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About the Authors

Jiawei Han is a Bliss Professor of Engineering in the Department of Computer Science at the University of Illinois at Urbana-Champaign. He has received numerous awards for his contributions on research into knowledge discovery and data mining, including ACM SIGKDD Innovation Award (2004), IEEE Computer Society Technical Achievement Award (2005), and IEEE W. Wallace McDowell Award (2009). He is a Fellow of ACM and IEEE. He served as founding Editor-in-Chief of *ACM Transactions on Knowledge Discovery from Data* (2006–2011) and as an editorial board member of several journals, including *IEEE Transactions on Knowledge and Data Engineering* and *Data Mining and Knowledge Discovery*.

Micheline Kamber has a master's degree in computer science (specializing in artificial intelligence) from Concordia University in Montreal, Quebec. She was an NSERC Scholar and has worked as a researcher at McGill University, Simon Fraser University, and in Switzerland. Her background in data mining and passion for writing in easy-to-understand terms help make this text a favorite of professionals, instructors, and students.

Jian Pei is currently an associate professor at the School of Computing Science, Simon Fraser University in British Columbia. He received a Ph.D. degree in computing science from Simon Fraser University in 2002 under Dr. Jiawei Han's supervision. He has published prolifically in the premier academic forums on data mining, databases, Web searching, and information retrieval and actively served the academic community. His publications have received thousands of citations and several prestigious awards. He is an associate editor of several data mining and data analytics journals.

2 Getting to Know Your Data

It's tempting to jump straight into mining, but first, we need to get the data ready. This involves having a closer look at attributes and data values. Real-world data are typically noisy, enormous in volume (often several gigabytes or more), and may originate from a hodgepodge of heterogenous sources. This chapter is about getting familiar with your data. Knowledge about your data is useful for data preprocessing (see Chapter 3), the first major task of the data mining process. You will want to know the following: What are the types of *attributes* or fields that make up your data? What kind of values does each attribute have? Which attributes are discrete, and which are continuous-valued? What do the data *look like*? How are the values distributed? Are there ways we can visualize the data to get a better sense of it all? Can we spot any outliers? Can we measure the similarity of some data objects with respect to others? Gaining such insight into the data will help with the subsequent analysis.

"*So what can we learn about our data that's helpful in data preprocessing?*" We begin in Section 2.1 by studying the various attribute types. These include nominal attributes, binary attributes, ordinal attributes, and numeric attributes. Basic *statistical descriptions* can be used to learn more about each attribute's values, as described in Section 2.2. Given a *temperature* attribute, for example, we can determine its **mean** (average value), **median** (middle value), and **mode** (most common value). These are **measures of central tendency**, which give us an idea of the "middle" or center of distribution.

Knowing such basic statistics regarding each attribute makes it easier to fill in missing values, smooth noisy values, and spot outliers during data preprocessing. Knowledge of the attributes and attribute values can also help in fixing inconsistencies incurred during data integration. Plotting the measures of central tendency shows us if the data are symmetric or skewed. Quantile plots, histograms, and scatter plots are other graphic displays of basic statistical descriptions. These can all be useful during data preprocessing and can provide insight into areas for mining.

The field of data visualization provides many additional techniques for viewing data through graphical means. These can help identify relations, trends, and biases "hidden" in unstructured data sets. Techniques may be as simple as scatter-plot matrices (where

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two attributes are mapped onto a 2-D grid) to more sophisticated methods such as treemaps (where a hierarchical partitioning of the screen is displayed based on the attribute values). Data visualization techniques are described in Section 2.3.

Finally, we may want to examine how similar (or dissimilar) data objects are. For example, suppose we have a database where the data objects are patients, described by their symptoms. We may want to find the similarity or dissimilarity between individual patients. Such information can allow us to find clusters of like patients within the data set. The similarity/dissimilarity between objects may also be used to detect outliers in the data, or to perform nearest-neighbor classification. (Clustering is the topic of Chapters 10 and 11, while nearest-neighbor classification is discussed in Chapter 9.) There are many measures for assessing similarity and dissimilarity. In general, such measures are referred to as proximity measures. Think of the proximity of two objects as a function of the *distance* between their attribute values, although proximity can also be calculated based on probabilities rather than actual distance. Measures of data proximity are described in Section 2.4.

In summary, by the end of this chapter, you will know the different attribute types and basic statistical measures to describe the central tendency and dispersion (spread) of attribute data. You will also know techniques to visualize attribute distributions and how to compute the similarity or dissimilarity between objects.

2.1 Data Objects and Attribute Types

Data sets are made up of data objects. A **data object** represents an entity—in a sales database, the objects may be customers, store items, and sales; in a medical database, the objects may be patients; in a university database, the objects may be students, professors, and courses. Data objects are typically described by attributes. Data objects can also be referred to as *samples, examples, instances, data points*, or *objects*. If the data objects are stored in a database, they are *data tuples*. That is, the rows of a database correspond to the data objects, and the columns correspond to the attributes. In this section, we define attributes and look at the various attribute types.

2.1.1 What Is an Attribute?

An **attribute** is a data field, representing a characteristic or feature of a data object. The nouns *attribute*, *dimension*, *feature*, and *variable* are often used interchangeably in the literature. The term *dimension* is commonly used in data warehousing. Machine learning literature tends to use the term *feature*, while statisticians prefer the term *variable*. Data mining and database professionals commonly use the term *attribute*, and we do here as well. Attributes describing a customer object can include, for example, *customer_ID*, *name*, and *address*. Observed values for a given attribute are known as *observations*. A set of attributes used to describe a given object is called an *attribute vector* (or *feature vector*). The distribution of data involving one attribute (or variable) is called *univariate*. A *bivariate* distribution involves two attributes, and so on.

The **type** of an attribute is determined by the set of possible values—nominal, binary, ordinal, or numeric—the attribute can have. In the following subsections, we introduce each type.

2.1.2 Nominal Attributes

Nominal means "relating to names." The values of a **nominal attribute** are symbols or *names of things*. Each value represents some kind of category, code, or state, and so nominal attributes are also referred to as **categorical**. The values do not have any meaningful order. In computer science, the values are also known as *enumerations*.

Example 2.1 **Nominal attributes.** Suppose that *hair_color* and *marital_status* are two attributes describing *person* objects. In our application, possible values for *hair_color* are *black*, *brown*, *blond*, *red*, *auburn*, *gray*, and *white*. The attribute *marital_status* can take on the values *single, married, divorced*, and *widowed*. Both *hair_color* and *marital_status* are nominal attributes. Another example of a nominal attribute is *occupation*, with the values *teacher, dentist, programmer, farmer*, and so on. ■

Although we said that the values of a nominal attribute are symbols or "names of things," it is possible to represent such symbols or "names" with numbers. With *hair_color*, for instance, we can assign a code of 0 for *black*, 1 for *brown*, and so on. Another example is *customor_ID*, with possible values that are all numeric. However, in such cases, the numbers are not intended to be used quantitatively. That is, mathematical operations on values of nominal attributes are not meaningful. It makes no sense to subtract one customer ID number from another, unlike, say, subtracting an age value from another (where *age* is a numeric attribute). Even though a nominal attribute may have integers as values, it is not considered a numeric attribute because the integers are not meant to be used quantitatively. We will say more on numeric attributes in Section 2.1.5.

Because nominal attribute values do not have any meaningful order about them and are not quantitative, it makes no sense to find the mean (average) value or median (middle) value for such an attribute, given a set of objects. One thing that is of interest, however, is the attribute's most commonly occurring value. This value, known as the *mode*, is one of the measures of central tendency. You will learn about measures of central tendency in Section 2.2.

2.1.3 Binary Attributes

A **binary attribute** is a nominal attribute with only two categories or states: 0 or 1, where 0 typically means that the attribute is absent, and 1 means that it is present. Binary attributes are referred to as **Boolean** if the two states correspond to *true* and *false*.

Example 2.2 **Binary attributes.** Given the attribute *smoker* describing a *patient* object, 1 indicates that the patient smokes, while 0 indicates that the patient does not. Similarly, suppose

the patient undergoes a medical test that has two possible outcomes. The attribute *medical_test* is binary, where a value of 1 means the result of the test for the patient is positive, while 0 means the result is negative. ■

A binary attribute is **symmetric** if both of its states are equally valuable and carry the same weight; that is, there is no preference on which outcome should be coded as 0 or 1. One such example could be the attribute *gender* having the states *male* and *female*.

A binary attribute is **asymmetric** if the outcomes of the states are not equally important, such as the *positive* and *negative* outcomes of a medical test for HIV. By convention, we code the most important outcome, which is usually the rarest one, by 1 (e.g., *HIV positive*) and the other by 0 (e.g., *HIV negative*).

2.1.4 Ordinal Attributes

An **ordinal attribute** is an attribute with possible values that have a meaningful order or *ranking* among them, but the magnitude between successive values is not known.

Example 2.3 **Ordinal attributes.** Suppose that *drink_size* corresponds to the size of drinks available at a fast-food restaurant. This nominal attribute has three possible values: *small, medium*, and *large*. The values have a meaningful sequence (which corresponds to increasing drink size); however, we cannot tell from the values *how much* bigger, say, a medium is than a large. Other examples of ordinal attributes include *grade* (e.g., *A+*, *A*, *A−*, *B+*, and so on) and *professional_rank*. Professional ranks can be enumerated in a sequential order: for example, *assistant*, *associate*, and *full* for professors, and *private, private first class, specialist, corporal, and sergeant* for army ranks.

Ordinal attributes are useful for registering subjective assessments of qualities that cannot be measured objectively; thus ordinal attributes are often used in surveys for ratings. In one survey, participants were asked to rate how satisfied they were as customers. Customer satisfaction had the following ordinal categories: *0: very dissatisfied, 1: somewhat dissatisfied, 2: neutral, 3: satisfied*, and *4: very satisfied.* ■

Ordinal attributes may also be obtained from the discretization of numeric quantities by splitting the value range into a finite number of ordered categories as described in Chapter 3 on data reduction.

The central tendency of an ordinal attribute can be represented by its mode and its median (the middle value in an ordered sequence), but the mean cannot be defined.

Note that nominal, binary, and ordinal attributes are *qualitative*. That is, they *describe* a feature of an object without giving an actual size or quantity. The values of such qualitative attributes are typically words representing categories. If integers are used, they represent computer codes for the categories, as opposed to measurable quantities (e.g., 0 for *small* drink size, 1 for *medium*, and 2 for *large*). In the following subsection we look at numeric attributes, which provide *quantitative* measurements of an object.

2.1.5 Numeric Attributes

A **numeric attribute** is *quantitative*; that is, it is a measurable quantity, represented in integer or real values. Numeric attributes can be *interval-scaled* or *ratio-scaled*.

Interval-Scaled Attributes

Interval-scaled attributes are measured on a scale of equal-size units. The values of interval-scaled attributes have order and can be positive, 0, or negative. Thus, in addition to providing a ranking of values, such attributes allow us to compare and quantify the *difference* between values.

Example 2.4 **Interval-scaled attributes.** A *temperature* attribute is interval-scaled. Suppose that we have the outdoor *temperature* value for a number of different days, where each day is an object. By ordering the values, we obtain a ranking of the objects with respect to *temperature*. In addition, we can quantify the difference between values. For example, a temperature of 20°C is five degrees higher than a temperature of 15°C. Calendar dates are another example. For instance, the years 2002 and 2010 are eight years apart. ■

Temperatures in Celsius and Fahrenheit do not have a true zero-point, that is, neither 0°C nor 0°F indicates "no temperature." (On the Celsius scale, for example, the unit of measurement is 1/100 of the difference between the melting temperature and the boiling temperature of water in atmospheric pressure.) Although we can compute the *difference* between temperature values, we cannot talk of one temperature value as being a *multiple* of another. Without a true zero, we cannot say, for instance, that 10°C is twice as warm as 5°C. That is, we cannot speak of the values in terms of ratios. Similarly, there is no true zero-point for calendar dates. (The year 0 does not correspond to the beginning of time.) This brings us to ratio-scaled attributes, for which a true zero-point exits.

Because interval-scaled attributes are numeric, we can compute their mean value, in addition to the median and mode measures of central tendency.

Ratio-Scaled Attributes

A **ratio-scaled attribute** is a numeric attribute with an inherent zero-point. That is, if a measurement is ratio-scaled, we can speak of a value as being a multiple (or ratio) of another value. In addition, the values are ordered, and we can also compute the difference between values, as well as the mean, median, and mode.

Example 2.5 **Ratio-scaled attributes.** Unlike temperatures in Celsius and Fahrenheit, the Kelvin (K) temperature scale has what is considered a true zero-point ($0°K = -273.15°C$): It is the point at which the particles that comprise matter have zero kinetic energy. Other examples of ratio-scaled attributes include *count* attributes such as *years_of_experience* (e.g., the objects are employees) and *number_of_words* (e.g., the objects are documents). Additional examples include attributes to measure weight, height, latitude and longitude

coordinates (e.g., when clustering houses), and monetary quantities (e.g., you are 100 times richer with $100 than with $1). ■

2.1.6 Discrete versus Continuous Attributes

In our presentation, we have organized attributes into nominal, binary, ordinal, and numeric types. There are many ways to organize attribute types. The types are not mutually exclusive.

Classification algorithms developed from the field of machine learning often talk of attributes as being either *discrete* or *continuous*. Each type may be processed differently. A **discrete attribute** has a finite or countably infinite set of values, which may or may not be represented as integers. The attributes *hair_color*, *smoker*, *medical_test*, and *drink_size* each have a finite number of values, and so are discrete. Note that discrete attributes may have numeric values, such as 0 and 1 for binary attributes or, the values 0 to 110 for the attribute *age*. An attribute is *countably infinite* if the set of possible values is infinite but the values can be put in a one-to-one correspondence with natural numbers. For example, the attribute *customer_ID* is countably infinite. The number of customers can grow to infinity, but in reality, the actual set of values is countable (where the values can be put in one-to-one correspondence with the set of integers). Zip codes are another example.

If an attribute is not discrete, it is **continuous**. The terms *numeric attribute* and *continuous attribute* are often used interchangeably in the literature. (This can be confusing because, in the classic sense, continuous values are real numbers, whereas numeric values can be either integers or real numbers.) In practice, real values are represented using a finite number of digits. Continuous attributes are typically represented as floating-point variables.

2.2 Basic Statistical Descriptions of Data

For data preprocessing to be successful, it is essential to have an overall picture of your data. Basic statistical descriptions can be used to identify properties of the data and highlight which data values should be treated as noise or outliers.

This section discusses three areas of basic statistical descriptions. We start with *measures of central tendency* (Section 2.2.1), which measure the location of the middle or center of a data distribution. Intuitively speaking, given an attribute, where do most of its values fall? In particular, we discuss the mean, median, mode, and midrange.

In addition to assessing the central tendency of our data set, we also would like to have an idea of the *dispersion of the data*. That is, how are the data spread out? The most common data dispersion measures are the *range*, *quartiles*, and *interquartile range*; the *five-number summary* and *boxplots*; and the *variance* and *standard deviation* of the data These measures are useful for identifying outliers and are described in Section 2.2.2.

Finally, we can use many graphic displays of basic statistical descriptions to visually inspect our data (Section 2.2.3). Most statistical or graphical data presentation software

packages include bar charts, pie charts, and line graphs. Other popular displays of data summaries and distributions include *quantile plots*, *quantile–quantile plots*, *histograms*, and *scatter plots*.

2.2.1 Measuring the Central Tendency: Mean, Median, and Mode

In this section, we look at various ways to measure the central tendency of data. Suppose that we have some attribute X, like *salary*, which has been recorded for a set of objects. Let $x_1, x_2, \ldots, x_N$ be the set of N observed values or *observations* for X. Here, these values may also be referred to as the data set (for X). If we were to plot the observations for *salary*, where would most of the values fall? This gives us an idea of the central tendency of the data. Measures of central tendency include the mean, median, mode, and midrange.

The most common and effective numeric measure of the "center" of a set of data is the *(arithmetic) mean*. Let $x_1, x_2, \ldots, x_N$ be a set of N values or *observations*, such as for some numeric attribute X, like *salary*. The **mean** of this set of values is

$$\bar{x} = \frac{\sum_{i=1}^{N} x_i}{N} = \frac{x_1 + x_2 + \cdots + x_N}{N}. \tag{2.1}$$

This corresponds to the built-in aggregate function, *average* (**avg()** in SQL), provided in relational database systems.

Example 2.6 **Mean.** Suppose we have the following values for *salary* (in thousands of dollars), shown in increasing order: 30, 36, 47, 50, 52, 52, 56, 60, 63, 70, 70, 110. Using Eq. (2.1), we have

$$\bar{x} = \frac{30 + 36 + 47 + 50 + 52 + 52 + 56 + 60 + 63 + 70 + 70 + 110}{12}$$
$$= \frac{696}{12} = 58.$$

Thus, the mean salary is $58,000. ■

Sometimes, each value x_i in a set may be associated with a weight w_i for $i = 1, \ldots, N$. The weights reflect the significance, importance, or occurrence frequency attached to their respective values. In this case, we can compute

$$\bar{x} = \frac{\sum_{i=1}^{N} w_i x_i}{\sum_{i=1}^{N} w_i} = \frac{w_1 x_1 + w_2 x_2 + \cdots + w_N x_N}{w_1 + w_2 + \cdots + w_N}. \tag{2.2}$$

This is called the **weighted arithmetic mean** or the **weighted average**.

Although the mean is the singlemost useful quantity for describing a data set, it is not always the best way of measuring the center of the data. A major problem with the mean is its sensitivity to extreme (e.g., outlier) values. Even a small number of extreme values can corrupt the mean. For example, the mean salary at a company may be substantially pushed up by that of a few highly paid managers. Similarly, the mean score of a class in an exam could be pulled down quite a bit by a few very low scores. To offset the effect caused by a small number of extreme values, we can instead use the **trimmed mean**, which is the mean obtained after chopping off values at the high and low extremes. For example, we can sort the values observed for *salary* and remove the top and bottom 2% before computing the mean. We should avoid trimming too large a portion (such as 20%) at both ends, as this can result in the loss of valuable information.

For skewed (asymmetric) data, a better measure of the center of data is the **median**, which is the middle value in a set of ordered data values. It is the value that separates the higher half of a data set from the lower half.

In probability and statistics, the median generally applies to numeric data; however, we may extend the concept to ordinal data. Suppose that a given data set of N values for an attribute X is sorted in increasing order. If N is odd, then the median is the *middle value* of the ordered set. If N is even, then the median is not unique; it is the two middlemost values and any value in between. If X is a numeric attribute in this case, by convention, the median is taken as the average of the two middlemost values.

