Лабораторная работа №4 по курсу "Интеллектуальный анализ данных"

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4.1 Кластеризация иерархическим алгоритмом

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt

from scipy.cluster import hierarchy
from scipy.spatial.distance import pdist
```

In [2]:
```
distance_mat = np.array([
    [0. ,  3.3,  3.2,  1.6,  4.8,  5.1],
    [3.3,  0.,   4.5,  3.25, 1.2,  2.6],
    [3.2,  4.5,  0. ,  1.4,  0.5,  2.3],
    [1.6,  3.25, 1.4,  0. ,  4.2,  1.8],
    [4.8,  1.2,  0.5,  4.2,  0.,   2.6],
    [5.1,  2.6,  2.3,  1.8 , 2.6,  0. ]
])
```

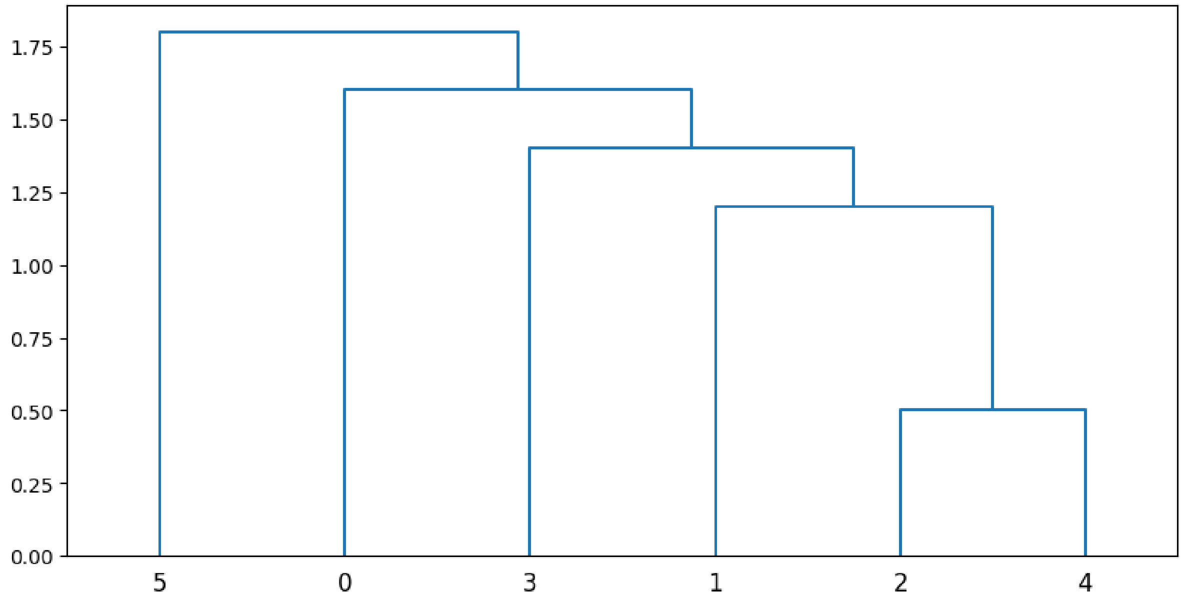
In [3]:
```
upper_triangle_dist_mat = np.array(
    [3.3, 3.2, 1.6, 4.8, 5.1, 4.5, 3.25, 1.2, 2.6, 1.4, 0.5, 2.3, 4.2, 1.8, 2.6]
)
```

Ближайший сосед

In [4]:
```
from sklearn.cluster import AgglomerativeClustering, ward_tree
```

In [5]:
```
Z = hierarchy.linkage(upper_triangle_dist_mat, "single")
```

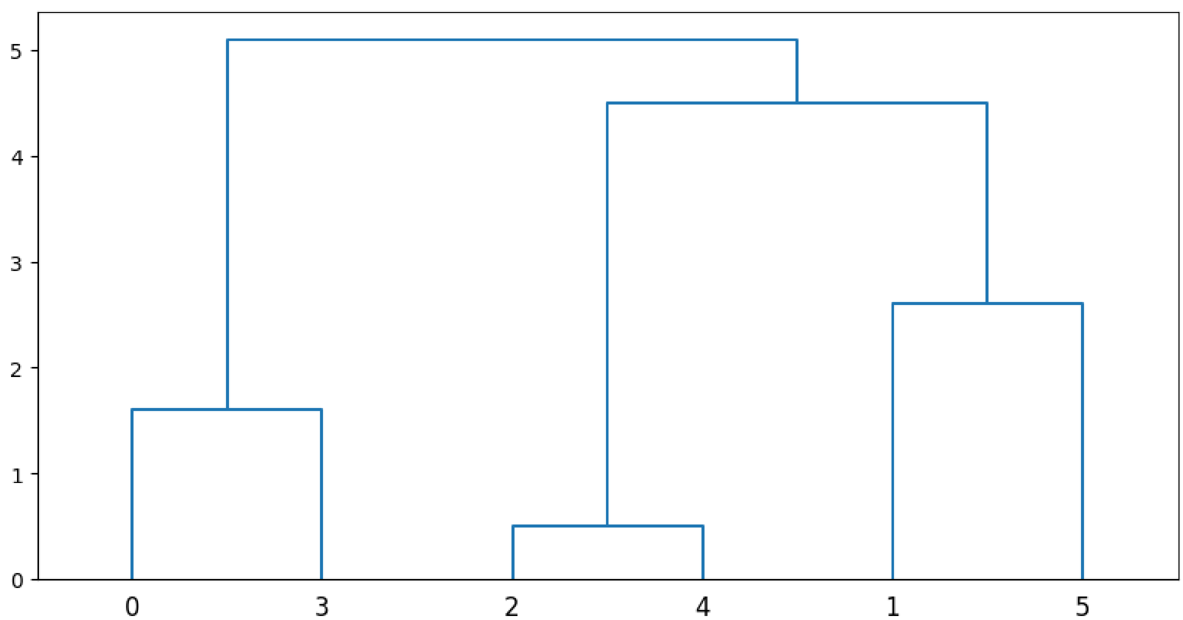
