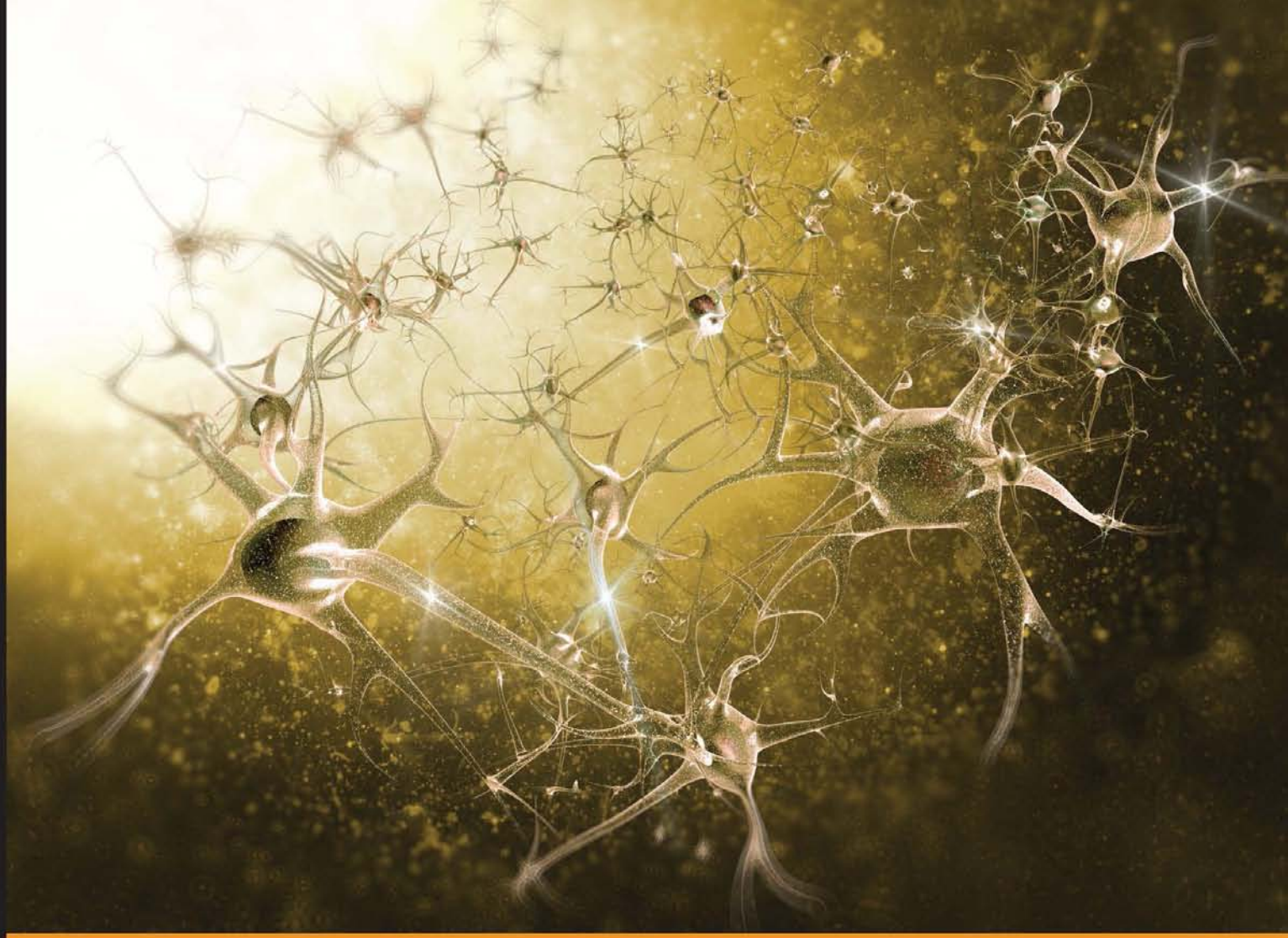

Community Experience Distilled

Python Machine Learning

Unlock deeper insights into machine learning with this vital guide to cutting-edge predictive analytics

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11
Working with Unlabeled Data – Clustering Analysis

In the previous chapters, we used supervised learning techniques to build machine learning models using data where the answer was already known—the class labels were already available in our training data. In this chapter, we will switch gears and explore cluster analysis, a category of **unsupervised learning** techniques that allows us to discover hidden structures in data where we do not know the right answer upfront. The goal of clustering is to find a natural grouping in data such that items in the same cluster are more similar to each other than those from different clusters.

Given its exploratory nature, clustering is an exciting topic and, in this chapter, you will learn about the following concepts that can help you to organize data into meaningful structures:

- Finding centers of similarity using the popular k-means algorithm
- Using a bottom-up approach to build hierarchical cluster trees
- Identifying arbitrary shapes of objects using a density-based clustering approach

Grouping objects by similarity using k-means

In this section, we will discuss one of the most popular **clustering** algorithms, **k-means**, which is widely used in academia as well as in industry. Clustering (or cluster analysis) is a technique that allows us to find groups of similar objects, objects that are more related to each other than to objects in other groups. Examples of business-oriented applications of clustering include the grouping of documents, music, and movies by different topics, or finding customers that share similar interests based on common purchase behaviors as a basis for recommendation engines.

As we will see in a moment, the k-means algorithm is extremely easy to implement but is also computationally very efficient compared to other clustering algorithms, which might explain its popularity. The k-means algorithm belongs to the category of prototype-based clustering. We will discuss two other categories of clustering, **hierarchical** and **density-based** clustering, later in this chapter. **Prototype-based** clustering means that each cluster is represented by a prototype, which can either be the **centroid** (*average*) of similar points with continuous features, or the **medoid** (the most *representative* or most frequently occurring point) in the case of categorical features. While k-means is very good at identifying clusters of spherical shape, one of the drawbacks of this clustering algorithm is that we have to specify the number of clusters *k* a priori. An inappropriate choice for *k* can result in poor clustering performance. Later in this chapter, we will discuss the **elbow** method and **silhouette plots**, which are useful techniques to evaluate the quality of a clustering to help us determine the optimal number of clusters *k*.

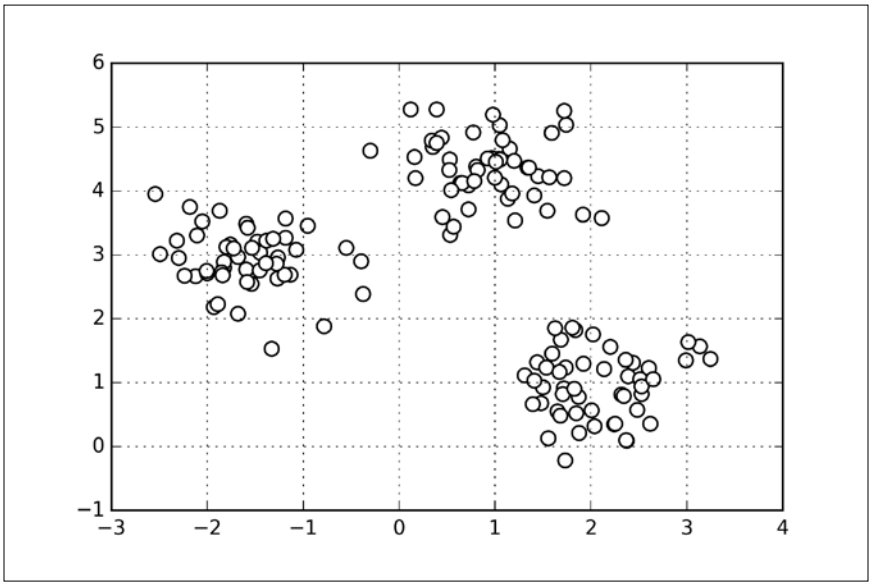
Although k-means clustering can be applied to data in higher dimensions, we will walk through the following examples using a simple two-dimensional dataset for the purpose of visualization:

```
>>> from sklearn.datasets import make_blobs
>>> X, y = make_blobs(n_samples=150,
...                   n_features=2,
...                   centers=3,
...                   cluster_std=0.5,
...                   shuffle=True,
...                   random_state=0)

>>> import matplotlib.pyplot as plt
>>> plt.scatter(X[:,0],
...             X[:,1],
...             c='white',
```

```
...             marker='o',
...             s=50)
>>> plt.grid()
>>> plt.show()
```

The dataset that we just created consists of 150 randomly generated points that are roughly grouped into three regions with higher density, which is visualized via a two-dimensional scatterplot:



In real-world applications of clustering, we do not have any ground truth category information about those samples; otherwise, it would fall into the category of supervised learning. Thus, our goal is to group the samples based on their feature similarities, which we can be achieved using the k-means algorithm that can be summarized by the following four steps:

1. Randomly pick *k* centroids from the sample points as initial cluster centers.
2. Assign each sample to the nearest centroid $\mu^{(j)}$, $j \in \{1,\ldots,k\}$.
3. Move the centroids to the center of the samples that were assigned to it.
4. Repeat the steps 2 and 3 until the cluster assignment do not change or a user-defined tolerance or a maximum number of iterations is reached.