Example 2.7 **Median.** Let's find the median of the data from Example 2.6. The data are already sorted in increasing order. There is an even number of observations (i.e., 12); therefore, the median is not unique. It can be any value within the two middlemost values of 52 and 56 (that is, within the sixth and seventh values in the list). By convention, we assign the average of the two middlemost values as the median; that is, $\frac{52+56}{2} = \frac{108}{2} = 54$. Thus, the median is \$54,000.

Suppose that we had only the first 11 values in the list. Given an odd number of values, the median is the middlemost value. This is the sixth value in this list, which has a value of \$52,000. ■

The median is expensive to compute when we have a large number of observations. For numeric attributes, however, we can easily *approximate* the value. Assume that data are grouped in intervals according to their x_i data values and that the frequency (i.e., number of data values) of each interval is known. For example, employees may be grouped according to their annual salary in intervals such as \$10–20,000, \$20–30,000, and so on. Let the interval that contains the median frequency be the *median interval*. We can approximate the median of the entire data set (e.g., the median salary) by interpolation using the formula

$$median = L_1 + \left(\frac{N/2 - \left(\sum freq\right)_l}{freq_{median}} \right) width, \tag{2.3}$$

where L_1 is the lower boundary of the median interval, N is the number of values in the entire data set, $\left(\sum freq\right)_l$ is the sum of the frequencies of all of the intervals that are

lower than the median interval, $freq_{median}$ is the frequency of the median interval, and *width* is the width of the median interval.

The *mode* is another measure of central tendency. The **mode** for a set of data is the value that occurs most frequently in the set. Therefore, it can be determined for qualitative and quantitative attributes. It is possible for the greatest frequency to correspond to several different values, which results in more than one mode. Data sets with one, two, or three modes are respectively called **unimodal**, **bimodal**, and **trimodal**. In general, a data set with two or more modes is **multimodal**. At the other extreme, if each data value occurs only once, then there is no mode.

Example 2.8 **Mode.** The data from Example 2.6 are bimodal. The two modes are $52,000 and $70,000. ■

For unimodal numeric data that are moderately skewed (asymmetrical), we have the following empirical relation:

$$mean - mode \approx 3 \times (mean - median). \tag{2.4}$$

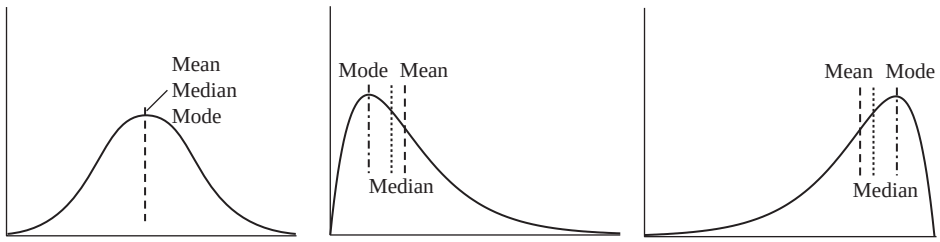
This implies that the mode for unimodal frequency curves that are moderately skewed can easily be approximated if the mean and median values are known.

The **midrange** can also be used to assess the central tendency of a numeric data set. It is the average of the largest and smallest values in the set. This measure is easy to compute using the SQL aggregate functions, max() and min().

Example 2.9 **Midrange.** The midrange of the data of Example 2.6 is $\frac{30,000+110,000}{2} = \$70,000$. ■

In a unimodal frequency curve with perfect **symmetric** data distribution, the mean, median, and mode are all at the same center value, as shown in Figure 2.1(a).

Data in most real applications are not symmetric. They may instead be either **positively skewed**, where the mode occurs at a value that is smaller than the median (Figure 2.1b), or **negatively skewed**, where the mode occurs at a value greater than the median (Figure 2.1c).



(a) Symmetric data **(b)** Positively skewed data **(c)** Negatively skewed data

Figure 2.1 Mean, median, and mode of symmetric versus positively and negatively skewed data.

2.2.2 Measuring the Dispersion of Data: Range, Quartiles, Variance, Standard Deviation, and Interquartile Range

We now look at measures to assess the dispersion or spread of numeric data. The measures include range, quantiles, quartiles, percentiles, and the interquartile range. The five-number summary, which can be displayed as a boxplot, is useful in identifying outliers. Variance and standard deviation also indicate the spread of a data distribution.

Range, Quartiles, and Interquartile Range

To start off, let's study the *range*, *quantiles*, *quartiles*, *percentiles*, and the *interquartile range* as measures of data dispersion.

Let $x_1, x_2, \ldots, x_N$ be a set of observations for some numeric attribute, X. The **range** of the set is the difference between the largest (max()) and smallest (min()) values.

Suppose that the data for attribute X are sorted in increasing numeric order. Imagine that we can pick certain data points so as to split the data distribution into equal-size consecutive sets, as in Figure 2.2. These data points are called *quantiles*. **Quantiles** are points taken at regular intervals of a data distribution, dividing it into essentially equal-size consecutive sets. (We say "essentially" because there may not be data values of X that divide the data into exactly equal-sized subsets. For readability, we will refer to them as equal.) The kth *q-quantile* for a given data distribution is the value x such that at most k/q of the data values are less than x and at most $(q-k)/q$ of the data values are more than x, where k is an integer such that $0 < k < q$. There are $q-1$ q-quantiles.

The 2-quantile is the data point dividing the lower and upper halves of the data distribution. It corresponds to the median. The 4-quantiles are the three data points that split the data distribution into four equal parts; each part represents one-fourth of the data distribution. They are more commonly referred to as **quartiles**. The 100-quantiles are more commonly referred to as **percentiles**; they divide the data distribution into 100 equal-sized consecutive sets. The median, quartiles, and percentiles are the most widely used forms of quantiles.

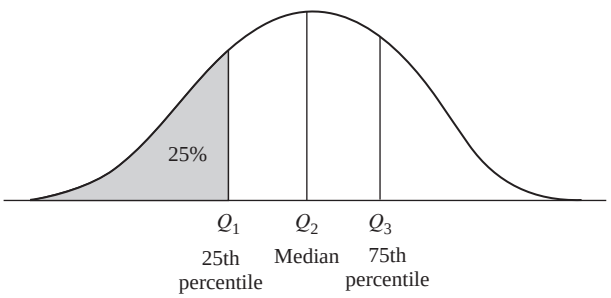


Figure 2.2 A plot of the data distribution for some attribute X. The quantiles plotted are quartiles. The three quartiles divide the distribution into four equal-size consecutive subsets. The second quartile corresponds to the median.

The quartiles give an indication of a distribution's center, spread, and shape. The **first quartile**, denoted by Q_1, is the 25th percentile. It cuts off the lowest 25% of the data. The **third quartile**, denoted by Q_3, is the 75th percentile—it cuts off the lowest 75% (or highest 25%) of the data. The second quartile is the 50th percentile. As the median, it gives the center of the data distribution.

The distance between the first and third quartiles is a simple measure of spread that gives the range covered by the middle half of the data. This distance is called the **interquartile range** (**IQR**) and is defined as

$$IQR = Q_3 - Q_1. \tag{2.5}$$

Example 2.10 **Interquartile range.** The quartiles are the three values that split the sorted data set into four equal parts. The data of Example 2.6 contain 12 observations, already sorted in increasing order. Thus, the quartiles for this data are the third, sixth, and ninth values, respectively, in the sorted list. Therefore, $Q_1 = \$47{,}000$ and Q_3 is $\$63{,}000$. Thus, the interquartile range is $IQR = 63 - 47 = \$16{,}000$. (Note that the sixth value is a median, $52,000, although this data set has two medians since the number of data values is even.) ■

Five-Number Summary, Boxplots, and Outliers

No single numeric measure of spread (e.g., *IQR*) is very useful for describing skewed distributions. Have a look at the symmetric and skewed data distributions of Figure 2.1. In the symmetric distribution, the median (and other measures of central tendency) splits the data into equal-size halves. This does not occur for skewed distributions. Therefore, it is more informative to also provide the two quartiles Q_1 and Q_3, along with the median. A common rule of thumb for identifying suspected **outliers** is to single out values falling at least $1.5 \times IQR$ above the third quartile or below the first quartile.

Because Q_1, the median, and Q_3 together contain no information about the endpoints (e.g., tails) of the data, a fuller summary of the shape of a distribution can be obtained by providing the lowest and highest data values as well. This is known as the *five-number summary*. The **five-number summary** of a distribution consists of the median (Q_2), the quartiles Q_1 and Q_3, and the smallest and largest individual observations, written in the order of *Minimum*, Q_1, *Median*, Q_3, *Maximum*.

Boxplots are a popular way of visualizing a distribution. A boxplot incorporates the five-number summary as follows:

- Typically, the ends of the box are at the quartiles so that the box length is the interquartile range.
- The median is marked by a line within the box.
- Two lines (called *whiskers*) outside the box extend to the smallest (*Minimum*) and largest (*Maximum*) observations.

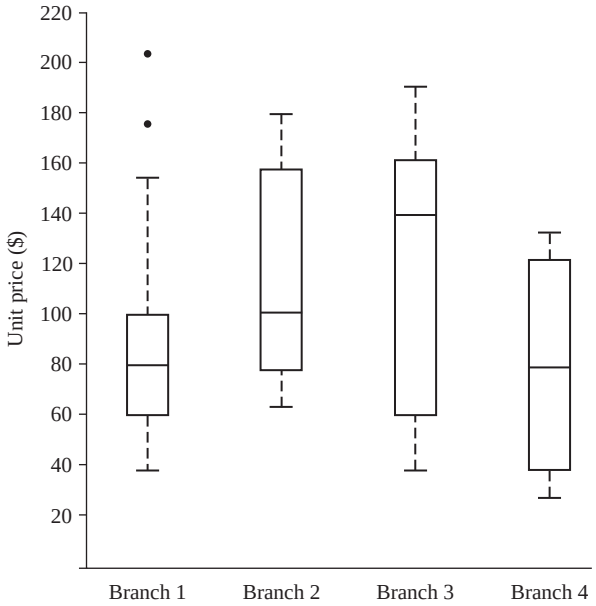


Figure 2.3 Boxplot for the unit price data for items sold at four branches of *AllElectronics* during a given time period.

When dealing with a moderate number of observations, it is worthwhile to plot potential outliers individually. To do this in a boxplot, the whiskers are extended to the extreme low and high observations *only if* these values are less than $1.5 \times IQR$ beyond the quartiles. Otherwise, the whiskers terminate at the most extreme observations occurring within $1.5 \times IQR$ of the quartiles. The remaining cases are plotted individually. Boxplots can be used in the comparisons of several sets of compatible data.

Example 2.11 **Boxplot.** Figure 2.3 shows boxplots for unit price data for items sold at four branches of *AllElectronics* during a given time period. For branch 1, we see that the median price of items sold is \$80, Q_1 is \$60, and Q_3 is \$100. Notice that two outlying observations for this branch were plotted individually, as their values of 175 and 202 are more than 1.5 times the IQR here of 40. ■

Boxplots can be computed in $O(n \log n)$ time. Approximate boxplots can be computed in linear or sublinear time depending on the quality guarantee required.

Variance and Standard Deviation

Variance and standard deviation are measures of data dispersion. They indicate how spread out a data distribution is. A low standard deviation means that the data observations tend to be very close to the mean, while a high standard deviation indicates that the data are spread out over a large range of values.

The **variance** of N observations, $x_1, x_2, \ldots, x_N$, for a numeric attribute X is

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2 = \left(\frac{1}{N}\sum_{i=1}^{N}x_i^2\right) - \bar{x}^2, \tag{2.6}$$

where $\bar{x}$ is the mean value of the observations, as defined in Eq. (2.1). The **standard deviation**, σ, of the observations is the square root of the variance, σ^2.

Example 2.12 **Variance and standard deviation.** In Example 2.6, we found $\bar{x} = \$58{,}000$ using Eq. (2.1) for the mean. To determine the variance and standard deviation of the data from that example, we set $N = 12$ and use Eq. (2.6) to obtain

$$\begin{aligned}\sigma^2 &= \frac{1}{12}(30^2 + 36^2 + 47^2 \ldots + 110^2) - 58^2\\ &\approx 379.17\\ \sigma &\approx \sqrt{379.17} \approx 19.47.\end{aligned}$$

■

The basic properties of the standard deviation, σ, as a measure of spread are as follows:

- σ measures spread about the mean and should be considered only when the mean is chosen as the measure of center.
- $\sigma = 0$ only when there is no spread, that is, when all observations have the same value. Otherwise, $\sigma > 0$.

Importantly, an observation is unlikely to be more than several standard deviations away from the mean. Mathematically, using Chebyshev's inequality, it can be shown that at least $\left(1 - \frac{1}{k^2}\right) \times 100\%$ of the observations are no more than k standard deviations from the mean. Therefore, the standard deviation is a good indicator of the spread of a data set.

The computation of the variance and standard deviation is scalable in large databases.

2.2.3 Graphic Displays of Basic Statistical Descriptions of Data

In this section, we study graphic displays of basic statistical descriptions. These include *quantile plots*, *quantile–quantile plots*, *histograms*, and *scatter plots*. Such graphs are helpful for the visual inspection of data, which is useful for data preprocessing. The first three of these show univariate distributions (i.e., data for one attribute), while scatter plots show bivariate distributions (i.e., involving two attributes).

Quantile Plot

In this and the following subsections, we cover common graphic displays of data distributions. A **quantile plot** is a simple and effective way to have a first look at a univariate data distribution. First, it displays all of the data for the given attribute (allowing the user

to assess both the overall behavior and unusual occurrences). Second, it plots quantile information (see Section 2.2.2). Let x_i, for $i = 1$ to N, be the data sorted in increasing order so that x_1 is the smallest observation and x_N is the largest for some ordinal or numeric attribute X. Each observation, x_i, is paired with a percentage, f_i, which indicates that approximately $f_i \times 100\%$ of the data are below the value, x_i. We say "approximately" because there may not be a value with exactly a fraction, f_i, of the data below x_i. Note that the 0.25 percentile corresponds to quartile Q_1, the 0.50 percentile is the median, and the 0.75 percentile is Q_3.

Let

$$f_i = \frac{i - 0.5}{N}. \tag{2.7}$$

These numbers increase in equal steps of $1/N$, ranging from $\frac{1}{2N}$ (which is slightly above 0) to $1 - \frac{1}{2N}$ (which is slightly below 1). On a quantile plot, x_i is graphed against f_i. This allows us to compare different distributions based on their quantiles. For example, given the quantile plots of sales data for two different time periods, we can compare their Q_1, median, Q_3, and other f_i values at a glance.

Example 2.13 **Quantile plot.** Figure 2.4 shows a quantile plot for the *unit price* data of Table 2.1. ■

Quantile–Quantile Plot

A **quantile–quantile plot**, or **q-q plot**, graphs the quantiles of one univariate distribution against the corresponding quantiles of another. It is a powerful visualization tool in that it allows the user to view whether there is a shift in going from one distribution to another.

Suppose that we have two sets of observations for the attribute or variable *unit price*, taken from two different branch locations. Let $x_1, \ldots, x_N$ be the data from the first branch, and $y_1, \ldots, y_M$ be the data from the second, where each data set is sorted in increasing order. If $M = N$ (i.e., the number of points in each set is the same), then we simply plot y_i against x_i, where y_i and x_i are both $(i - 0.5)/N$ quantiles of their respective data sets. If $M < N$ (i.e., the second branch has fewer observations than the first), there can be only M points on the q-q plot. Here, y_i is the $(i - 0.5)/M$ quantile of the y

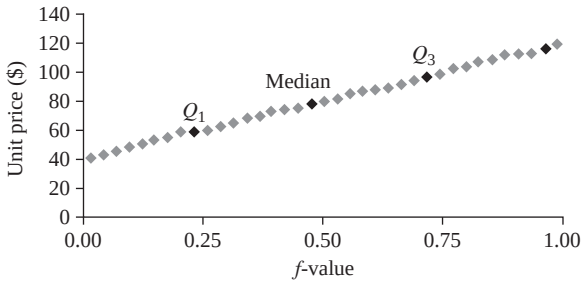


Figure 2.4 A quantile plot for the unit price data of Table 2.1.

Table 2.1 A Set of Unit Price Data for Items Sold at a Branch of *AllElectronics*

Unit price ($)	*Count of items sold*
40	275
43	300
47	250
—	—
74	360
75	515
78	540
—	—
115	320
117	270
120	350

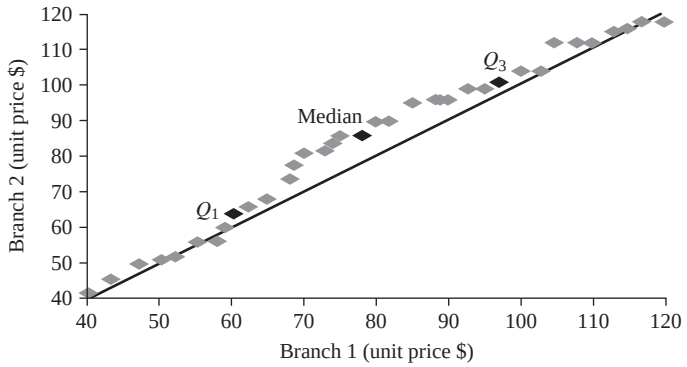


Figure 2.5 A q-q plot for unit price data from two *AllElectronics* branches.

data, which is plotted against the $(i - 0.5)/M$ quantile of the x data. This computation typically involves interpolation.

Example 2.14 **Quantile–quantile plot.** Figure 2.5 shows a quantile–quantile plot for *unit price* data of items sold at two branches of *AllElectronics* during a given time period. Each point corresponds to the same quantile for each data set and shows the unit price of items sold at branch 1 versus branch 2 for that quantile. (To aid in comparison, the straight line represents the case where, for each given quantile, the unit price at each branch is the same. The darker points correspond to the data for Q_1, the median, and Q_3, respectively.)

We see, for example, that at Q_1, the unit price of items sold at branch 1 was slightly less than that at branch 2. In other words, 25% of items sold at branch 1 were less than or

equal to \$60, while 25% of items sold at branch 2 were less than or equal to \$64. At the 50th percentile (marked by the median, which is also Q_2), we see that 50% of items sold at branch 1 were less than \$78, while 50% of items at branch 2 were less than \$85. In general, we note that there is a shift in the distribution of branch 1 with respect to branch 2 in that the unit prices of items sold at branch 1 tend to be lower than those at branch 2. ■

Histograms

Histograms (or **frequency histograms**) are at least a century old and are widely used. "Histos" means pole or mast, and "gram" means chart, so a histogram is a chart of poles. Plotting histograms is a graphical method for summarizing the distribution of a given attribute, X. If X is nominal, such as *automobile_model* or *item_type*, then a pole or vertical bar is drawn for each known value of X. The height of the bar indicates the frequency (i.e., count) of that X value. The resulting graph is more commonly known as a **bar chart**.

