CHAPTER 7

# Clustering

Clustering is the process of finding meaningful groups in data. In clustering, the objective is not to predict a target class variable, but to simply capture the possible natural groupings in the data. For example, the customers of a company can be grouped based on purchase behavior. In the past few years, clustering has even found a use in political elections (Pearson & Cooper, 2012). The prospective electoral voters can be clustered into different groups so that candidates can tailor the messages to resonate within each group. the difference between classification and clustering can be illustrated with an example. Categorizing a *given* voter as a "soccer mom" (a known user group) or not, based on previously available labeled data, is supervised learning—Classification. Segregating a population of electorates into different groups, based on similar demographics is unsupervised learning—Clustering. The process of identifying whether a data point belongs to a particular known group is classification. The process of dividing the dataset into meaningful groups is clustering. In mostcases, one would not know ahead what groups to look for and, thus, the inferred groups might be difficult to explain. The task of clustering can be used in two different classes of applications: to *describe* a given dataset and as a *preprocessing* step for other data science algorithms.

## CLUSTERING TO DESCRIBE THE DATA

The most common application of clustering is to explore the data and find all the possible meaningful groups in the data. Clustering a company's customer records can yield a few groups in such a way that customers within a group are more like each other than customers belonging to a different group. Depending on the clustering technique used, the number of groups or clusters is either user-defined or automatically determined by the algorithm from the dataset. Since clustering is not about predicting the membership of a customer in a well-defined meaningful group (e.g., frequent high-volume purchaser), the similarities of customers within a group need



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to be carefully investigated to make sense of the group as a whole. Some of the common applications of clustering to describe the underlying natural structure of data are:

1. ***Marketing:*** Finding the common groups of customers based on all past customer behaviors, and/or purchase patterns. This task is helpful to segment the customers, identify prototype customers (description of a typical customer of a group), and to tailor a marketing message to the customers in a group.
2. ***Document clustering:*** One common text mining task is to automatically group documents (or text blobs) into groups of similar topics. Document clustering provides a way of identifying key topics, comprehending and summarizing these clustered groups rather than having to read through whole documents. Document clustering is used for routing customer support incidents, online content sites, forensic investigations, etc.
3. ***Session grouping:*** In web analytics, clustering is helpful to understand common groups of clickstream patterns and to discover different kinds of clickstream profiles. One clickstream profile may be that of a customer who knows what they want and proceeds straight to checkout. Another profile may be that of a customer who has researched the products, read through customer reviews, and then makes a purchase during a later session. Clustering the web sessions by profile helps the e-commerce company provide features fitting each customer profile.

## CLUSTERING FOR PREPROCESSING

Since a clustering process considers all the attributes of the dataset and *reduces* the information to a cluster, which is really another attribute (i.e., the ID of the cluster to which a record would belong to), clustering can be used as a data compression technique. The output of clustering is the cluster ID for each record and it can be used as an input variable for other data science tasks. Hence, clustering can be employed as a preprocessing technique for other data science processes. In general, clustering can be used for two types of preprocessing:

1. ***Clustering to reduce dimensionality:*** In an n-dimensional dataset (n number of attributes), the computational complexity is proportional to the number of dimensions or "*n*." With clustering, *n*-dimensional attributes can be converted or reduced to one categorical attribute—"Cluster ID." This reduces the complexity, although there will be some loss of information because of the dimensionality reduction to one

single attribute. Chapter 14, Feature Selection provides an in-depth look at feature selection techniques.

2. ***Clustering for object reduction:*** Assume that the number of customers for an organization is in the millions and the number of cluster groups is 100. For each of these 100 cluster groups, one "poster child" customer can be identified that represents the typical characteristics of all the customers in that cluster group. The poster child customer can be an actual customer or a fictional customer. The prototype of a cluster is the most common representation of all the customers in a group. Reducing millions of customer records to 100 prototype records provides an obvious benefit. In some applications, instead of processing millions of records, just the prototypes can be processed for further classification or regression tasks. This greatly reduces the record count and the dataset can be made appropriate for classification by algorithms like *k*-nearest neighbor (*k*-NN) where computation complexity depends on the number of records.

## TYPES OF CLUSTERING TECHNIQUES

Regardless of the types of clustering applications, the clustering process seeks to find groupings in data, in such a way that data points within a cluster are more *similar* to each other than to data points in the other clusters (Witten & Frank, 2005). One common way of measuring similarity is the Euclidean distance measurement in *n*-dimensional space. In Fig. 7.1 all data points in Cluster 2 are closer to other data points in Cluster 2 than to other data points in Cluster 1. Before explaining the different ways to implement clustering, the different types of clusters have to be defined. Based on a data point's membership to an identified group, a cluster can be:

- ***Exclusive or strict partitioning clusters***: Each data object belongs to one exclusive cluster, like the example shown in Fig. 7.1. This is the most common type of cluster.
- ***Overlapping clusters***: The cluster groups are not exclusive, and each data object may belong to more than one cluster. These are also known as multi-view clusters. For example, a customer of a company can be grouped in a high-profit customer cluster and a high-volume customer cluster at the same time.
- ***Hierarchical clusters***: Each child cluster can be merged to form a parent cluster. For example, the most profitable customer cluster can be further divided into a long-term customer cluster and a cluster with new customers with high-value purchases.

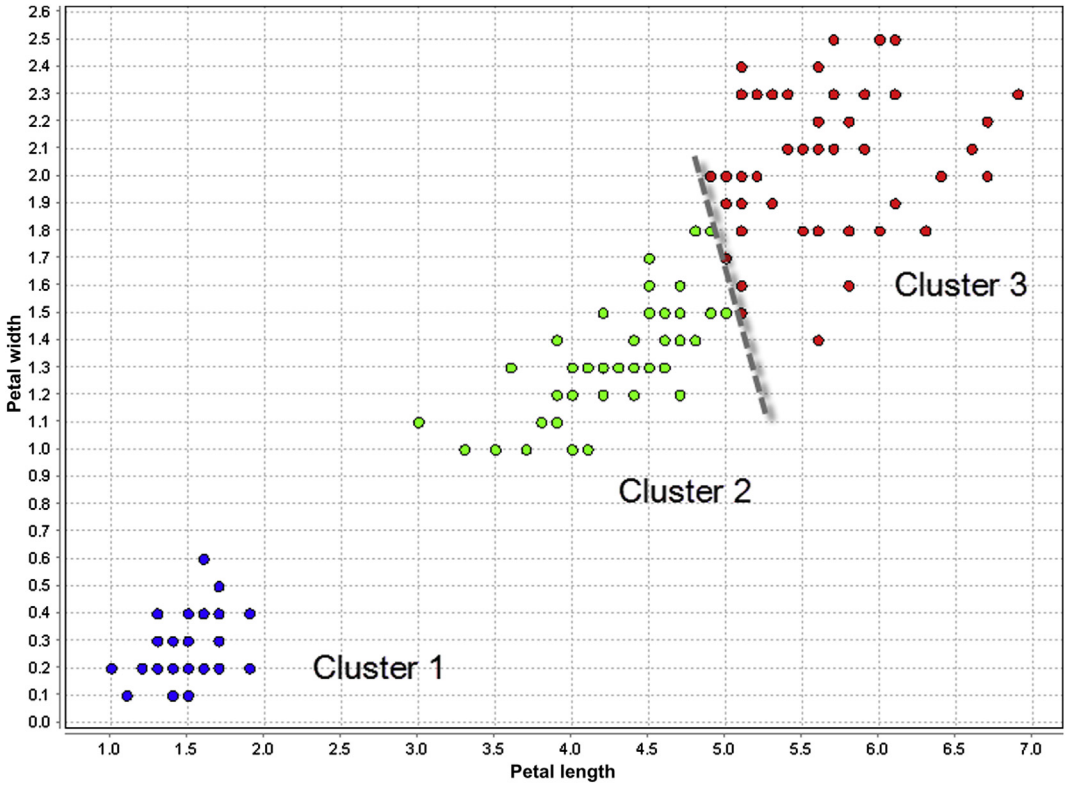



**FIGURE 7.1**
Example of a clustering of the Iris dataset without class labels.

- ***Fuzzy or probabilistic clusters***: Each data point belongs to all cluster groups with varying degrees of membership from 0 to 1. For example, in a dataset with clusters A, B, C, and D, a data point can be associated with all the clusters with degree A = 0.5, B = 0.1, C = 0.4, and D = 0. Instead of a definite association of a data point with one cluster, fuzzy clustering associates a probability of membership to all the clusters.

Clustering techniques can also be classified based on the algorithmic approach used to find clusters in the dataset. Each of these classes of clustering algorithms differ based on what relationship they leverage between the data objects.

- ***Prototype-based clustering***: In the prototype-based clustering, each cluster is represented by a central data object, also called a prototype. The prototype of each cluster is usually the center of the cluster, hence, this clustering is also called centroid clustering or center-based clustering. For example, in clustering customer segments, each customer

cluster will have a central prototype customer and customers with similar properties are associated with the prototype customer of a cluster.

- ***Density clustering*:** In Fig. 7.1, it can be observed that clusters occupy the area where there are more data points per unit space and are separated by sparse space. A cluster can also be defined as a dense region where data objects are concentrated surrounded by a low-density area where data objects are sparse. Each dense area can be assigned a cluster and the low-density area can be discarded as noise. In this form of clustering not all data objects are clustered since noise objects are unassigned to any cluster.
- ***Hierarchical clustering*:** Hierarchical clustering is a process where a cluster hierarchy is created based on the distance between data points. The output of a hierarchical clustering is a *dendrogram*: a tree diagram that shows different clusters at any point of precision which is specified by the user. There are two approaches to create a hierarchy of clusters. A bottom-up approach is where each data point is considered a cluster, and the clusters are merged to finally form one massive cluster. The top-down approach is where the dataset is considered one cluster and they are recursively divided into different sub-clusters until individual data objects are defined as separate clusters. Hierarchical clustering is useful when the data size is limited. A level of interactive feedback is required to cut the dendrogram tree to a given level of precision.
- ***Model-based clustering*:** Model-based clustering gets its foundation from statistics and probability distribution models; this technique is also called distribution-based clustering. A cluster can be thought of as a grouping that has the data points belonging to the same probability distribution. Hence, each cluster can be represented by a distribution model (like Gaussian or Poisson), where the parameter of the distribution can be iteratively optimized between the cluster data and the model. With this approach, the entire dataset can be represented by a mixture of distribution models. *Mixture of Gaussians* is one of the model-based clustering techniques used where a fixed number of distributions are initialized, and parameters are optimized to fit the cluster data.

In the rest of the chapter, the common implementations of clustering will be discussed. First, *k*-means clustering will be covered, which is a kind of prototype-clustering technique. This is followed by the Density-Based Spatial Clustering of Applications with Noise (DBSCAN), which provides a view into density clustering, and the chapter is concluded with an explanation of a novel approach called self-organizing maps (SOMs).

## SEGMENTING CUSTOMER RECORDS

All business entities record most of their interactions with customers, including but not limited to monetary transactions, customer service, customer location and details, online interactions, product usage, and warranty and service information. Take the telecommunications industry as an example. Telecommunications companies have now evolved to provide multiple services to different types of customers by packaging products like phones, wireless, internet, data communications, corporate backbones, entertainment content, home security, etc. To better understand customers, whose numbers often range in the millions, it is necessary to combine multiple datasets about the customers and their interactions with each product. The vastness of the number and variety of attributes in the dataset provides both an opportunity and challenge to better know their customers (Berry & Linoff, 2000a,b). One logical way to understand the customer beyond straightforward classifications like customer type (residential, corporate, government, etc.) or revenue volume (high-, medium-, and low-revenue customers), is to segment the customer based on usage patterns, demographics, geography, and behavior patterns for product usage.

For a customer segmentation task, the data need to be prepared in such a way that each record (row) is associated with each customer and the columns contain all the attributes about the customer, including demographics, address, products used, revenue details, usage details of the product, call volume, type of calls, call duration, time of calls, etc. Table 7.1 shows an example structure of a denormalized customer dataset. Preparing this dataset is going to be a time-consuming task. One of the obvious methods of segmentation is stratifying based on any of the existing attributes. For example, one can segment the data based on a customer's geographical location.

A clustering algorithm consumes this data and groups the customers with similar patterns into clusters based on all the attributes. Based on the data, clustering could be based on a combination of call usage, data patterns, and monthly bills. The resulting clusters could be a group of customers who have low data usage but with high bills at a location where there is weak cellular coverage, which may indicate dissatisfied customers.

The clustering algorithm doesn't explicitly provide the reason for clustering and doesn't intuitively label the cluster groups. While clustering can be performed using a large number of attributes, it is up to the practitioner to carefully select the attributes that will be relevant for clustering. Automated feature selection methods can reduce the dimensions for a clustering exercise. Clustering could be iteratively developed further by selecting or ignoring other attributes in the customer dataset.

