plot_kmeans_digits

A demo of K-Means clustering on the handwritten digits data

In this example we compare the various initialization strategies for K-means in terms of runtime and quality of the results.

As the ground truth is known here, we also apply different cluster quality metrics to judge the goodness of fit of the cluster labels to the ground truth.

Cluster quality metrics evaluated (see `clustering_evaluation` for definitions and discussions of the metrics):

```
 =========== ========================================================
Shorthand    full name
=========== ========================================================
homo         homogeneity score
compl        completeness score
v-meas       V measure
ARI          adjusted Rand index
AMI          adjusted mutual information
silhouette   silhouette coefficient
=========== ========================================================
```

Load the dataset

We will start by loading the `digits` dataset. This dataset contains handwritten digits from 0 to 9. In the context of clustering, one would like to group images such that the handwritten digits on the image are the same.

```
In [9]: import numpy as np
        from sklearn.datasets import load_digits

        data, labels = load_digits(return_X_y=True)
        (n_samples, n_features), n_digits = data.shape, np.unique(labels).size

        print(f"# digits: {n_digits}; # samples: {n_samples}; # features {n_features}")
```

```
# digits: 10; # samples: 1797; # features 64
```

Define our evaluation benchmark

We will first our evaluation benchmark. During this benchmark, we intend to compare different initialization methods for KMeans. Our benchmark will:

- create a pipeline which will scale the data using a :class: `~sklearn.preprocessing.StandardScaler` ;
- train and time the pipeline fitting;
- measure the performance of the clustering obtained via different metrics.

In [10]:
```python
from time import time
from sklearn import metrics
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler


def bench_k_means(kmeans, name, data, labels):
    """Benchmark to evaluate the KMeans initialization methods.

    Parameters
    ----------
    kmeans : KMeans instance
        A :class:`~sklearn.cluster.KMeans` instance with the initialization
        already set.
    name : str
        Name given to the strategy. It will be used to show the results in a
        table.
    data : ndarray of shape (n_samples, n_features)
        The data to cluster.
    labels : ndarray of shape (n_samples,)
        The labels used to compute the clustering metrics which requires some
        supervision.
    """
    t0 = time()
    estimator = make_pipeline(StandardScaler(), kmeans).fit(data)
    fit_time = time() - t0
    results = [name, fit_time, estimator[-1].inertia_]

    # Define the metrics which require only the true labels and estimator
    # labels
    clustering_metrics = [
        metrics.homogeneity_score,
        metrics.completeness_score,
        metrics.v_measure_score,
        metrics.adjusted_rand_score,
        metrics.adjusted_mutual_info_score,
    ]
    results += [m(labels, estimator[-1].labels_) for m in clustering_metrics]

    # The silhouette score requires the full dataset
    results += [
        metrics.silhouette_score(data, estimator[-1].labels_,
                                      metric="euclidean", sample_size=300,)
    ]

    # Show the results
    formatter_result = ("{:9s}\t{:.3f}s\t{:.0f}\t{:.3f}\t{:.3f}"
                        "\t{:.3f}\t{:.3f}\t{:.3f}\t{:.3f}")
    print(formatter_result.format(*results))
```

Run the benchmark

We will compare three approaches:

- an initialization using `kmeans++` . This method is stochastic and we will run the initialization 4 times;
- a random initialization. This method is stochastic as well and we will run the initialization 4 times;
- an initialization based on a :class: `~sklearn.decomposition.PCA` projection. Indeed, we will use the components of the :class: `~sklearn.decomposition.PCA` to initialize KMeans. This method is deterministic and a single initialization suffice.

In [11]:
```
from sklearn.cluster import KMeans
from sklearn.decomposition import PCA

print(82 * '_')
print('init\t\ttime\tinertia\thomo\tcompl\tv-meas\tARI\tAMI\tsilhouette')

kmeans = KMeans(init="k-means++", n_clusters=n_digits, n_init=4,
                random_state=0)
bench_k_means(kmeans=kmeans, name="k-means++", data=data, labels=labels)

kmeans = KMeans(init="random", n_clusters=n_digits, n_init=4, random_state=0)
bench_k_means(kmeans=kmeans, name="random", data=data, labels=labels)

pca = PCA(n_components=n_digits).fit(data)
kmeans = KMeans(init=pca.components_, n_clusters=n_digits, n_init=1)
bench_k_means(kmeans=kmeans, name="PCA-based", data=data, labels=labels)

print(82 * '_')
```

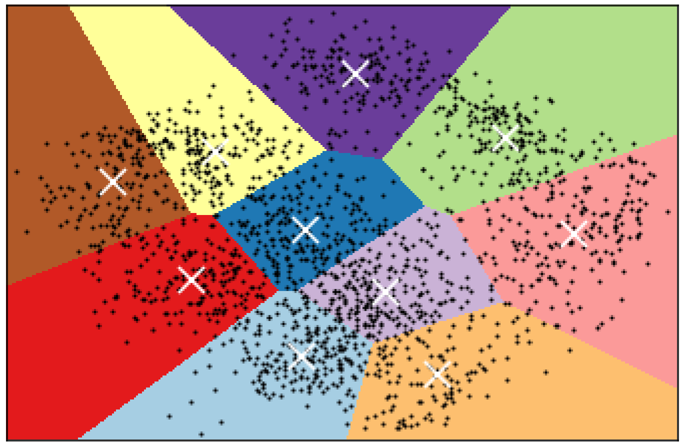
```
__________________________________________________________________________________
init		time	inertia	homo	compl	v-meas	ARI	AMI	silhouette
k-means++	0.112s	69485	0.613	0.660	0.636	0.482	0.632	0.170
random   	0.048s	69952	0.545	0.616	0.578	0.415	0.574	0.144
PCA-based	0.024s	72686	0.636	0.658	0.647	0.521	0.643	0.142
__________________________________________________________________________________
```

Visualize the results on PCA-reduced data

- :class: `~sklearn.decomposition.PCA` allows to project the data from the original 64-dimensional space into a lower dimensional space.
- Subsequently, we can use :class: `~sklearn.decomposition.PCA` to project into a 2-dimensional space and plot the data and the clusters in this new space.