In [6]:
```
plt.figure(figsize=(10, 5))
dn = hierarchy.dendrogram(Z, color_threshold=0.5)
```



Наиболее удаленный сосед

In [7]:
```
Z = hierarchy.linkage(upper_triangle_dist_mat, "complete")
```

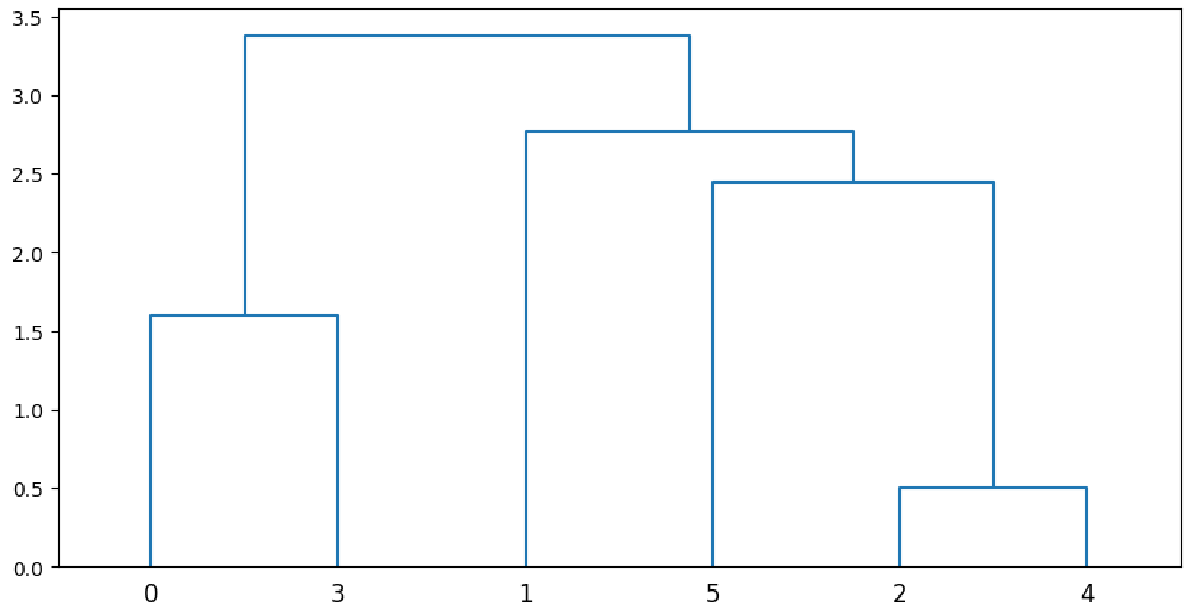
In [8]:
```
plt.figure(figsize=(10, 5))
dn = hierarchy.dendrogram(Z, color_threshold=0.5)
```



Средняя связь

In [9]:
```
Z = hierarchy.linkage(upper_triangle_dist_mat, "average")
```

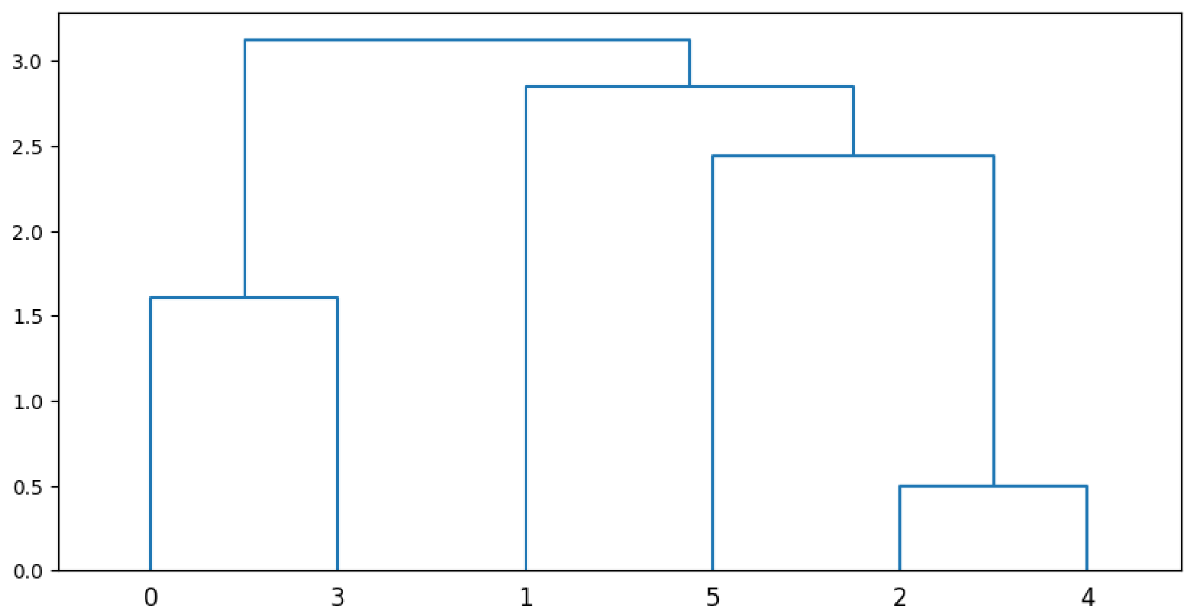
In [10]:
```
plt.figure(figsize=(10, 5))
dn = hierarchy.dendrogram(Z, color_threshold=0.5)
```



Центроидный метод

In [11]:
```
Z = hierarchy.linkage(upper_triangle_dist_mat, "centroid")
```

In [12]:
```
plt.figure(figsize=(10, 5))
dn = hierarchy.dendrogram(Z, color_threshold=0.5)
```



Сравнение результатов

Используем метрику оценки Silhouette

In [13]:
```
import pandas as pd
from sklearn import datasets, metrics
from sklearn.cluster import AgglomerativeClustering
```