**Table 7.1** Dataset for Customer Segmentation

| Customer ID | Location | Demographics | Call Usage | Data Usage (MB) | Monthly Bill ($) |
|---|---|---|---|---|---|
| 01 | San Jose, CA | Male | 1400 | 200 | 75.23 |
| 02 | Miami, FL | Female | 2103 | 5000 | 125.78 |
| 03 | Los Angeles, CA | Male | 292 | 2000 | 89.90 |
| 04 | San Jose, CA | Female | 50 | 40 | 59.34 |

## 7.1 *K*-MEANS CLUSTERING

*k*-Means clustering is a prototype-based clustering method where the dataset is divided into *k*-clusters. *k*-Means clustering is one of the simplest and most commonly used clustering algorithms. In this technique, the user specifies the number of clusters ($k$) that need to be grouped in the dataset.

The objective of *k*-means clustering is to find a *prototype* data point for each cluster; all the data points are then assigned to the nearest prototype, which then forms a cluster. The prototype is called as the *centroid*, the center of the cluster. The center of the cluster can be the mean of all data objects in the cluster, as in *k*-means, or the most represented data object, as in *k*-medoid clustering. The cluster centroid or mean data object does not have to be a real data point in the dataset and can be an imaginary data point that represents the characteristics of all the data points within the cluster.

The *k*-means clustering algorithm is based on the works of Stuart Lloyd and E.W. Forgy (Lloyd, 1982) and is sometimes referred to as the Lloyd–Forgy algorithm or Lloyd's algorithm. Visually, the *k*-means algorithm divides the data space into *k* partitions or boundaries, where the centroid in each partition is the prototype of the clusters. The data objects inside a partition belong to the cluster. These partitions are also called *Voronoi partitions*, and each prototype is a seed in a Voronoi partition. A Voronoi partition is a process of segmenting a space into regions, around a set of points called seeds. All other points are then associated to the nearest seed and the points associated with the seed from a unique partition. Fig. 7.2 shows a sample Voronoi partition around seeds marked as black dots.

*k*-Means clustering creates *k* partitions in *n*-dimensional space, where *n* is the number of attributes in a given dataset. To partition the dataset, a proximity measure has to be defined. The most commonly used measure for a numeric attribute is the Euclidean distance. Fig. 7.3 illustrates the clustering of the Iris dataset with only the petal length and petal width attributes. This Iris dataset is two-dimensional (selected for easy visual explanation), with numeric attributes and *k* specified as 3. The outcome of *k*-means clustering provides a clear partition space for Cluster 1 and a narrow space for the other two clusters, Cluster 2 and Cluster 3.

### 7.1.1 How It Works

The logic of finding *k*-clusters within a given dataset is rather simple and always converges to a solution. However, the final result in most cases will be locally optimal where the solution will not converge to the best global solution. The process of *k*-means clustering is similar to Voronoi iteration, where the objective is to divide a space into cells around points. The difference is Voronoi iteration partitions the space, whereas, *k*-means clustering partitions the points in data space. Take the example of a two-dimensional dataset (Fig. 7.4). The step-by-step process of finding three clusters is provided below (Tan, Michael, & Kumar, 2005).

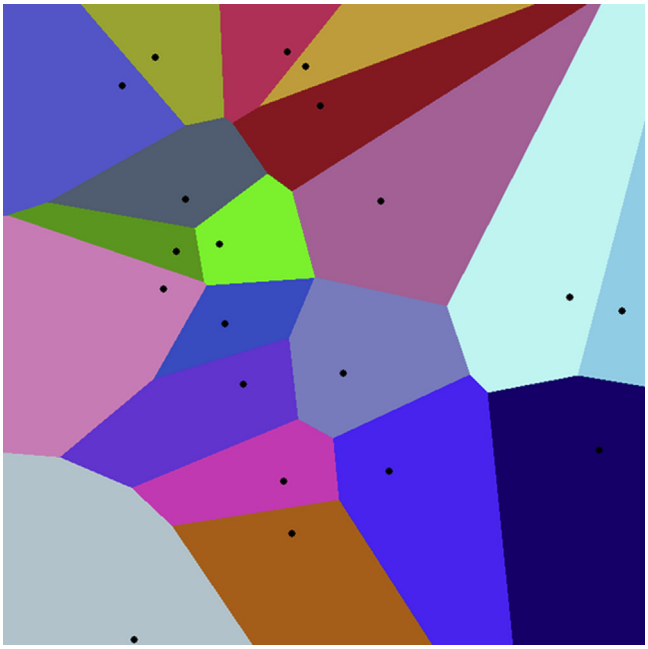


**FIGURE 7.2**
Voronoi partition "Euclidean Voronoi Diagram" by Raincomplex—personal work. Licensed under Creative Commons Zero, Public Domain Dedication via Wikimedia Commons. http://commons.wikimedia.org/wiki/File:Euclidean_Voronoi_Diagram.png#mediaviewer/File:Euclidean_Voronoi_Diagram.png.[1])

### *Step 1: Initiate Centroids*

The first step in $k$-means algorithm is to initiate $k$ random centroids. The number of clusters $k$ should be specified by the user. In this case, three centroids are initiated in a given data space. In Fig. 7.5, each initial centroid is given a shape (with a circle to differentiate centroids from other data points) so that data points assigned to a centroid can be indicated by the same shape.

### *Step 2: Assign Data Points*

Once centroids have been initiated, all the data points are now assigned to the nearest centroid to form a cluster. In this context the "nearest" is calculated by a proximity measure. Euclidean distance measurement is the most common proximity measure, though other measures like the Manhattan measure and Jaccard coefficient can be used. The Euclidean distance between two data points $X$ $(x_1, x_2, \ldots, x_n)$ and $C$ $(c_1, c_2, \ldots, c_n)$ with $n$ attributes is given by (7.1)

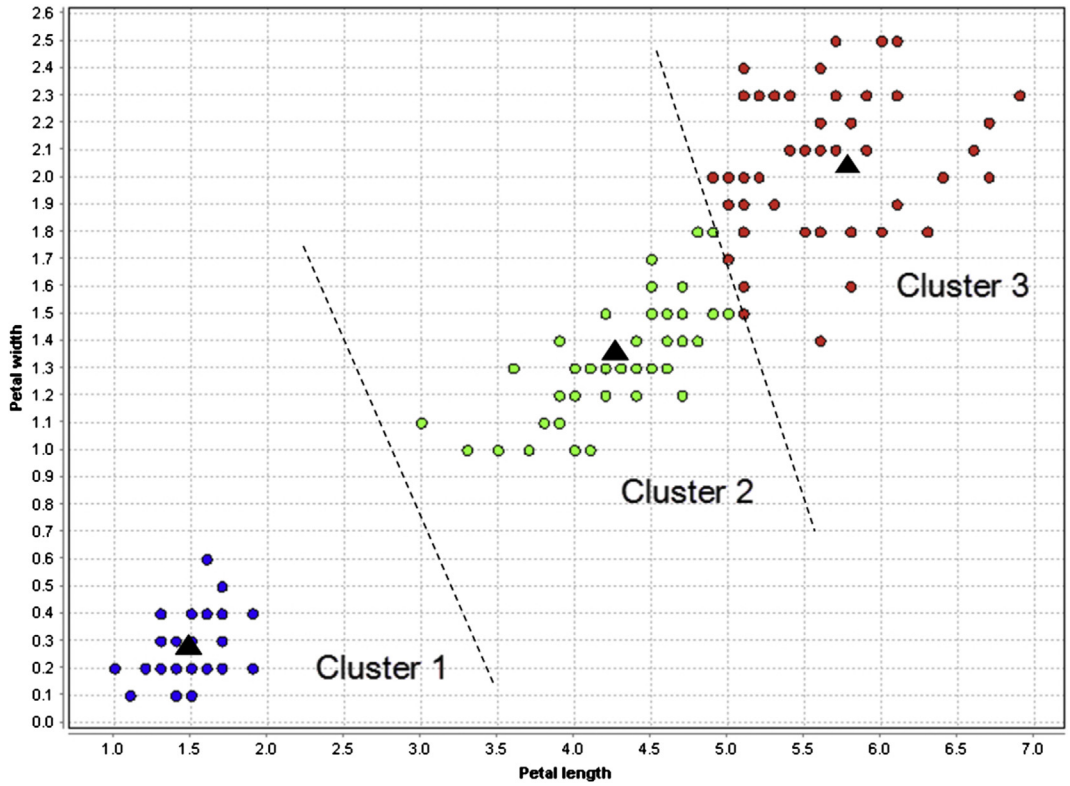



**FIGURE 7.3**
Prototype-based clustering and boundaries.

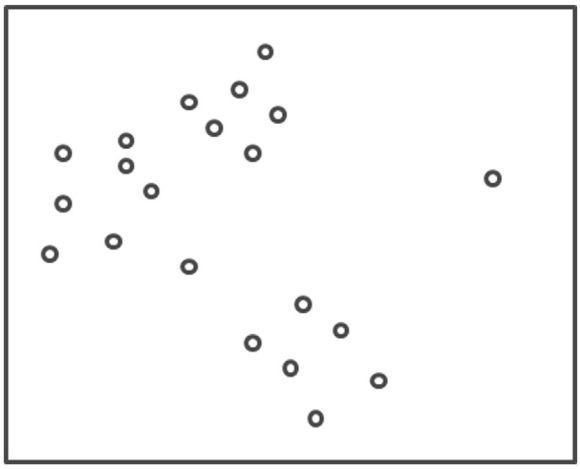


**FIGURE 7.4**
Dataset with two dimensions.

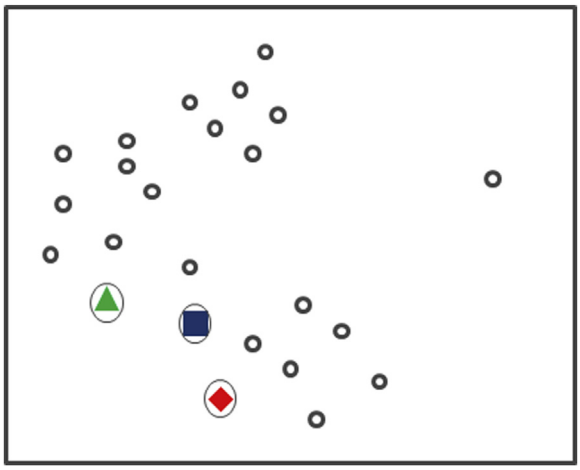


**FIGURE 7.5**
Initial random centroids.

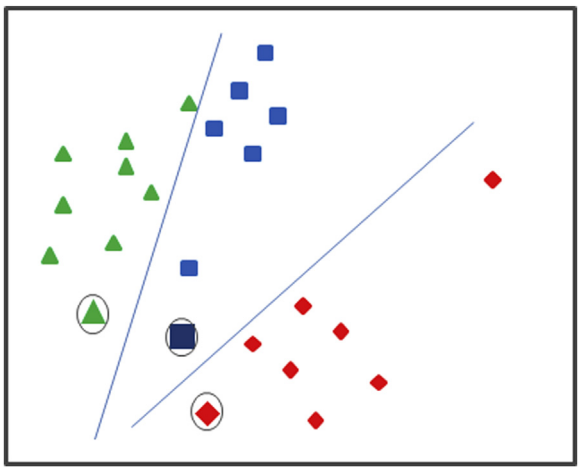


**FIGURE 7.6**
Assignment of data points to nearest centroids.

$$\text{Distance d} = \sqrt{(x_1 - c_1)^2 + (x_2 - c_2)^2 + \ldots + (x_n - c_n)^2} \tag{7.1}$$

All the data points associated to a centroid now have the same shape as their corresponding centroid as shown in Fig. 7.6. This step also leads to partitioning of data space into Voronoi partitions, with lines shown as boundaries.

### *Step 3: Calculate New Centroids*

For each cluster, a new centroid can now be calculated, which is also the prototype of each cluster group. This new centroid is the most representative data point of all data points in the cluster. Mathematically, this step can be expressed as minimizing the sum of squared errors (SSEs) of all data points in a cluster to the centroid of the cluster. The overall objective of the step is to minimize the SSEs of individual clusters. The SSE of a cluster can be calculated using Eq. (7.2).

$$\text{SSE} = \sum_{i=1}^{k} \sum_{x_j \in C_i} \left\| x_j - \mu_i \right\|^2 \tag{7.2}$$

where $C_i$ is the $i^{\text{th}}$ cluster, $j$ are the data points in a given cluster, $\mu_i$ is the centroid for $i^{\text{th}}$ cluster, and $x_j$ is a specific data object. The centroid with minimal SSE for the given cluster $i$ is the new mean of the cluster. The mean of the cluster can be calculated using (7.3)

$$\mu_i = \frac{1}{j_i} \sum_{x \in c_i} X \tag{7.3}$$

where $X$ is the data object vector $(x_1, x_2, \ldots, x_n)$. In the case of $k$-means clustering, the new centroid will be the mean of all the data points. $k$-Medoid clustering is a variation of $k$-means clustering, where the median is calculated instead of the mean. Fig. 7.7 shows the location of the new centroids.