In [12]:
```python
import matplotlib.pyplot as plt

reduced_data = PCA(n_components=2).fit_transform(data)
kmeans = KMeans(init="k-means++", n_clusters=n_digits, n_init=4)
kmeans.fit(reduced_data)

# Step size of the mesh. Decrease to increase the quality of the VQ.
h = .02     # point in the mesh [x_min, x_max]x[y_min, y_max].

# Plot the decision boundary. For that, we will assign a color to each
x_min, x_max = reduced_data[:, 0].min() - 1, reduced_data[:, 0].max() + 1
y_min, y_max = reduced_data[:, 1].min() - 1, reduced_data[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))

# Obtain labels for each point in mesh. Use last trained model.
Z = kmeans.predict(np.c_[xx.ravel(), yy.ravel()])

# Put the result into a color plot
Z = Z.reshape(xx.shape)
plt.figure(1)
plt.clf()
plt.imshow(Z, interpolation="nearest",
           extent=(xx.min(), xx.max(), yy.min(), yy.max()),
           cmap=plt.cm.Paired, aspect="auto", origin="lower")

plt.plot(reduced_data[:, 0], reduced_data[:, 1], 'k.', markersize=2)
# Plot the centroids as a white X
centroids = kmeans.cluster_centers_
plt.scatter(centroids[:, 0], centroids[:, 1], marker="x", s=169, linewidths=3,
            color="w", zorder=10)
plt.title("K-means clustering on the digits dataset (PCA-reduced data)\n"
          "Centroids are marked with white cross")
plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)
plt.xticks(())
plt.yticks(())
plt.show()
```

K-means clustering on the digits dataset (PCA-reduced data)
Centroids are marked with white cross



```
In [ ]:
```

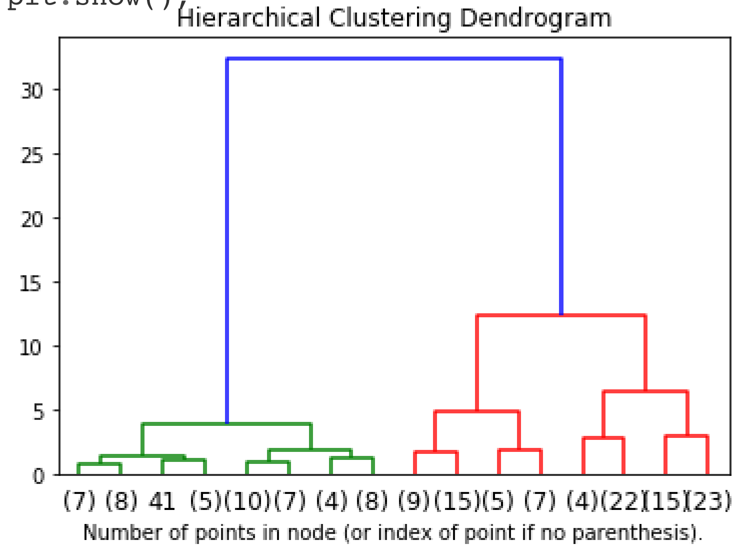
plot_agglomerative_dendrogram

Plot Hierarchical Clustering Dendrogram

This example plots the corresponding dendrogram of a hierarchical clustering using AgglomerativeClustering and the dendrogram method available in scipy.

In [2]:
```
import numpy as np

from matplotlib import pyplot as plt
from scipy.cluster.hierarchy import dendrogram
from sklearn.datasets import load_iris
from sklearn.cluster import AgglomerativeClustering


def plot_dendrogram(model, **kwargs):
    # Create linkage matrix and then plot the dendrogram

    # create the counts of samples under each node
    counts = np.zeros(model.children_.shape[0])
    n_samples = len(model.labels_)
    for i, merge in enumerate(model.children_):
        current_count = 0
        for child_idx in merge:
            if child_idx < n_samples:
                current_count += 1  # leaf node
            else:
                current_count += counts[child_idx - n_samples]
        counts[i] = current_count

    linkage_matrix = np.column_stack([model.children_, model.distances_,
                                      counts]).astype(float)

    # Plot the corresponding dendrogram
    dendrogram(linkage_matrix, **kwargs)


iris = load_iris()
X = iris.data

# setting distance_threshold=0 ensures we compute the full tree.
model = AgglomerativeClustering(distance_threshold=0, n_clusters=None)

model = model.fit(X)
plt.title('Hierarchical Clustering Dendrogram')

# plot the top three levels of the dendrogram
plot_dendrogram(model, truncate_mode='level', p=3)
```

```
plt.xlabel("Number of points in node (or index of point if no parenthesis).")
plt.show();
```



```
In [ ]:
```