If X is numeric, the term *histogram* is preferred. The range of values for X is partitioned into disjoint consecutive subranges. The subranges, referred to as *buckets* or *bins*, are disjoint subsets of the data distribution for X. The range of a bucket is known as the **width**. Typically, the buckets are of equal width. For example, a *price* attribute with a value range of \$1 to \$200 (rounded up to the nearest dollar) can be partitioned into subranges 1 to 20, 21 to 40, 41 to 60, and so on. For each subrange, a bar is drawn with a height that represents the total count of items observed within the subrange. Histograms and partitioning rules are further discussed in Chapter 3 on data reduction.

Example 2.15 **Histogram.** Figure 2.6 shows a histogram for the data set of Table 2.1, where buckets (or bins) are defined by equal-width ranges representing \$20 increments and the frequency is the count of items sold. ■

Although histograms are widely used, they may not be as effective as the quantile plot, q-q plot, and boxplot methods in comparing groups of univariate observations.

Scatter Plots and Data Correlation

A **scatter plot** is one of the most effective graphical methods for determining if there appears to be a relationship, pattern, or trend between two numeric attributes. To construct a scatter plot, each pair of values is treated as a pair of coordinates in an algebraic sense and plotted as points in the plane. Figure 2.7 shows a scatter plot for the set of data in Table 2.1.

The scatter plot is a useful method for providing a first look at bivariate data to see clusters of points and outliers, or to explore the possibility of correlation relationships. Two attributes, X, and Y, are **correlated** if one attribute implies the other. Correlations can be positive, negative, or null (uncorrelated). Figure 2.8 shows examples of positive and negative correlations between two attributes. If the plotted points pattern slopes

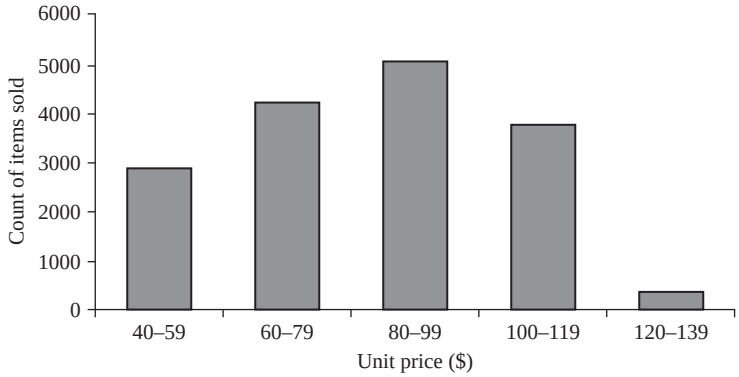


Figure 2.6 A histogram for the Table 2.1 data set.

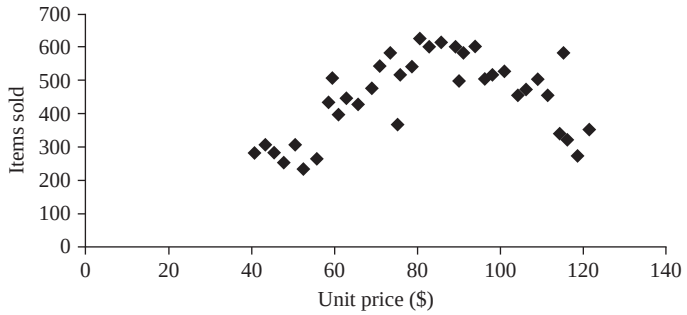


Figure 2.7 A scatter plot for the Table 2.1 data set.

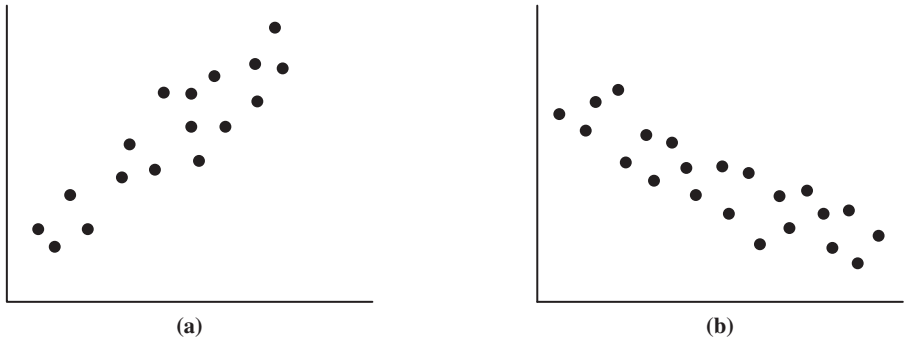


Figure 2.8 Scatter plots can be used to find (a) positive or (b) negative correlations between attributes.

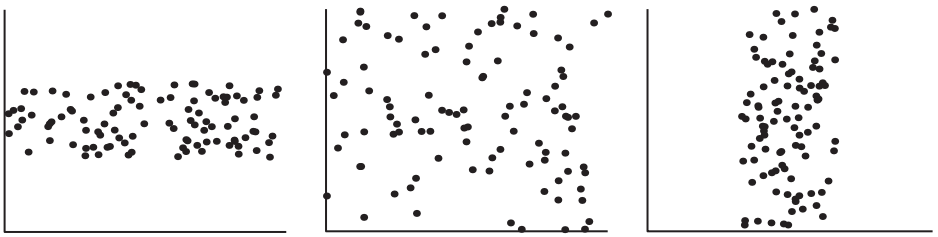


Figure 2.9 Three cases where there is no observed correlation between the two plotted attributes in each of the data sets.

from lower left to upper right, this means that the values of X increase as the values of Y increase, suggesting a *positive correlation* (Figure 2.8a). If the pattern of plotted points slopes from upper left to lower right, the values of X increase as the values of Y decrease, suggesting a *negative correlation* (Figure 2.8b). A line of best fit can be drawn to study the correlation between the variables. Statistical tests for correlation are given in Chapter 3 on data integration (Eq. (3.3)). Figure 2.9 shows three cases for which there is no correlation relationship between the two attributes in each of the given data sets. Section 2.3.2 shows how scatter plots can be extended to n attributes, resulting in a *scatter-plot matrix*.

In conclusion, basic data descriptions (e.g., measures of central tendency and measures of dispersion) and graphic statistical displays (e.g., quantile plots, histograms, and scatter plots) provide valuable insight into the overall behavior of your data. By helping to identify noise and outliers, they are especially useful for data cleaning.

2.3 Data Visualization

How can we convey data to users effectively? **Data visualization** aims to communicate data clearly and effectively through graphical representation. Data visualization has been used extensively in many applications—for example, at work for reporting, managing business operations, and tracking progress of tasks. More popularly, we can take advantage of visualization techniques to discover data relationships that are otherwise not easily observable by looking at the raw data. Nowadays, people also use data visualization to create fun and interesting graphics.

In this section, we briefly introduce the basic concepts of data visualization. We start with multidimensional data such as those stored in relational databases. We discuss several representative approaches, including pixel-oriented techniques, geometric projection techniques, icon-based techniques, and hierarchical and graph-based techniques. We then discuss the visualization of complex data and relations.

2.3.1 Pixel-Oriented Visualization Techniques

A simple way to visualize the value of a dimension is to use a pixel where the color of the pixel reflects the dimension's value. For a data set of m dimensions, **pixel-oriented techniques** create m windows on the screen, one for each dimension. The m dimension values of a record are mapped to m pixels at the corresponding positions in the windows. The colors of the pixels reflect the corresponding values.

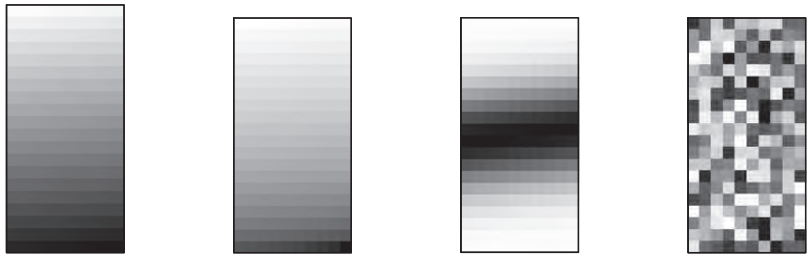
Inside a window, the data values are arranged in some global order shared by all windows. The global order may be obtained by sorting all data records in a way that's meaningful for the task at hand.

Example 2.16 **Pixel-oriented visualization.** *AllElectronics* maintains a customer information table, which consists of four dimensions: *income*, *credit_limit*, *transaction_volume*, and *age*. Can we analyze the correlation between *income* and the other attributes by visualization?

We can sort all customers in income-ascending order, and use this order to lay out the customer data in the four visualization windows, as shown in Figure 2.10. The pixel colors are chosen so that the smaller the value, the lighter the shading. Using pixel-based visualization, we can easily observe the following: *credit_limit* increases as *income* increases; customers whose income is in the middle range are more likely to purchase more from *AllElectronics*; there is no clear correlation between *income* and *age*. ■

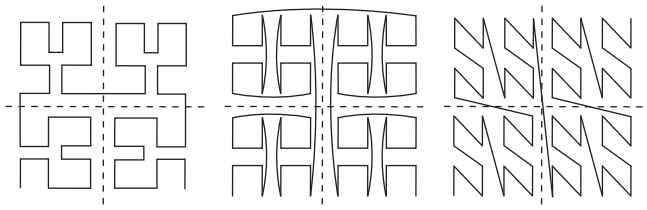
In pixel-oriented techniques, data records can also be ordered in a query-dependent way. For example, given a point query, we can sort all records in descending order of similarity to the point query.

Filling a window by laying out the data records in a linear way may not work well for a wide window. The first pixel in a row is far away from the last pixel in the previous row, though they are next to each other in the global order. Moreover, a pixel is next to the one above it in the window, even though the two are not next to each other in the global order. To solve this problem, we can lay out the data records in a space-filling curve



(a) *income* **(b)** *credit_limit* **(c)** *transaction_volume* **(d)** *age*

Figure 2.10 Pixel-oriented visualization of four attributes by sorting all customers in *income* ascending order.



(a) Hilbert curve **(b)** Gray code **(c)** Z-curve

Figure 2.11 Some frequently used 2-D space-filling curves.

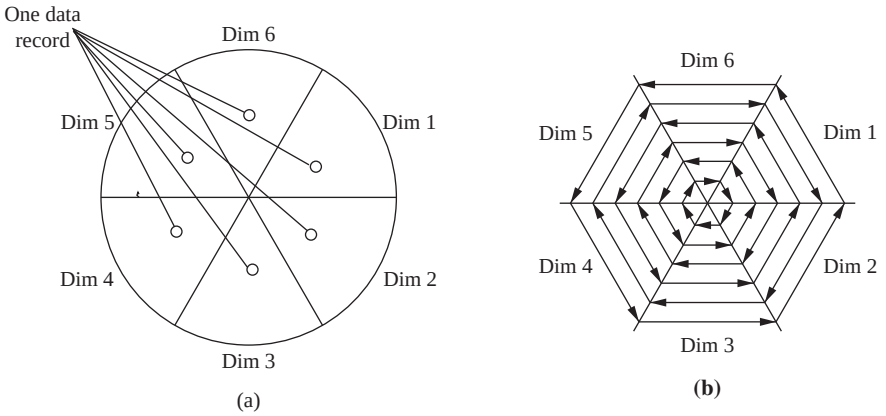


Figure 2.12 The circle segment technique. (a) Representing a data record in circle segments. (b) Laying out pixels in circle segments.

to fill the windows. A *space-filling curve* is a curve with a range that covers the entire n-dimensional unit hypercube. Since the visualization windows are 2-D, we can use any 2-D space-filling curve. Figure 2.11 shows some frequently used 2-D space-filling curves.

Note that the windows do not have to be rectangular. For example, the *circle segment technique* uses windows in the shape of segments of a circle, as illustrated in Figure 2.12. This technique can ease the comparison of dimensions because the dimension windows are located side by side and form a circle.

2.3.2 Geometric Projection Visualization Techniques

A drawback of pixel-oriented visualization techniques is that they cannot help us much in understanding the distribution of data in a multidimensional space. For example, they do not show whether there is a dense area in a multidimensional subspace. **Geometric**

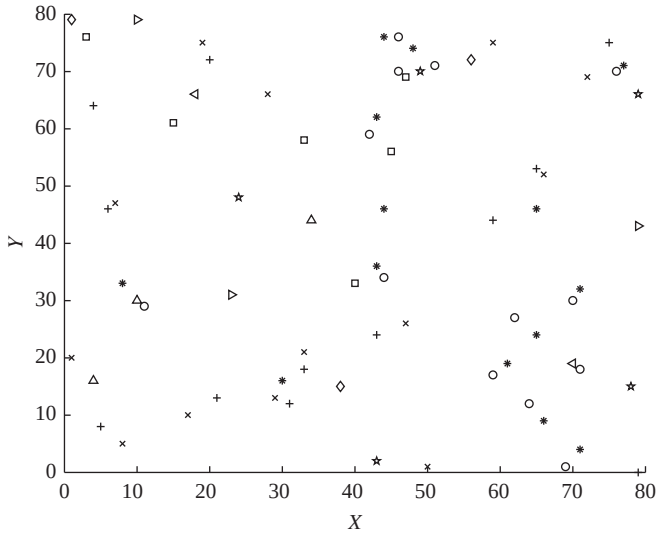


Figure 2.13 Visualization of a 2-D data set using a scatter plot. *Source: www.cs.sfu.ca/jpei/publications/rareevent-geoinformatica06.pdf*.

projection techniques help users find interesting projections of multidimensional data sets. The central challenge the geometric projection techniques try to address is how to visualize a high-dimensional space on a 2-D display.

A **scatter plot** displays 2-D data points using Cartesian coordinates. A third dimension can be added using different colors or shapes to represent different data points. Figure 2.13 shows an example, where X and Y are two spatial attributes and the third dimension is represented by different shapes. Through this visualization, we can see that points of types "+" and "×" tend to be colocated.

A 3-D scatter plot uses three axes in a Cartesian coordinate system. If it also uses color, it can display up to 4-D data points (Figure 2.14).

For data sets with more than four dimensions, scatter plots are usually ineffective. The **scatter-plot matrix** technique is a useful extension to the scatter plot. For an n-dimensional data set, a scatter-plot matrix is an $n \times n$ grid of 2-D scatter plots that provides a visualization of each dimension with every other dimension. Figure 2.15 shows an example, which visualizes the Iris data set. The data set consists of 450 samples from each of three species of Iris flowers. There are five dimensions in the data set: length and width of sepal and petal, and species.

The scatter-plot matrix becomes less effective as the dimensionality increases. Another popular technique, called parallel coordinates, can handle higher dimensionality. To visualize n-dimensional data points, the **parallel coordinates** technique draws n equally spaced axes, one for each dimension, parallel to one of the display axes.

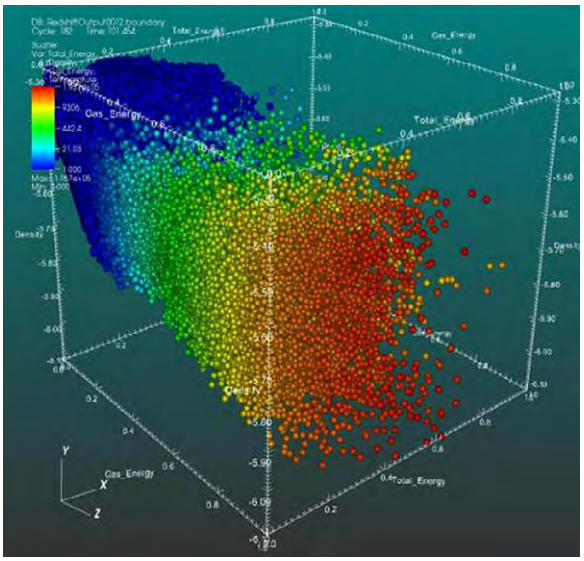


Figure 2.14 Visualization of a 3-D data set using a scatter plot. *Source: http://upload.wikimedia.org/wikipedia/commons/c/c4/Scatter_plot.jpg.*

A data record is represented by a polygonal line that intersects each axis at the point corresponding to the associated dimension value (Figure 2.16).

A major limitation of the parallel coordinates technique is that it cannot effectively show a data set of many records. Even for a data set of several thousand records, visual clutter and overlap often reduce the readability of the visualization and make the patterns hard to find.

2.3.3 Icon-Based Visualization Techniques

Icon-based visualization techniques use small icons to represent multidimensional data values. We look at two popular icon-based techniques: *Chernoff faces* and *stick figures.*

Chernoff faces were introduced in 1973 by statistician Herman Chernoff. They display multidimensional data of up to 18 variables (or dimensions) as a cartoon human face (Figure 2.17). Chernoff faces help reveal trends in the data. Components of the face, such as the eyes, ears, mouth, and nose, represent values of the dimensions by their shape, size, placement, and orientation. For example, dimensions can be mapped to the following facial characteristics: eye size, eye spacing, nose length, nose width, mouth curvature, mouth width, mouth openness, pupil size, eyebrow slant, eye eccentricity, and head eccentricity.

Chernoff faces make use of the ability of the human mind to recognize small differences in facial characteristics and to assimilate many facial characteristics at once.