Now the next question is *how do we measure similarity between objects?* We can define similarity as the opposite of distance, and a commonly used distance for clustering samples with continuous features is the **squared Euclidean distance** between two points *x* and *y* in *m-dimensional* space:

$$d(\boldsymbol{x}, \boldsymbol{y})^2 = \sum_{j=1}^{m} \left(x_j - y_j \right)^2 = \left\| \boldsymbol{x} - \boldsymbol{y} \right\|_2^2$$

Note that, in the preceding equation, the index *j* refers to the *jth* dimension (feature column) of the sample points *x* and *y*. In the rest of this section, we will use the superscripts *i* and *j* to refer to the sample index and cluster index, respectively.

Based on this Euclidean distance metric, we can describe the k-means algorithm as a simple optimization problem, an iterative approach for minimizing the **within-cluster sum of squared errors** (**SSE**), which is sometimes also called **cluster inertia**:

$$SSE = \sum_{i=1}^{n} \sum_{j=1}^{k} w^{(i,j)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(j)} \right\|_2^2$$

Here, $\boldsymbol{\mu}^{(j)}$ is the representative point (centroid) for cluster *j*, and $w^{(i,j)} = 1$ if the sample $\boldsymbol{x}^{(i)}$ is in cluster *j*; $w^{(i,j)} = 0$ otherwise.

Now that you have learned how the simple k-means algorithm works, let's apply it to our sample dataset using the `KMeans` class from scikit-learn's `cluster` module:

```
>>> from sklearn.cluster import KMeans
>>> km = KMeans(n_clusters=3,
...             init='random',
...             n_init=10,
...             max_iter=300,
...             tol=1e-04,
...             random_state=0)
>>> y_km = km.fit_predict(X)
```

Using the preceding code, we set the number of desired clusters to `3`; specifying the number of clusters a priori is one of the limitations of k-means. We set `n_init=10` to run the k-means clustering algorithms 10 times independently with different random centroids to choose the final model as the one with the lowest SSE. Via the `max_iter` parameter, we specify the maximum number of iterations for each single run (here, `300`). Note that the k-means implementation in scikit-learn stops early if it converges before the maximum number of iterations is reached.

However, it is possible that k-means does not reach convergence for a particular run, which can be problematic (computationally expensive) if we choose relatively large values for `max_iter`. One way to deal with convergence problems is to choose larger values for `tol`, which is a parameter that controls the tolerance with regard to the changes in the within-cluster sum-squared-error to declare convergence. In the preceding code, we chose a tolerance of `1e-04` (=0.0001).

K-means++

So far, we discussed the classic k-means algorithm that uses a random seed to place the initial centroids, which can sometimes result in bad clusterings or slow convergence if the initial centroids are chosen poorly. One way to address this issue is to run the k-means algorithm multiple times on a dataset and choose the best performing model in terms of the SSE. Another strategy is to place the initial centroids far away from each other via the **k-means++** algorithm, which leads to better and more consistent results than the classic k-means (D. Arthur and S. Vassilvitskii. k-means++: *The Advantages of Careful Seeding*. In Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms, pages 1027–1035. Society for Industrial and Applied Mathematics, 2007).

The initialization in k-means++ can be summarized as follows:

1. Initialize an empty set $\mathbf{M}$ to store the k centroids being selected.
2. Randomly choose the first centroid $\boldsymbol{\mu}^{(j)}$ from the input samples and assign it to $\mathbf{M}$.
3. For each sample $\boldsymbol{x}^{(i)}$ that is not in $\mathbf{M}$, find the minimum squared distance $d\left(\boldsymbol{x}^{(i)}, \mathbf{M}\right)^2$ to any of the centroids in $\mathbf{M}$.
4. To randomly select the next centroid $\boldsymbol{\mu}^{(p)}$, use a weighted probability distribution equal to $\frac{d\left(\boldsymbol{\mu}^{(p)}, \mathbf{M}\right)^2}{\sum_i d\left(\boldsymbol{x}^{(i)}, \mathbf{M}\right)^2}$.
5. Repeat steps 2 and 3 until k centroids are chosen.
6. Proceed with the classic k-means algorithm.

To use k-means++ with scikit-learn's `KMeans` object, we just need to set the `init` parameter to `k-means++` (the default setting) instead of `random`.

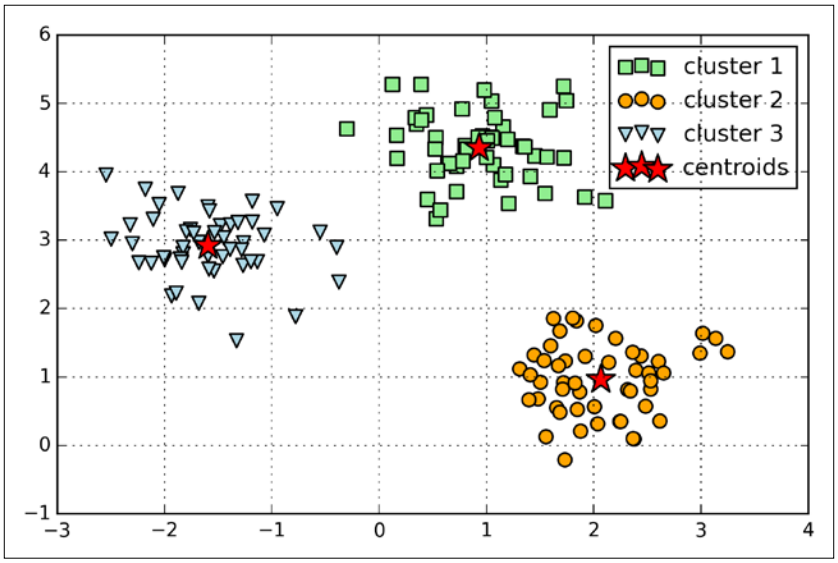
Another problem with k-means is that one or more clusters can be empty. Note that this problem does not exist for k-medoids or fuzzy C-means, an algorithm that we will discuss in the next subsection. However, this problem is accounted for in the current k-means implementation in scikit-learn. If a cluster is empty, the algorithm will search for the sample that is farthest away from the centroid of the empty cluster. Then it will reassign the centroid to be this farthest point.

When we are applying k-means to real-world data using a Euclidean distance metric, we want to make sure that the features are measured on the same scale and apply z-score standardization or min-max scaling if necessary.

After we predicted the cluster labels `y_km` and discussed the challenges of the k-means algorithm, let's now visualize the clusters that k-means identified in the dataset together with the cluster centroids. These are stored under the `centers_` attribute of the fitted `KMeans` object:

```
>>> plt.scatter(X[y_km==0,0],
...             X[y_km ==0,1],
...             s=50,
...             c='lightgreen',
...             marker='s',
...             label='cluster 1')
>>> plt.scatter(X[y_km ==1,0],
...             X[y_km ==1,1],
...             s=50,
...             c='orange',
...             marker='o',
...             label='cluster 2')
>>> plt.scatter(X[y_km ==2,0],
...             X[y_km ==2,1],
...             s=50,
...             c='lightblue',
...             marker='v',
...             label='cluster 3')
>>> plt.scatter(km.cluster_centers_[:,0],
...             km.cluster_centers_[:,1],
...             s=250,
...             marker='*',
...             c='red',
...             label='centroids')
>>> plt.legend()
>>> plt.grid()
>>> plt.show()
```

In the following scatterplot, we can see that k-means placed the three centroids at the center of each sphere, which looks like a reasonable grouping given this dataset:



Although k-means worked well on this toy dataset, we need to note some of the main challenges of k-means. One of the drawbacks of k-means is that we have to specify the number of clusters *k* a priori, which may not always be so obvious in real-world applications, especially if we are working with a higher dimensional dataset that cannot be visualized. The other properties of k-means are that clusters do not overlap and are not hierarchical, and we also assume that there is at least one item in each cluster.