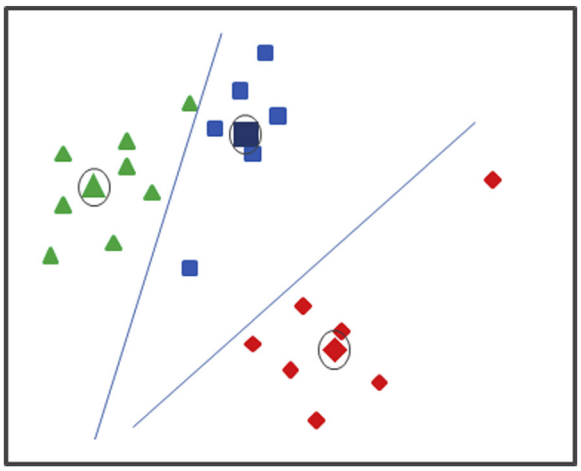


**FIGURE 7.7**
New centroids.

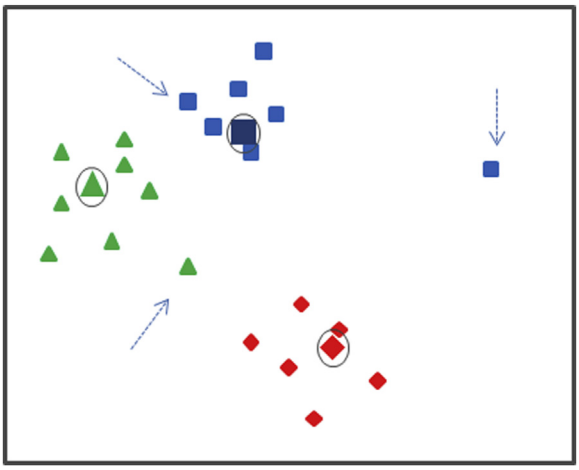


**FIGURE 7.8**
Assignment of data points to new centroids.

### *Step 4: Repeat Assignment and Calculate New Centroids*

Once the new centroids have been identified, assigning data points to the nearest centroid is repeated until all the data points are reassigned to new centroids. In Fig. 7.8, note the change in assignment of three data points that belonged to different clusters in the previous step.

### *Step 5: Termination*

Step 3—calculating new centroids, and step 4—assigning data points to new centroids, are repeated until no further change in assignment of data points happens. In other words, no significant change in centroids are noted. The final centroids are declared the prototypes of the clusters and they are used to describe the whole clustering model. Each data point in the dataset is now tied with a new clustering ID attribute that identifies the cluster.

### *Special Cases*

Even though *k*-means clustering is simple and easy to implement, one of the key drawbacks of *k*-means clustering is that the algorithm seeks to find a *local optimum*, which may not yield globally optimal clustering. In this approach, the algorithm starts with an initial configuration (centroids) and continuously improves to find the best solution possible for that initial configuration. Since the solution is optimal to the initial configuration (locally optimal), there might be a better optimal solution if the initial configuration changes. The locally optimal solution may not be the most optimal solution for the given clustering problem. Hence, the success of a *k*-means algorithm much depends on the initiation of centroids. This limitation can be

addressed by having multiple random initiations; in each run one could measure the cohesiveness of the clusters by a *performance criterion*. The clustering run with the best performance metric can be chosen as the final run. Evaluation of clustering is discussed in the next section. Some key issues to be considered in *k*-means clustering are:

- ***Initiation:*** The final clustering grouping depends on the random initiator and the nature of the dataset. When random initiation is used, one can run the entire clustering process (also called "runs") with a different set of random initiators and find the clustering process that has minimal total SSE. Another technique is hierarchical clustering, where each cluster is in turn split into multiple clusters and, thereby, minimal SSE is achieved. Hierarchical clustering is further divided into agglomerative or bottom-up clustering and divisive or top-down clustering, depending on how the clustering is initiated. Agglomerative clustering starts with each data point as an individual cluster and proceeds to combine data points into clusters. Divisive clustering starts with the whole dataset as one big cluster and proceeds to split that into multiple clusters.
- ***Empty clusters:*** One possibility in *k*-means clustering is the formation of empty clusters in which no data objects are associated. If empty clusters are formed, a new centroid can be introduced in the cluster that has the highest SSE, thereby, splitting the cluster that contributes to the highest SSE or selecting a new centroid that is at the farthest point away from any other centroid.
- ***Outliers:*** Since SSE is used as an objective function, *k*-means clustering is susceptible to outliers; they drift the centroid away from the representative data points in a cluster. Hence, the prototype is no longer the best representative of the clusters it represents. While outliers can be eliminated with preprocessing techniques, in some applications finding outliers or a group of outliers is the objective of clustering, similar to identifying fraudulent transactions.
- ***Post-processing:*** Since *k*-means clustering seeks to be locally optimal, a few post-processing techniques can be introduced to force a new solution that has less SSE. One could always increase the number of clusters, *k*, and reduce SSE. But, this technique can start overfitting the dataset and yield less useful information. There are a few approaches that can be deployed, such as bisecting the cluster that has the highest SSE and merging two clusters into one even if SSE increases slightly.

### *Evaluation of Clusters*

Evaluation of *k*-means clustering is different from regression and classification algorithms because in clustering there are no known external labels for

comparison. The evaluation parameter will have to be developed from the very dataset that is being evaluated. This is called unsupervised or internal evaluation. Evaluation of clustering can be as simple as computing total SSE. Good models will have low SSE within the cluster and low overall SSE among all clusters. SSE can also be referred to as the average within-cluster distance and can be calculated for each cluster and then averaged for all the clusters.

Another commonly used evaluation measure is the Davies–Bouldin index (Davies & Bouldin, 1979). The Davies–Bouldin index is a measure of uniqueness of the clusters and takes into consideration both cohesiveness of the cluster (distance between the data points and center of the cluster) and separation between the clusters. It is the function of the ratio of within-cluster separation to the separation between the clusters. The lower the value of the Davies–Bouldin index, the better the clustering. However, both SSE and the Davies–Bouldin index have the limitation of not guaranteeing better clustering when they have lower scores.

### 7.1.2 How to Implement

*k*-Means clustering implementation in RapidMiner is simple and straightforward with one operator for modeling and one for unsupervised evaluation. In the modeling step, the parameter for the number of clusters, *k*, is specified as desired. The output model is a list of centroids for each cluster and a new attribute is attached to the original input dataset with the cluster ID. The cluster label is appended to the original dataset for each data point and can be visually evaluated after the clustering. A model evaluation step is required to calculate the average cluster distance and Davies–Bouldin index.

For this implementation, the Iris dataset will be used with four attributes and 150 data objects (Fisher, 1936). Even though a class label is not needed for clustering, it was kept for later explanation to see if identified clusters from an unlabeled dataset are similar to natural clusters of species in the dataset.

#### *Step 1: Data Preparation*

*k*-Means clustering accepts both numeric and polynominal data types; however, the distance measures are more effective with numeric data types. The number of attributes increases the dimension space for clustering. In this example the number of attributes has been limited to two by selecting petal width (a3) and petal length (a4) using the *Select attribute* operator as shown in Fig. 7.9. It is easy to visualize the mechanics of *k*-means algorithm by looking at two-dimensional plots for clustering. In practical implementations, clustering datasets will have more attributes.

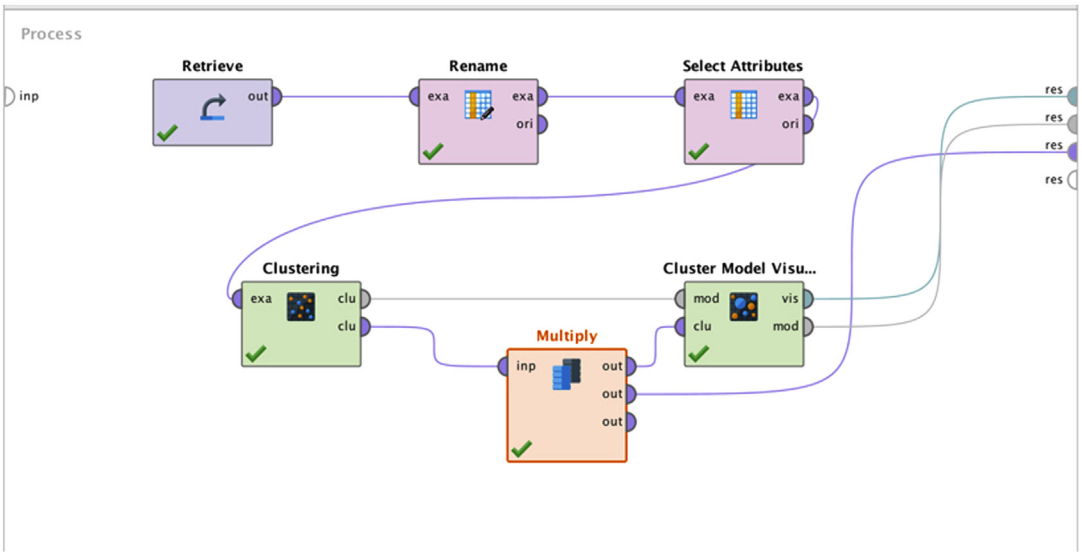



**FIGURE 7.9**
Data science process for *k*-means clustering.

### *Step 2: Clustering Operator and Parameters*

The *k*-means modeling operator is available in the Modeling > Clustering and Segmentation folder of RapidMiner. These parameters can be configured in the model operator:

- *k*: *k* is the desired number of clusters.
- *Add cluster as attribute*: Append cluster labels (IDs) into the original dataset. Turning on this option is recommended for later analysis.
- *Max runs*: Since the effectiveness of *k*-means clustering is dependent on random initial centroids, multiple runs are required to select the clustering with the lowest SSE. The number of such runs can be specified here.
- *Measure type*: The proximity measure can be specified in this parameter. The default and most common measurement is Euclidean distance (L2). Other options here are Manhattan distance (L1), Jaccard coefficient, and cosine similarity for document data. Please refer to Chapter 4, Classification section *k*-NN for description on distance measures.
- *Max optimization steps*: This parameter specifies the number of iterations of assigning data objects to centroids and calculating new centroids.

The output of the modeling step includes the cluster model with *k* centroid data objects and the initial dataset appended with cluster labels. Cluster labels are named generically such as cluster_0, cluster_1,. . ., cluster_$k-1$.

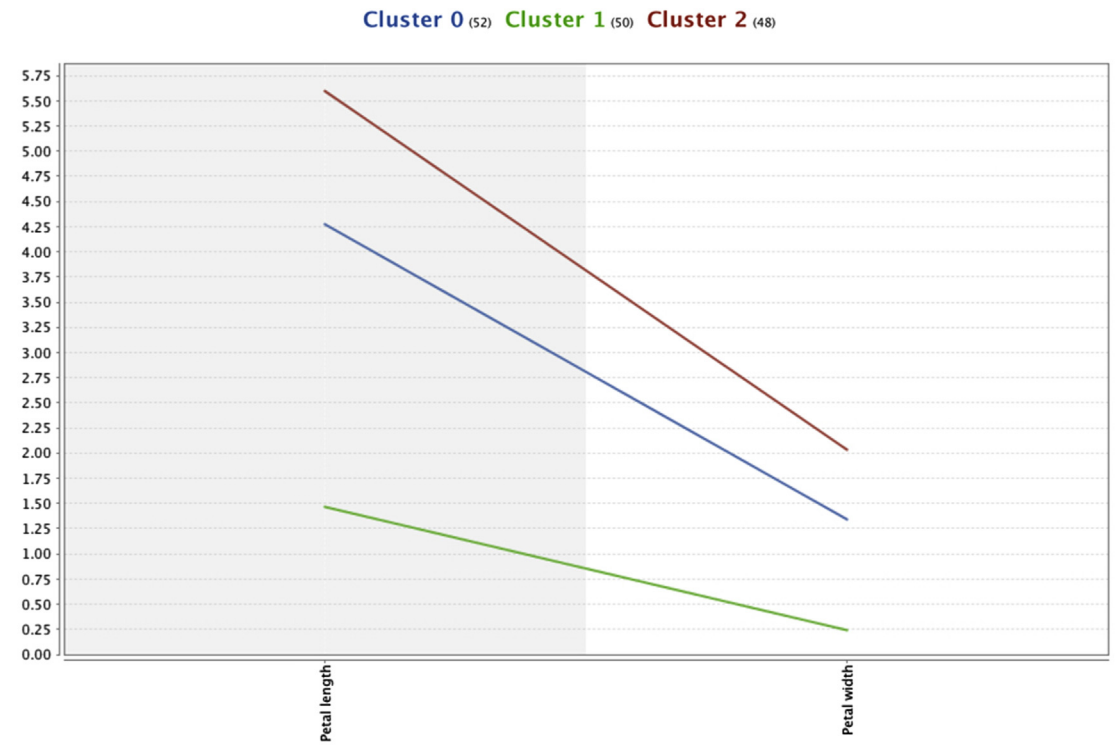
### Step 3: Evaluation

Since the attributes used in the dataset are numeric, the effectiveness of clustering groups need to be evaluated using SSE and the Davies–Bouldin index. In RapidMiner, the *Cluster Model Visualizer* operator under Modeling > Segmentation is available for a performance evaluation of cluster groups and visualization. *Cluster Model Visualizer* operator needs both inputs from the modeling step: cluster centroid vector (model) and the labeled dataset. The two measurement outputs of the evaluation are average cluster distance and the Davies–Bouldin index.