```
data = datasets.load_digits()
X, y = data.data, data.target

n_clusters = 6


algorithms = []
for i in range(2, n_clusters):
    algorithms.append(AgglomerativeClustering(n_clusters=i, metric='precomputed', l
    algorithms.append(AgglomerativeClustering(n_clusters=i, metric='precomputed', l
    algorithms.append(AgglomerativeClustering(n_clusters=i, metric='precomputed', l

data = []
for algo in algorithms:
    algo.fit(distance_mat)
    data.append(
        (
            {
                "Silhouette": metrics.silhouette_score(distance_mat, algo.labels_)
            }
        )
    )

results = pd.DataFrame(
    data=data,
    columns=["Silhouette"],
    index=[
        'Single, n = 2', 'Complete, n = 2', 'Average, n = 2',
        'Single, n = 3', 'Complete, n = 3', 'Average, n = 3',
        'Single, n = 4', 'Complete, n = 4', 'Average, n = 4',
        'Single, n = 5', 'Complete, n = 5', 'Average, n = 5',
    ],
)

results
```

Out[13]:

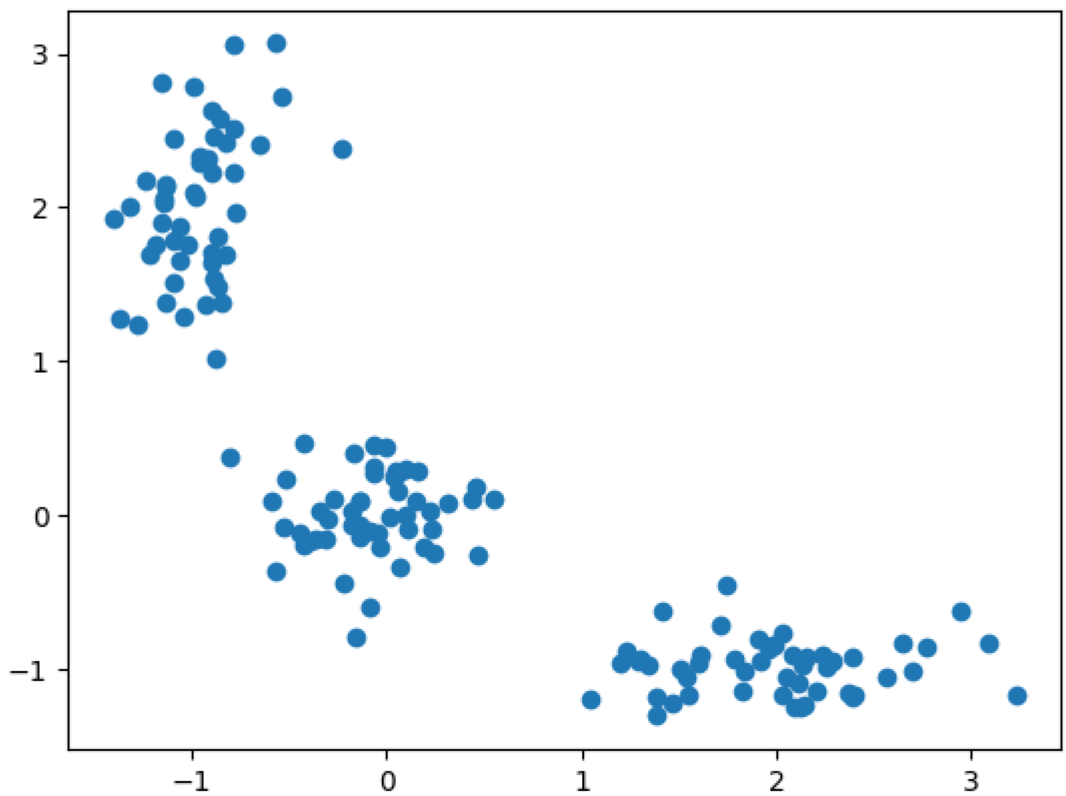
	Silhouette
Single, n = 2	-0.099914
Complete, n = 2	0.247890
Average, n = 2	0.247890
Single, n = 3	-0.107858
Complete, n = 3	0.146005
Average, n = 3	0.125300
Single, n = 4	-0.037944
Complete, n = 4	0.070679
Average, n = 4	0.070679
Single, n = 5	0.000967
Complete, n = 5	0.000967
Average, n = 5	0.000967

Пример кластеризации большого искусственного датасета:

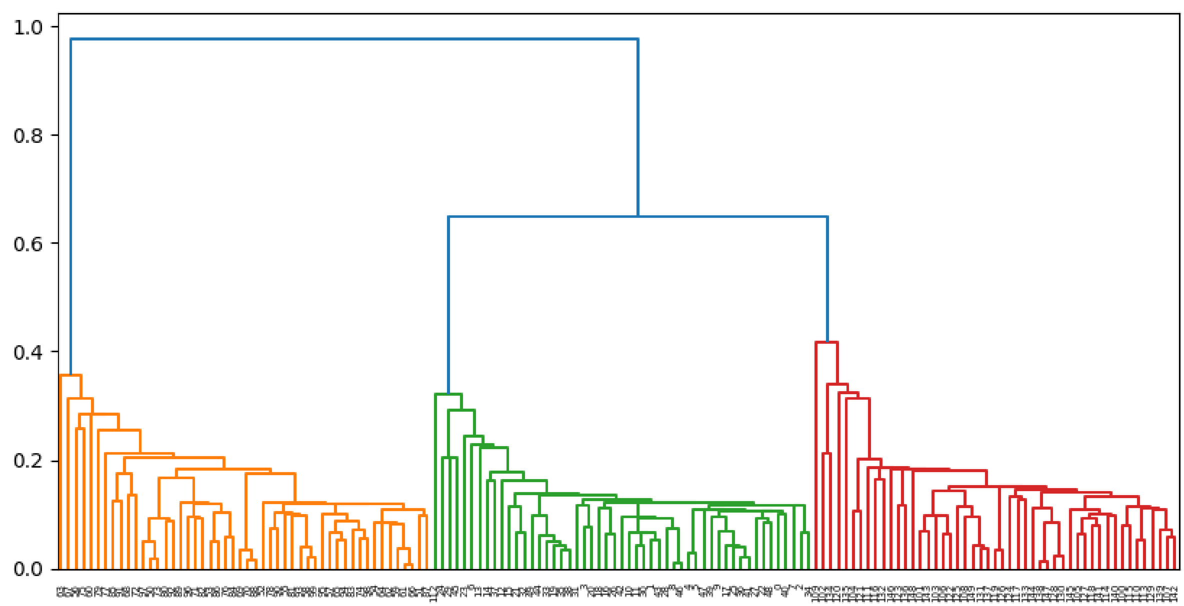
In [18]:
```
X = np.zeros((150, 2))

np.random.seed(seed=42)
X[:50, 0] = np.random.normal(loc=0.0, scale=0.3, size=50)
X[:50, 1] = np.random.normal(loc=0.0, scale=0.3, size=50)

X[50:100, 0] = np.random.normal(loc=2.0, scale=0.5, size=50)
X[50:100, 1] = np.random.normal(loc=-1.0, scale=0.2, size=50)