Hard versus soft clustering

Hard clustering describes a family of algorithms where each sample in a dataset is assigned to exactly one cluster, as in the k-means algorithm that we discussed in the previous subsection. In contrast, algorithms for **soft clustering** (sometimes also called **fuzzy clustering**) assign a sample to one or more clusters. A popular example of soft clustering is the **fuzzy C-means** (**FCM**) algorithm (also called **soft k-means** or **fuzzy k-means**). The original idea goes back to the 1970s where Joseph C. Dunn first proposed an early version of fuzzy clustering to improve k-means (J. C. Dunn. *A Fuzzy Relative of the Isodata Process and its Use in Detecting Compact Well-separated Clusters*. 1973). Almost a decade later, James C. Bedzek published his work on the improvements of the fuzzy clustering algorithm, which is now known as the FCM algorithm (J. C. Bezdek. *Pattern Recognition with Fuzzy Objective Function Algorithms*. Springer Science & Business Media, 2013).

The FCM procedure is very similar to k-means. However, we replace the hard cluster assignment by probabilities for each point belonging to each cluster. In k-means, we could express the cluster membership of a sample x by a sparse vector of binary values:

$$\begin{bmatrix} \boldsymbol{\mu}^{(1)} \rightarrow 0 \\ \boldsymbol{\mu}^{(2)} \rightarrow 1 \\ \boldsymbol{\mu}^{(3)} \rightarrow 0 \end{bmatrix}$$

Here, the index position with value 1 indicates the cluster centroid $\boldsymbol{\mu}^{(j)}$ the sample is assigned to (assuming $k = 3,\ j \in \{1, 2, 3\}$). In contrast, a membership vector in FCM could be represented as follows:

$$\begin{bmatrix} \boldsymbol{\mu}^{(1)} \rightarrow 0.1 \\ \boldsymbol{\mu}^{(2)} \rightarrow 0.85 \\ \boldsymbol{\mu}^{(3)} \rightarrow 0.05 \end{bmatrix}$$

Here, each value falls in the range [0, 1] and represents a probability of membership to the respective cluster centroid. The sum of the memberships for a given sample is equal to 1. Similarly to the k-means algorithm, we can summarize the FCM algorithm in four key steps:

1. Specify the number of k centroids and randomly assign the cluster memberships for each point.
2. Compute the cluster centroids $\boldsymbol{\mu}^{(j)},\ j \in \{1,\ldots,k\}$.
3. Update the cluster memberships for each point.
4. Repeat steps 2 and 3 until the membership coefficients do not change or a user-defined tolerance or a maximum number of iterations is reached.

The objective function of FCM—we abbreviate it by J_m—looks very similar to the **within cluster sum-squared-error** that we minimize in k-means:

$$J_m = \sum_{i=1}^{n} \sum_{j=1}^{k} w^{m(i,j)} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(j)} \right\|_2^2,\ m \in [1, \infty)$$

However, note that the membership indicator $w^{(i,j)}$ is not a binary value as in k-means ($w^{(i,j)} \in \{0,1\}$) but a real value that denotes the cluster membership probability ($w^{(i,j)} \in [0,1]$). You also may have noticed that we added an additional exponent to $w^{(i,j)}$; the exponent m, any number greater or equal to 1 (typically $m = 2$), is the so-called **fuzziness coefficient** (or simply **fuzzifier**) that controls the degree of **fuzziness**. The larger the value of $\boldsymbol{m}$, the smaller the cluster membership $w^{(i,j)}$ becomes, which leads to fuzzier clusters. The cluster membership probability itself is calculated as follows:

$$w^{(i,j)} = \left[\sum_{p=1}^{k} \left(\frac{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(j)} \right\|_2}{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(p)} \right\|_2} \right)^{\frac{2}{m-1}} \right]^{-1}$$

For example, if we chose three cluster centers as in the previous k-means example, we could calculate the membership of the $\boldsymbol{x}^{(i)}$ sample belonging to the $\mu^{(j)}$ cluster as:

$$w^{(i,j)} = \left[\left(\frac{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(j)} \right\|_2}{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(1)} \right\|_2} \right)^{\frac{2}{m-1}} + \left(\frac{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(j)} \right\|_2}{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(2)} \right\|_2} \right)^{\frac{2}{m-1}} + \left(\frac{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(j)} \right\|_2}{\left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}^{(3)} \right\|_2} \right)^{\frac{2}{m-1}} \right]^{-1}$$

The center $\mu^{(j)}$ of a cluster itself is calculated as the mean of all samples in the cluster weighted by the membership degree of belonging to its own cluster:

$$\boldsymbol{\mu}^{(j)} = \frac{\sum_{i=1}^{n} w^{m(i,j)} \boldsymbol{x}^{(i)}}{\sum_{i=1}^{n} w^{m(i,j)}}$$

Just by looking at the equation to calculate the cluster memberships, it is intuitive to say that each iteration in FCM is more expensive than an iteration in k-means. However, FCM typically requires fewer iterations overall to reach convergence. Unfortunately, the FCM algorithm is currently not implemented in scikit-learn. However, it has been found in practice that both k-means and FCM produce very similar clustering outputs, as described in a study by Soumi Ghosh and Sanjay K. Dubey (S. Ghosh and S. K. Dubey. *Comparative Analysis of k-means and Fuzzy c-means Algorithms*. IJACSA, 4:35–38, 2013).

Using the elbow method to find the optimal number of clusters

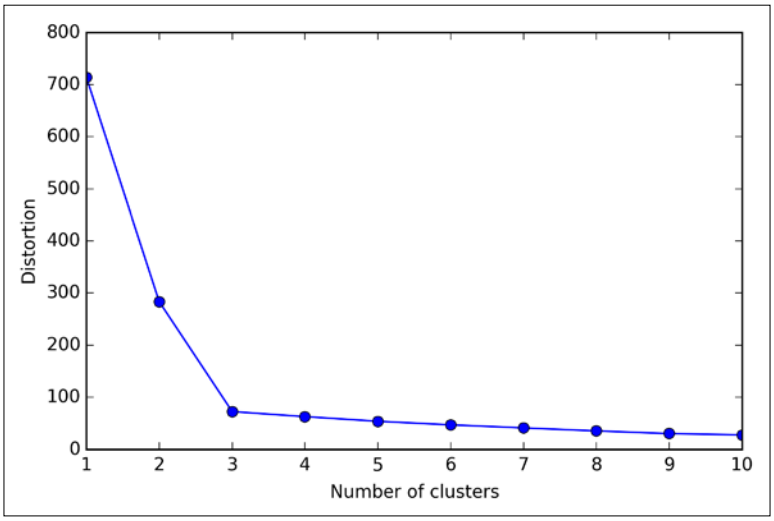
One of the main challenges in unsupervised learning is that we do not know the definitive answer. We don't have the ground truth class labels in our dataset that allow us to apply the techniques that we used in *Chapter 6, Learning Best Practices for Model Evaluation and Hyperparameter Tuning*, in order to evaluate the performance of a supervised model. Thus, in order to quantify the quality of clustering, we need to use intrinsic metrics—such as the within-cluster SSE (distortion) that we discussed earlier in this chapter—to compare the performance of different k-means clusterings. Conveniently, we don't need to compute the within-cluster SSE explicitly as it is already accessible via the `inertia_` attribute after fitting a `KMeans` model:

```
>>> print('Distortion: %.2f' % km.inertia_)
Distortion: 72.48
```

Based on the within-cluster SSE, we can use a graphical tool, the so-called **elbow** method, to estimate the optimal number of clusters *k* for a given task. Intuitively, we can say that, if *k* increases, the distortion will decrease. This is because the samples will be closer to the centroids they are assigned to. The idea behind the elbow method is to identify the value of *k* where the distortion begins to increase most rapidly, which will become more clear if we plot distortion for different values of *k*:

```
>>> distortions = []
>>> for i in range(1, 11):
...     km = KMeans(n_clusters=i,
...                 init='k-means++',
...                 n_init=10,
...                 max_iter=300,
...                 random_state=0)
>>>     km.fit(X)
>>>     distortions.append(km.inertia_)
>>> plt.plot(range(1,11), distortions, marker='o')
>>> plt.xlabel('Number of clusters')
>>> plt.ylabel('Distortion')
>>> plt.show()
```