### Step 4: Execution and Interpretation

After the outputs from the *performance* operator have been connected to the result ports, the data science process can be executed. These outputs can be observed from results window:

- ***Cluster Model (Clustering):*** The model output contains the centroid for each of the *k*-clusters, along with their attribute values. As shown in Fig. 7.10, in the text view and folder view sections, all the data objects associated with the each cluster can be seen. The centroid plot view provides the parallel chart view (Chapter 3: Data Exploration) of the centroids. A large separation between centroids is desirable, because well-separated clusters divide the dataset cleanly.
- ***Labeled example set:*** The appended dataset has some of the most important information on clustering. The generic Iris dataset of 150 observations is clustered in three groups. The cluster value is appended as a new special polynominal attribute and takes a generic label format. In the scatterplot view of this output dataset, the *x*- and *y*-axes can be configured to be attributes of the original dataset, petal length and petal width. In the plot in Fig. 7.11, it can be noted how the algorithm identified clusters. This output can be compared against the original label (Iris species). and only five data points in the border of I. *versicolor* and I. *virginica* are mis-clustered! The *k*-means clustering process identified the different species in the dataset almost exactly.
- ***Visualizer and Performance vector:*** The output of the Cluster Model Visualizer shows the centroid charts, table, scatter plots, heatmaps, and performance evaluation metrics like average distance measured and the Davies–Bouldin index (Fig. 7.12). This step can be used to compare multiple clustering processes with different parameters. In advanced implementations, it is possible to determine the value of "*k*" using *Optimize Parameters* operator, based on the number of looped clustering runs with various values of *k*. Amongst multiple clustering runs each with a distinct value for *k*, the *k* value with the lowest average-within-centroid distance or Davies–Bouldin index is selected as the most optimal.




| Cluster | Petal length | Petal width |
|---|---|---|
| Cluster 0 | 4.269 | 1.342 |
| Cluster 1 | 1.464 | 0.244 |
| Cluster 2 | 5.596 | 2.037 |

**FIGURE 7.10**
*k*-Means clustering centroids output.

The *k*-means clustering algorithm is simple, easy to implement, and easy to interpret. Although the algorithm can effectively handle an *n*-dimensional dataset, the operation will be expensive with a higher number of iterations and runs. One of the key limitations of *k*-means is that it relies on the user to assign the value of *k* (Berry & Linoff, 2000a,2000b). The number of clusters in the dataset will be unknown to begin with and an arbitrary number can limit the ability to find the right number of natural clusters in the dataset. There are a variety of methods to estimate the right number for *k*, ranging from the Bayesian Information Criterion to hierarchical methods that increase the value of *k* until the data points assigned to the cluster are Gaussian (Hamerly & Elkan, 2003). For a start, it is recommended to use a

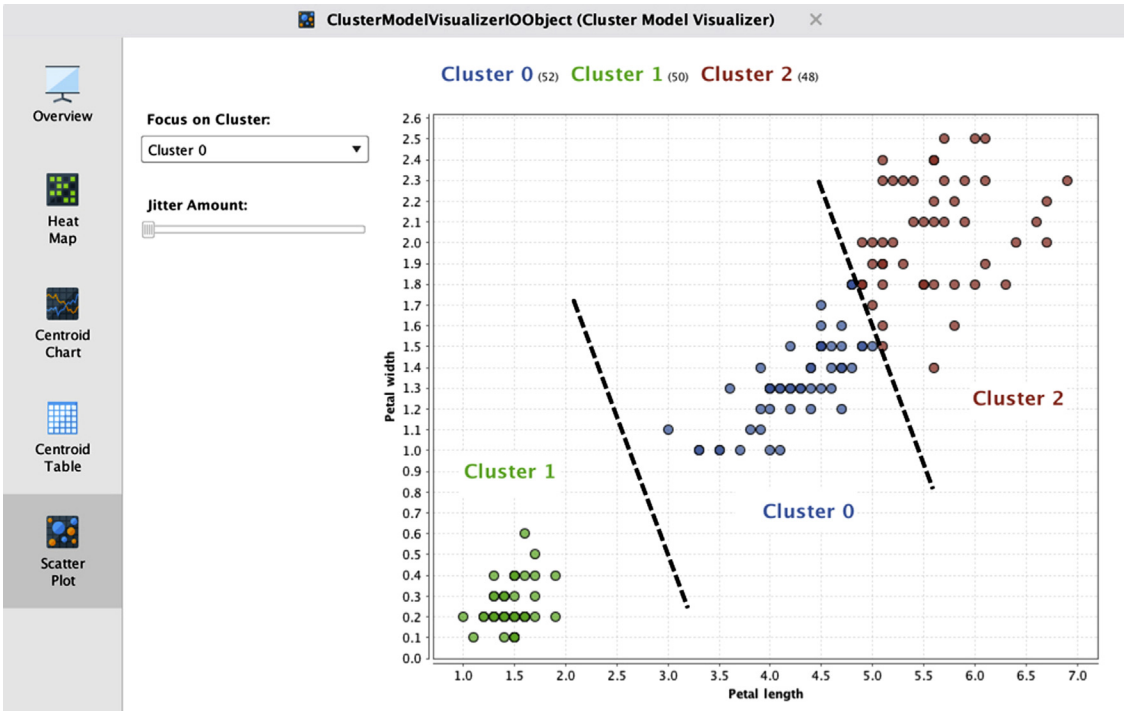



**FIGURE 7.11**
*k*-Means clustering visual output.

value of $k$ in the low single digits and increasing it until it fits. Clustering using density methods will help provide an idea into the number of clusters and could be used as a value of $k$ in $k$-means clustering.

Since the centroid prototype approach is used, $k$-means tends to find globular clusters in the dataset. However, natural clusters can be of all shapes and sizes. The presence of outliers possesses a challenge in the modeling of $k$-means clustering. The simplicity of the $k$-means clustering technique makes it a great choice for quick evaluation of globular clusters and as a preprocessing technique for data science modeling and for dimensionality reduction.

## 7.2 DBSCAN CLUSTERING

A cluster can also be defined as an area of high concentration (or density) of data objects surrounded by areas of low concentration (or density) of data objects. A density-clustering algorithm identifies clusters in the data based on the measurement of the density distribution in $n$-dimensional space. Unlike

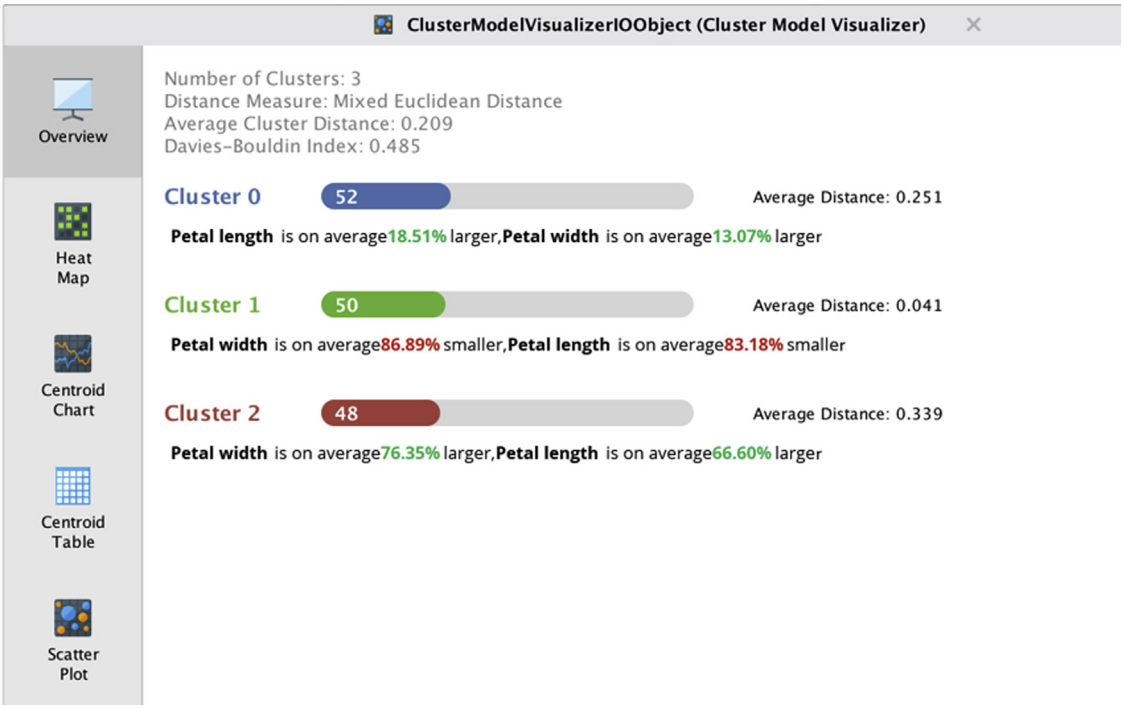



**FIGURE 7.12**
Performance measures of *k*-means clustering.

centroid methods, specifying the number of the cluster parameters ($k$) is not necessary for density-based algorithms. Thus, density-based clustering can serve as an important data exploration technique. DBSCAN is one of the most commonly used density-clustering algorithms (Ester, Kriegel, Sander, & Xu,1996). To understand how the algorithm works, the concept of density in a data space first needs to be defined.

Density can be defined as the number of data points in a unit $n$-dimensional space. The number of dimensions $n$ is the number of attributes in a dataset. To simplify the visualization and to further understand how the model works, consider a two-dimensional space or a dataset with two numeric attributes. From looking at the dataset represented in Fig. 7.13, it can be visually concluded that the density in the top-left section is higher than the density in top-right, bottom-left, and bottom-right sections. Technically, density relates to the number of points in unit space, in this case a quadrant. Wherever there is high-density space amongst relatively low-density spaces, there is a cluster.

One can also measure density within a circular space around a point as in Fig. 7.14. The number of points within a circular space with radius $\varepsilon$

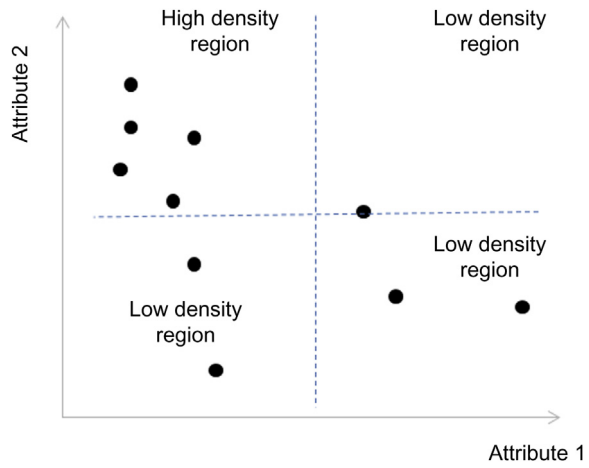



**FIGURE 7.13**
Dataset with two attributes.

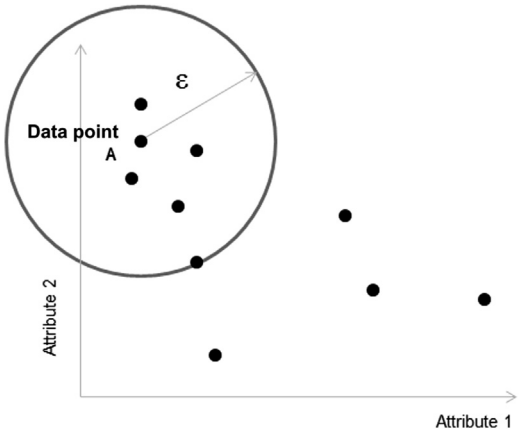



**FIGURE 7.14**
Density of a data point within radius $\varepsilon$.

(epsilon) around a data point A is six. This measure is called center-based density since the space considered is globular with the center being the point that is considered.

### 7.2.1 How It Works

The DBSCAN algorithm creates clusters by identifying high-density and low-density space within the dataset. Similar to *k*-means clustering, it is preferred

that the attributes are numeric because distance calculation is still used. The algorithm can be reduced to three steps: defining threshold density, classification of data points, and clustering (Tan et al., 2005).

### Step 1: Defining Epsilon and MinPoints

The DBSCAN algorithm starts with calculation of a density for all data points in a dataset, with a given fixed radius $\varepsilon$ (epsilon). To determine whether a neighborhood is high-density or low-density, a threshold of data points (MinPoints) will have to be defined, above which the neighborhood is considered high-density. In Fig. 7.14, the number of data points inside the space is defined by radius $\varepsilon$. If MinPoints is defined as 5, the space $\varepsilon$ surrounding data point A is considered a high-density region. Both $\varepsilon$ and MinPoints are user-defined parameters and can be altered for a dataset.

### Step 2: Classification of Data Points

In a dataset, with a given $\varepsilon$ and MinPoints, all data points can be defined into three buckets (Fig. 7.15):

- *Core points*: All the data points inside the high-density region of at least one data point are considered a core point. A high-density region is a space where there are at least *MinPoints* data points within a radius of $\varepsilon$ for any data point.
- *Border points*: Border points sit on the circumference of radius $\varepsilon$ from a data point. A border point is the boundary between high-density and

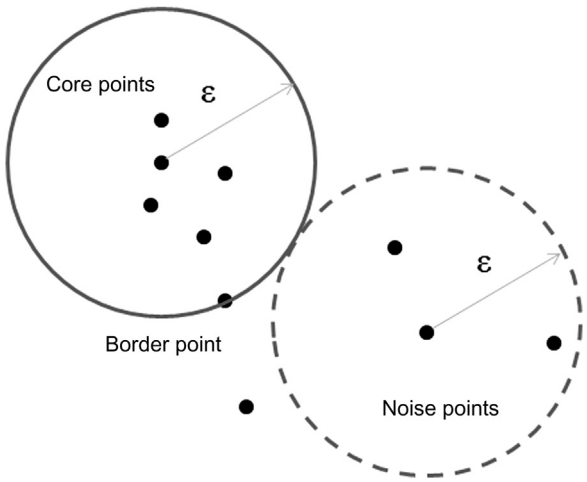



**FIGURE 7.15**
Core, border, and density points.

low-density space. Border points are counted within the high-density space calculation.