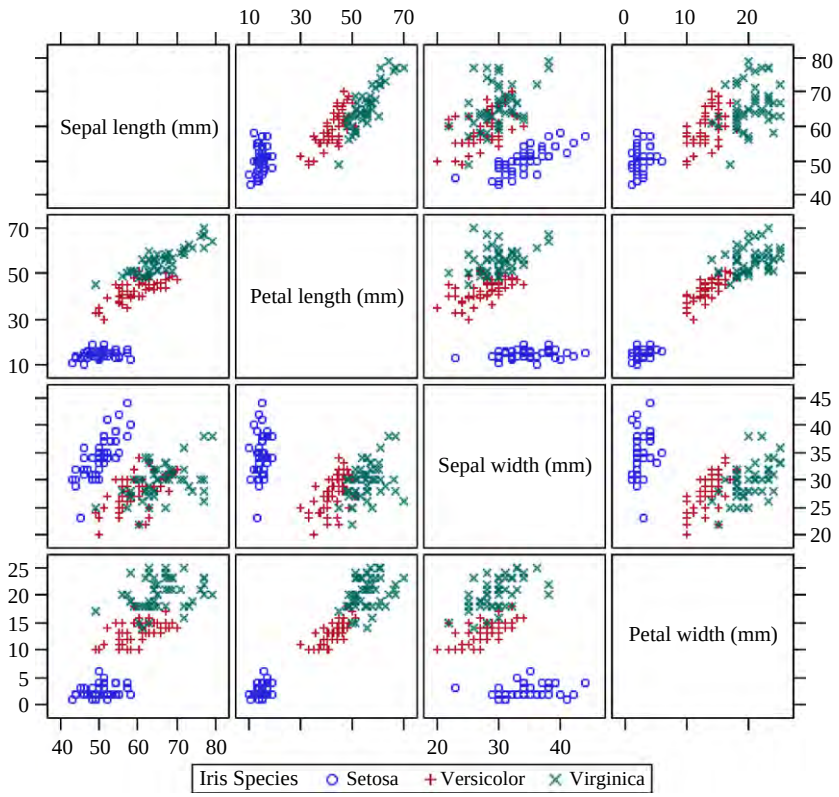


Figure 2.15 Visualization of the Iris data set using a scatter-plot matrix. *Source:* *http://support.sas.com/documentation/cdl/en/grstatproc/61948/HTML/default/images/gsgscmat.gif*.

Viewing large tables of data can be tedious. By condensing the data, Chernoff faces make the data easier for users to digest. In this way, they facilitate visualization of regularities and irregularities present in the data, although their power in relating multiple relationships is limited. Another limitation is that specific data values are not shown. Furthermore, facial features vary in perceived importance. This means that the similarity of two faces (representing two multidimensional data points) can vary depending on the order in which dimensions are assigned to facial characteristics. Therefore, this mapping should be carefully chosen. Eye size and eyebrow slant have been found to be important.

Asymmetrical Chernoff faces were proposed as an extension to the original technique. Since a face has vertical symmetry (along the y-axis), the left and right side of a face are identical, which wastes space. Asymmetrical Chernoff faces double the number of facial characteristics, thus allowing up to 36 dimensions to be displayed.

The **stick figure** visualization technique maps multidimensional data to five-piece stick figures, where each figure has four limbs and a body. Two dimensions are mapped to the display (x and y) axes and the remaining dimensions are mapped to the angle

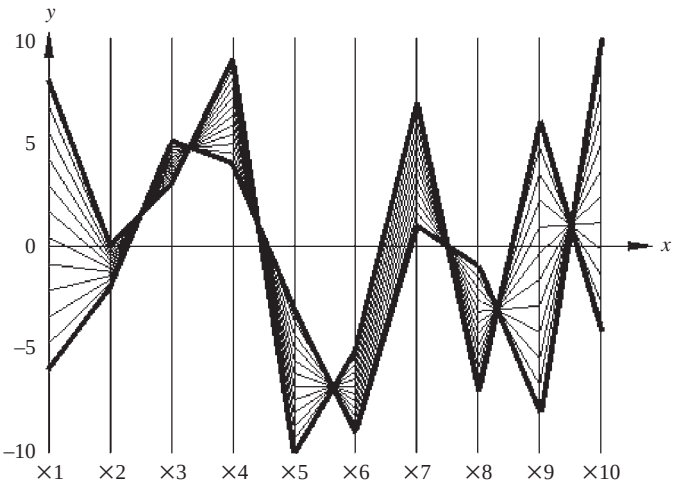


Figure 2.16 Here is a visualization that uses parallel coordinates. *Source: www.stat.columbia.edu/~cook/movabletype/archives/2007/10/parallel_coordi.thml.*

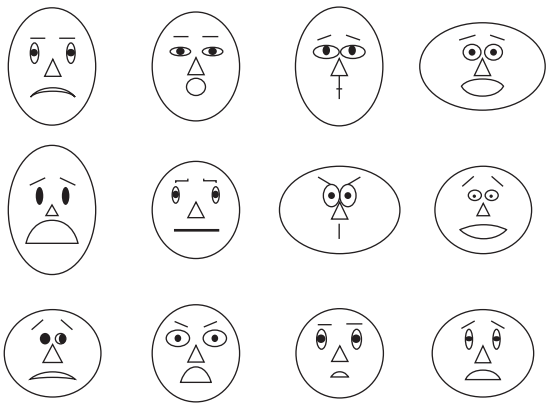


Figure 2.17 Chernoff faces. Each face represents an n-dimensional data point ($n \leq 18$).

and/or length of the limbs. Figure 2.18 shows census data, where *age* and *income* are mapped to the display axes, and the remaining dimensions (*gender, education*, and so on) are mapped to stick figures. If the data items are relatively dense with respect to the two display dimensions, the resulting visualization shows texture patterns, reflecting data trends.

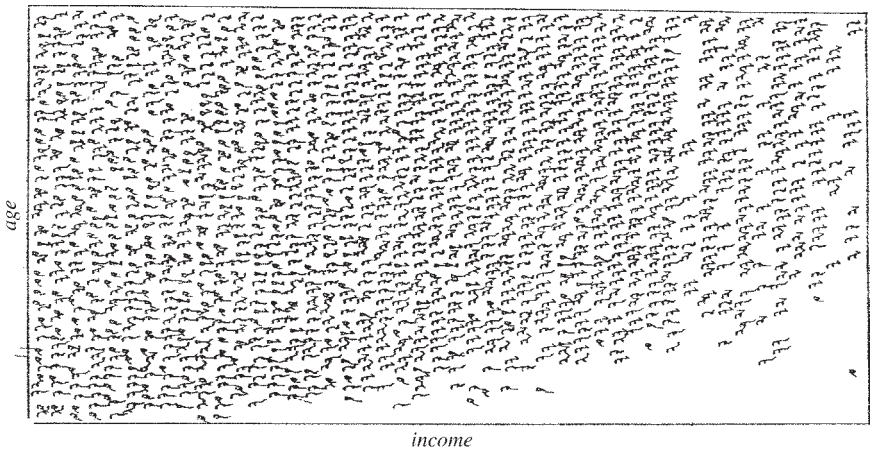


Figure 2.18 Census data represented using stick figures. *Source:* Professor G. Grinstein, Department of Computer Science, University of Massachusetts at Lowell.

2.3.4 Hierarchical Visualization Techniques

The visualization techniques discussed so far focus on visualizing multiple dimensions simultaneously. However, for a large data set of high dimensionality, it would be difficult to visualize all dimensions at the same time. **Hierarchical visualization techniques** partition all dimensions into subsets (i.e., subspaces). The subspaces are visualized in a hierarchical manner.

"Worlds-within-Worlds," also known as *n*-Vision, is a representative hierarchical visualization method. Suppose we want to visualize a 6-D data set, where the dimensions are $F, X_1, \ldots, X_5$. We want to observe how dimension F changes with respect to the other dimensions. We can first fix the values of dimensions X_3, X_4, X_5 to some selected values, say, c_3, c_4, c_5. We can then visualize F, X_1, X_2 using a 3-D plot, called a *world*, as shown in Figure 2.19. The position of the origin of the inner world is located at the point (c_3, c_4, c_5) in the outer world, which is another 3-D plot using dimensions X_3, X_4, X_5. A user can interactively change, in the outer world, the location of the origin of the inner world. The user then views the resulting changes of the inner world. Moreover, a user can vary the dimensions used in the inner world and the outer world. Given more dimensions, more levels of worlds can be used, which is why the method is called "worlds-within-worlds."

As another example of hierarchical visualization methods, **tree-maps** display hierarchical data as a set of nested rectangles. For example, Figure 2.20 shows a tree-map visualizing Google news stories. All news stories are organized into seven categories, each shown in a large rectangle of a unique color. Within each category (i.e., each rectangle at the top level), the news stories are further partitioned into smaller subcategories.

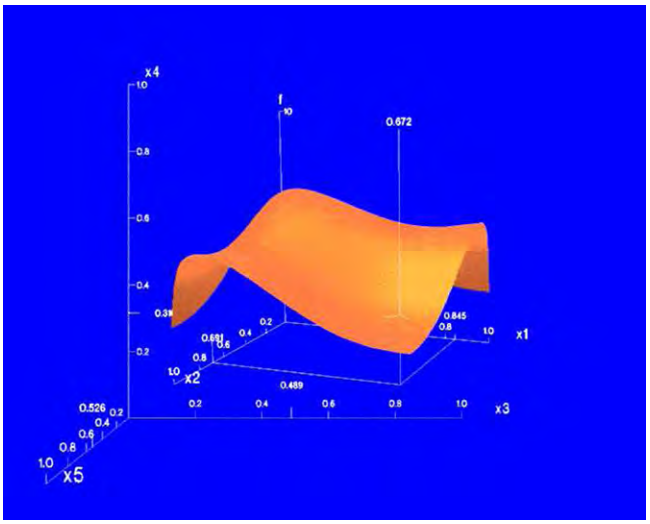


Figure 2.19 "Worlds-within-Worlds" (also known as *n*-Vision). *Source: http://graphics.cs.columbia.edu/projects/AutoVisual/images/1.dipstick.5.gif.*

2.3.5 Visualizing Complex Data and Relations

In early days, visualization techniques were mainly for numeric data. Recently, more and more non-numeric data, such as text and social networks, have become available. Visualizing and analyzing such data attracts a lot of interest.

There are many new visualization techniques dedicated to these kinds of data. For example, many people on the Web tag various objects such as pictures, blog entries, and product reviews. A **tag cloud** is a visualization of statistics of user-generated tags. Often, in a tag cloud, tags are listed alphabetically or in a user-preferred order. The importance of a tag is indicated by font size or color. Figure 2.21 shows a tag cloud for visualizing the popular tags used in a Web site.

Tag clouds are often used in two ways. First, in a tag cloud for a single item, we can use the size of a tag to represent the number of times that the tag is applied to this item by different users. Second, when visualizing the tag statistics on multiple items, we can use the size of a tag to represent the number of items that the tag has been applied to, that is, the popularity of the tag.

In addition to complex data, complex relations among data entries also raise challenges for visualization. For example, Figure 2.22 uses a disease influence graph to visualize the correlations between diseases. The nodes in the graph are diseases, and the size of each node is proportional to the prevalence of the corresponding disease. Two nodes are linked by an edge if the corresponding diseases have a strong correlation. The width of an edge is proportional to the strength of the correlation pattern of the two corresponding diseases.

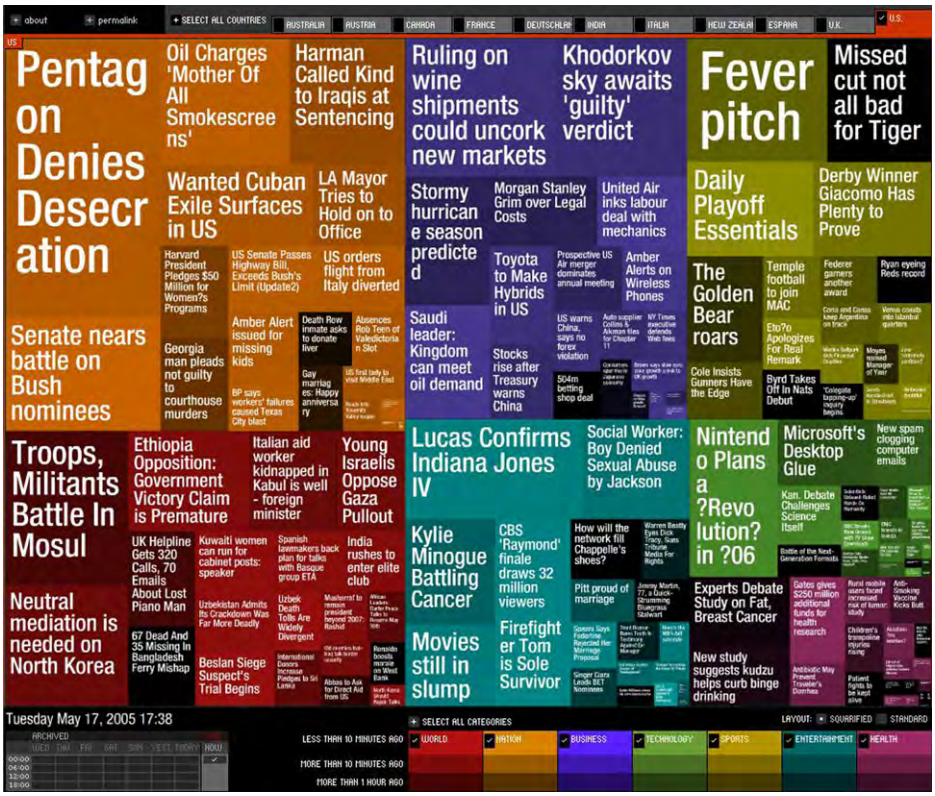


Figure 2.20 Newsmap: Use of tree-maps to visualize Google news headline stories. *Source: www.cs.umd.edu/class/spring2005/cmsc838s/viz4all/ss/newsmap.png.*

In summary, visualization provides effective tools to explore data. We have introduced several popular methods and the essential ideas behind them. There are many existing tools and methods. Moreover, visualization can be used in data mining in various aspects. In addition to visualizing data, visualization can be used to represent the data mining process, the patterns obtained from a mining method, and user interaction with the data. Visual data mining is an important research and development direction.

2.4 Measuring Data Similarity and Dissimilarity

In data mining applications, such as clustering, outlier analysis, and nearest-neighbor classification, we need ways to assess how alike or unalike objects are in comparison to one another. For example, a store may want to search for clusters of *customer* objects, resulting in groups of customers with similar characteristics (e.g., similar income, area of residence, and age). Such information can then be used for marketing. A **cluster** is

Figure 2.21 Using a tag cloud to visualize popular Web site tags. *Source:* A snapshot of *www.flickr.com/photos/tags/*, January 23, 2010.

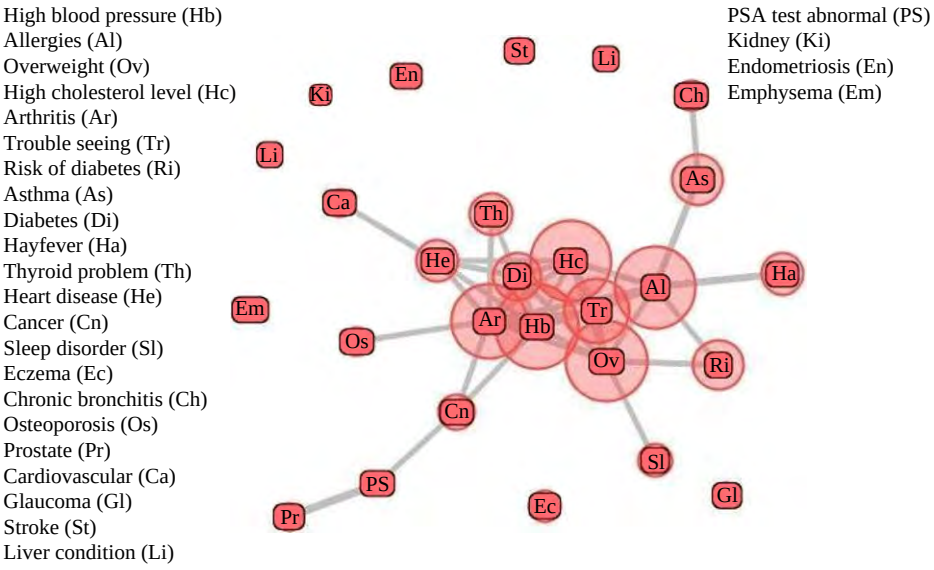


Figure 2.22 Disease influence graph of people at least 20 years old in the NHANES data set.

a collection of data objects such that the objects within a cluster are *similar* to one another and *dissimilar* to the objects in other clusters. Outlier analysis also employs clustering-based techniques to identify potential outliers as objects that are highly dissimilar to others. Knowledge of object similarities can also be used in nearest-neighbor classification schemes where a given object (e.g., a *patient*) is assigned a class label (relating to, say, a *diagnosis*) based on its similarity toward other objects in the model.

This section presents similarity and dissimilarity measures, which are referred to as measures of *proximity*. Similarity and dissimilarity are related. A similarity measure for two objects, i and j, will typically return the value 0 if the objects are unalike. The higher the similarity value, the greater the similarity between objects. (Typically, a value of 1 indicates complete similarity, that is, the objects are identical.) A dissimilarity measure works the opposite way. It returns a value of 0 if the objects are the same (and therefore, far from being dissimilar). The higher the dissimilarity value, the more dissimilar the two objects are.

In Section 2.4.1 we present two data structures that are commonly used in the above types of applications: the *data matrix* (used to store the data objects) and the *dissimilarity matrix* (used to store dissimilarity values for pairs of objects). We also switch to a different notation for data objects than previously used in this chapter since now we are dealing with objects described by more than one attribute. We then discuss how object dissimilarity can be computed for objects described by *nominal* attributes (Section 2.4.2), by *binary* attributes (Section 2.4.3), by *numeric* attributes (Section 2.4.4), by *ordinal* attributes (Section 2.4.5), or by combinations of these attribute types (Section 2.4.6). Section 2.4.7 provides similarity measures for very long and sparse data vectors, such as term-frequency vectors representing documents in information retrieval. Knowing how to compute dissimilarity is useful in studying attributes and will also be referenced in later topics on clustering (Chapters 10 and 11), outlier analysis (Chapter 12), and nearest-neighbor classification (Chapter 9).

2.4.1 Data Matrix versus Dissimilarity Matrix

In Section 2.2, we looked at ways of studying the central tendency, dispersion, and spread of observed values for some attribute X. Our objects there were one-dimensional, that is, described by a single attribute. In this section, we talk about objects described by *multiple* attributes. Therefore, we need a change in notation. Suppose that we have n objects (e.g., persons, items, or courses) described by p attributes (also called *measurements* or *features*, such as age, height, weight, or gender). The objects are $x_1 = (x_{11}, x_{12}, \ldots, x_{1p})$, $x_2 = (x_{21}, x_{22}, \ldots, x_{2p})$, and so on, where x_{ij} is the value for object x_i of the jth attribute. For brevity, we hereafter refer to object x_i as object i. The objects may be tuples in a relational database, and are also referred to as *data samples* or *feature vectors*.

Main memory-based clustering and nearest-neighbor algorithms typically operate on either of the following two data structures:

- **Data matrix** (or *object-by-attribute structure*): This structure stores the n data objects in the form of a relational table, or n-by-p matrix (n objects $\times p$ attributes):

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}. \tag{2.8}$$

Each row corresponds to an object. As part of our notation, we may use f to index through the p attributes.