As we can see in the following plot, the *elbow* is located at $k = 3$, which provides evidence that $k = 3$ is indeed a good choice for this dataset:



Quantifying the quality of clustering via silhouette plots

Another intrinsic metric to evaluate the quality of a clustering is **silhouette analysis**, which can also be applied to clustering algorithms other than k-means that we will discuss later in this chapter. Silhouette analysis can be used as a graphical tool to plot a measure of how tightly grouped the samples in the clusters are. To calculate the **silhouette coefficient** of a single sample in our dataset, we can apply the following three steps:

1. Calculate the cluster cohesion $a^{(i)}$ as the average distance between a sample $\boldsymbol{x}^{(i)}$ and all other points in the same cluster.
2. Calculate the cluster separation $b^{(i)}$ from the next closest cluster as the average distance between the sample $\boldsymbol{x}^{(i)}$ and all samples in the nearest cluster.
3. Calculate the silhouette $s^{(i)}$ as the difference between cluster cohesion and separation divided by the greater of the two, as shown here:

$$s^{(i)} = \frac{b^{(i)} - a^{(i)}}{\max\left\{b^{(i)}, a^{(i)}\right\}}$$

The silhouette coefficient is bounded in the range -1 to 1. Based on the preceding formula, we can see that the silhouette coefficient is 0 if the cluster separation and cohesion are equal ($b^{(i)} = a^{(i)}$). Furthermore, we get close to an ideal silhouette coefficient of 1 if $b^{(i)} >> a^{(i)}$, since $b^{(i)}$ quantifies how dissimilar a sample is to other clusters, and $a^{(i)}$ tells us how similar it is to the other samples in its own cluster, respectively.

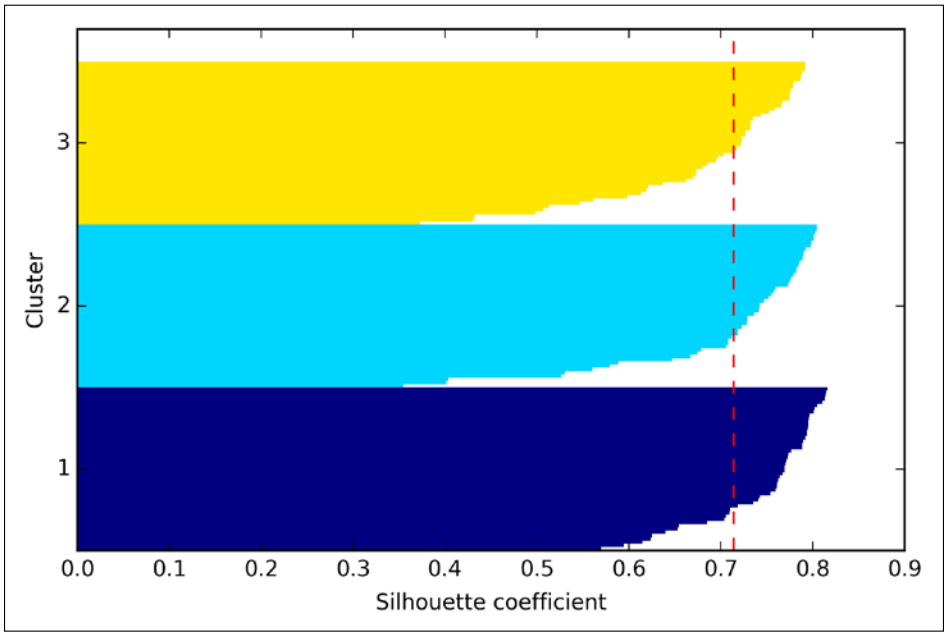
The silhouette coefficient is available as `silhouette_samples` from scikit-learn's `metric` module, and optionally the `silhouette_scores` can be imported. This calculates the average silhouette coefficient across all samples, which is equivalent to `numpy.mean(silhouette_samples(...))`. By executing the following code, we will now create a plot of the silhouette coefficients for a k-means clustering with $k = 3$:

```
>>> km = KMeans(n_clusters=3,
...             init='k-means++',
...             n_init=10,
...             max_iter=300,
...             tol=1e-04,
...             random_state=0)
>>> y_km = km.fit_predict(X)

>>> import numpy as np
>>> from matplotlib import cm
>>> from sklearn.metrics import silhouette_samples
>>> cluster_labels = np.unique(y_km)
>>> n_clusters = cluster_labels.shape[0]
>>> silhouette_vals = silhouette_samples(X,
...                                      y_km,
...                                      metric='euclidean')
>>> y_ax_lower, y_ax_upper = 0, 0
>>> yticks = []
>>> for i, c in enumerate(cluster_labels):
...     c_silhouette_vals = silhouette_vals[y_km == c]
...     c_silhouette_vals.sort()
...     y_ax_upper += len(c_silhouette_vals)
...     color = cm.jet(i / n_clusters)
...     plt.barh(range(y_ax_lower, y_ax_upper),
...              c_silhouette_vals,
...              height=1.0,
...              edgecolor='none',
...              color=color)
...     yticks.append((y_ax_lower + y_ax_upper) / 2)
...     y_ax_lower += len(c_silhouette_vals)
>>> silhouette_avg = np.mean(silhouette_vals)
>>> plt.axvline(silhouette_avg,
...             color="red",
...             linestyle="--")
>>> plt.yticks(yticks, cluster_labels + 1)
```

```
>>> plt.ylabel('Cluster')
>>> plt.xlabel('Silhouette coefficient')
>>> plt.show()
```

Through a visual inspection of the silhouette plot, we can quickly scrutinize the sizes of the different clusters and identify clusters that contain *outliers*:



As we can see in the preceding silhouette plot, our silhouette coefficients are not even close to 0, which can be an indicator of a good clustering. Furthermore, to summarize the goodness of our clustering, we added the average silhouette coefficient to the plot (dotted line).

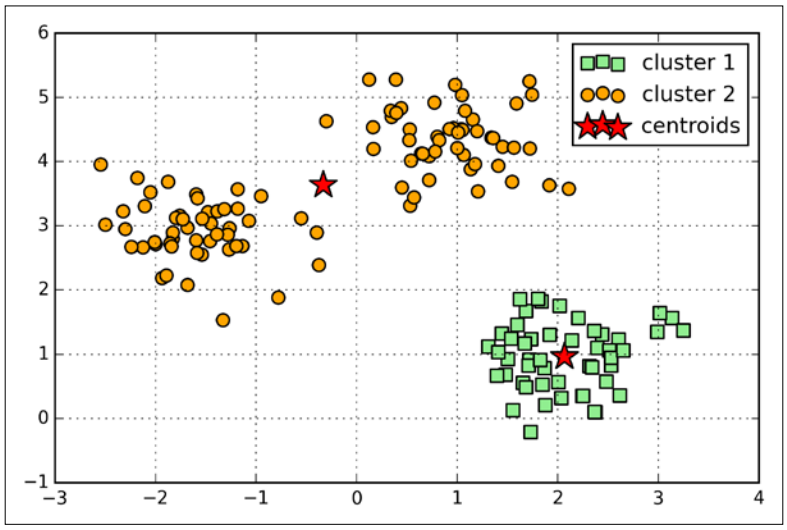
To see how a silhouette plot looks for a relatively *bad* clustering, let's seed the k-means algorithm with two centroids only:

```
>>> km = KMeans(n_clusters=2,
...             init='k-means++',
...             n_init=10,
...             max_iter=300,
...             tol=1e-04,
...             random_state=0)
>>> y_km = km.fit_predict(X)

>>> plt.scatter(X[y_km==0,0],
...             X[y_km==0,1],
...             s=50, c='lightgreen',
```

```
...             marker='s',
...             label='cluster 1')
>>> plt.scatter(X[y_km==1,0],
...             X[y_km==1,1],
...             s=50,
...             c='orange',
...             marker='o',
...             label='cluster 2')
>>> plt.scatter(km.cluster_centers_[:,0],
...             km.cluster_centers_[:,1],
...             s=250,
...             marker='*',
...             c='red',
...             label='centroids')
>>> plt.legend()
>>> plt.grid()
>>> plt.show()
```

As we can see in the following scatterplot, one of the centroids falls between two of the three spherical groupings of the sample points. Although the clustering does not look completely terrible, it is suboptimal.