X[100:150, 0] = np.random.normal(loc=-1.0, scale=0.2, size=50)
X[100:150, 1] = np.random.normal(loc=2.0, scale=0.5, size=50)
```

In [19]:
```
plt.scatter(X[:, 0], X[:, 1])
```

Out[19]:
```
<matplotlib.collections.PathCollection at 0x29259f04f10>
```



In [20]:
```
distance_mat = pdist(X)
Z = hierarchy.linkage(distance_mat, "single")
plt.figure(figsize=(10, 5))
dn = hierarchy.dendrogram(Z, color_threshold=0.5)
```



4.2 Кластеризация методом k-средних

6 вариант

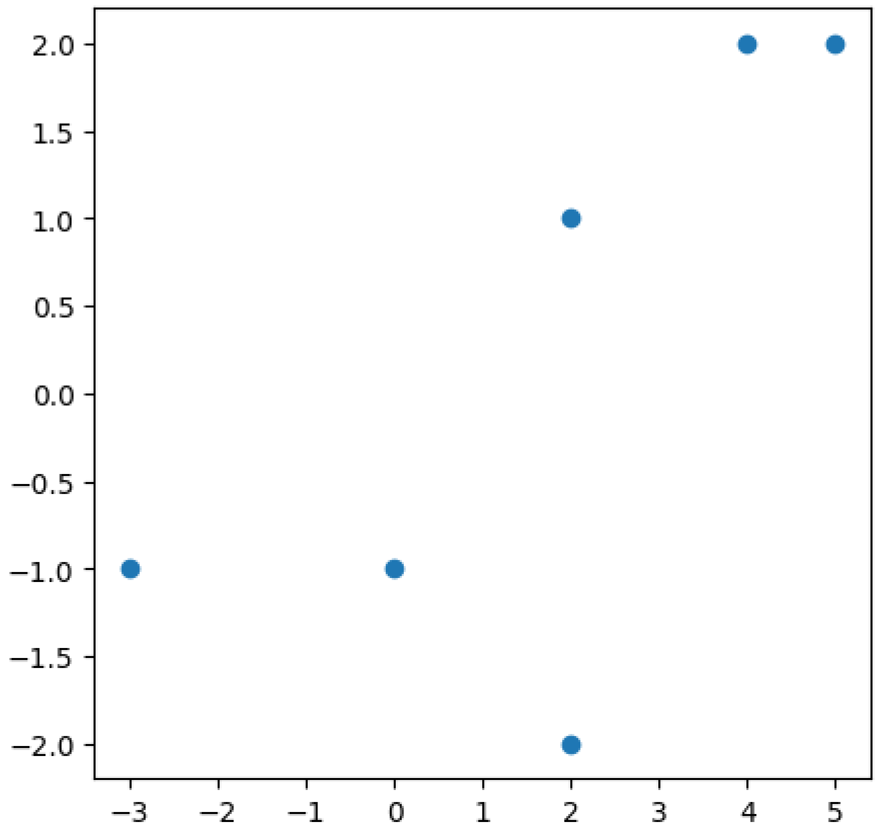
In [21]:
```
from scipy.spatial.distance import cdist
```

```python
from sklearn.cluster import KMeans
```

In [22]:
```python
X = np.array(
    [
        [2, 1], [5, 2], [-3, -1], [4, 2], [0, -1], [2, -2]
    ]
)
```

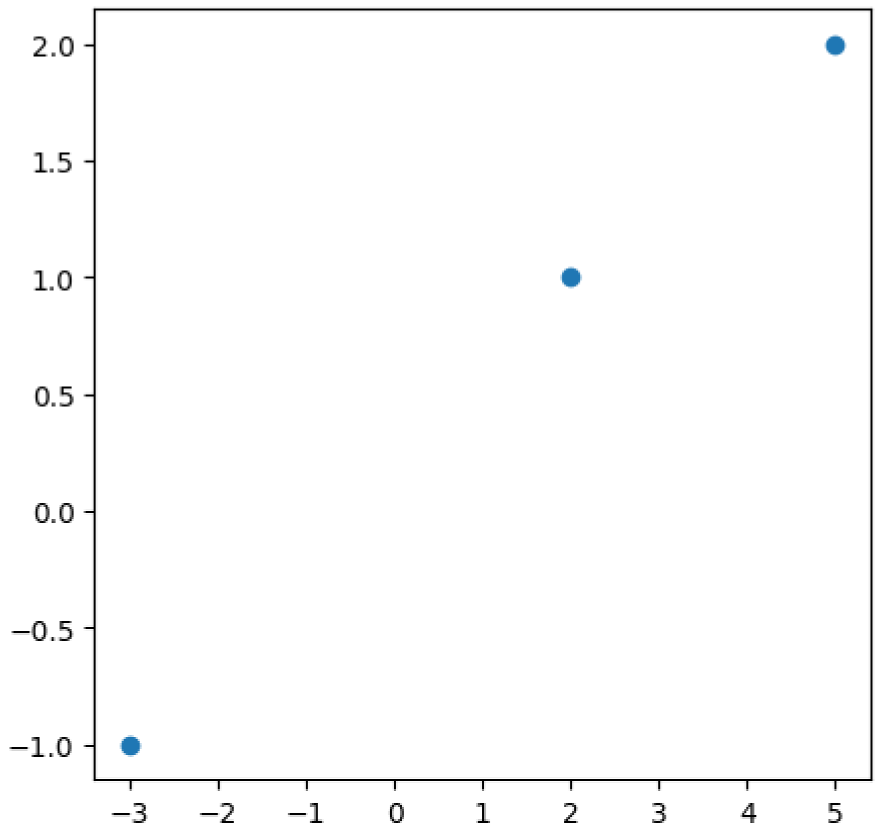
In [23]:
```python
plt.figure(figsize=(5, 5))
plt.scatter(X[:, 0], X[:, 1])
```

Out[23]: <matplotlib.collections.PathCollection at 0x29259d74550>



In [24]:
```python
centroids = np.array([X[0, :], X[1, :], X[2, :]])