- **Dissimilarity matrix** (or *object-by-object structure*): This structure stores a collection of proximities that are available for all pairs of n objects. It is often represented by an n-by-n table:

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}, \tag{2.9}$$

where $d(i, j)$ is the measured **dissimilarity** or "difference" between objects i and j. In general, $d(i, j)$ is a non-negative number that is close to 0 when objects i and j are highly similar or "near" each other, and becomes larger the more they differ. Note that $d(i, i) = 0$; that is, the difference between an object and itself is 0. Furthermore, $d(i, j) = d(j, i)$. (For readability, we do not show the $d(j, i)$ entries; the matrix is symmetric.) Measures of dissimilarity are discussed throughout the remainder of this chapter.

Measures of similarity can often be expressed as a function of measures of dissimilarity. For example, for nominal data,

$$sim(i, j) = 1 - d(i, j), \tag{2.10}$$

where $sim(i, j)$ is the similarity between objects i and j. Throughout the rest of this chapter, we will also comment on measures of similarity.

A data matrix is made up of two entities or "things," namely rows (for objects) and columns (for attributes). Therefore, the data matrix is often called a **two-mode** matrix. The dissimilarity matrix contains one kind of entity (dissimilarities) and so is called a **one-mode** matrix. Many clustering and nearest-neighbor algorithms operate on a dissimilarity matrix. Data in the form of a data matrix can be transformed into a dissimilarity matrix before applying such algorithms.

2.4.2 Proximity Measures for Nominal Attributes

A nominal attribute can take on two or more states (Section 2.1.2). For example, *map_color* is a nominal attribute that may have, say, five states: *red, yellow, green, pink*, and *blue*.

Let the number of states of a nominal attribute be M. The states can be denoted by letters, symbols, or a set of integers, such as $1, 2, \ldots, M$. Notice that such integers are used just for data handling and do not represent any specific ordering.

"How is dissimilarity computed between objects described by nominal attributes?" The dissimilarity between two objects i and j can be computed based on the ratio of mismatches:

$$d(i, j) = \frac{p - m}{p}, \tag{2.11}$$

where m is the number of *matches* (i.e., the number of attributes for which i and j are in the same state), and p is the total number of attributes describing the objects. Weights can be assigned to increase the effect of m or to assign greater weight to the matches in attributes having a larger number of states.

Example 2.17 **Dissimilarity between nominal attributes.** Suppose that we have the sample data of Table 2.2, except that only the *object-identifier* and the attribute *test-1* are available, where *test-1* is nominal. (We will use *test-2* and *test-3* in later examples.) Let's compute the dissimilarity matrix (Eq. 2.9), that is,

$$\begin{bmatrix} 0 & & & \\ d(2,1) & 0 & & \\ d(3,1) & d(3,2) & 0 & \\ d(4,1) & d(4,2) & d(4,3) & 0 \end{bmatrix}.$$

Since here we have one nominal attribute, *test-1*, we set $p = 1$ in Eq. (2.11) so that $d(i, j)$ evaluates to 0 if objects i and j match, and 1 if the objects differ. Thus, we get

$$\begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ 1 & 1 & 0 & \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

From this, we see that all objects are dissimilar except objects 1 and 4 (i.e., $d(4,1) = 0$). ■

Table 2.2 A Sample Data Table Containing Attributes of Mixed Type

Object Identifier	*test-1 (nominal)*	*test-2 (ordinal)*	*test-3 (numeric)*
1	code A	excellent	45
2	code B	fair	22
3	code C	good	64
4	code A	excellent	28

Alternatively, similarity can be computed as

$$sim(i, j) = 1 - d(i, j) = \frac{m}{p}. \tag{2.12}$$

Proximity between objects described by nominal attributes can be computed using an alternative encoding scheme. Nominal attributes can be encoded using asymmetric binary attributes by creating a new binary attribute for each of the M states. For an object with a given state value, the binary attribute representing that state is set to 1, while the remaining binary attributes are set to 0. For example, to encode the nominal attribute *map_color*, a binary attribute can be created for each of the five colors previously listed. For an object having the color *yellow*, the *yellow* attribute is set to 1, while the remaining four attributes are set to 0. Proximity measures for this form of encoding can be calculated using the methods discussed in the next subsection.

2.4.3 Proximity Measures for Binary Attributes

Let's look at dissimilarity and similarity measures for objects described by either *symmetric* or *asymmetric binary attributes*.

Recall that a binary attribute has only one of two states: 0 and 1, where 0 means that the attribute is absent, and 1 means that it is present (Section 2.1.3). Given the attribute *smoker* describing a patient, for instance, 1 indicates that the patient smokes, while 0 indicates that the patient does not. Treating binary attributes as if they are numeric can be misleading. Therefore, methods specific to binary data are necessary for computing dissimilarity.

"*So, how can we compute the dissimilarity between two binary attributes?*" One approach involves computing a dissimilarity matrix from the given binary data. If all binary attributes are thought of as having the same weight, we have the 2×2 contingency table of Table 2.3, where q is the number of attributes that equal 1 for both objects i and j, r is the number of attributes that equal 1 for object i but equal 0 for object j, s is the number of attributes that equal 0 for object i but equal 1 for object j, and t is the number of attributes that equal 0 for both objects i and j. The total number of attributes is p, where $p = q + r + s + t$.

Recall that for symmetric binary attributes, each state is equally valuable. Dissimilarity that is based on symmetric binary attributes is called **symmetric binary dissimilarity**. If objects i and j are described by symmetric binary attributes, then the

Table 2.3 Contingency Table for Binary Attributes

		Object j		
		1	0	sum
Object i	1	q	r	$q+r$
	0	s	t	$s+t$
	sum	$q+s$	$r+t$	p

dissimilarity between i and j is

$$d(i, j) = \frac{r + s}{q + r + s + t}. \tag{2.13}$$

For asymmetric binary attributes, the two states are not equally important, such as the *positive* (1) and *negative* (0) outcomes of a disease test. Given two asymmetric binary attributes, the agreement of two 1s (a positive match) is then considered more significant than that of two 0s (a negative match). Therefore, such binary attributes are often considered "monary" (having one state). The dissimilarity based on these attributes is called **asymmetric binary dissimilarity**, where the number of negative matches, t, is considered unimportant and is thus ignored in the following computation:

$$d(i, j) = \frac{r + s}{q + r + s}. \tag{2.14}$$

Complementarily, we can measure the difference between two binary attributes based on the notion of similarity instead of dissimilarity. For example, the **asymmetric binary similarity** between the objects i and j can be computed as

$$sim(i, j) = \frac{q}{q + r + s} = 1 - d(i, j). \tag{2.15}$$

The coefficient $sim(i, j)$ of Eq. (2.15) is called the **Jaccard coefficient** and is popularly referenced in the literature.

When both symmetric and asymmetric binary attributes occur in the same data set, the mixed attributes approach described in Section 2.4.6 can be applied.

Example 2.18 **Dissimilarity between binary attributes.** Suppose that a patient record table (Table 2.4) contains the attributes *name, gender, fever, cough, test-1, test-2, test-3*, and *test-4*, where *name* is an object identifier, *gender* is a symmetric attribute, and the remaining attributes are asymmetric binary.

For asymmetric attribute values, let the values Y (*yes*) and P (*positive*) be set to 1, and the value N (*no* or *negative*) be set to 0. Suppose that the distance between objects

Table 2.4 Relational Table Where Patients Are Described by Binary Attributes

name	*gender*	*fever*	*cough*	*test-1*	*test-2*	*test-3*	*test-4*
Jack	M	Y	N	P	N	N	N
Jim	M	Y	Y	N	N	N	N
Mary	F	Y	N	P	N	P	N
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

(patients) is computed based only on the asymmetric attributes. According to Eq. (2.14), the distance between each pair of the three patients—Jack, Mary, and Jim—is

$$d(Jack, Jim) = \frac{1+1}{1+1+1} = 0.67,$$

$$d(Jack, Mary) = \frac{0+1}{2+0+1} = 0.33,$$

$$d(Jim, Mary) = \frac{1+2}{1+1+2} = 0.75.$$

These measurements suggest that Jim and Mary are unlikely to have a similar disease because they have the highest dissimilarity value among the three pairs. Of the three patients, Jack and Mary are the most likely to have a similar disease. ■

2.4.4 Dissimilarity of Numeric Data: Minkowski Distance

In this section, we describe distance measures that are commonly used for computing the dissimilarity of objects described by numeric attributes. These measures include the *Euclidean, Manhattan*, and *Minkowski distances.*

In some cases, the data are normalized before applying distance calculations. This involves transforming the data to fall within a smaller or common range, such as $[-1, 1]$ or $[0.0, 1.0]$. Consider a *height* attribute, for example, which could be measured in either meters or inches. In general, expressing an attribute in smaller units will lead to a larger range for that attribute, and thus tend to give such attributes greater effect or "weight." Normalizing the data attempts to give all attributes an equal weight. It may or may not be useful in a particular application. Methods for normalizing data are discussed in detail in Chapter 3 on data preprocessing.

The most popular distance measure is **Euclidean distance** (i.e., straight line or "as the crow flies"). Let $i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jp})$ be two objects described by p numeric attributes. The Euclidean distance between objects i and j is defined as

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}. \tag{2.16}$$

Another well-known measure is the **Manhattan (or city block) distance**, named so because it is the distance in blocks between any two points in a city (such as 2 blocks down and 3 blocks over for a total of 5 blocks). It is defined as

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{ip} - x_{jp}|. \tag{2.17}$$

Both the Euclidean and the Manhattan distance satisfy the following mathematical properties:

Non-negativity: $d(i, j) \geq 0$: Distance is a non-negative number.

Identity of indiscernibles: $d(i, i) = 0$: The distance of an object to itself is 0.

Symmetry: $d(i, j) = d(j, i)$: Distance is a symmetric function.

Triangle inequality: $d(i, j) \leq d(i, k) + d(k, j)$: Going directly from object i to object j in space is no more than making a detour over any other object k.

A measure that satisfies these conditions is known as **metric**. Please note that the non-negativity property is implied by the other three properties.

Example 2.19 **Euclidean distance and Manhattan distance.** Let $\boldsymbol{x_1} = (1, 2)$ and $\boldsymbol{x_2} = (3, 5)$ represent two objects as shown in Figure 2.23. The Euclidean distance between the two is $\sqrt{2^2 + 3^2} = 3.61$. The Manhattan distance between the two is $2 + 3 = 5$. ■

Minkowski distance is a generalization of the Euclidean and Manhattan distances. It is defined as

$$d(i, j) = \sqrt[h]{|x_{i1} - x_{j1}|^h + |x_{i2} - x_{j2}|^h + \cdots + |x_{ip} - x_{jp}|^h}, \tag{2.18}$$

where h is a real number such that $h \geq 1$. (Such a distance is also called L_p **norm** in some literature, where the symbol p refers to our notation of h. We have kept p as the number of attributes to be consistent with the rest of this chapter.) It represents the Manhattan distance when $h = 1$ (i.e., L_1 norm) and Euclidean distance when $h = 2$ (i.e., L_2 norm).

The **supremum distance** (also referred to as $\boldsymbol{L_{max}}$, $\boldsymbol{L_\infty}$ **norm** and as the **Chebyshev distance**) is a generalization of the Minkowski distance for $h \to \infty$. To compute it, we find the attribute f that gives the maximum difference in values between the two objects. This difference is the supremum distance, defined more formally as:

$$d(i, j) = \lim_{h \to \infty} \left(\sum_{f=1}^{p} |x_{if} - x_{jf}|^h \right)^{\frac{1}{h}} = \max_{f}^{p} |x_{if} - x_{jf}|. \tag{2.19}$$

The L^∞ norm is also known as the *uniform norm*.

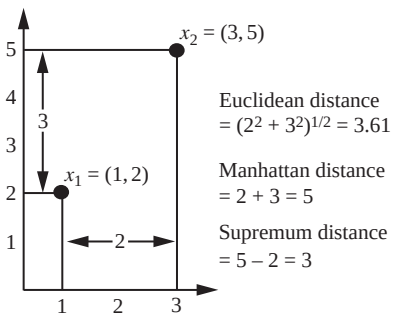


Figure 2.23 Euclidean, Manhattan, and supremum distances between two objects.

Example 2.20 **Supremum distance.** Let's use the same two objects, $\boldsymbol{x_1} = (1, 2)$ and $\boldsymbol{x_2} = (3, 5)$, as in Figure 2.23. The second attribute gives the greatest difference between values for the objects, which is $5 - 2 = 3$. This is the supremum distance between both objects. ■

If each attribute is assigned a weight according to its perceived importance, the **weighted Euclidean distance** can be computed as

$$d(i, j) = \sqrt{w_1|x_{i1} - x_{j1}|^2 + w_2|x_{i2} - x_{j2}|^2 + \cdots + w_m|x_{ip} - x_{jp}|^2}. \tag{2.20}$$

Weighting can also be applied to other distance measures as well.

2.4.5 Proximity Measures for Ordinal Attributes

The values of an ordinal attribute have a meaningful order or ranking about them, yet the magnitude between successive values is unknown (Section 2.1.4). An example includes the sequence *small*, *medium*, *large* for a *size* attribute. Ordinal attributes may also be obtained from the discretization of numeric attributes by splitting the value range into a finite number of categories. These categories are organized into ranks. That is, the range of a numeric attribute can be mapped to an ordinal attribute f having M_f states. For example, the range of the interval-scaled attribute *temperature* (in Celsius) can be organized into the following states: -30 to -10, -10 to 10, 10 to 30, representing the categories *cold temperature*, *moderate temperature*, and *warm temperature*, respectively. Let M represent the number of possible states that an ordinal attribute can have. These ordered states define the ranking $1, \ldots, M_f$.

"*How are ordinal attributes handled?*" The treatment of ordinal attributes is quite similar to that of numeric attributes when computing dissimilarity between objects. Suppose that f is an attribute from a set of ordinal attributes describing n objects. The dissimilarity computation with respect to f involves the following steps:

1. The value of f for the ith object is x_{if}, and f has M_f ordered states, representing the ranking $1, \ldots, M_f$. Replace each x_{if} by its corresponding rank, $r_{if} \in \{1, \ldots, M_f\}$.
2. Since each ordinal attribute can have a different number of states, it is often necessary to map the range of each attribute onto [0.0, 1.0] so that each attribute has equal weight. We perform such data normalization by replacing the rank r_{if} of the ith object in the fth attribute by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}. \tag{2.21}$$

3. Dissimilarity can then be computed using any of the distance measures described in Section 2.4.4 for numeric attributes, using z_{if} to represent the f value for the ith object.

Example 2.21 **Dissimilarity between ordinal attributes.** Suppose that we have the sample data shown earlier in Table 2.2, except that this time only the *object-identifier* and the continuous ordinal attribute, *test-2*, are available. There are three states for *test-2*: *fair*, *good*, and *excellent*, that is, $M_f = 3$. For step 1, if we replace each value for *test-2* by its rank, the four objects are assigned the ranks 3, 1, 2, and 3, respectively. Step 2 normalizes the ranking by mapping rank 1 to 0.0, rank 2 to 0.5, and rank 3 to 1.0. For step 3, we can use, say, the Euclidean distance (Eq. 2.16), which results in the following dissimilarity matrix:

$$\begin{bmatrix} 0 & & & \\ 1.0 & 0 & & \\ 0.5 & 0.5 & 0 & \\ 0 & 1.0 & 0.5 & 0 \end{bmatrix}.$$

Therefore, objects 1 and 2 are the most dissimilar, as are objects 2 and 4 (i.e., $d(2,1) = 1.0$ and $d(4,2) = 1.0$). This makes intuitive sense since objects 1 and 4 are both *excellent*. Object 2 is *fair*, which is at the opposite end of the range of values for *test-2*. ■

Similarity values for ordinal attributes can be interpreted from dissimilarity as $sim(i,j) = 1 - d(i,j)$.

2.4.6 Dissimilarity for Attributes of Mixed Types

Sections 2.4.2 through 2.4.5 discussed how to compute the dissimilarity between objects described by attributes of the same type, where these types may be either *nominal*, *symmetric binary*, *asymmetric binary*, *numeric*, or *ordinal*. However, in many real databases, objects are described by a *mixture* of attribute types. In general, a database can contain all of these attribute types.

"*So, how can we compute the dissimilarity between objects of mixed attribute types?*" One approach is to group each type of attribute together, performing separate data mining (e.g., clustering) analysis for each type. This is feasible if these analyses derive compatible results. However, in real applications, it is unlikely that a separate analysis per attribute type will generate compatible results.

A more preferable approach is to process all attribute types together, performing a single analysis. One such technique combines the different attributes into a single dissimilarity matrix, bringing all of the meaningful attributes onto a common scale of the interval [0.0, 1.0].

Suppose that the data set contains p attributes of mixed type. The dissimilarity $d(i, j)$ between objects i and j is defined as

$$d(i,j) = \frac{\sum_{f=1}^{p} \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{p} \delta_{ij}^{(f)}}, \tag{2.22}$$

where the indicator $\delta_{ij}^{(f)} = 0$ if either (1) x_{if} or x_{jf} is missing (i.e., there is no measurement of attribute f for object i or object j), or (2) $x_{if} = x_{jf} = 0$ and attribute f is asymmetric binary; otherwise, $\delta_{ij}^{(f)} = 1$. The contribution of attribute f to the dissimilarity between i and j (i.e., $d_{ij}^{(f)}$) is computed dependent on its type:

- If f is numeric: $d_{ij}^{(f)} = \frac{|x_{if} - x_{jf}|}{max_h x_{hf} - min_h x_{hf}}$, where h runs over all nonmissing objects for attribute f.
- If f is nominal or binary: $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$; otherwise, $d_{ij}^{(f)} = 1$.
- If f is ordinal: compute the ranks r_{if} and $z_{if} = \frac{r_{if} - 1}{M_f - 1}$, and treat z_{if} as numeric.

These steps are identical to what we have already seen for each of the individual attribute types. The only difference is for numeric attributes, where we normalize so that the values map to the interval [0.0, 1.0]. Thus, the dissimilarity between objects can be computed even when the attributes describing the objects are of different types.