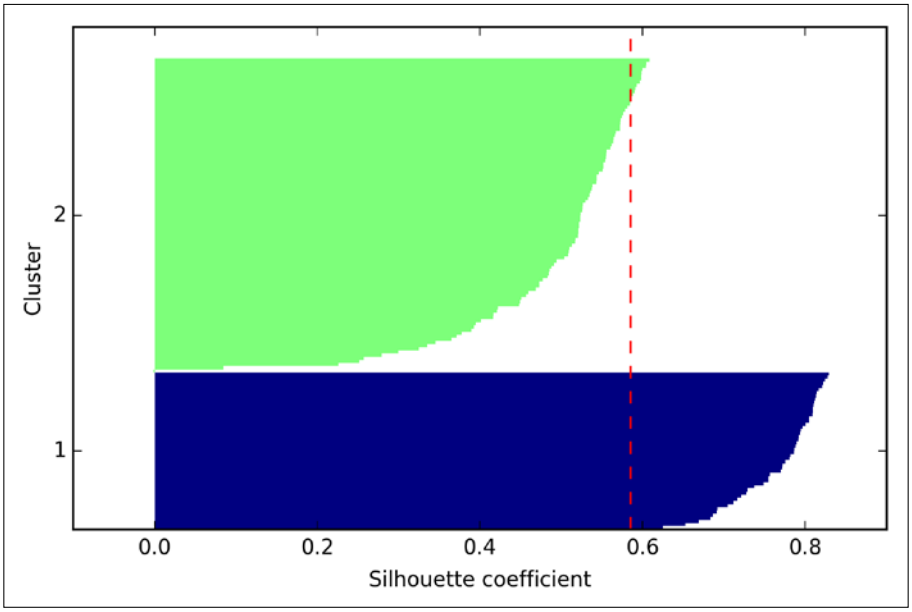


Next we create the silhouette plot to evaluate the results. Please keep in mind that we typically do not have the luxury of visualizing datasets in two-dimensional scatterplots in real-world problems, since we typically work with data in higher dimensions:

```
>>> cluster_labels = np.unique(y_km)
>>> n_clusters = cluster_labels.shape[0]
>>> silhouette_vals = silhouette_samples(X,
```

```
...                                          y_km,
...                                          metric='euclidean')
>>> y_ax_lower, y_ax_upper = 0, 0
yticks = []
>>> for i, c in enumerate(cluster_labels):
...     c_silhouette_vals = silhouette_vals[y_km == c]
...     c_silhouette_vals.sort()
...     y_ax_upper += len(c_silhouette_vals)
...     color = cm.jet(i / n_clusters)
...     plt.barh(range(y_ax_lower, y_ax_upper),
...              c_silhouette_vals,
...              height=1.0,
...              edgecolor='none',
...              color=color)
...     yticks.append((y_ax_lower + y_ax_upper) / 2)
...     y_ax_lower += len(c_silhouette_vals)
>>> silhouette_avg = np.mean(silhouette_vals)
>>> plt.axvline(silhouette_avg, color="red", linestyle="--")
>>> plt.yticks(yticks, cluster_labels + 1)
>>> plt.ylabel('Cluster')
>>> plt.xlabel('Silhouette coefficient')
>>> plt.show()
```

As we can see in the resulting plot, the silhouettes now have visibly different lengths and width, which yields further evidence for a suboptimal clustering:

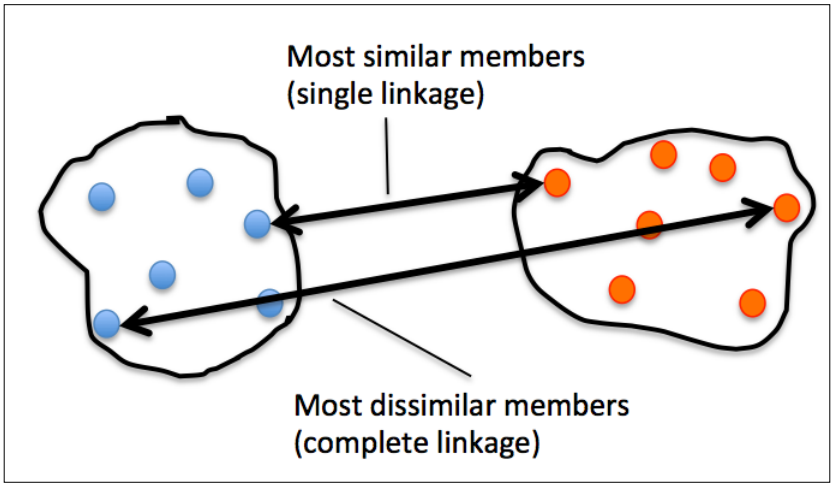


Organizing clusters as a hierarchical tree

In this section, we will take a look at an alternative approach to prototype-based clustering: **hierarchical clustering**. One advantage of hierarchical clustering algorithms is that it allows us to plot **dendrograms** (visualizations of a binary hierarchical clustering), which can help with the interpretation of the results by creating meaningful taxonomies. Another useful advantage of this hierarchical approach is that we do not need to specify the number of clusters upfront.

The two main approaches to hierarchical clustering are **agglomerative** and **divisive** hierarchical clustering. In divisive hierarchical clustering, we start with one cluster that encompasses all our samples, and we iteratively split the cluster into smaller clusters until each cluster only contains one sample. In this section, we will focus on agglomerative clustering, which takes the opposite approach. We start with each sample as an individual cluster and merge the closest pairs of clusters until only one cluster remains.

The two standard algorithms for agglomerative hierarchical clustering are **single linkage** and **complete linkage**. Using single linkage, we compute the distances between the most similar members for each pair of clusters and merge the two clusters for which the distance between the most similar members is the smallest. The complete linkage approach is similar to single linkage but, instead of comparing the most similar members in each pair of clusters, we compare the most dissimilar members to perform the merge. This is shown in the following diagram:



Other commonly used algorithms for agglomerative hierarchical clustering include **average linkage** and **Ward's linkage**. In average linkage, we merge the cluster pairs based on the minimum average distances between all group members in the two clusters. In Ward's method, those two clusters that lead to the minimum increase of the total within-cluster SSE are merged.

In this section, we will focus on agglomerative clustering using the complete linkage approach. This is an iterative procedure that can be summarized by the following steps:

1. Compute the distance matrix of all samples.
2. Represent each data point as a singleton cluster.
3. Merge the two closest clusters based on the distance of the most dissimilar (distant) members.
4. Update the similarity matrix.
5. Repeat steps 2 to 4 until one single cluster remains.

Now we will discuss how to compute the distance matrix (step 1). But first, let's generate some random sample data to work with. The rows represent different observations (IDs 0 to 4), and the columns are the different features (X, Y, Z) of those samples:

```
>>> import pandas as pd
>>> import numpy as np
>>> np.random.seed(123)
>>> variables = ['X', 'Y', 'Z']
>>> labels = ['ID_0','ID_1','ID_2','ID_3','ID_4']
>>> X = np.random.random_sample([5,3])*10
>>> df = pd.DataFrame(X, columns=variables, index=labels)
>>> df
```

After executing the preceding code, we should now see the following distance matrix:

	X	Y	Z
ID_0	6.964692	2.861393	2.268515
ID_1	5.513148	7.194690	4.231065
ID_2	9.807642	6.848297	4.809319
ID_3	3.921175	3.431780	7.290497
ID_4	4.385722	0.596779	3.980443

Performing hierarchical clustering on a distance matrix

To calculate the distance matrix as input for the hierarchical clustering algorithm, we will use the `pdist` function from SciPy's `spatial.distance` submodule:

```
>>> from scipy.spatial.distance import pdist, squareform
>>> row_dist = pd.DataFrame(squareform(
...             pdist(df, metric='euclidean')),
...             columns=labels, index=labels)
>>> row_dist
```

Using the preceding code, we calculated the Euclidean distance between each pair of sample points in our dataset based on the features X, Y, and Z. We provided the condensed distance matrix—returned by `pdist`—as input to the `squareform` function to create a symmetrical matrix of the pair-wise distances, as shown here:

	ID_0	ID_1	ID_2	ID_3	ID_4
ID_0	0.000000	4.973534	5.516653	5.899885	3.835396
ID_1	4.973534	0.000000	4.347073	5.104311	6.698233
ID_2	5.516653	4.347073	0.000000	7.244262	8.316594
ID_3	5.899885	5.104311	7.244262	0.000000	4.382864
ID_4	3.835396	6.698233	8.316594	4.382864	0.000000

Next we will apply the complete linkage agglomeration to our clusters using the `linkage` function from SciPy's `cluster.hierarchy` submodule, which returns a so-called **linkage matrix**.