plt.figure(figsize=(5, 5))
plt.scatter(centroids[:, 0], centroids[:, 1])
```

Out[24]: <matplotlib.collections.PathCollection at 0x29259ef4090>

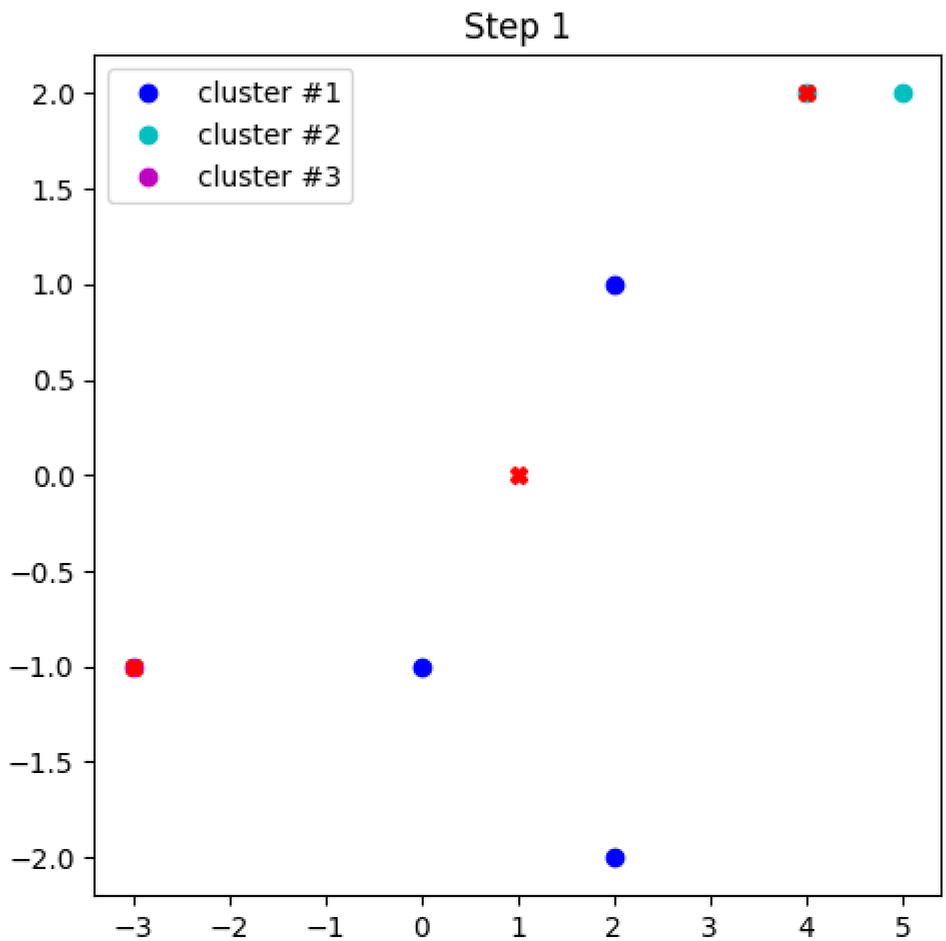


In [28]:

```
cent_history = []
cent_history.append(centroids)

for i in range(3):
    distances = cdist(X, centroids)
    labels = distances.argmin(axis=1)

    centroids = centroids.copy()
    centroids[0, :] = np.mean(X[labels == 0, :], axis=0)
    centroids[1, :] = np.mean(X[labels == 1, :], axis=0)
    centroids[2, :] = np.mean(X[labels == 2, :], axis=0)

    cent_history.append(centroids)
```

In [29]:

```
plt.figure(figsize=(12, 12))
for i in range(1):
    distances = cdist(X, cent_history[i])
    labels = distances.argmin(axis=1)