- *Noise points*: Any point that is neither a core point nor border point is called a noise point. They form a low-density region around the high-density region.

### Step 3: Clustering

Once all data points in the dataset are classified into density points, clustering is a straightforward task. Groups of core points form distinct clusters. If two core points are within $\varepsilon$ of each other, then both core points are within the same cluster. All these clustered core points form a cluster, which is surrounded by low-density noise points. All noise points form low-density regions around the high-density cluster, and noise points are not classified in any cluster. Since DBSCAN is a partial clustering algorithm, a few data points are left unlabeled or associated to a default noise cluster.

### Optimizing Parameters

One of the key advantages of using a density algorithm is that there is no need for specifying the number of clusters ($k$). Clusters are automatically found in the dataset. However, there is an issue with selecting the distance parameter $\varepsilon$ and a minimum threshold (MinPoints) to identify the dense region. One technique used to estimate optimal parameters for the DBSCAN clustering algorithm relates to the $k$-NN algorithm. The initial values of the parameter can be estimated by building a $k$-distribution graph. For a user-specified value of $k$ (say, four data points), the distance of the $k$-th NN can be calculated for a data point. If the data point is a core point in a high-density region, then the distance of the $k$-th NN will be smaller. For a noise point, the distance will be larger. Similarly, the $k$-distance can be calculated for all data points in a dataset. A $k$-distance distribution graph can be built by arranging all the $k$-distance values of individual data points in descending order, as shown in Fig. 7.16. This arrangement is similar to Pareto charts. Points on the right-hand side of the chart will belong to data points inside a cluster, because the distance is smaller. In most datasets, the value of $k$-distance sharply rises after a particular value. The distance at which the chart rises will be the optimal value $\varepsilon$ (epsilon) and the value of $k$ can be used for MinPoints.

### Special Cases: Varying Densities

The DBSCAN algorithm partitions data based on a certain threshold density. This approach creates an issue when a dataset contains areas of varying data density. The dataset in Fig. 7.17 has four distinct regions numbered from 1−4. Region 1 is the high-density area A, regions 2 and 4 are of medium-density B, and between them is region 3, which is extremely low-density C. If

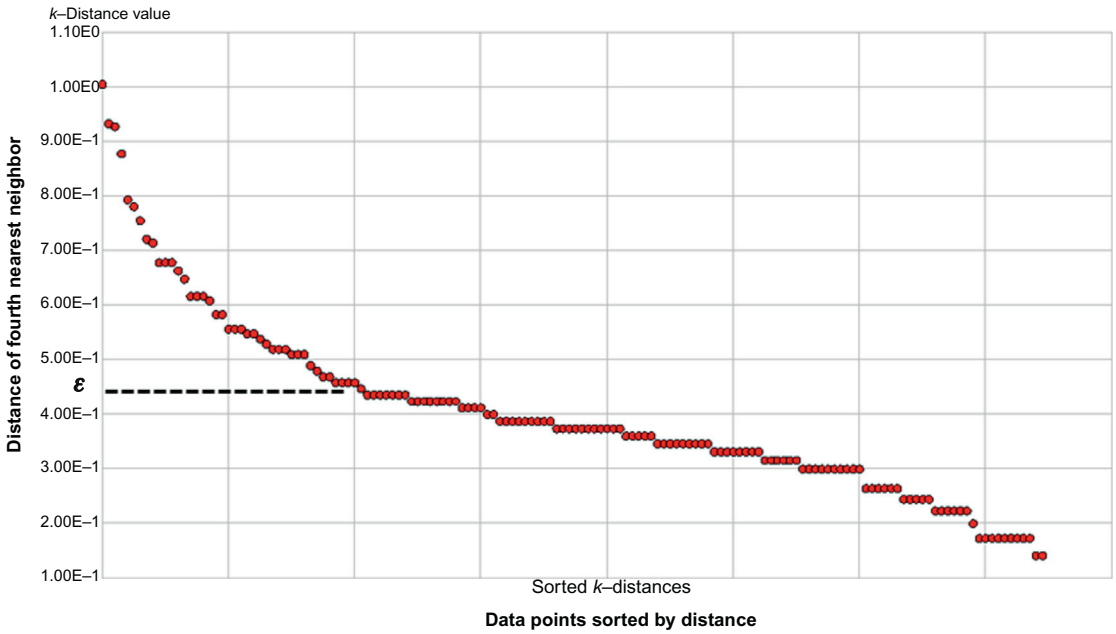



**FIGURE 7.16**
*k*-Distribution chart for the Iris dataset with $k = 4$.

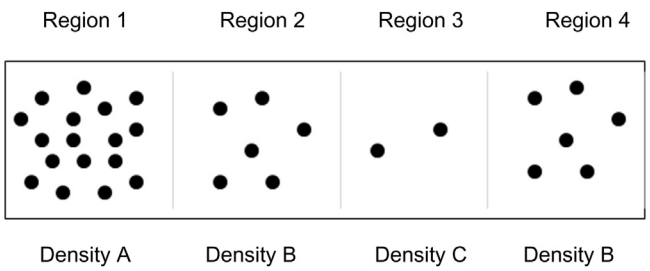



**FIGURE 7.17**
Dataset with varying densities.

the density threshold parameters are tuned in such a way as to partition and identify region 1, then regions 2 and 4 (with density B) will be considered noise, along with region 3. Even though region 4 with density B is next to an extremely low-density area and clearly identifiable visually, the DBSCAN algorithm will classify regions 2 through 4 as noise. The *k*-means clustering algorithm is better at partitioning datasets with varying densities.

### 7.2.2 How to Implement

The implementation of the DBSCAN algorithm is supported in RapidMiner through the DBSCAN modeling operator. The DBSCAN operator accepts numeric and polynominal datasets with provisions for user-specified $\varepsilon$ (epsilon) and MinPoints parameters. Here are the implementation steps.

#### *Step 1: Data Preparation*

As with the *k*-means section, the number of attributes in the dataset will be limited to a3 and a4 (petal length and petal width) using the *Select Attribute* operator, so that the cluster can be visualized and the clustering process better understood.

#### *Step 2: Clustering Operator and Parameters*

The modeling operator is available in the Modeling > Clustering and Segmentation folder and is labeled DBSCAN. These parameters can be configured in the model operator:

- *Epsilon ($\varepsilon$)*: Size of the high-density neighborhood. The default value is 1.
- *MinPoints*: Minimum number of data objects within the epsilon neighborhood to qualify as a cluster.
- *Distance measure*: The proximity measure can be specified in this parameter. The default and most common measurement is Euclidean distance. Other options here are Manhattan distance, Jaccard coefficient, and cosine similarity for document data. Please refer to Chapter 4, Classification for a summary of different distance measures.
- *Add cluster as attributes*: To append cluster labels into the original dataset. This option is recommended for later analysis.

#### *Step 3: Evaluation*

Similar to *k*-means clustering implementation, the effectiveness of clustering groups can be evaluated using average within-cluster distance. In RapidMiner, the *Cluster Density Performance* operator under Evaluation > Clustering is available for performance evaluation of cluster groups generated by Density algorithms. The clustering model and labeled dataset are connected to *performance* operator for cluster evaluation. Additionally, to aid the calculation, *performance* operator expects Similarity Measure objects. A similarity measure vector is a distance measure of every example data object with the other data object. The similarity measure can be calculated by using *Data to Similarity* Operator on the example dataset.

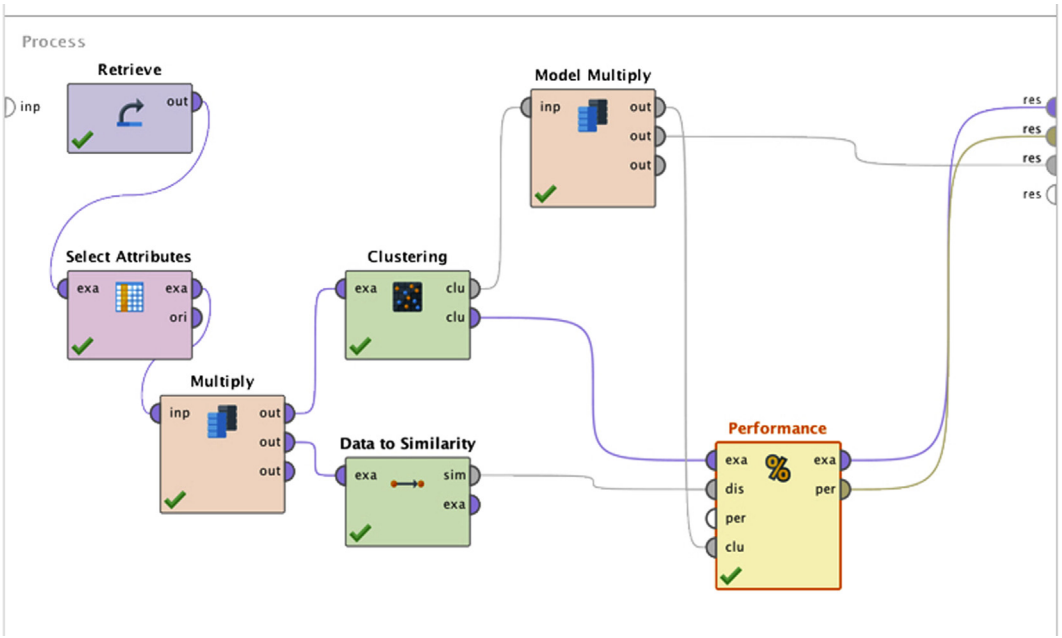



**FIGURE 7.18**
Data science process with density clustering.

### *Step 4: Execution and Interpretation*

After the outputs from the *performance* operator have been connected to the result ports, as shown in Fig. 7.18, the model can be executed. The result output can be observed as:

1. *Model*: The cluster model output contains information on the number of clusters found in the dataset (Cluster 1, Cluster 2, etc.) and data objects identified as noise points (Cluster 0). If no noise points are found, then Cluster 0 is an empty cluster. As shown in Fig. 7.19, the Folder view and Graph view from the output window provide the visualization of data points classified under different clusters.
2. *Clustered example set*: The example set now has a clustering label that can be used for further analysis and visualization. In the scatterplot view of this dataset (Fig. 7.20), *x*- and *y*-axes can be configured to be attributes of the original dataset, petal length and petal width. The Color Column can be configured to be the new cluster label. In the plot, it can be noted how the algorithm found two clusters within the example set. The I. *setosa* species data objects have clear high-density areas but there is a density bridge between the I. *versicolor* and I. *virginica* species data points. There is no clear low-density area to