However, before we call the `linkage` function, let's take a careful look at the function documentation:

```
>>> from scipy.cluster.hierarchy import linkage
>>> help(linkage)
[…]
Parameters:
  y : ndarray
    A condensed or redundant distance matrix. A condensed
    distance matrix is a flat array containing the upper
    triangular of the distance matrix. This is the form
    that pdist returns. Alternatively, a collection of m
    observation vectors in n dimensions may be passed as
    an m by n array.

  method : str, optional
    The linkage algorithm to use. See the Linkage Methods
    section below for full descriptions.

  metric : str, optional
    The distance metric to use. See the distance.pdist
    function for a list of valid distance metrics.

 Returns:
  Z : ndarray
    The hierarchical clustering encoded as a linkage matrix.
[…]
```

Based on the function description, we conclude that we can use a condensed distance matrix (upper triangular) from the `pdist` function as an input attribute. Alternatively, we could also provide the initial data array and use the `euclidean` metric as a function argument in `linkage`. However, we should not use the squareform distance matrix that we defined earlier, since it would yield different distance values from those expected. To sum it up, the three possible scenarios are listed here:

- **Incorrect approach**: In this approach, we use the squareform distance matrix. The code is as follows:

```
>>> from scipy.cluster.hierarchy import linkage
>>> row_clusters = linkage(row_dist,
...                        method='complete',
...                        metric='euclidean')
```

- **Correct approach**: In this approach, we use the condensed distance matrix. The code is as follows:

```
>>> row_clusters = linkage(pdist(df, metric='euclidean'),
...                        method='complete')
```

- **Correct approach**: In this approach, we use the input sample matrix. The code is as follows:

```
>>> row_clusters = linkage(df.values,
...                        method='complete',
...                        metric='euclidean')
```

To take a closer look at the clustering results, we can turn them to a pandas `DataFrame` (best viewed in IPython Notebook) as follows:

```
>>> pd.DataFrame(row_clusters,
...      columns=['row label 1',
...               'row label 2',
...               'distance',
...               'no. of items in clust.'],
...      index=['cluster %d' %(i+1) for i in
...             range(row_clusters.shape[0])])
```

As shown in the following table, the linkage matrix consists of several rows where each row represents one merge. The first and second columns denote the most dissimilar members in each cluster, and the third row reports the distance between those members. The last column returns the count of the members in each cluster.

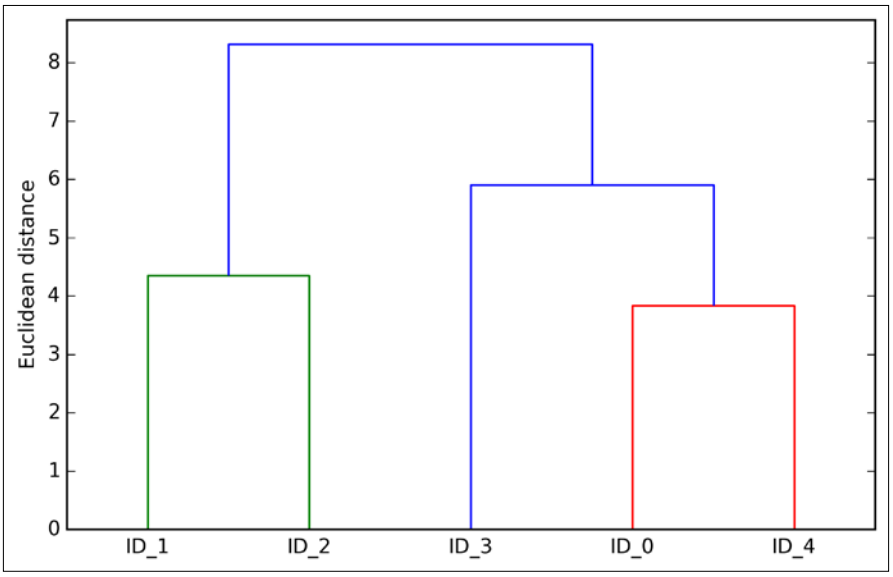
	row label 1	row label 2	distance	no. of items in clust.
cluster 1	0	4	3.835396	2
cluster 2	1	2	4.347073	2
cluster 3	3	5	5.899885	3
cluster 4	6	7	8.316594	5

Now that we have computed the linkage matrix, we can visualize the results in the form of a dendrogram:

```
>>> from scipy.cluster.hierarchy import dendrogram
# make dendrogram black (part 1/2)
# from scipy.cluster.hierarchy import set_link_color_palette
# set_link_color_palette(['black'])
```

```
>>> row_dendr = dendrogram(row_clusters,
...                        labels=labels,
...                        # make dendrogram black (part 2/2)
...                        # color_threshold=np.inf
...                        )
>>> plt.tight_layout()
>>> plt.ylabel('Euclidean distance')
>>> plt.show()
```

If you are executing the preceding code or reading the e-book version of this book, you will notice that the branches in the resulting dendrogram are shown in different colors. The coloring scheme is derived from a list of matplotlib colors that are cycled for the distance thresholds in the dendrogram. For example, to display the dendrograms in black, you can uncomment the respective sections that I inserted in the preceding code.



Such a dendrogram summarizes the different clusters that were formed during the agglomerative hierarchical clustering; for example, we can see that the samples **ID_0** and **ID_4**, followed by **ID_1** and **ID_2**, are the most similar ones based on the Euclidean distance metric.

Attaching dendrograms to a heat map

In practical applications, hierarchical clustering dendrograms are often used in combination with a **heat map**, which allows us to represent the individual values in the sample matrix with a color code. In this section, we will discuss how to attach a dendrogram to a heat map plot and order the rows in the heat map correspondingly.

However, attaching a dendrogram to a heat map can be a little bit tricky, so let's go through this procedure step by step:

1. We create a new `figure` object and define the *x* axis position, *y* axis position, width, and height of the dendrogram via the `add_axes` attribute. Furthermore, we rotate the dendrogram 90 degrees counter-clockwise. The code is as follows:

```
>>> fig = plt.figure(figsize=(8,8))
>>> axd = fig.add_axes([0.09,0.1,0.2,0.6])
>>> row_dendr = dendrogram(row_clusters, orientation='right')
```

2. Next we reorder the data in our initial `DataFrame` according to the clustering labels that can be accessed from the dendrogram object, which is essentially a Python dictionary, via the `leaves` key. The code is as follows:

```
>>> df_rowclust = df.ix[row_dendr['leaves'][::-1]]
```

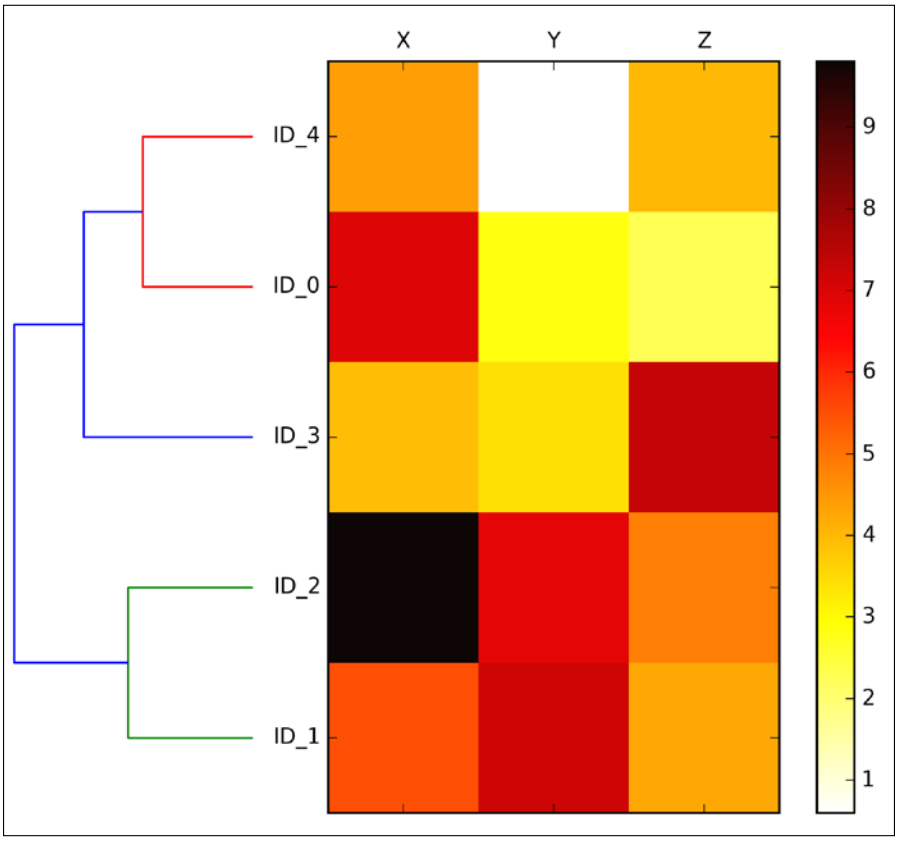
3. Now we construct the heat map from the reordered `DataFrame` and position it right next to the dendrogram:

```
>>> axm = fig.add_axes([0.23,0.1,0.6,0.6])
>>> cax = axm.matshow(df_rowclust,
...                   interpolation='nearest', cmap='hot_r')
```