Example 2.22 **Dissimilarity between attributes of mixed type.** Let's compute a dissimilarity matrix for the objects in Table 2.2. Now we will consider *all* of the attributes, which are of different types. In Examples 2.17 and 2.21, we worked out the dissimilarity matrices for each of the individual attributes. The procedures we followed for *test-1* (which is nominal) and *test-2* (which is ordinal) are the same as outlined earlier for processing attributes of mixed types. Therefore, we can use the dissimilarity matrices obtained for *test-1* and *test-2* later when we compute Eq. (2.22). First, however, we need to compute the dissimilarity matrix for the third attribute, *test-3* (which is numeric). That is, we must compute $d_{ij}^{(3)}$. Following the case for numeric attributes, we let $max_h x_h = 64$ and $min_h x_h = 22$. The difference between the two is used in Eq. (2.22) to normalize the values of the dissimilarity matrix. The resulting dissimilarity matrix for *test-3* is

$$\begin{bmatrix} 0 & & & \\ 0.55 & 0 & & \\ 0.45 & 1.00 & 0 & \\ 0.40 & 0.14 & 0.86 & 0 \end{bmatrix}.$$

We can now use the dissimilarity matrices for the three attributes in our computation of Eq. (2.22). The indicator $\delta_{ij}^{(f)} = 1$ for each of the three attributes, f. We get, for example, $d(3, 1) = \frac{1(1) + 1(0.50) + 1(0.45)}{3} = 0.65$. The resulting dissimilarity matrix obtained for the

data described by the three attributes of mixed types is:

$$\begin{bmatrix} 0 & & & \\ 0.85 & 0 & & \\ 0.65 & 0.83 & 0 & \\ 0.13 & 0.71 & 0.79 & 0 \end{bmatrix}.$$

From Table 2.2, we can intuitively guess that objects 1 and 4 are the most similar, based on their values for *test*-1 and *test*-2. This is confirmed by the dissimilarity matrix, where $d(4, 1)$ is the lowest value for any pair of different objects. Similarly, the matrix indicates that objects 1 and 2 are the least similar. ■

2.4.7 Cosine Similarity

A document can be represented by thousands of attributes, each recording the frequency of a particular word (such as a keyword) or phrase in the document. Thus, each document is an object represented by what is called a *term-frequency vector*. For example, in Table 2.5, we see that *Document1* contains five instances of the word *team*, while *hockey* occurs three times. The word *coach* is absent from the entire document, as indicated by a count value of 0. Such data can be highly asymmetric.

Term-frequency vectors are typically very long and **sparse** (i.e., they have many 0 values). Applications using such structures include information retrieval, text document clustering, biological taxonomy, and gene feature mapping. The traditional distance measures that we have studied in this chapter do not work well for such sparse numeric data. For example, two term-frequency vectors may have many 0 values in common, meaning that the corresponding documents do not share many words, but this does not make them similar. We need a measure that will focus on the words that the two documents *do* have in common, and the occurrence frequency of such words. In other words, we need a measure for numeric data that ignores zero-matches.

Cosine similarity is a measure of similarity that can be used to compare documents or, say, give a ranking of documents with respect to a given vector of query words. Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be two vectors for comparison. Using the cosine measure as a

Table 2.5 Document Vector or Term-Frequency Vector

Document	*team*	*coach*	*hockey*	*baseball*	*soccer*	*penalty*	*score*	*win*	*loss*	*season*
Document1	5	0	3	0	2	0	0	2	0	0
Document2	3	0	2	0	1	1	0	1	0	1
Document3	0	7	0	2	1	0	0	3	0	0
Document4	0	1	0	0	1	2	2	0	3	0

similarity function, we have

$$sim(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x} \cdot \boldsymbol{y}}{||\boldsymbol{x}|| ||\boldsymbol{y}||}, \tag{2.23}$$

where $||\boldsymbol{x}||$ is the Euclidean norm of vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_p)$, defined as $\sqrt{x_1^2 + x_2^2 + \cdots + x_p^2}$. Conceptually, it is the length of the vector. Similarly, $||\boldsymbol{y}||$ is the Euclidean norm of vector $\boldsymbol{y}$. The measure computes the cosine of the angle between vectors $\boldsymbol{x}$ and $\boldsymbol{y}$. A cosine value of 0 means that the two vectors are at 90 degrees to each other (orthogonal) and have no match. The closer the cosine value to 1, the smaller the angle and the greater the match between vectors. Note that because the cosine similarity measure does not obey all of the properties of Section 2.4.4 defining metric measures, it is referred to as a *nonmetric measure*.

Example 2.23 **Cosine similarity between two term-frequency vectors.** Suppose that $\boldsymbol{x}$ and $\boldsymbol{y}$ are the first two term-frequency vectors in Table 2.5. That is, $\boldsymbol{x} = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0)$ and $\boldsymbol{y} = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1)$. How similar are $\boldsymbol{x}$ and $\boldsymbol{y}$? Using Eq. (2.23) to compute the cosine similarity between the two vectors, we get:

$$\begin{aligned}
\boldsymbol{x}^t \cdot \boldsymbol{y} &= 5 \times 3 + 0 \times 0 + 3 \times 2 + 0 \times 0 + 2 \times 1 + 0 \times 1 + 0 \times 0 + 2 \times 1 \\
&\quad + 0 \times 0 + 0 \times 1 = 25 \\
||\boldsymbol{x}|| &= \sqrt{5^2 + 0^2 + 3^2 + 0^2 + 2^2 + 0^2 + 0^2 + 2^2 + 0^2 + 0^2} = 6.48 \\
||\boldsymbol{y}|| &= \sqrt{3^2 + 0^2 + 2^2 + 0^2 + 1^2 + 1^2 + 0^2 + 1^2 + 0^2 + 1^2} = 4.12 \\
sim(\boldsymbol{x}, \boldsymbol{y}) &= 0.94
\end{aligned}$$

Therefore, if we were using the cosine similarity measure to compare these documents, they would be considered quite similar. ■

When attributes are binary-valued, the cosine similarity function can be interpreted in terms of shared features or attributes. Suppose an object $\boldsymbol{x}$ possesses the ith attribute if $x_i = 1$. Then $\boldsymbol{x}^t \cdot \boldsymbol{y}$ is the number of attributes possessed (i.e., shared) by both $\boldsymbol{x}$ and $\boldsymbol{y}$, and $|\boldsymbol{x}||\boldsymbol{y}|$ is the *geometric mean* of the number of attributes possessed by $\boldsymbol{x}$ and the number possessed by $\boldsymbol{y}$. Thus, $sim(\boldsymbol{x}, \boldsymbol{y})$ is a measure of relative possession of common attributes.

A simple variation of cosine similarity for the preceding scenario is

$$sim(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x} \cdot \boldsymbol{y}}{\boldsymbol{x} \cdot \boldsymbol{x} + \boldsymbol{y} \cdot \boldsymbol{y} - \boldsymbol{x} \cdot \boldsymbol{y}}, \tag{2.24}$$

which is the ratio of the number of attributes shared by $\boldsymbol{x}$ and $\boldsymbol{y}$ to the number of attributes possessed by $\boldsymbol{x}$ or $\boldsymbol{y}$. This function, known as the **Tanimoto coefficient** or **Tanimoto distance**, is frequently used in information retrieval and biology taxonomy.

2.5 Summary

- Data sets are made up of data objects. A **data object** represents an entity. Data objects are described by attributes. Attributes can be nominal, binary, ordinal, or numeric.
- The values of a **nominal** (or **categorical**) **attribute** are symbols or names of things, where each value represents some kind of category, code, or state.
- **Binary attributes** are nominal attributes with only two possible states (such as 1 and 0 or true and false). If the two states are equally important, the attribute is *symmetric*; otherwise it is *asymmetric*.
- An **ordinal attribute** is an attribute with possible values that have a meaningful order or ranking among them, but the magnitude between successive values is not known.
- A **numeric attribute** is *quantitative* (i.e., it is a measurable quantity) represented in integer or real values. Numeric attribute types can be *interval-scaled* or *ratio-scaled*. The values of an **interval-scaled attribute** are measured in fixed and equal units. **Ratio-scaled attributes** are numeric attributes with an inherent zero-point. Measurements are ratio-scaled in that we can speak of values as being an order of magnitude larger than the unit of measurement.
- **Basic statistical descriptions** provide the analytical foundation for data preprocessing. The basic statistical measures for data summarization include *mean, weighted mean, median*, and *mode* for measuring the central tendency of data; and *range, quantiles, quartiles, interquartile range, variance*, and *standard deviation* for measuring the dispersion of data. Graphical representations (e.g., *boxplots, quantile plots, quantile–quantile plots, histograms*, and *scatter plots*) facilitate visual inspection of the data and are thus useful for data preprocessing and mining.
- **Data visualization** techniques may be *pixel-oriented, geometric-based, icon-based*, or *hierarchical*. These methods apply to multidimensional relational data. Additional techniques have been proposed for the visualization of complex data, such as text and social networks.
- Measures of object **similarity** and **dissimilarity** are used in data mining applications such as clustering, outlier analysis, and nearest-neighbor classification. Such measures of *proximity* can be computed for each attribute type studied in this chapter, or for combinations of such attributes. Examples include the *Jaccard coefficient* for asymmetric binary attributes and *Euclidean*, *Manhattan*, *Minkowski*, and *supremum* distances for numeric attributes. For applications involving sparse numeric data vectors, such as term-frequency vectors, the *cosine measure* and the *Tanimoto coefficient* are often used in the assessment of similarity.

2.6 Exercises

2.1 Give three additional commonly used statistical measures that are not already illustrated in this chapter for the characterization of *data dispersion*. Discuss how they can be computed efficiently in large databases.

2.2 Suppose that the data for analysis includes the attribute *age*. The *age* values for the data tuples are (in increasing order) 13, 15, 16, 16, 19, 20, 20, 21, 22, 22, 25, 25, 25, 25, 30, 33, 33, 35, 35, 35, 35, 36, 40, 45, 46, 52, 70.

(a) What is the *mean* of the data? What is the *median*?

(b) What is the *mode* of the data? Comment on the data's modality (i.e., bimodal, trimodal, etc.).

(c) What is the *midrange* of the data?

(d) Can you find (roughly) the first quartile (Q_1) and the third quartile (Q_3) of the data?

(e) Give the *five-number summary* of the data.

(f) Show a *boxplot* of the data.

(g) How is a *quantile–quantile plot* different from a *quantile plot*?

2.3 Suppose that the values for a given set of data are grouped into intervals. The intervals and corresponding frequencies are as follows:

age	*frequency*
1–5	200
6–15	450
16–20	300
21–50	1500
51–80	700
81–110	44

Compute an *approximate median* value for the data.

2.4 Suppose that a hospital tested the age and body fat data for 18 randomly selected adults with the following results:

age	23	23	27	27	39	41	47	49	50
%fat	9.5	26.5	7.8	17.8	31.4	25.9	27.4	27.2	31.2
age	52	54	54	56	57	58	58	60	61
%fat	34.6	42.5	28.8	33.4	30.2	34.1	32.9	41.2	35.7

(a) Calculate the mean, median, and standard deviation of *age* and *%fat*.

(b) Draw the boxplots for *age* and *%fat*.

(c) Draw a *scatter plot* and a *q-q plot* based on these two variables.

2.5 Briefly outline how to compute the dissimilarity between objects described by the following:

(a) Nominal attributes

(b) Asymmetric binary attributes

(c) Numeric attributes
(d) Term-frequency vectors

2.6 Given two objects represented by the tuples (22, 1, 42, 10) and (20, 0, 36, 8):

(a) Compute the *Euclidean distance* between the two objects.
(b) Compute the *Manhattan distance* between the two objects.
(c) Compute the *Minkowski distance* between the two objects, using $q = 3$.
(d) Compute the *supremum distance* between the two objects.

2.7 The *median* is one of the most important holistic measures in data analysis. Propose several methods for median approximation. Analyze their respective complexity under different parameter settings and decide to what extent the real value can be approximated. Moreover, suggest a heuristic strategy to balance between accuracy and complexity and then apply it to all methods you have given.

2.8 It is important to define or select similarity measures in data analysis. However, there is no commonly accepted subjective similarity measure. Results can vary depending on the similarity measures used. Nonetheless, seemingly different similarity measures may be equivalent after some transformation.

Suppose we have the following 2-D data set:

	A_1	A_2
$\boldsymbol{x_1}$	1.5	1.7
$\boldsymbol{x_2}$	2	1.9
$\boldsymbol{x_3}$	1.6	1.8
$\boldsymbol{x_4}$	1.2	1.5
$\boldsymbol{x_5}$	1.5	1.0

(a) Consider the data as 2-D data points. Given a new data point, $\boldsymbol{x} = (1.4, 1.6)$ as a query, rank the database points based on similarity with the query using Euclidean distance, Manhattan distance, supremum distance, and cosine similarity.
(b) Normalize the data set to make the norm of each data point equal to 1. Use Euclidean distance on the transformed data to rank the data points.

2.7 Bibliographic Notes

Methods for descriptive data summarization have been studied in the statistics literature long before the onset of computers. Good summaries of statistical descriptive data mining methods include Freedman, Pisani, and Purves [FPP07] and Devore [Dev95]. For

statistics-based visualization of data using boxplots, quantile plots, quantile–quantile plots, scatter plots, and loess curves, see Cleveland [Cle93].

Pioneering work on data visualization techniques is described in *The Visual Display of Quantitative Information* [Tuf83], *Envisioning Information* [Tuf90], and *Visual Explanations: Images and Quantities, Evidence and Narrative* [Tuf97], all by Tufte, in addition to *Graphics and Graphic Information Processing* by Bertin [Ber81], *Visualizing Data* by Cleveland [Cle93], and *Information Visualization in Data Mining and Knowledge Discovery* edited by Fayyad, Grinstein, and Wierse [FGW01].

Major conferences and symposiums on visualization include *ACM Human Factors in Computing Systems (CHI)*, *Visualization*, and the *International Symposium on Information Visualization*. Research on visualization is also published in *Transactions on Visualization and Computer Graphics*, *Journal of Computational and Graphical Statistics*, and *IEEE Computer Graphics and Applications*.

Many graphical user interfaces and visualization tools have been developed and can be found in various data mining products. Several books on data mining (e.g., *Data Mining Solutions* by Westphal and Blaxton [WB98]) present many good examples and visual snapshots. For a survey of visualization techniques, see "Visual techniques for exploring databases" by Keim [Kei97].

Similarity and distance measures among various variables have been introduced in many textbooks that study cluster analysis, including Hartigan [Har75]; Jain and Dubes [JD88]; Kaufman and Rousseeuw [KR90]; and Arabie, Hubert, and de Soete [AHS96]. Methods for combining attributes of different types into a single dissimilarity matrix were introduced by Kaufman and Rousseeuw [KR90].

10 Cluster Analysis: Basic Concepts and Methods

Imagine that you are the Director of Customer Relationships at *AllElectronics*, and you have five managers working for you. You would like to organize all the company's customers into five groups so that each group can be assigned to a different manager. Strategically, you would like that the customers in each group are as similar as possible. Moreover, two given customers having very different business patterns should not be placed in the same group. Your intention behind this business strategy is to develop customer relationship campaigns that specifically target each group, based on common features shared by the customers per group. What kind of data mining techniques can help you to accomplish this task?

Unlike in classification, the class label (or *group_ID*) of each customer is unknown. You need to *discover* these groupings. Given a large number of customers and many attributes describing customer profiles, it can be very costly or even infeasible to have a human study the data and manually come up with a way to partition the customers into strategic groups. You need a *clustering* tool to help.

Clustering is the process of grouping a set of data objects into multiple groups or *clusters* so that objects within a cluster have high similarity, but are very dissimilar to objects in other clusters. Dissimilarities and similarities are assessed based on the attribute values describing the objects and often involve distance measures.[1] Clustering as a data mining tool has its roots in many application areas such as biology, security, business intelligence, and Web search.

This chapter presents the basic concepts and methods of cluster analysis. In Section 10.1, we introduce the topic and study the requirements of clustering methods for massive amounts of data and various applications. You will learn several basic clustering techniques, organized into the following categories: *partitioning methods* (Section 10.2), *hierarchical methods* (Section 10.3), *density-based methods* (Section 10.4), and *grid-based methods* (Section 10.5). In Section 10.6, we briefly discuss how to evaluate

[1] Data similarity and dissimilarity are discussed in detail in Section 2.4. You may want to refer to that section for a quick review.

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clustering methods. A discussion of advanced methods of clustering is reserved for Chapter 11.

10.1 Cluster Analysis

This section sets up the groundwork for studying cluster analysis. Section 10.1.1 defines cluster analysis and presents examples of where it is useful. In Section 10.1.2, you will learn aspects for comparing clustering methods, as well as requirements for clustering. An overview of basic clustering techniques is presented in Section 10.1.3.

10.1.1 What Is Cluster Analysis?

Cluster analysis or simply **clustering** is the process of partitioning a set of data objects (or observations) into subsets. Each subset is a **cluster**, such that objects in a cluster are similar to one another, yet dissimilar to objects in other clusters. The set of clusters resulting from a cluster analysis can be referred to as a **clustering**. In this context, different clustering methods may generate different clusterings on the same data set. The partitioning is not performed by humans, but by the clustering algorithm. Hence, clustering is useful in that it can lead to the discovery of previously unknown groups within the data.

Cluster analysis has been widely used in many applications such as business intelligence, image pattern recognition, Web search, biology, and security. In business intelligence, clustering can be used to organize a large number of customers into groups, where customers within a group share strong similar characteristics. This facilitates the development of business strategies for enhanced customer relationship management. Moreover, consider a consultant company with a large number of projects. To improve project management, clustering can be applied to partition projects into categories based on similarity so that project auditing and diagnosis (to improve project delivery and outcomes) can be conducted effectively.

In image recognition, clustering can be used to discover clusters or "subclasses" in handwritten character recognition systems. Suppose we have a data set of handwritten digits, where each digit is labeled as either 1, 2, 3, and so on. Note that there can be a large variance in the way in which people write the same digit. Take the number 2, for example. Some people may write it with a small circle at the left bottom part, while some others may not. We can use clustering to determine subclasses for "2," each of which represents a variation on the way in which 2 can be written. Using multiple models based on the subclasses can improve overall recognition accuracy.

Clustering has also found many applications in Web search. For example, a keyword search may often return a very large number of hits (i.e., pages relevant to the search) due to the extremely large number of web pages. Clustering can be used to organize the search results into groups and present the results in a concise and easily accessible way. Moreover, clustering techniques have been developed to cluster documents into topics, which are commonly used in information retrieval practice.

As a data mining function, cluster analysis can be used as a standalone tool to gain insight into the distribution of data, to observe the characteristics of each cluster, and to focus on a particular set of clusters for further analysis. Alternatively, it may serve as a preprocessing step for other algorithms, such as characterization, attribute subset selection, and classification, which would then operate on the detected clusters and the selected attributes or features.