    plt.subplot(2, 2, i + 1)
    plt.plot(X[labels == 0, 0], X[labels == 0, 1], "bo", label="cluster #1")
    plt.plot(X[labels == 1, 0], X[labels == 1, 1], "co", label="cluster #2")
    plt.plot(X[labels == 2, 0], X[labels == 2, 1], "mo", label="cluster #3")
    plt.plot(cent_history[i][:, 0], cent_history[i][:, 1], "rX")
    plt.legend(loc=0)
    plt.title("Step {:}".format(i + 1));
```

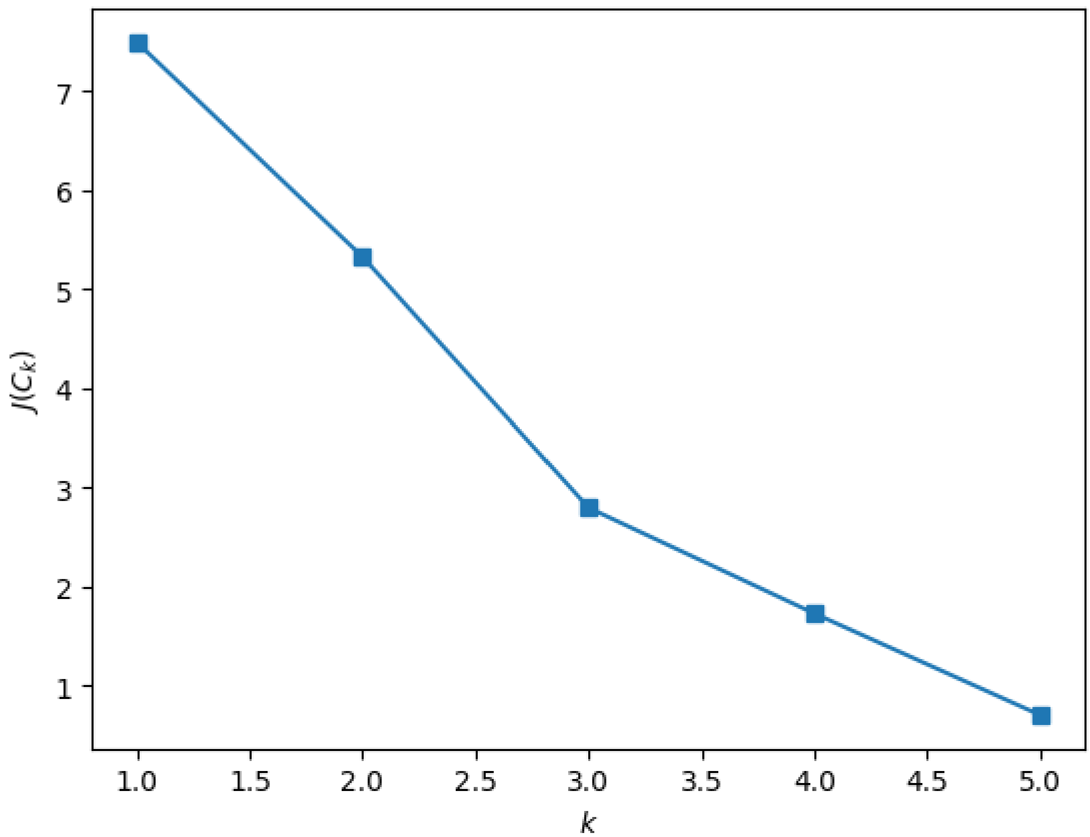


Выбор оптимального числа кластеров

In [30]:
```
inertia = []
for k in range(1, 6):
    kmeans = KMeans(n_clusters=k, random_state=1, n_init='auto').fit(X)
    inertia.append(np.sqrt(kmeans.inertia_))
```

График величины 'Inertia' уменьшает скорость убывания в тот момент когда количество кластеров оптимальное

In [31]:
```
plt.plot(range(1, 6), inertia, marker="s")
plt.xlabel("$k$")
plt.ylabel("$J(C_k)$");
```



4.3 Кластеризация ирисов Фишера

In [44]:
```
from sklearn.mixture import GaussianMixture