4. Finally we will modify the aesthetics of the heat map by removing the axis ticks and hiding the axis spines. Also, we will add a color bar and assign the feature and sample names to the *x* and *y* axis tick labels, respectively. The code is as follows:

```
>>> axd.set_xticks([])
>>> axd.set_yticks([])
>>> for i in axd.spines.values():
...     i.set_visible(False)
>>> fig.colorbar(cax)
>>> axm.set_xticklabels(['']  + list(df_rowclust.columns))
>>> axm.set_yticklabels(['']  + list(df_rowclust.index))
>>> plt.show()
```

After following the previous steps, the heat map should be displayed with the dendrogram attached:



As we can see, the row order in the heat map reflects the clustering of the samples in the dendrogram. In addition to a simple dendrogram, the color-coded values of each sample and feature in the heat map provide us with a nice summary of the dataset.

Applying agglomerative clustering via scikit-learn

In this section, we saw how to perform agglomerative hierarchical clustering using SciPy. However, there is also an `AgglomerativeClustering` implementation in scikit-learn, which allows us to choose the number of clusters that we want to return. This is useful if we want to prune the hierarchical cluster tree. By setting the `n_cluster` parameter to `2`, we will now cluster the samples into two groups using the same complete linkage approach based on the Euclidean distance metric as before:

```
>>> from sklearn.cluster import AgglomerativeClustering
>>> ac = AgglomerativeClustering(n_clusters=2,
...                              affinity='euclidean',
...                              linkage='complete')
>>> labels = ac.fit_predict(X)
>>> print('Cluster labels: %s' % labels)
Cluster labels: [0 1 1 0 0]
```

Looking at the predicted cluster labels, we can see that the first, fourth, and fifth sample (**ID_0**, **ID_3**, and **ID_4**) were assigned to one cluster (`0`), and the samples **ID_1** and **ID_2** were assigned to a second cluster (`1`), which is consistent with the results that we can observe in the dendrogram.

Locating regions of high density via DBSCAN

Although we can't cover the vast number of different clustering algorithms in this chapter, let's at least introduce one more approach to clustering: **Density-based Spatial Clustering of Applications with Noise** (**DBSCAN**). The notion of density in DBSCAN is defined as the number of points within a specified radius ε.

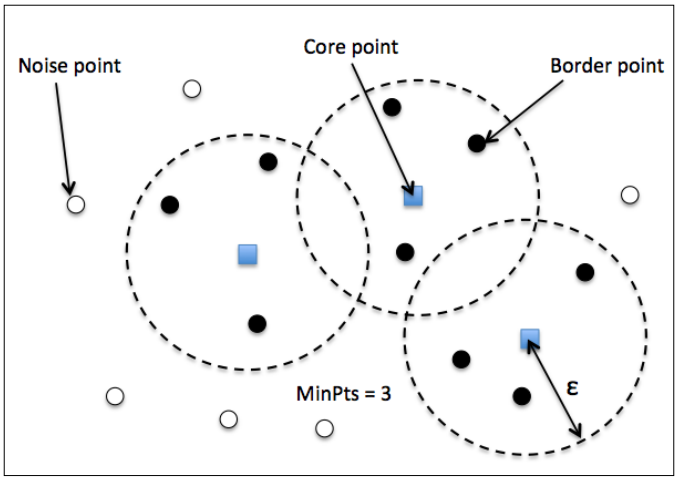
In DBSCAN, a special label is assigned to each sample (point) using the following criteria:

- A point is considered as **core point** if at least a specified number (MinPts) of neighboring points fall within the specified radius ε
- A **border point** is a point that has fewer neighbors than MinPts within ε, but lies within the ε radius of a core point
- All other points that are neither core nor border points are considered as **noise points**

After labeling the points as core, border, or noise points, the DBSCAN algorithm can be summarized in two simple steps:

1. Form a separate cluster for each core point or a connected group of core points (core points are connected if they are no farther away than ε).
2. Assign each border point to the cluster of its corresponding core point.

To get a better understanding of what the result of DBSCAN can look like before jumping to the implementation, let's summarize what you have learned about core points, border points, and noise points in the following figure:

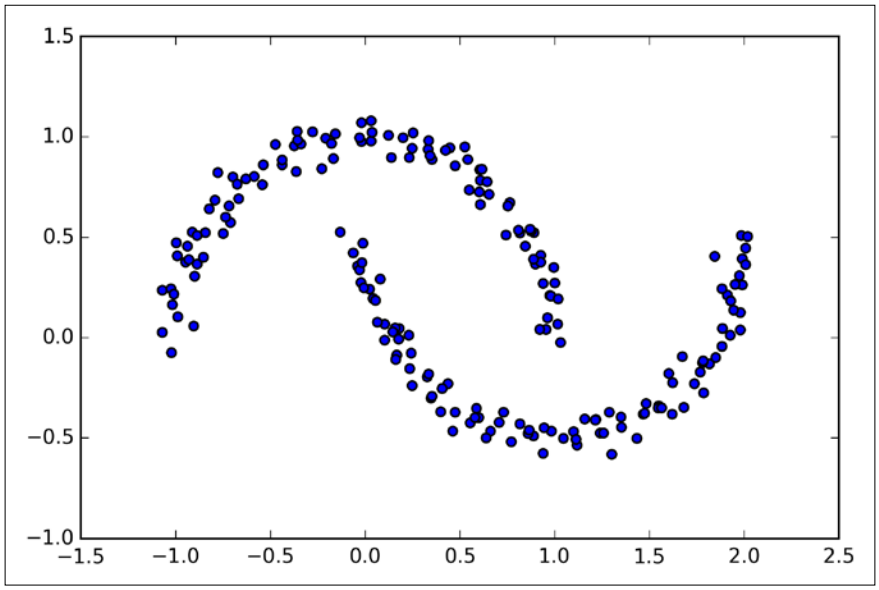


One of the main advantages of using DBSCAN is that it does not assume that the clusters have a spherical shape as in k-means. Furthermore, DBSCAN is different from k-means and hierarchical clustering in that it doesn't necessarily assign each point to a cluster but is capable of removing noise points.