Because a cluster is a collection of data objects that are similar to one another within the cluster and dissimilar to objects in other clusters, a cluster of data objects can be treated as an implicit class. In this sense, clustering is sometimes called **automatic classification**. Again, a critical difference here is that clustering can automatically find the groupings. This is a distinct advantage of cluster analysis.

Clustering is also called **data segmentation** in some applications because clustering partitions large data sets into groups according to their *similarity*. Clustering can also be used for **outlier detection**, where outliers (values that are "far away" from any cluster) may be more interesting than common cases. Applications of outlier detection include the detection of credit card fraud and the monitoring of criminal activities in electronic commerce. For example, exceptional cases in credit card transactions, such as very expensive and infrequent purchases, may be of interest as possible fraudulent activities. Outlier detection is the subject of Chapter 12.

Data clustering is under vigorous development. Contributing areas of research include data mining, statistics, machine learning, spatial database technology, information retrieval, Web search, biology, marketing, and many other application areas. Owing to the huge amounts of data collected in databases, cluster analysis has recently become a highly active topic in data mining research.

As a branch of statistics, cluster analysis has been extensively studied, with the main focus on *distance-based cluster analysis*. Cluster analysis tools based on *k*-means, *k*-medoids, and several other methods also have been built into many statistical analysis software packages or systems, such as S-Plus, SPSS, and SAS. In machine learning, recall that classification is known as supervised learning because the class label information is given, that is, the learning algorithm is supervised in that it is told the class membership of each training tuple. Clustering is known as **unsupervised learning** because the class label information is not present. For this reason, clustering is a form of **learning by observation**, rather than *learning by examples*. In data mining, efforts have focused on finding methods for efficient and effective cluster analysis in *large databases*. Active themes of research focus on the *scalability* of clustering methods, the effectiveness of methods for clustering *complex shapes* (e.g., nonconvex) and *types of data* (e.g., text, graphs, and images), *high-dimensional* clustering techniques (e.g., clustering objects with thousands of features), and methods for clustering *mixed numerical and nominal data* in large databases.

10.1.2 Requirements for Cluster Analysis

Clustering is a challenging research field. In this section, you will learn about the requirements for clustering as a data mining tool, as well as aspects that can be used for comparing clustering methods.

The following are typical requirements of clustering in data mining.

- **Scalability**: Many clustering algorithms work well on small data sets containing fewer than several hundred data objects; however, a large database may contain millions or even billions of objects, particularly in Web search scenarios. Clustering on only a sample of a given large data set may lead to biased results. Therefore, highly scalable clustering algorithms are needed.
- **Ability to deal with different types of attributes**: Many algorithms are designed to cluster numeric (interval-based) data. However, applications may require clustering other data types, such as binary, nominal (categorical), and ordinal data, or mixtures of these data types. Recently, more and more applications need clustering techniques for complex data types such as graphs, sequences, images, and documents.
- **Discovery of clusters with arbitrary shape**: Many clustering algorithms determine clusters based on Euclidean or Manhattan distance measures (Chapter 2). Algorithms based on such distance measures tend to find spherical clusters with similar size and density. However, a cluster could be of any shape. Consider sensors, for example, which are often deployed for environment surveillance. Cluster analysis on sensor readings can detect interesting phenomena. We may want to use clustering to find the frontier of a running forest fire, which is often not spherical. It is important to develop algorithms that can detect clusters of arbitrary shape.
- **Requirements for domain knowledge to determine input parameters**: Many clustering algorithms require users to provide domain knowledge in the form of input parameters such as the desired number of clusters. Consequently, the clustering results may be sensitive to such parameters. Parameters are often hard to determine, especially for high-dimensionality data sets and where users have yet to grasp a deep understanding of their data. Requiring the specification of domain knowledge not only burdens users, but also makes the quality of clustering difficult to control.
- **Ability to deal with noisy data**: Most real-world data sets contain outliers and/or missing, unknown, or erroneous data. Sensor readings, for example, are often noisy—some readings may be inaccurate due to the sensing mechanisms, and some readings may be erroneous due to interferences from surrounding transient objects. Clustering algorithms can be sensitive to such noise and may produce poor-quality clusters. Therefore, we need clustering methods that are robust to noise.
- **Incremental clustering and insensitivity to input order**: In many applications, incremental updates (representing newer data) may arrive at any time. Some clustering algorithms cannot incorporate incremental updates into existing clustering structures and, instead, have to recompute a new clustering from scratch. Clustering algorithms may also be sensitive to the input data order. That is, given a set of data objects, clustering algorithms may return dramatically different clusterings depending on the order in which the objects are presented. Incremental clustering algorithms and algorithms that are insensitive to the input order are needed.

- **Capability of clustering high-dimensionality data**: A data set can contain numerous dimensions or attributes. When clustering documents, for example, each keyword can be regarded as a dimension, and there are often thousands of keywords. Most clustering algorithms are good at handling low-dimensional data such as data sets involving only two or three dimensions. Finding clusters of data objects in a high-dimensional space is challenging, especially considering that such data can be very sparse and highly skewed.
- **Constraint-based clustering**: Real-world applications may need to perform clustering under various kinds of constraints. Suppose that your job is to choose the locations for a given number of new automatic teller machines (ATMs) in a city. To decide upon this, you may cluster households while considering constraints such as the city's rivers and highway networks and the types and number of customers per cluster. A challenging task is to find data groups with good clustering behavior that satisfy specified constraints.
- **Interpretability and usability**: Users want clustering results to be interpretable, comprehensible, and usable. That is, clustering may need to be tied in with specific semantic interpretations and applications. It is important to study how an application goal may influence the selection of clustering features and clustering methods.

The following are orthogonal aspects with which clustering methods can be compared:

- **The partitioning criteria**: In some methods, all the objects are partitioned so that no hierarchy exists among the clusters. That is, all the clusters are at the same level conceptually. Such a method is useful, for example, for partitioning customers into groups so that each group has its own manager. Alternatively, other methods partition data objects hierarchically, where clusters can be formed at different semantic levels. For example, in text mining, we may want to organize a corpus of documents into multiple general topics, such as "politics" and "sports," each of which may have subtopics, For instance, "football," "basketball," "baseball," and "hockey" can exist as subtopics of "sports." The latter four subtopics are at a lower level in the hierarchy than "sports."
- **Separation of clusters**: Some methods partition data objects into mutually exclusive clusters. When clustering customers into groups so that each group is taken care of by one manager, each customer may belong to only one group. In some other situations, the clusters may not be exclusive, that is, a data object may belong to more than one cluster. For example, when clustering documents into topics, a document may be related to multiple topics. Thus, the topics as clusters may not be exclusive.
- **Similarity measure**: Some methods determine the similarity between two objects by the distance between them. Such a distance can be defined on Euclidean space,

a road network, a vector space, or any other space. In other methods, the similarity may be defined by connectivity based on density or contiguity, and may not rely on the absolute distance between two objects. Similarity measures play a fundamental role in the design of clustering methods. While distance-based methods can often take advantage of optimization techniques, density- and continuity-based methods can often find clusters of arbitrary shape.

- **Clustering space**: Many clustering methods search for clusters within the entire given data space. These methods are useful for low-dimensionality data sets. With high-dimensional data, however, there can be many irrelevant attributes, which can make similarity measurements unreliable. Consequently, clusters found in the full space are often meaningless. It's often better to instead search for clusters within different subspaces of the same data set. *Subspace clustering* discovers clusters and subspaces (often of low dimensionality) that manifest object similarity.

To conclude, clustering algorithms have several requirements. These factors include scalability and the ability to deal with different types of attributes, noisy data, incremental updates, clusters of arbitrary shape, and constraints. Interpretability and usability are also important. In addition, clustering methods can differ with respect to the partitioning level, whether or not clusters are mutually exclusive, the similarity measures used, and whether or not subspace clustering is performed.

10.1.3 Overview of Basic Clustering Methods

There are many clustering algorithms in the literature. It is difficult to provide a crisp categorization of clustering methods because these categories may overlap so that a method may have features from several categories. Nevertheless, it is useful to present a relatively organized picture of clustering methods. In general, the major fundamental clustering methods can be classified into the following categories, which are discussed in the rest of this chapter.

Partitioning methods: Given a set of n objects, a partitioning method constructs k partitions of the data, where each partition represents a cluster and $k \leq n$. That is, it divides the data into k groups such that each group must contain at least one object. In other words, partitioning methods conduct one-level partitioning on data sets. The basic partitioning methods typically adopt *exclusive cluster separation*. That is, each object must belong to exactly one group. This requirement may be relaxed, for example, in fuzzy partitioning techniques. References to such techniques are given in the bibliographic notes (Section 10.9).

Most partitioning methods are distance-based. Given k, the number of partitions to construct, a partitioning method creates an initial partitioning. It then uses an **iterative relocation technique** that attempts to improve the partitioning by moving objects from one group to another. The general criterion of a good partitioning is that objects in the same cluster are "close" or related to each other, whereas objects in different clusters are "far apart" or very different. There are various kinds of other

criteria for judging the quality of partitions. Traditional partitioning methods can be extended for subspace clustering, rather than searching the full data space. This is useful when there are many attributes and the data are sparse.

Achieving global optimality in partitioning-based clustering is often computationally prohibitive, potentially requiring an exhaustive enumeration of all the possible partitions. Instead, most applications adopt popular heuristic methods, such as greedy approaches like the *k-means* and the *k-medoids* algorithms, which progressively improve the clustering quality and approach a local optimum. These heuristic clustering methods work well for finding spherical-shaped clusters in small- to medium-size databases. To find clusters with complex shapes and for very large data sets, partitioning-based methods need to be extended. Partitioning-based clustering methods are studied in depth in Section 10.2.

Hierarchical methods: A hierarchical method creates a hierarchical decomposition of the given set of data objects. A hierarchical method can be classified as being either *agglomerative* or *divisive*, based on how the hierarchical decomposition is formed. The *agglomerative approach*, also called the *bottom-up* approach, starts with each object forming a separate group. It successively merges the objects or groups close to one another, until all the groups are merged into one (the topmost level of the hierarchy), or a termination condition holds. The *divisive approach*, also called the *top-down* approach, starts with all the objects in the same cluster. In each successive iteration, a cluster is split into smaller clusters, until eventually each object is in one cluster, or a termination condition holds.

Hierarchical clustering methods can be distance-based or density- and continuity-based. Various extensions of hierarchical methods consider clustering in subspaces as well.

Hierarchical methods suffer from the fact that once a step (merge or split) is done, it can never be undone. This rigidity is useful in that it leads to smaller computation costs by not having to worry about a combinatorial number of different choices. Such techniques cannot correct erroneous decisions; however, methods for improving the quality of hierarchical clustering have been proposed. Hierarchical clustering methods are studied in Section 10.3.

Density-based methods: Most partitioning methods cluster objects based on the distance between objects. Such methods can find only spherical-shaped clusters and encounter difficulty in discovering clusters of arbitrary shapes. Other clustering methods have been developed based on the notion of *density*. Their general idea is to continue growing a given cluster as long as the density (number of objects or data points) in the "neighborhood" exceeds some threshold. For example, for each data point within a given cluster, the neighborhood of a given radius has to contain at least a minimum number of points. Such a method can be used to filter out noise or outliers and discover clusters of arbitrary shape.

Density-based methods can divide a set of objects into multiple exclusive clusters, or a hierarchy of clusters. Typically, density-based methods consider exclusive clusters only, and do not consider fuzzy clusters. Moreover, density-based methods can be extended from full space to subspace clustering. Density-based clustering methods are studied in Section 10.4.

Grid-based methods: Grid-based methods quantize the object space into a finite number of cells that form a grid structure. All the clustering operations are performed on the grid structure (i.e., on the quantized space). The main advantage of this approach is its fast processing time, which is typically independent of the number of data objects and dependent only on the number of cells in each dimension in the quantized space.

Using grids is often an efficient approach to many spatial data mining problems, including clustering. Therefore, grid-based methods can be integrated with other clustering methods such as density-based methods and hierarchical methods. Grid-based clustering is studied in Section 10.5.

These methods are briefly summarized in Figure 10.1. Some clustering algorithms integrate the ideas of several clustering methods, so that it is sometimes difficult to classify a given algorithm as uniquely belonging to only one clustering method category. Furthermore, some applications may have clustering criteria that require the integration of several clustering techniques.

In the following sections, we examine each clustering method in detail. Advanced clustering methods and related issues are discussed in Chapter 11. In general, the notation used is as follows. Let D be a data set of n objects to be clustered. An object is described by d variables, where each variable is also called an attribute or a dimension,

Method	General Characteristics
Partitioning methods	– Find mutually exclusive clusters of spherical shape – Distance-based – May use mean or medoid (etc.) to represent cluster center – Effective for small- to medium-size data sets
Hierarchical methods	– Clustering is a hierarchical decomposition (i.e., multiple levels) – Cannot correct erroneous merges or splits – May incorporate other techniques like microclustering or consider object "linkages"
Density-based methods	– Can find arbitrarily shaped clusters – Clusters are dense regions of objects in space that are separated by low-density regions – Cluster density: Each point must have a minimum number of points within its "neighborhood" – May filter out outliers
Grid-based methods	– Use a multiresolution grid data structure – Fast processing time (typically independent of the number of data objects, yet dependent on grid size)

Figure 10.1 Overview of clustering methods discussed in this chapter. Note that some algorithms may combine various methods.

and therefore may also be referred to as a *point* in a d-dimensional object space. Objects are represented in bold italic font (e.g., $\boldsymbol{p}$).

10.2 Partitioning Methods

The simplest and most fundamental version of cluster analysis is partitioning, which organizes the objects of a set into several exclusive groups or clusters. To keep the problem specification concise, we can assume that the number of clusters is given as background knowledge. This parameter is the starting point for partitioning methods.

Formally, given a data set, D, of n objects, and k, the number of clusters to form, a **partitioning algorithm** organizes the objects into k partitions ($k \leq n$), where each partition represents a cluster. The clusters are formed to optimize an objective partitioning criterion, such as a dissimilarity function based on distance, so that the objects within a cluster are "similar" to one another and "dissimilar" to objects in other clusters in terms of the data set attributes.

In this section you will learn the most well-known and commonly used partitioning methods—k-means (Section 10.2.1) and k-medoids (Section 10.2.2). You will also learn several variations of these classic partitioning methods and how they can be scaled up to handle large data sets.

10.2.1 *k*-Means: A Centroid-Based Technique

Suppose a data set, D, contains n objects in Euclidean space. Partitioning methods distribute the objects in D into k clusters, $C_1, \ldots, C_k$, that is, $C_i \subset D$ and $C_i \cap C_j = \emptyset$ for $(1 \leq i, j \leq k)$. An objective function is used to assess the partitioning quality so that objects within a cluster are similar to one another but dissimilar to objects in other clusters. This is, the objective function aims for high intracluster similarity and low intercluster similarity.

A centroid-based partitioning technique uses the *centroid* of a cluster, C_i, to represent that cluster. Conceptually, the centroid of a cluster is its center point. The centroid can be defined in various ways such as by the mean or medoid of the objects (or points) assigned to the cluster. The difference between an object $\boldsymbol{p} \in C_i$ and $\boldsymbol{c_i}$, the representative of the cluster, is measured by $dist(\boldsymbol{p}, \boldsymbol{c_i})$, where $dist(\boldsymbol{x}, \boldsymbol{y})$ is the Euclidean distance between two points $\boldsymbol{x}$ and $\boldsymbol{y}$. The quality of cluster C_i can be measured by the **within-cluster variation**, which is the sum of *squared error* between all objects in C_i and the centroid $\boldsymbol{c_i}$, defined as

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} dist(\boldsymbol{p}, \boldsymbol{c_i})^2, \tag{10.1}$$

where E is the sum of the squared error for all objects in the data set; $\boldsymbol{p}$ is the point in space representing a given object; and $\boldsymbol{c_i}$ is the centroid of cluster C_i (both $\boldsymbol{p}$ and $\boldsymbol{c_i}$ are multidimensional). In other words, for each object in each cluster, the distance from

the object to its cluster center is squared, and the distances are summed. This objective function tries to make the resulting k clusters as compact and as separate as possible.

Optimizing the within-cluster variation is computationally challenging. In the worst case, we would have to enumerate a number of possible partitionings that are exponential to the number of clusters, and check the within-cluster variation values. It has been shown that the problem is NP-hard in general Euclidean space even for two clusters (i.e., $k = 2$). Moreover, the problem is NP-hard for a general number of clusters k even in the 2-D Euclidean space. If the number of clusters k and the dimensionality of the space d are fixed, the problem can be solved in time $O(n^{dk+1} \log n)$, where n is the number of objects. To overcome the prohibitive computational cost for the exact solution, greedy approaches are often used in practice. A prime example is the k-means algorithm, which is simple and commonly used.

"*How does the* k*-means algorithm work?*" The k-means algorithm defines the centroid of a cluster as the mean value of the points within the cluster. It proceeds as follows. First, it randomly selects k of the objects in D, each of which initially represents a cluster mean or center. For each of the remaining objects, an object is assigned to the cluster to which it is the most similar, based on the Euclidean distance between the object and the cluster mean. The k-means algorithm then iteratively improves the within-cluster variation. For each cluster, it computes the new mean using the objects assigned to the cluster in the previous iteration. All the objects are then reassigned using the updated means as the new cluster centers. The iterations continue until the assignment is stable, that is, the clusters formed in the current round are the same as those formed in the previous round. The k-means procedure is summarized in Figure 10.2.

Algorithm: *k*-means. The k-means algorithm for partitioning, where each cluster's center is represented by the mean value of the objects in the cluster.

Input:

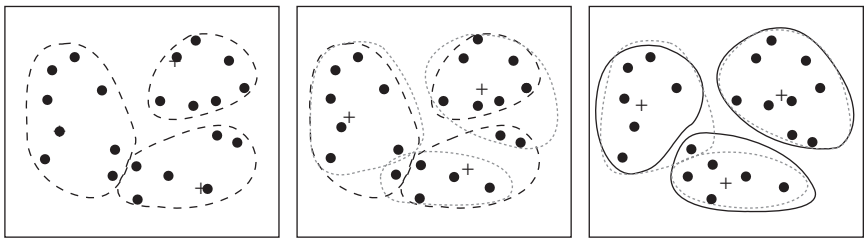
- k: the number of clusters,
- D: a data set containing n objects.

Output: A set of k clusters.

Method:

(1) arbitrarily choose k objects from D as the initial cluster centers;
(2) **repeat**
(3) (re)assign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster;
(4) update the cluster means, that is, calculate the mean value of the objects for each cluster;
(5) **until** no change;

Figure 10.2 The k-means partitioning algorithm.



