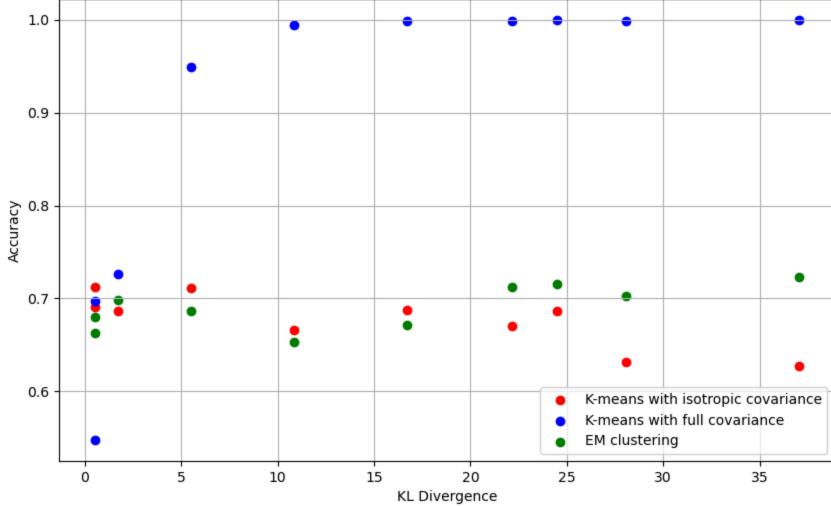


Plots for Run 3



Total Dots: 30

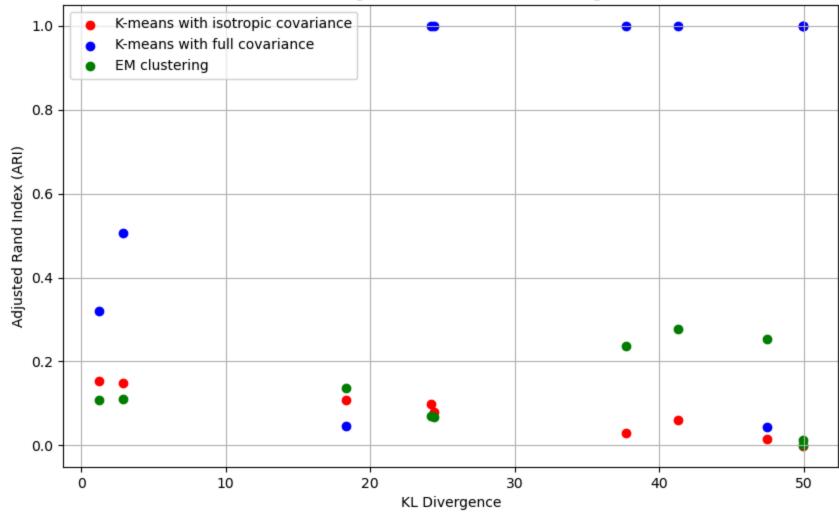




```
In [107... kmeans_iso_ari = [result['ari'] for result in results['kmeans_with_isotropic']]
   kmeans_full_ari = [result['ari'] for result in results['kmeans_full']]
   em_ari = [result['ari'] for result in results['em_clustering']]
   kl_divergence = results['KL_divergence']
```

Total Dots: 30





```
In [114... kmeans_iso_accuracy = [result['accuracy'] for result in results['kmeans_with_isotropic']]
kmeans_iso_ari = [result['ari'] for result in results['kmeans_with_isotropic']]
kmeans_full_accuracy = [result['accuracy'] for result in results['kmeans_full']]
kmeans_full_ari = [result['ari'] for result in results['kmeans_full']]
em_accuracy = [result['accuracy'] for result in results['em_clustering']]
em_ari = [result['ari'] for result in results['em_clustering']]
```

```
kl_divergence = results['KL_divergence']
df = pd.DataFrame({
    "Run": [i + 1 for i in range(10)],
    "KIso(Accuracy)": kmeans_iso_accuracy,
    "KIso(ARI)": kmeans_iso_ari,
    "KFull(Accuracy)": kmeans_full_accuracy,
    "KFull(ARI)": kmeans_full_ari,
   "EM(Accuracy)": em_accuracy,
   "EM(ARI)": em_ari,
    "KL Divergence": kl_divergence
})
pd.set option('display.max columns', None)
pd.set_option('display.expand_frame_repr', False)
print(df)
  Run KIso(Accuracy) KIso(ARI) KFull(Accuracy) KFull(ARI) EM(Accuracy)
                                                                           EM(ARI) KL Divergence
                0.622 0.058595
                                                                    0.734 0.218413
                                                                                        33.854417
                                           0.654
                                                   0.093957
    2
                0.562 0.014391
                                                   1.000000
                                                                    0.572 0.019774
                                                                                        48.573051
1
                                           1.000
    3
                0.615 0.051951
                                           1.000
                                                   1.000000
                                                                    0.583 0.026587
                                                                                        44.934097
                0.542 0.006066
    4
                                           1.000
                                                   1.000000
                                                                    0.757 0.263633
                                                                                        49.247311
    5
                0.583
                       0.026593
                                                   1.000000
                                                                    0.723 0.198353
                                                                                        43.191435
                                           1.000
5
                                                                    0.705 0.167435
    6
                0.642 0.079736
                                           1.000
                                                   1.000000
                                                                                        26.753354
                0.619 0.055700
                                                                    0.705 0.167467
                                                                                        29.052020
6
    7
                                           0.687
                                                   0.139016
    8
                0.644 0.082032
                                           0.554
                                                   0.010677
                                                                    0.707 0.170692
                                                                                        16.306208
                                                                    0.761 0.271922
8
    9
                0.572 0.019755
                                                                                        48.028811
                                           1.000
                                                   1.000000
   10
                0.702 0.162378
                                           0.988
                                                   0.952528
                                                                    0.672 0.117591
                                                                                        10.277155
```