For a more illustrative example, let's create a new dataset of half-moon-shaped structures to compare k-means clustering, hierarchical clustering, and DBSCAN:

```
>>> from sklearn.datasets import make_moons
>>> X, y = make_moons(n_samples=200,
...                   noise=0.05,
...                   random_state=0)
>>> plt.scatter(X[:,0], X[:,1])
>>> plt.show()
```

As we can see in the resulting plot, there are two visible, half-moon-shaped groups consisting of 100 sample points each:

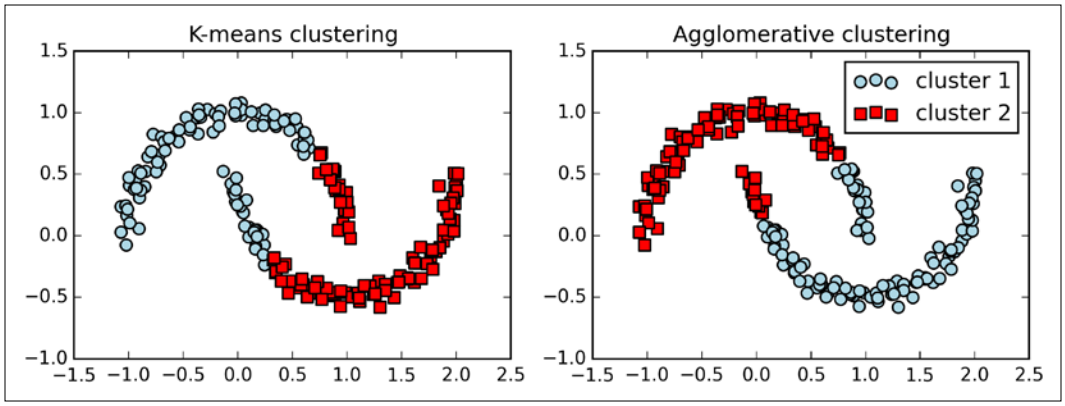


We will start by using the k-means algorithm and complete linkage clustering to see whether one of those previously discussed clustering algorithms can successfully identify the half-moon shapes as separate clusters. The code is as follows:

```
>>> f, (ax1, ax2) = plt.subplots(1, 2, figsize=(8,3))
>>> km = KMeans(n_clusters=2,
...             random_state=0)
>>> y_km = km.fit_predict(X)
>>> ax1.scatter(X[y_km==0,0],
...             X[y_km==0,1],
...             c='lightblue',
...             marker='o',
...             s=40,
...             label='cluster 1')
>>> ax1.scatter(X[y_km==1,0],
...             X[y_km==1,1],
...             c='red',
...             marker='s',
...             s=40,
...             label='cluster 2')
>>> ax1.set_title('K-means clustering')
>>> ac = AgglomerativeClustering(n_clusters=2,
```

```
...                                affinity='euclidean',
...                                linkage='complete')
>>> y_ac = ac.fit_predict(X)
>>> ax2.scatter(X[y_ac==0,0],
...             X[y_ac==0,1],
...             c='lightblue',
...             marker='o',
...             s=40,
...             label='cluster 1')
>>> ax2.scatter(X[y_ac==1,0],
...             X[y_ac==1,1],
...             c='red',
...             marker='s',
...             s=40,
...             label='cluster 2')
>>> ax2.set_title('Agglomerative clustering')
>>> plt.legend()
>>> plt.show()
```

Based on the visualized clustering results, we can see that the k-means algorithm is unable to separate the two clusters, and the hierarchical clustering algorithm was challenged by those complex shapes:

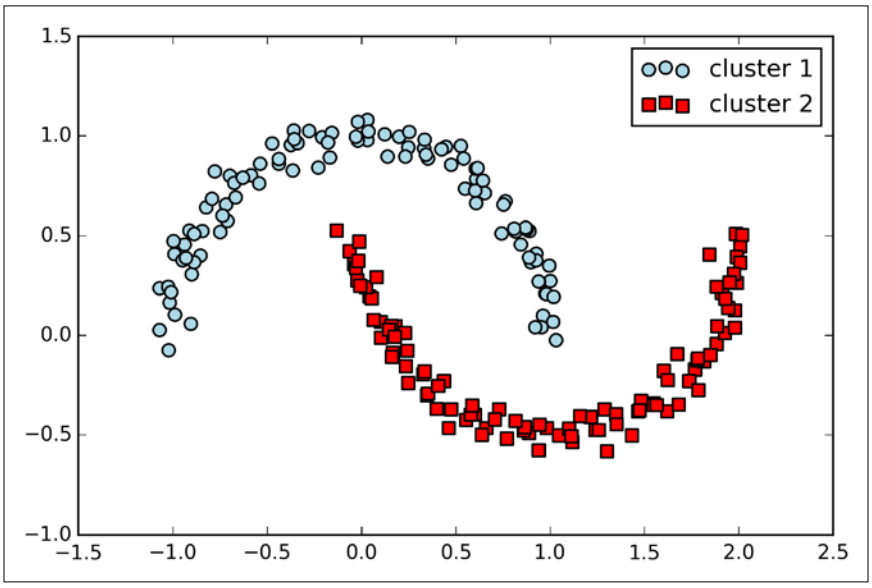


Finally, let's try the DBSCAN algorithm on this dataset to see if it can find the two half-moon-shaped clusters using a density-based approach:

```
>>> from sklearn.cluster import DBSCAN
>>> db = DBSCAN(eps=0.2,
...             min_samples=5,
...             metric='euclidean')
>>> y_db = db.fit_predict(X)
```

```
>>> plt.scatter(X[y_db==0,0],
...             X[y_db==0,1],
...             c='lightblue',
...             marker='o',
...             s=40,
...             label='cluster 1')
>>> plt.scatter(X[y_db==1,0],
...             X[y_db==1,1],
...             c='red',
...             marker='s',
...             s=40,
...             label='cluster 2')
>>> plt.legend()
>>> plt.show()
```

The DBSCAN algorithm can successfully detect the half-moon shapes, which highlights one of the strengths of DBSCAN (clustering data of arbitrary shapes)



However, we should also note some of the disadvantages of DBSCAN. With an increasing number of features in our dataset—given a fixed size training set—the negative effect of the *curse of dimensionality* increases. This is especially a problem if we are using the Euclidean distance metric. However, the problem of the *curse of dimensionality* is not unique to DBSCAN; it also affects other clustering algorithms that use the Euclidean distance metric, for example, the k-means and hierarchical clustering algorithms. In addition, we have two hyperparameters in DBSCAN (MinPts and ε) that need to be optimized to yield good clustering results. Finding a good combination of MinPts and ε can be problematic if the density differences in the dataset are relatively large.

So far, we saw three of the most fundamental categories of clustering algorithms: prototype-based clustering with k-means, agglomerative hierarchical clustering, and density-based clustering via DBSCAN. However, I also want to mention a fourth class of more advanced clustering algorithms that we have not covered in this chapter: **graph-based clustering**. Probably the most prominent members of the graph-based clustering family are **spectral clustering algorithms**. Although there are many different implementations of spectral clustering, they all have in common that they use the eigenvectors of a similarity matrix to derive the cluster relationships. Since spectral clustering is beyond the scope of this book, you can read the excellent tutorial by Ulrike von Luxburg to learn more about this topic (U. Von Luxburg. *A Tutorial on Spectral Clustering*. Statistics and computing, 17(4):395–416, 2007). It is freely available from arXiv at `http://arxiv.org/pdf/0711.0189v1.pdf`.

Note that, in practice, it is not always obvious which algorithm will perform best on a given dataset, especially if the data comes in multiple dimensions that make it hard or impossible to visualize. Furthermore, it is important to emphasize that a successful clustering does not only depend on the algorithm and its hyperparameters. Rather, the choice of an appropriate distance metric and the use of domain knowledge that can help guide the experimental setup can be even more important.

Summary

In this chapter, you learned about three different clustering algorithms that can help us with the discovery of hidden structures or information in data. We started this chapter with a prototype-based approach, k-means, which clusters samples into spherical shapes based on a specified number of cluster centroids. Since clustering is an unsupervised method, we do not enjoy the luxury of ground truth labels to evaluate the performance of a model. Thus, we looked at useful intrinsic performance metrics such as the elbow method or silhouette analysis as an attempt to quantify the quality of clustering.

We then looked at a different approach to clustering: agglomerative hierarchical clustering. Hierarchical clustering does not require specifying the number of clusters upfront, and the result can be visualized in a dendrogram representation, which can help with the interpretation of the results. The last clustering algorithm that we saw in this chapter was DBSCAN, an algorithm that groups points based on local densities and is capable of handling outliers and identifying nonglobular shapes.

After this excursion into the field of unsupervised learning, it is now about time to introduce some of the most exciting machine learning algorithms for supervised learning: multilayer artificial neural networks. After their recent resurgence, neural networks are once again the hottest topic in machine learning research. Thanks to the recently developed deep learning algorithms, neural networks are conceived as state-of-the-art for many complex tasks such as image classification and speech recognition. In *Chapter 12*, *Training Artificial Neural Networks for Image Recognition*, we will construct our own multilayer neural network from scratch. In *Chapter 13*, *Parallelizing Neural Network Training with Theano*, we will introduce powerful libraries that can help us to train complex network architectures most efficiently.