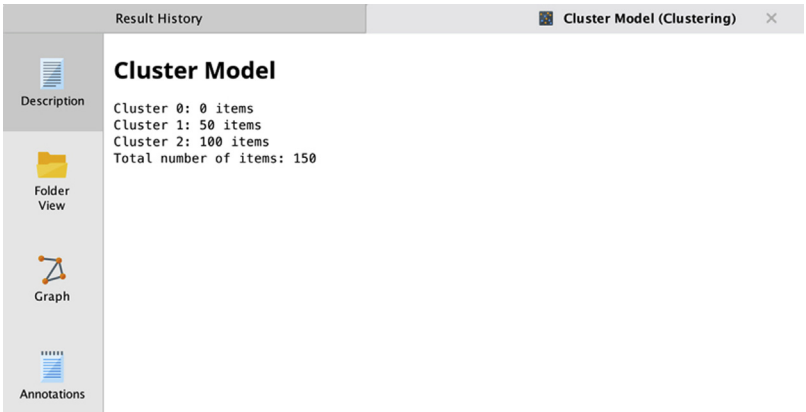



**FIGURE 7.19**
Density-clustering model output.

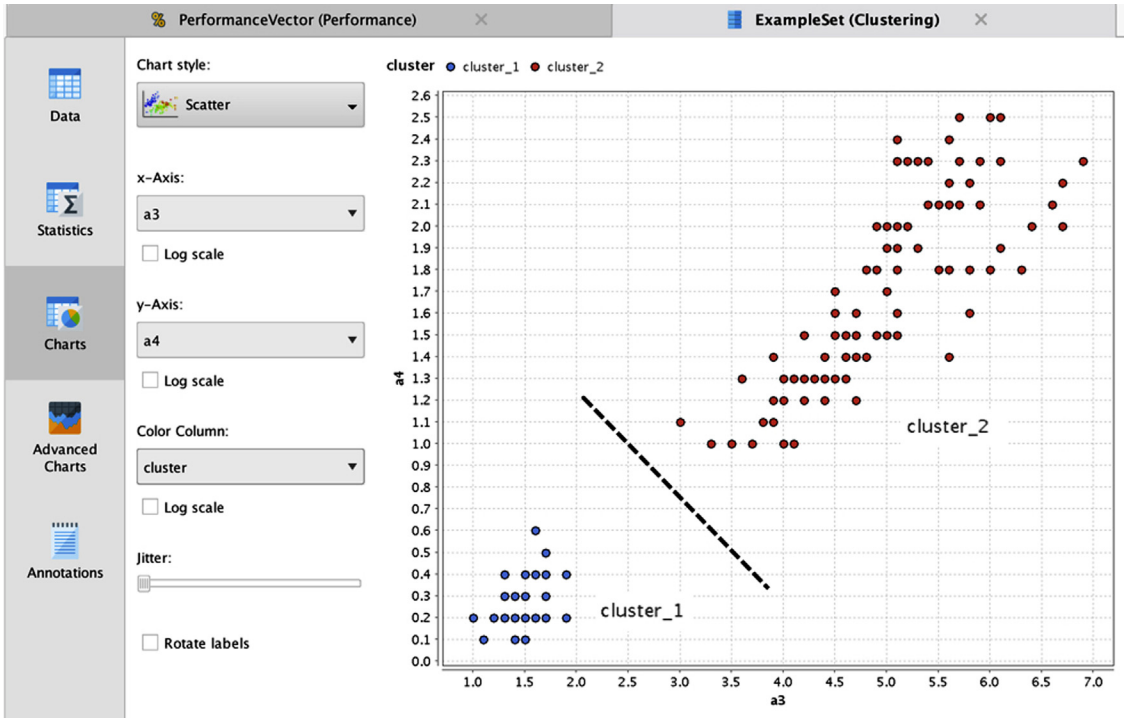



**FIGURE 7.20**
Density-clustering visual output.

partition these two species of data points. Hence, I. *versicolor* and I. *virginica* natural clusters are combined to one artificial predicted cluster. The epsilon and MinPoints parameters can be adjusted to find different results for the clustering.

3. *Performance vector*: The performance vector window shows the average distance within each cluster and the average of all clusters. The average distance is the distance between all the data points within the cluster divided by number of data points. These measures can be used to compare the performance of multiple model runs.

The main attraction of using DBSCAN clustering is that one does not have to specify the value of k, the number of clusters to be identified. In many practical applications, the number of clusters to be discovered will be unknown, like finding unique customers or electoral segments. DBSCAN uses variations in the density of the data distribution to find the concentration of structures in the data. These clusters can be of any shape and they are not confined to globular structures as in the k-means approach. But the density algorithms run into the risk of finding bridges between two natural clusters and merging them into one cluster.

Since the density-clustering technique yields partial clustering, DBSCAN ignores noise and outlier data points and they are not clustered in the final results. The inability to identify varying densities within a dataset is one of the major limitations of the DBSCAN clustering technique. Centroid methods are more successful at finding varying density patterns in a dataset. A dataset with a high number of attributes will have processing challenges with density-clustering methods. Given the complementary pros and cons of the k-means and DBSCAN methods, it is advisable to cluster the dataset by both methods and understand the patterns of both result sets.

## 7.3 SELF-ORGANIZING MAPS

A self-organizing map (SOM) is a powerful visual clustering technique that evolved from a combination of neural networks and prototype-based clustering. A SOM is a form of neural network where the output is an organized visual matrix, usually a two-dimensional grid with rows and columns. The objective of this neural network is to transfer all input data objects with $n$ attributes ($n$ dimensions) to the output lattice in such a way that objects next to each other are closely related to each other. Two examples of SOM layouts are provided in Fig. 7.21. This two-dimensional matrix becomes an exploration tool in identifying the clusters of objects related to each other by visual examination. A key distinction in this neural network is the absence of an output target function to optimize or predict, hence, it is an unsupervised learning algorithm. SOMs effectively arrange the data points in a lower

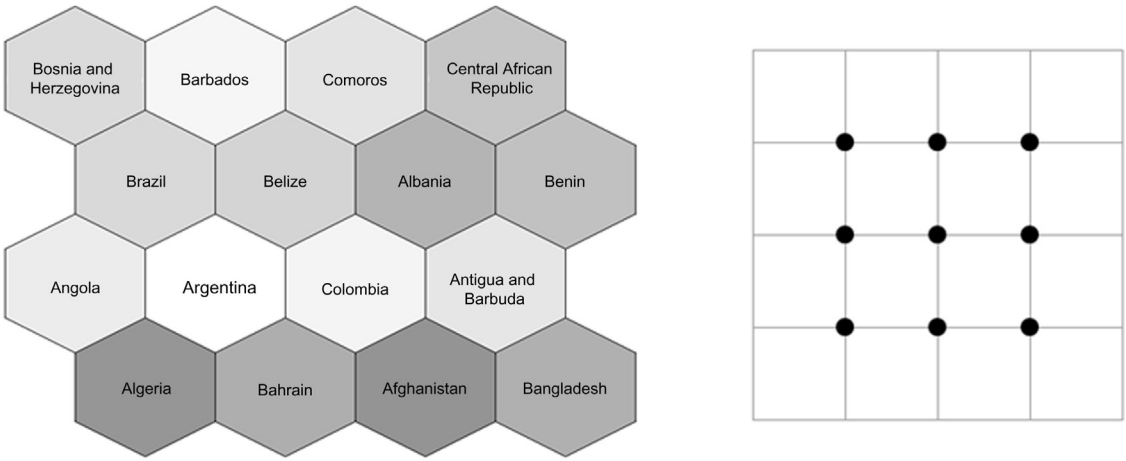



**FIGURE 7.21**
Self-organizing maps of countries by GDP data using a (A) hexagonal grid and (B) rectangular lattice. *GDP*, Gross domestic product.

dimensional space, thereby, aiding in the visualization of high-dimensional data through a low-dimensional space.

SOMs are relevant to clustering because the most common SOM output is a two-dimensional grid with data objects placed next to each other based on their similarity to one another. Objects related to each other are placed in close proximity. SOMs differ from other clustering techniques because there is no explicit clustering labels assigned to data objects. Data objects are arranged based on their attribute proximity and the task of clustering is left to visual analysis by the user. Hence, SOM is used as a *visual* clustering and data exploration technique (Germano, 1999).

SOMs were first proposed by Kohonen (1982) and, hence, this technique is also known as Kohonen networks; it is sometimes also referred to by a more specific name, self-organizing feature maps. SOM methodology is used to project data objects from *data space*, mostly in *n* dimensions, to *grid space*, usually resulting in two dimensions. Though other output formats are possible, the most common output formats for SOMs are: (1) a hexagonal lattice or a (2) rectangular grid as shown in Fig. 7.21. Each data point from the dataset occupies a cell or a node in the output lattice, with arrangement constraints depending on the similarity of data points. Each cell in the SOM grid, called a *neuron*, corresponds to one or a group of data points. In a hexagonal grid, each neuron has six neighbors while a rectangular lattice has four neighbors.

SOMs are commonly used in comparing data points with a large number of numeric attributes. The objective of this kind of analysis is to compare the

relative features of data objects in a simple two-dimensional setting where the placement of objects is related to each other. In Fig. 7.21A, the SOM compares relative gross domestic product (GDP) data from different countries where countries with similar GDP profiles are placed either in the same cells or next to each other. All similar countries around a particular cell can be considered a grouping. Although the individual data objects (countries) do not have a cluster membership, the placement of objects together aides in visual data analysis. This application is also called competitive SOMs.

### 7.3.1 How It Works

The algorithm for a SOM is similar to centroid-based clustering but with a neural network foundation. Since a SOM is essentially a neural network, the model accepts only numerical attributes. However, there is no target variable in SOM because it is an unsupervised learning model. The objective of the algorithm is to find a set of centroids (neurons) to represent the cluster but with topological constraints. The topology refers to an arrangement of centroids in the output grid. All the data objects from the dataset are assigned to each centroid. Centroids closer to each other in the grid are more closely "related" to each other than to centroids further away in the grid. A SOM converts numbers from the data space to a grid space with additional inter-topology relationships.

#### *Step 1: Topology Specification*

The first step for a SOM is specifying the topology of the output. Even though multi-dimensional output is possible, two-dimensional rows and columns with either a rectangular lattice or a hexagonal lattice are commonly used in SOMs to aid in the visual discovery of clustering. One advantage in using a hexagonal lattice is that each node or centroid can have six neighbors, two more than in a rectangular lattice. Hence, in a hexagonal lattice, the association of a data point with another data point can be more precise than for a rectangular grid. The number of centroids can be specified by providing the number of rows and columns in the grid. The number of centroids is the product of the number of rows and columns in the grid. Fig. 7.22 shows a hexagonal lattice SOM.

#### *Step 2: Initialize Centroids*

A SOM starts the process by initializing the centroids. The initial centroids are values of random data objects from the dataset. This is similar to initializing centroids in *k*-means clustering.

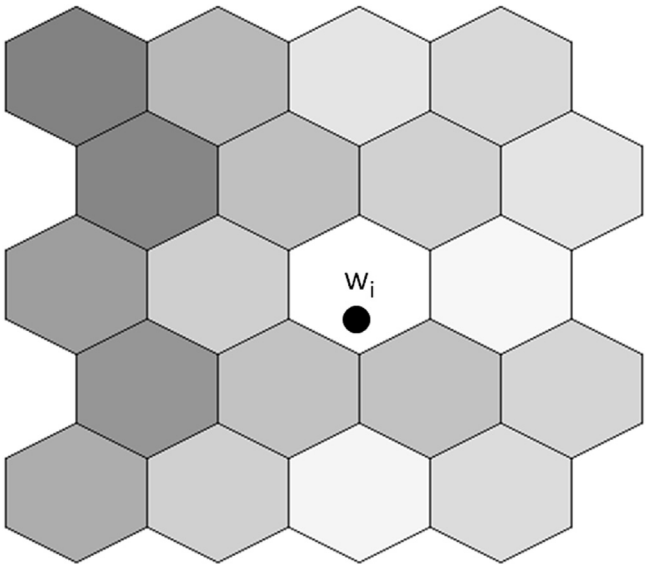



**FIGURE 7.22**
Weight of the centroid is updated.

### *Step 3: Assignment of Data Objects*

After centroids are selected and placed on the grid in the intersection of rows and columns, data objects are selected one by one and assigned to the nearest centroid. The nearest centroid can be calculated using a distance function like Euclidean distance for numeric data or a cosine measure for document or binary data.

### *Step 4: Centroid Update*

The centroid update is the most significant and distinct step in the SOM algorithm and is repeated for every data object. The centroid update has two related sub-steps.

The first sub-step is to update the closest centroid. The objective of the method is to update the data values of the nearest centroid of the data object, proportional to the difference between the centroid and the data object. This is similar to updating weights in the back-propagation algorithm of neural networks. In the neural network section of Chapter 4, Classification, how the weights of neurons are updated based on the error difference between the predicted and actual values was discussed. Similarly, in the context of a SOM, the values of centroids are updated. In fact, centroids are considered neurons in a SOM. Through this update, the closest centroid moves closer to the data object in the data space.

The centroid update step is repeated for a number of iterations, usually in the thousands. Denote $t$ as the $t^{th}$ iteration of the update where the data point $d(t)$ is picked up. Let $w_1$, $w_2$, $w_3$, …, $w_k$ represent all the centroids in the grid space. Fig. 7.22 shows the lattice with centroid weight. Let $r$ and $c$ be the number of rows and columns in the grid. Then $k$ will be equal to $r * c$. Let $w_i$ be the nearest centroid for a data object $d(t)$. During iteration $t$, the nearest centroid $w_i$ is updated using Eq. (7.4).

$$w_i(t+1) = w_i(t) + f_i(t) \times [d(t) - w_i(t)] \tag{7.4}$$

The effect of the update is determined by the difference between the centroid and the data point in the data space and the neighborhood function $f_i(t)$. The neighborhood function decreases for every iteration so that there are no drastic changes made in the final iteration. In addition to updating the nearest primary centroid, all other centroids in the grid space neighborhood of the primary centroid are updated as well. This will be reviewed in more detail in the next sub-step.