from sklearn import datasets
from sklearn.decomposition import PCA
from sklearn.metrics import accuracy_score, classification_report

import pandas as pd
```

In [34]:
```
iris = datasets.load_iris()
```

Загрузка датасета в пандас:

In [36]:
```
df = pd.DataFrame(data= np.c_[iris['data'], iris['target']],
                  columns= iris['feature_names'] + ['target'])

df
```

Out[36]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
0	5.1	3.5	1.4	0.2	0.0
1	4.9	3.0	1.4	0.2	0.0
2	4.7	3.2	1.3	0.2	0.0
3	4.6	3.1	1.5	0.2	0.0
4	5.0	3.6	1.4	0.2	0.0
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	2.0
146	6.3	2.5	5.0	1.9	2.0
147	6.5	3.0	5.2	2.0	2.0
148	6.2	3.4	5.4	2.3	2.0
149	5.9	3.0	5.1	1.8	2.0

150 rows × 5 columns

In [37]:

```
X = df.drop(['target'], axis=1)
```

In [38]:

```
target = df['target'].values
target = np.int16(target)
```

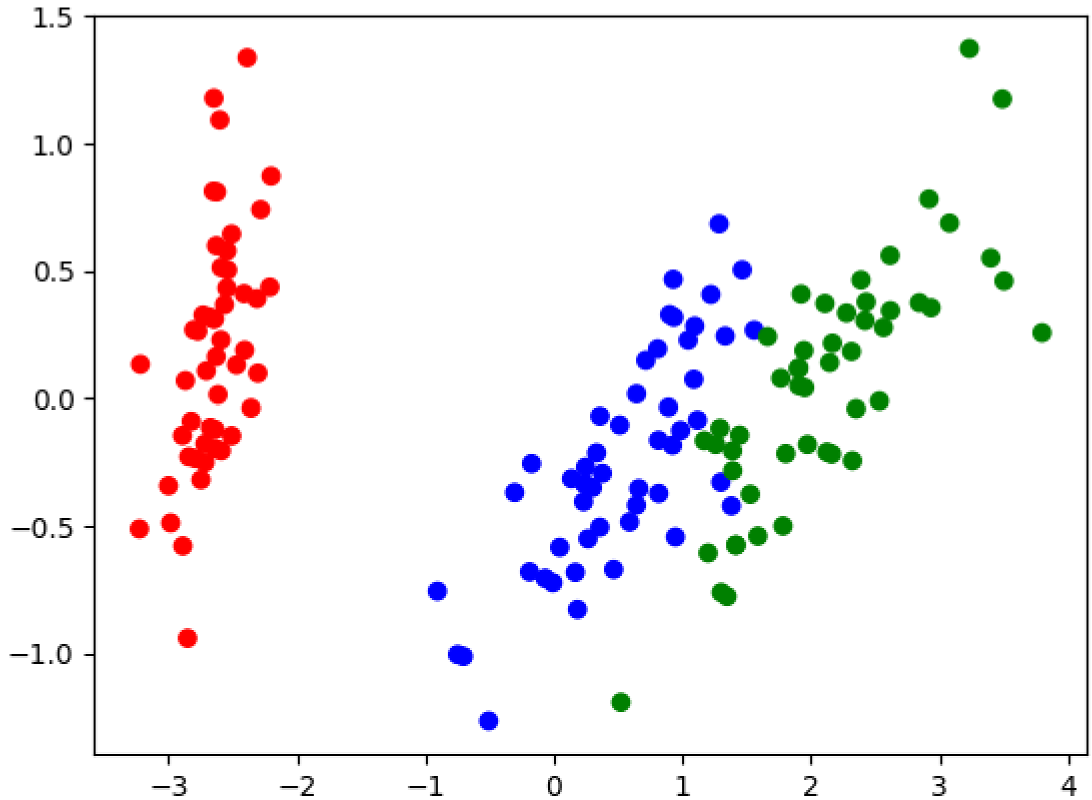
PCA

In [39]:

```
pca = PCA(n_components=2)
X_2d = pca.fit_transform(X)

color_map = {
    '0': 'r',
    '1': 'b',
    '2': 'g'
}

colors = []
for i in range(target.shape[0]):
    colors.append(color_map[f'{target[i]}'])

plt.scatter(X_2d[:, 0], X_2d[:, 1], c=colors)
```

Out[39]:

```
<matplotlib.collections.PathCollection at 0x2925a1ac290>
```



In [40]:
```
gm = GaussianMixture(n_components=3).fit(X)
```

In [41]:
```
y_pred = gm.predict(X)
```

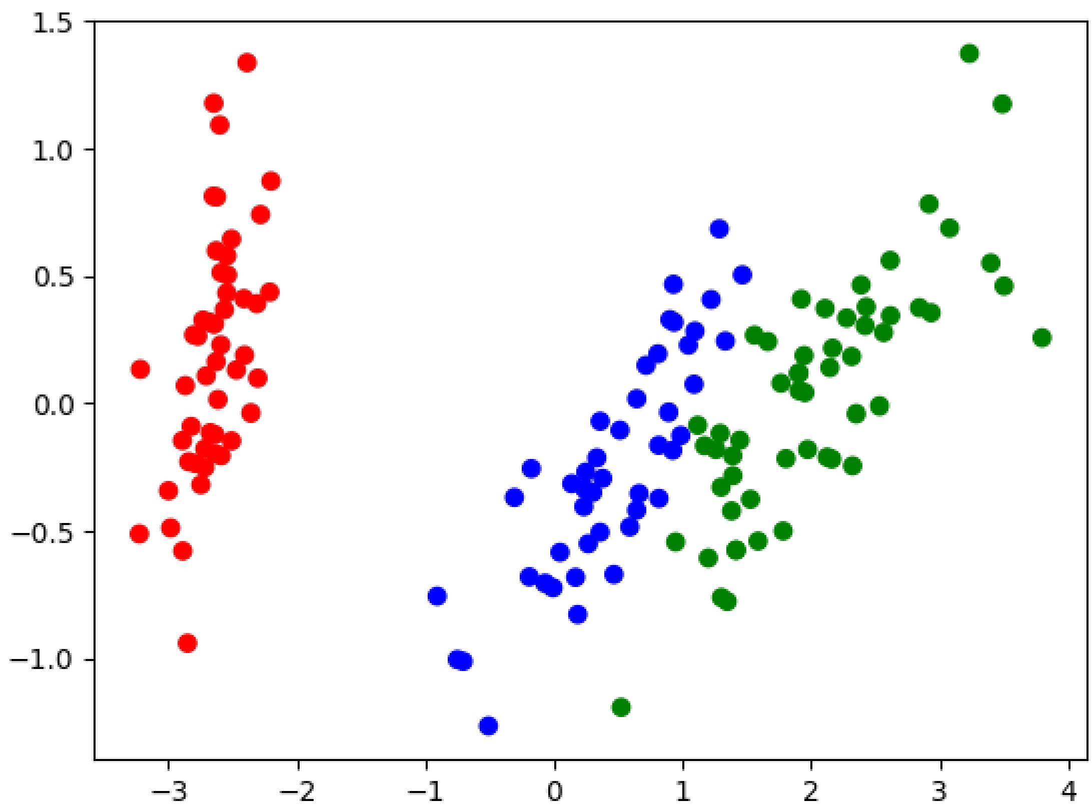
In [45]:
```
print(classification_report(target, y_pred))
```

```
              precision    recall  f1-score   support

           0       1.00      1.00      1.00        50
           1       1.00      0.90      0.95        50
           2       0.91      1.00      0.95        50

    accuracy                           0.97       150
   macro avg       0.97      0.97      0.97       150
weighted avg       0.97      0.97      0.97       150
```

Визулизация через PCA:

In [46]:
```
colors = []
for i in range(target.shape[0]):
    colors.append(color_map[f'{y_pred[i]}'])

plt.scatter(X_2d[:, 0], X_2d[:, 1], c=colors)
```

Out[46]:
```
<matplotlib.collections.PathCollection at 0x2925b59c290>
```


1.5
1.0
0.5
0.0
−0.5
−1.0
−3
−2
−1
0
1
2
3
4