The second sub-step is to update all centroids in the grid space neighborhood as shown in Fig. 7.23. The neighborhood update step has to be proportional to the distance from the closest centroid to the centroid that is being updated. The update function has to be stronger when the distance is closer. Taking into account time decay and distance between neighborhood centroids, a Gaussian function is commonly used for:

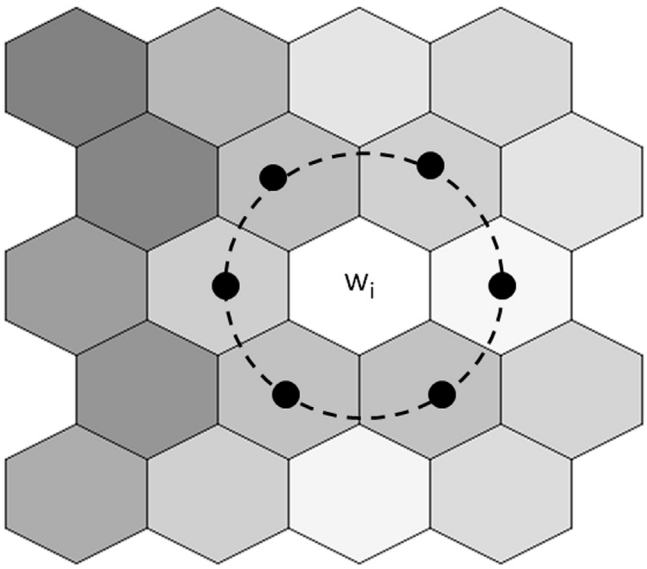



**FIGURE 7.23**
The weight of the neighborhood centroids are updated.

$$f_i(t) = \lambda_i(t) e^{\left(-\frac{(g_i - g_j)^2}{2\sigma^2}\right)} \tag{7.5}$$

where $\lambda_i(t)$ is the learning rate function that takes a value between 0 and 1 and decays for every iteration. Usually it is either a linear rate function or an inverse of the time function. The variable in the exponential parameter $g_i - g_j$ is the distance between the centroid being updated and the nearest centroid of the data point in the grid space. The variable $\sigma$ determines the radius of the centroid update or the neighborhood effect. By updating the entire neighborhood of centroids in the grid, the SOM self-organizes the centroid lattice. Effectively, the SOM converts data from the data space to a location-constrained grid space.

#### *Step 5: Termination*

The entire algorithm is continued until no significant centroid updates take place in each run or until the specified number of run count is reached. The selection of the data object can be repeated if the dataset size is small. Like with many data science algorithms, a SOM tends to converge to a solution in most cases but doesn't guarantee an optimal solution. To tackle this problem, it is necessary to have multiple runs with various initiation measures and to compare the results.

#### *Step 6: Mapping a New Data Object*

A SOM model itself is a valuable visualization tool that can describe the relationship between data objects and be used for visual clustering. After the grids with the desired number of centroids have been built, any new data object can be quickly given a location on the grid space, based on its proximity to the centroids. The characteristics of new data objects can be further understood by studying the neighbors.

### 7.3.2 How to Implement

SOM can be implemented in a few different ways in RapidMiner, with varied functionality and resulting output.

- *Data exploration chart*: In Chapter 3, Data Exploration, the SOM chart was reviewed as one of the data exploration techniques. In RapidMiner, any dataset connected to a result port has a SOM chart feature under the Chart tab. This is a quick and easy method where the number of rows and columns can be specified, and a SOM chart can be rendered.
- *Data Transformation > Attribute set reduction > SOM Operator*: The *SOM* operator available under the Data Transformation folder is used to reduce the number of dimensions in the dataset. It is similar to the

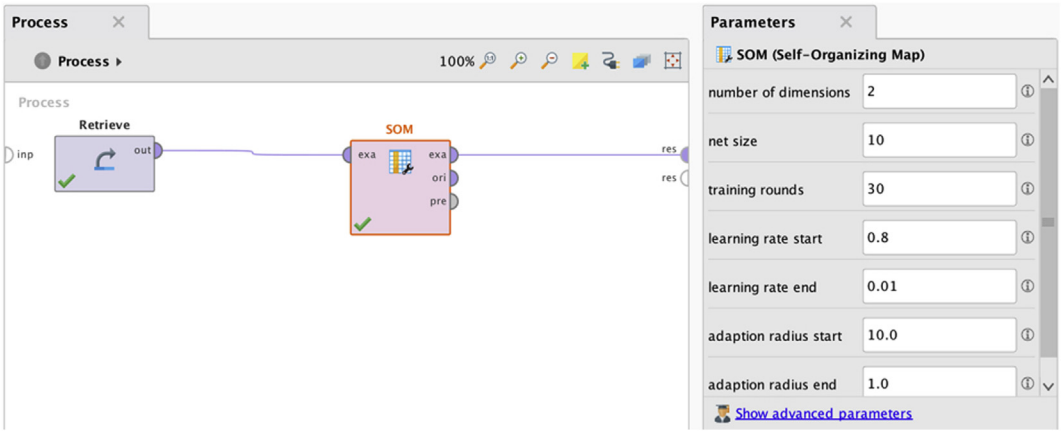



**FIGURE 7.24**
SOM in data transformation. *SOM*, Self-organizing map.

application of principal component analysis where the dataset is reduced to a lower dimensionality. In theory, a SOM can help reduce the data to any number of dimensions below the dimension count of the dataset. In this operator, the number of desired output dimensions can be specified in the parameters, as shown in Fig. 7.24. The net size parameter indicates the unique values in each of the SOM dimensions. There is no visual output for this operator and in two dimensions, only a square topography can be achieved through the *SOM data transformation* operator.

- *RapidMiner Extension > SOM Modeling Operator*: The *SOM modeling* operator is available in the SOM extension (Motl, 2012) and offers rich SOM visuals. SOM extensions will be used for the rest of this implementation section, so installing the SOM extension is recommended before proceeding further.

RapidMiner provides a marketplace platform called Extensions for specialized data science tasks which has operators, data science algorithms, data transformation operators, and visual exploration tools. The extensions can be installed and uninstalled easily from Help > Updates and Extensions. SOM is one of the extensions, along with text mining, the R extension, Recommenders, Weka extension, etc. Extensions will be used in the upcoming chapters.

The dataset used in this section is the relative GDP information by country (IMF, 2012) from the *World Economic Outlook Database October 2012* by the International Monetary Fund. The dataset has 186 records, one for each country, and four attributes in percentage of GDP: relative GDP invested, relative GDP saved, government revenue, and current account balance. Fig. 7.25 shows the actual raw data for a few rows and Fig. 7.26 shows the quartile plot for all the attributes.

| Row No. | Country | Current account balance | General government revenue | Gross national savings | Total investment |
|---|---|---|---|---|---|
| 1 | Afghanistan | 3.877 | 21.977 | 30.398 | 26.521 |
| 2 | Albania | −11.372 | 25.835 | 14.509 | 25.886 |
| 3 | Algeria | 7.489 | 36.458 | 48.947 | 41.428 |
| 4 | Angola | 9.024 | 43.479 | 21.692 | 12.668 |
| 5 | Antigua and... | −13.109 | 22.430 | 16.194 | 29.303 |
| 6 | Argentina | 0.658 | 37.199 | 22.595 | 24.451 |
| 7 | Armenia | −14.653 | 20.970 | 16.660 | 31.313 |
| 8 | Australia | −2.870 | 31.846 | 23.925 | 26.794 |
| 9 | Austria | 3.009 | 48.105 | 24.611 | 21.602 |
| 10 | Azerbaijan | 28.423 | 45.652 | 46.955 | 18.532 |

**FIGURE 7.25**
GDP by country dataset. *GDP*, Gross domestic product.

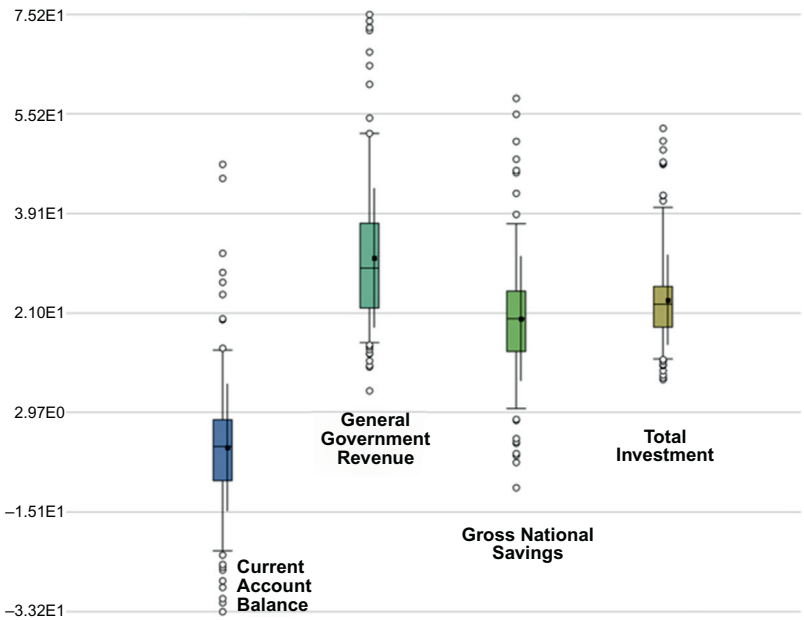



**FIGURE 7.26**
GDP by country: box-whisker (quartile) plot for all four attributes. *GDP*, Gross domestic product.

The objective of the clustering is to compare and contrast countries based on their percentage of GDP invested and saved, government revenue, and current account balance. Note that they are not compared using the size of the economy through absolute GDP but by the size of investment, national savings, current account, and the size of government relative to the country's GDP. The goal of this modeling exercise is to arrange countries in a grid so that countries with similar characteristics of investing, savings, size of government, and current accounts are placed next to each other. The four-dimensional information is being compressed into a two-dimensional map or grid. The dataset and RapidMiner process can be accessed from the companion site of the book at www.IntroDataScience.com.

### Step 1: Data Preparation

As a neural network, a SOM cannot accept polynominal or categorical attributes because centroid updates and distance calculations work only with numeric values. Polynominal data can be either ignored with information loss or converted to a numeric attribute using the *Nominal to Numerical* type conversion operator available in RapidMiner. The country attribute is set as a label using Set role operator. In this dataset, there are records (each record is a country) where there is no data in few attributes. Neural networks cannot handle missing values and, hence, they need to be replaced by either zero or the minimum or average value for the attribute using the *Replace Missing Value* operator. In this example the average was chosen as the default missing value.

### Step 2: SOM Modeling Operator and Parameters

The *SOM modeling extension* operator is available in the Self-Organizing Map folder, labeled with the same name. Please note that the SOM folder is visible only when the SOM extension has been installed. The coming parameters can be configured in the model operator. The modeling operator accepts the example set with numeric data and a label attribute if applicable. In this example set, the country name is a label attribute. Fig. 7.27 shows the RapidMiner process for developing a SOM model.

- *Training Rounds*: Defaults to 1000. This value indicates the number of training rounds for the data object selection process.
- *Net Size*: Indicates whether the grid size should be specified by the user or automatically approximated by the system. In this exercise select user input for *X* and *Y*.
- *Net Size X*: Specifies the number of columns in the grid (horizontal direction). This is the same as the possible values for the SOM_0 attribute in the output. In this example this value will be set to 10.

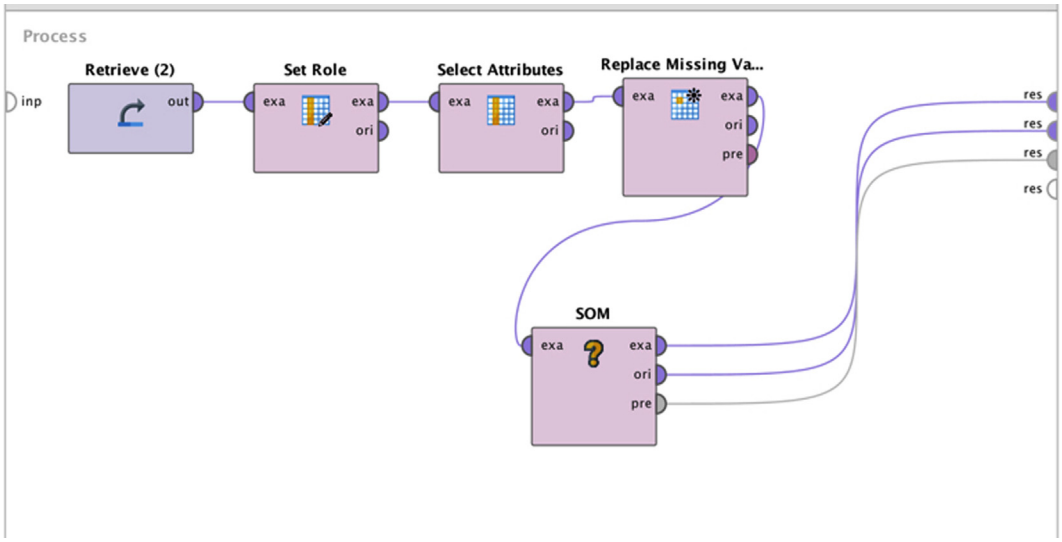



**FIGURE 7.27**
Clustering with SOM. *SOM*, Self-organizing map.

- *Net Size Y*: Specifies the number of rows in the grid (vertical direction). This also indicates the values for the SOM_1 attribute in the output grid. In this example this value will be set to 10.
- *Learning Rate*: The neural network learning parameter ($\lambda$), which takes a value from 0 to 1. The value of $\lambda$ determines how sensitive the change in weight is to the previous weights. A value closer to 0 means the new weight would be mostly based on previous weight and an $\lambda$ closer to 1 means that the weight would be mainly based on error correction. The initial $\lambda$ will be assigned as 0.9 (see Section 4.5 on Neural Networks).
- *Learning Rate function*: The learning rate function in a neural network is a time decay function of the learning process. The default and most commonly used time decay function is the inverse of time.

### *Step 3: Execution and Interpretation*

The RapidMiner process can be saved and executed. The output of the *SOM modeling* operator consists of a visual model and a grid dataset. The visual model is a lattice with centroids and mapped data points. The grid dataset output is the example set labeled with location coordinates for each record in the grid lattice.

### *Visual Model*

The visual model of the SOM displays the most recognizable form of SOM in a hexagonal grid format. The size of the grid is configured by the input parameters that set the net size of *X* and *Y*. There are several advanced visualization styles available in the Visualization results window. The SOM visual output can be customized using these parameters:

- *Visualization Style*: This selection controls the visual layout and background color of the SOM hexagons. The value of the selected measure is represented as a background gradient color. The default, U-Matrix, presents a background gradient color proportional to the distance of the central data points in adjacent hexagons. The P-Matrix option shows the number of example data points through the background gradient color. The selection of an individual attribute name for the visualization style renders the background gradient proportional to the value of the selected attribute. The visualization style selection does not rearrange the data points assigned to hexagons.
- *Label*: Selection shows the attribute value selected in the hexagons.
- *Color Schema*: Selection of monochrome or color scheme.

Fig. 7.28 shows a SOM with the default selection of the label as Country and the visualization style as U-Matrix. It can be observed how countries are

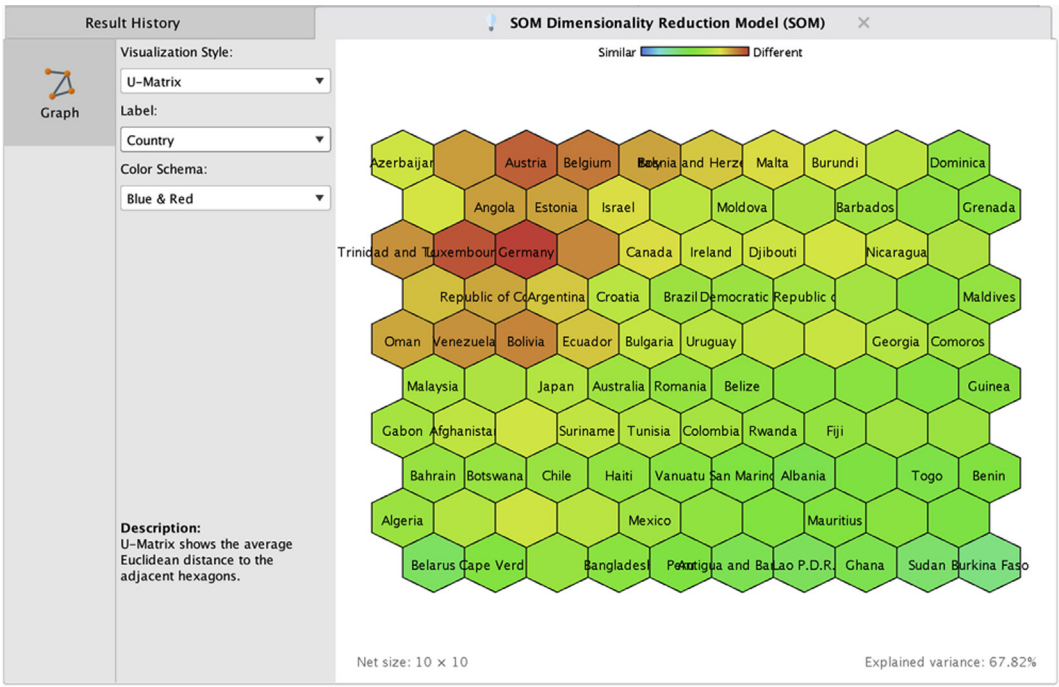



**FIGURE 7.28**
SOM output in the hexagonal grid. *SOM*, Self-organizing map.

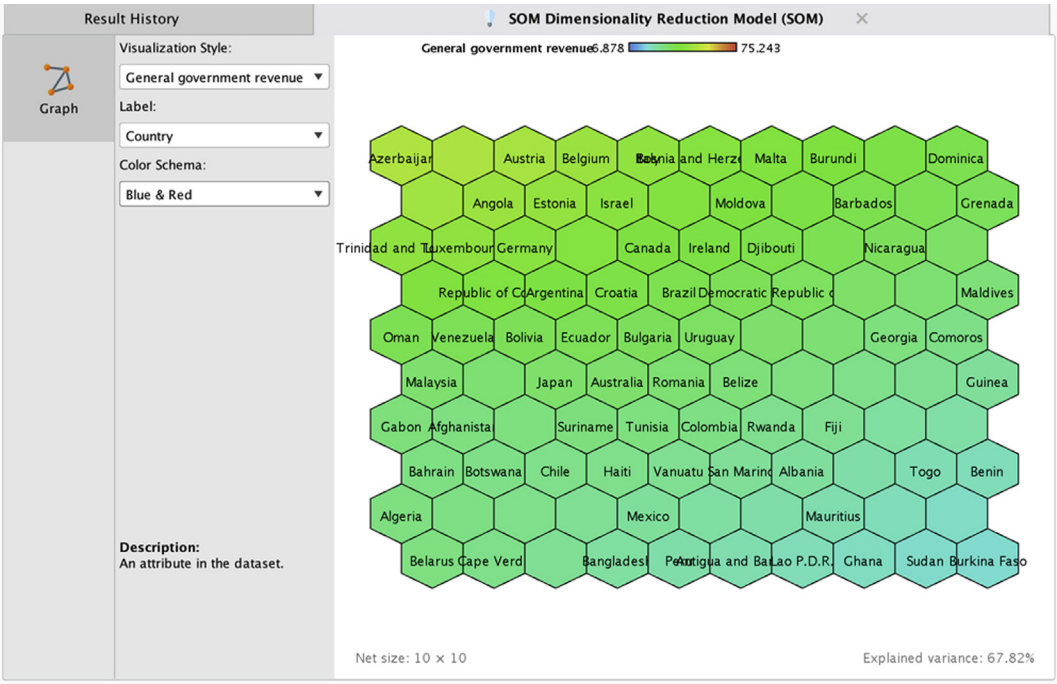



**FIGURE 7.29**
SOM output with color overlay related to government revenue. *SOM*, Self-organizing map.

placed on the grid based on their relationship with each other, as evaluated by the four economic metrics in relation to GDP. Countries with similar characteristics are placed closer to each other than to others in the grid. If more than one country belongs to a centroid (hexagon), then the label of one country closer to the centroid is displayed on the grid. The grid locations of all the counties are listed in the location coordinates section of the results window.

A few interesting patterns in the data can be observed by changing the visualization style as a metric in the dataset. In Fig. 7.29, government revenue as percentage of GDP is used and visually, countries with high government revenue as a percentage of GDP is displayed on the top-left side of the grid (e.g., Belgium with 48%) and countries with low government revenue are at bottom of the grid (Bangladesh 11%).

Fig. 7.30 shows the national savings rate visualization in the SOM; countries with a high savings rate (Algeria 49%) are concentrated on the left side and countries with a low savings rate (Maldives 2%) are concentrated on the right side of the SOM.

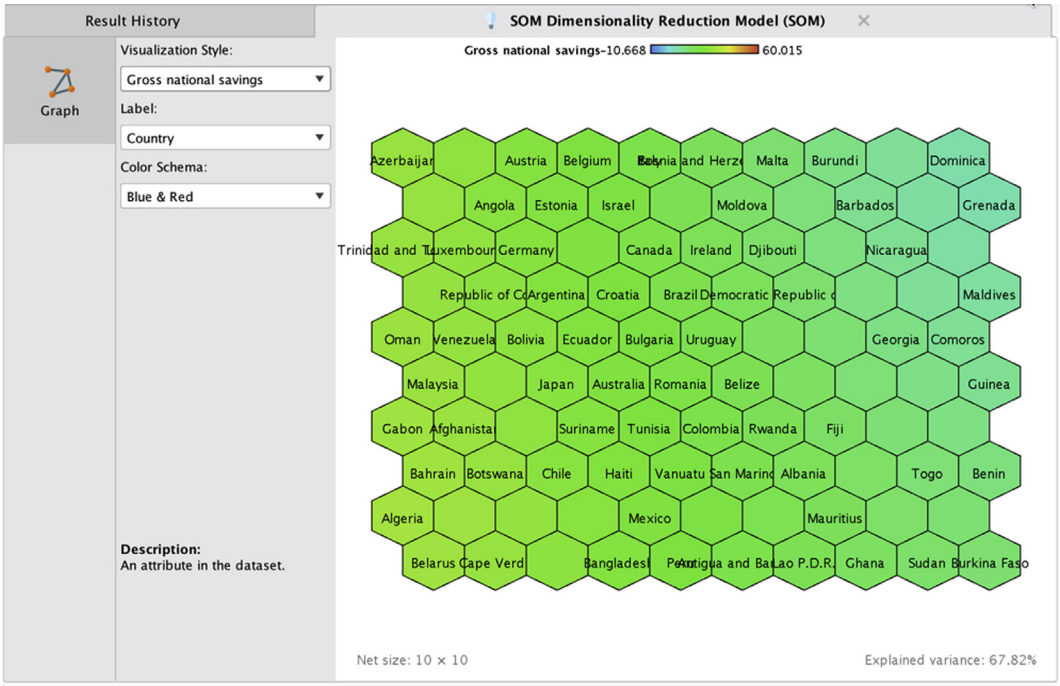


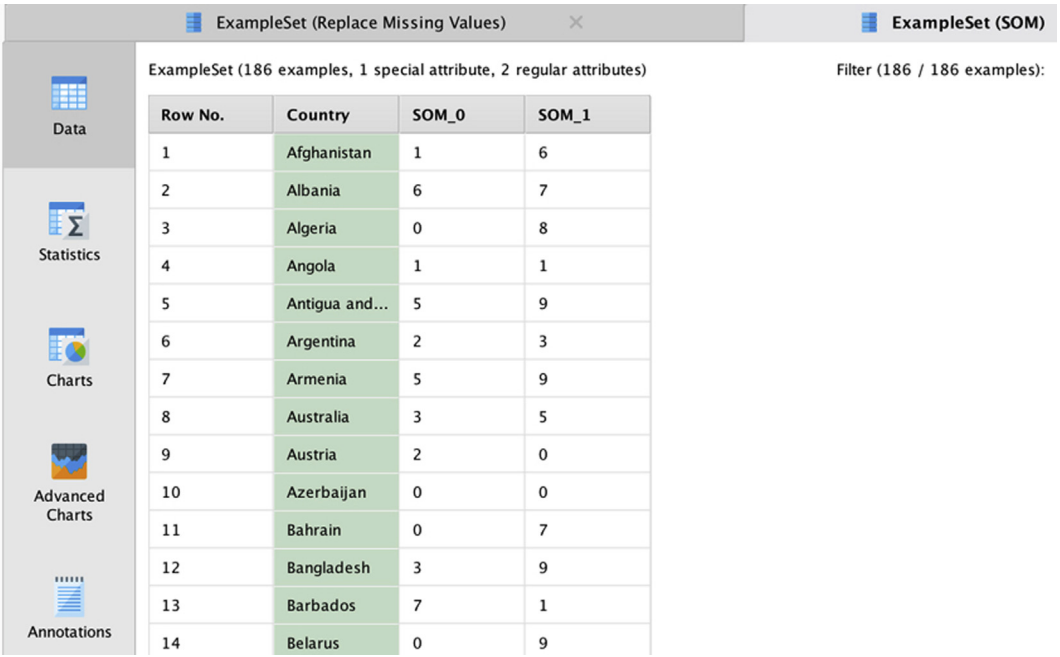

**FIGURE 7.30**
SOM output with color overlay related to national savings rate. *SOM*, Self-organizing map.

### *Location Coordinates*

The second output of the *SOM* operator contains the location coordinates of the *x*- and *y*-axes of grid with labels SOM_0 and SOM_1. The coordinate values of location range from 0 to net size—1, as specified in the model parameters, since all data objects, in this case countries, are assigned to a specific location in the grid. This output, as shown in Fig. 7.31, can be further used for post-processing such as distance calculation of locations between countries in the grid space.

### *Conclusion*

The methodology of SOMs is derived from the foundations of both neural network and prototype-clustering approaches. SOMs are an effective visual clustering tool to understand high-dimensional numeric data. They reduce the features of the dataset to two or three features, which is used to specify the topology of the layout. Hence, SOMs are predominantly used as a visual discovery and data exploration technique. Some of the applications of SOMs include the methods that are used in conjunction with other data science techniques such as graph mining (Resta, 2012), text mining (Liu, Liu, & Wang, 2012), speech recognition (Kohonen, 1988), etc.




| Row No. | Country | SOM_0 | SOM_1 |
|---|---|---|---|
| 1 | Afghanistan | 1 | 6 |
| 2 | Albania | 6 | 7 |
| 3 | Algeria | 0 | 8 |
| 4 | Angola | 1 | 1 |
| 5 | Antigua and... | 5 | 9 |
| 6 | Argentina | 2 | 3 |
| 7 | Armenia | 5 | 9 |
| 8 | Australia | 3 | 5 |
| 9 | Austria | 2 | 0 |
| 10 | Azerbaijan | 0 | 0 |
| 11 | Bahrain | 0 | 7 |
| 12 | Bangladesh | 3 | 9 |
| 13 | Barbados | 7 | 1 |
| 14 | Belarus | 0 | 9 |

**FIGURE 7.31**
SOM output with location coordinates. *SOM*, Self-organizing map.

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