(a) Initial clustering **(b)** Iterate **(c)** Final clustering

Figure 10.3 Clustering of a set of objects using the *k*-means method; for (b) update cluster centers and reassign objects accordingly (the mean of each cluster is marked by a +).

Example 10.1 **Clustering by *k*-means partitioning.** Consider a set of objects located in 2-D space, as depicted in Figure 10.3(a). Let $k = 3$, that is, the user would like the objects to be partitioned into three clusters.

According to the algorithm in Figure 10.2, we arbitrarily choose three objects as the three initial cluster centers, where cluster centers are marked by a +. Each object is assigned to a cluster based on the cluster center to which it is the nearest. Such a distribution forms silhouettes encircled by dotted curves, as shown in Figure 10.3(a).

Next, the cluster centers are updated. That is, the mean value of each cluster is recalculated based on the current objects in the cluster. Using the new cluster centers, the objects are redistributed to the clusters based on which cluster center is the nearest. Such a redistribution forms new silhouettes encircled by dashed curves, as shown in Figure 10.3(b).

This process iterates, leading to Figure 10.3(c). The process of iteratively reassigning objects to clusters to improve the partitioning is referred to as *iterative relocation*. Eventually, no reassignment of the objects in any cluster occurs and so the process terminates. The resulting clusters are returned by the clustering process. ■

The *k*-means method is not guaranteed to converge to the global optimum and often terminates at a local optimum. The results may depend on the initial random selection of cluster centers. (You will be asked to give an example to show this as an exercise.) To obtain good results in practice, it is common to run the *k*-means algorithm multiple times with different initial cluster centers.

The time complexity of the *k*-means algorithm is $O(nkt)$, where n is the total number of objects, k is the number of clusters, and t is the number of iterations. Normally, $k \ll n$ and $t \ll n$. Therefore, the method is relatively scalable and efficient in processing large data sets.

There are several variants of the *k*-means method. These can differ in the selection of the initial *k*-means, the calculation of dissimilarity, and the strategies for calculating cluster means.

The *k*-means method can be applied only when the mean of a set of objects is defined. This may not be the case in some applications such as when data with nominal attributes are involved. The ***k*-modes method** is a variant of *k*-means, which extends the *k*-means paradigm to cluster nominal data by replacing the means of clusters with modes. It uses new dissimilarity measures to deal with nominal objects and a frequency-based method to update modes of clusters. The *k*-means and the *k*-modes methods can be integrated to cluster data with mixed numeric and nominal values.

The necessity for users to specify *k*, the number of clusters, in advance can be seen as a disadvantage. There have been studies on how to overcome this difficulty, however, such as by providing an approximate range of *k* values, and then using an analytical technique to determine the best *k* by comparing the clustering results obtained for the different *k* values. The *k*-means method is not suitable for discovering clusters with nonconvex shapes or clusters of very different size. Moreover, it is sensitive to noise and outlier data points because a small number of such data can substantially influence the mean value.

"*How can we make the* k*-means algorithm more scalable?*" One approach to making the *k*-means method more efficient on large data sets is to use a good-sized set of samples in clustering. Another is to employ a filtering approach that uses a spatial hierarchical data index to save costs when computing means. A third approach explores the microclustering idea, which first groups nearby objects into "microclusters" and then performs *k*-means clustering on the microclusters. Microclustering is further discussed in Section 10.3.

10.2.2 *k*-Medoids: A Representative Object-Based Technique

The *k*-means algorithm is sensitive to outliers because such objects are far away from the majority of the data, and thus, when assigned to a cluster, they can dramatically distort the mean value of the cluster. This inadvertently affects the assignment of other objects to clusters. This effect is particularly exacerbated due to the use of the *squared*-error function of Eq. (10.1), as observed in Example 10.2.

Example 10.2 A drawback of *k*-means. Consider six points in 1-D space having the values $1, 2, 3, 8, 9, 10$, and 25, respectively. Intuitively, by visual inspection we may imagine the points partitioned into the clusters $\{1, 2, 3\}$ and $\{8, 9, 10\}$, where point 25 is excluded because it appears to be an outlier. How would *k*-means partition the values? If we apply *k*-means using $k = 2$ and Eq. (10.1), the partitioning $\{\{1, 2, 3\}, \{8, 9, 10, 25\}\}$ has the within-cluster variation

$$(1-2)^2 + (2-2)^2 + (3-2)^2 + (8-13)^2 + (9-13)^2 + (10-13)^2 + (25-13)^2 = 196,$$

given that the mean of cluster $\{1, 2, 3\}$ is 2 and the mean of $\{8, 9, 10, 25\}$ is 13. Compare this to the partitioning $\{\{1, 2, 3, 8\}, \{9, 10, 25\}\}$, for which *k*-means computes the within-cluster variation as

$$\begin{aligned}(1-3.5)^2 + (2-3.5)^2 + (3-3.5)^2 + (8-3.5)^2 + (9-14.67)^2 \\ + (10-14.67)^2 + (25-14.67)^2 = 189.67,\end{aligned}$$

given that 3.5 is the mean of cluster $\{1,2,3,8\}$ and 14.67 is the mean of cluster $\{9,10,25\}$. The latter partitioning has the lowest within-cluster variation; therefore, the k-means method assigns the value 8 to a cluster different from that containing 9 and 10 due to the outlier point 25. Moreover, the center of the second cluster, 14.67, is substantially far from all the members in the cluster. ■

"*How can we modify the k-means algorithm to diminish such sensitivity to outliers?*" Instead of taking the mean value of the objects in a cluster as a reference point, we can pick actual objects to represent the clusters, using one representative object per cluster. Each remaining object is assigned to the cluster of which the representative object is the most similar. The partitioning method is then performed based on the principle of minimizing the sum of the dissimilarities between each object $\boldsymbol{p}$ and its corresponding representative object. That is, an **absolute-error criterion** is used, defined as

$$E = \sum_{i=1}^{k} \sum_{\boldsymbol{p} \in C_i} dist(\boldsymbol{p}, \boldsymbol{o_i}), \tag{10.2}$$

where E is the sum of the absolute error for all objects $\boldsymbol{p}$ in the data set, and $\boldsymbol{o_i}$ is the representative object of C_i. This is the basis for the ***k*-medoids method**, which groups n objects into k clusters by minimizing the absolute error (Eq. 10.2).

When $k = 1$, we can find the exact median in $O(n^2)$ time. However, when k is a general positive number, the k-medoid problem is NP-hard.

The **Partitioning Around Medoids (PAM)** algorithm (see Figure 10.5 later) is a popular realization of k-medoids clustering. It tackles the problem in an iterative, greedy way. Like the k-means algorithm, the initial representative objects (called seeds) are chosen arbitrarily. We consider whether replacing a representative object by a nonrepresentative object would improve the clustering quality. All the possible replacements are tried out. The iterative process of replacing representative objects by other objects continues until the quality of the resulting clustering cannot be improved by any replacement. This quality is measured by a cost function of the average dissimilarity between an object and the representative object of its cluster.

Specifically, let $\boldsymbol{o_1}, \ldots, \boldsymbol{o_k}$ be the current set of representative objects (i.e., medoids). To determine whether a nonrepresentative object, denoted by $\boldsymbol{o_{random}}$, is a good replacement for a current medoid $\boldsymbol{o_j}$ $(1 \leq j \leq k)$, we calculate the distance from every object $\boldsymbol{p}$ to the closest object in the set $\{\boldsymbol{o_1}, \ldots, \boldsymbol{o_{j-1}}, \boldsymbol{o_{random}}, \boldsymbol{o_{j+1}}, \ldots, \boldsymbol{o_k}\}$, and use the distance to update the cost function. The reassignments of objects to $\{\boldsymbol{o_1}, \ldots, \boldsymbol{o_{j-1}}, \boldsymbol{o_{random}}, \boldsymbol{o_{j+1}}, \ldots, \boldsymbol{o_k}\}$ are simple. Suppose object $\boldsymbol{p}$ is currently assigned to a cluster represented by medoid $\boldsymbol{o_j}$ (Figure 10.4a or b). Do we need to reassign $\boldsymbol{p}$ to a different cluster if $\boldsymbol{o_j}$ is being replaced by $\boldsymbol{o_{random}}$? Object $\boldsymbol{p}$ needs to be reassigned to either $\boldsymbol{o_{random}}$ or some other cluster represented by $\boldsymbol{o_i}$ $(i \neq j)$, whichever is the closest. For example, in Figure 10.4(a), $\boldsymbol{p}$ is closest to $\boldsymbol{o_i}$ and therefore is reassigned to $\boldsymbol{o_i}$. In Figure 10.4(b), however, $\boldsymbol{p}$ is closest to $\boldsymbol{o_{random}}$ and so is reassigned to $\boldsymbol{o_{random}}$. What if, instead, $\boldsymbol{p}$ is currently assigned to a cluster represented by some other object $\boldsymbol{o_i}$, $i \neq j$?

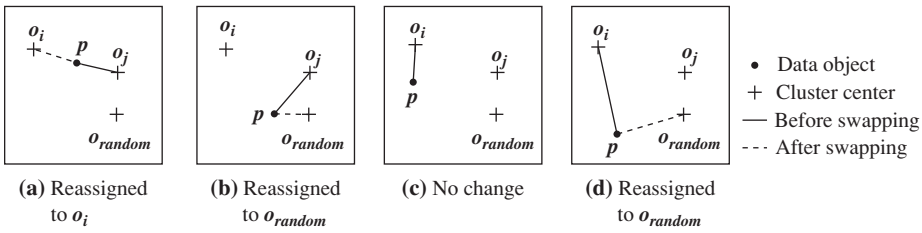


Figure 10.4 Four cases of the cost function for k-medoids clustering.

Object $\boldsymbol{o}$ remains assigned to the cluster represented by $\boldsymbol{o_i}$ as long as $\boldsymbol{o}$ is still closer to $\boldsymbol{o_i}$ than to $\boldsymbol{o_{random}}$ (Figure 10.4c). Otherwise, $\boldsymbol{o}$ is reassigned to $\boldsymbol{o_{random}}$ (Figure 10.4d).

Each time a reassignment occurs, a difference in absolute error, E, is contributed to the cost function. Therefore, the cost function calculates the *difference* in absolute-error value if a current representative object is replaced by a nonrepresentative object. The total cost of swapping is the sum of costs incurred by all nonrepresentative objects. If the total cost is negative, then $\boldsymbol{o_j}$ is replaced or swapped with $\boldsymbol{o_{random}}$ because the actual absolute-error E is reduced. If the total cost is positive, the current representative object, $\boldsymbol{o_j}$, is considered acceptable, and nothing is changed in the iteration.

"*Which method is more robust—k-means or k-medoids?*" The k-medoids method is more robust than k-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean. However, the complexity of each iteration in the k-medoids algorithm is $O(k(n-k)^2)$. For large values of n and k, such computation becomes very costly, and much more costly than the k-means method. Both methods require the user to specify k, the number of clusters.

"*How can we scale up the k-medoids method?*" A typical k-medoids partitioning algorithm like PAM (Figure 10.5) works effectively for small data sets, but does not scale well for large data sets. To deal with larger data sets, a *sampling*-based method called **CLARA** (**Clustering LARge Applications**) can be used. Instead of taking the whole data set into consideration, CLARA uses a random sample of the data set. The PAM algorithm is then applied to compute the best medoids from the sample. Ideally, the sample should closely represent the original data set. In many cases, a large sample works well if it is created so that each object has equal probability of being selected into the sample. The representative objects (medoids) chosen will likely be similar to those that would have been chosen from the whole data set. CLARA builds clusterings from multiple random samples and returns the best clustering as the output. The complexity of computing the medoids on a random sample is $O(ks^2 + k(n-k))$, where s is the size of the sample, k is the number of clusters, and n is the total number of objects. CLARA can deal with larger data sets than PAM.

The effectiveness of CLARA depends on the sample size. Notice that PAM searches for the best k-medoids among a given data set, whereas CLARA searches for the best k-medoids among the *selected sample* of the data set. CLARA cannot find a good clustering if any of the best sampled medoids is far from the best k-medoids. If an object

Algorithm: *k*-medoids. PAM, a *k*-medoids algorithm for partitioning based on medoid or central objects.

Input:

- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

Output: A set of *k* clusters.

Method:

(1) arbitrarily choose *k* objects in *D* as the initial representative objects or seeds;
(2) **repeat**
(3) assign each remaining object to the cluster with the nearest representative object;
(4) randomly select a nonrepresentative object, o_{random};
(5) compute the total cost, *S*, of swapping representative object, o_j, with o_{random};
(6) **if** $S < 0$ **then** swap o_j with o_{random} to form the new set of *k* representative objects;
(7) **until** no change;

Figure 10.5 PAM, a *k*-medoids partitioning algorithm.

is one of the best *k*-medoids but is not selected during sampling, CLARA will never find the best clustering. (You will be asked to provide an example demonstrating this as an exercise.)

"*How might we improve the quality and scalability of CLARA?*" Recall that when searching for better medoids, PAM examines every object in the data set against every current medoid, whereas CLARA confines the candidate medoids to only a random sample of the data set. A randomized algorithm called **CLARANS** (Clustering Large Applications based upon RANdomized Search) presents a trade-off between the cost and the effectiveness of using samples to obtain clustering.

First, it randomly selects *k* objects in the data set as the current medoids. It then randomly selects a current medoid $\boldsymbol{x}$ and an object $\boldsymbol{y}$ that is not one of the current medoids. Can replacing $\boldsymbol{x}$ by $\boldsymbol{y}$ improve the absolute-error criterion? If yes, the replacement is made. CLARANS conducts such a randomized search *l* times. The set of the current medoids after the *l* steps is considered a local optimum. CLARANS repeats this randomized process *m* times and returns the best local optimal as the final result.

10.3 Hierarchical Methods

While partitioning methods meet the basic clustering requirement of organizing a set of objects into a number of exclusive groups, in some situations we may want to partition our data into groups at different levels such as in a hierarchy. A **hierarchical clustering method** works by grouping data objects into a hierarchy or "tree" of clusters.

Representing data objects in the form of a hierarchy is useful for data summarization and visualization. For example, as the manager of human resources at *AllElectronics*,

you may organize your employees into major groups such as executives, managers, and staff. You can further partition these groups into smaller subgroups. For instance, the general group of staff can be further divided into subgroups of senior officers, officers, and trainees. All these groups form a hierarchy. We can easily summarize or characterize the data that are organized into a hierarchy, which can be used to find, say, the average salary of managers and of officers.

Consider handwritten character recognition as another example. A set of handwriting samples may be first partitioned into general groups where each group corresponds to a unique character. Some groups can be further partitioned into subgroups since a character may be written in multiple substantially different ways. If necessary, the hierarchical partitioning can be continued recursively until a desired granularity is reached.

In the previous examples, although we partitioned the data hierarchically, we did not assume that the data have a hierarchical structure (e.g., managers are at the same level in our *AllElectronics* hierarchy as staff). Our use of a hierarchy here is just to summarize and represent the underlying data in a compressed way. Such a hierarchy is particularly useful for data visualization.

Alternatively, in some applications we may believe that the data bear an underlying hierarchical structure that we want to discover. For example, hierarchical clustering may uncover a hierarchy for *AllElectronics* employees structured on, say, salary. In the study of evolution, hierarchical clustering may group animals according to their biological features to uncover evolutionary paths, which are a hierarchy of species. As another example, grouping configurations of a strategic game (e.g., chess or checkers) in a hierarchical way may help to develop game strategies that can be used to train players.

In this section, you will study hierarchical clustering methods. Section 10.3.1 begins with a discussion of agglomerative versus divisive hierarchical clustering, which organize objects into a hierarchy using a bottom-up or top-down strategy, respectively. Agglomerative methods start with individual objects as clusters, which are iteratively merged to form larger clusters. Conversely, divisive methods initially let all the given objects form one cluster, which they iteratively split into smaller clusters.

Hierarchical clustering methods can encounter difficulties regarding the selection of merge or split points. Such a decision is critical, because once a group of objects is merged or split, the process at the next step will operate on the newly generated clusters. It will neither undo what was done previously, nor perform object swapping between clusters. Thus, merge or split decisions, if not well chosen, may lead to low-quality clusters. Moreover, the methods do not scale well because each decision of merge or split needs to examine and evaluate many objects or clusters.

A promising direction for improving the clustering quality of hierarchical methods is to integrate hierarchical clustering with other clustering techniques, resulting in **multiple-phase** (or **multiphase**) **clustering**. We introduce two such methods, namely BIRCH and Chameleon. BIRCH (Section 10.3.3) begins by partitioning objects hierarchically using tree structures, where the leaf or low-level nonleaf nodes can be viewed as "microclusters" depending on the resolution scale. It then applies other

clustering algorithms to perform macroclustering on the microclusters. Chameleon (Section 10.3.4) explores dynamic modeling in hierarchical clustering.

There are several orthogonal ways to categorize hierarchical clustering methods. For instance, they may be categorized into *algorithmic* methods, *probabilistic* methods, and *Bayesian* methods. Agglomerative, divisive, and multiphase methods are *algorithmic*, meaning they consider data objects as deterministic and compute clusters according to the deterministic distances between objects. Probabilistic methods use probabilistic models to capture clusters and measure the quality of clusters by the fitness of models. We discuss probabilistic hierarchical clustering in Section 10.3.5. *Bayesian methods* compute a distribution of possible clusterings. That is, instead of outputting a single deterministic clustering over a data set, they return a group of clustering structures and their probabilities, conditional on the given data. Bayesian methods are considered an advanced topic and are not discussed in this book.

10.3.1 Agglomerative versus Divisive Hierarchical Clustering

A hierarchical clustering method can be either *agglomerative* or *divisive*, depending on whether the hierarchical decomposition is formed in a bottom-up (merging) or top-down (splitting) fashion. Let's have a closer look at these strategies.

An **agglomerative hierarchical clustering method** uses a bottom-up strategy. It typically starts by letting each object form its own cluster and iteratively merges clusters into larger and larger clusters, until all the objects are in a single cluster or certain termination conditions are satisfied. The single cluster becomes the hierarchy's root. For the merging step, it finds the two clusters that are closest to each other (according to some similarity measure), and combines the two to form one cluster. Because two clusters are merged per iteration, where each cluster contains at least one object, an agglomerative method requires at most n iterations.

A **divisive hierarchical clustering method** employs a top-down strategy. It starts by placing all objects in one cluster, which is the hierarchy's root. It then divides the root cluster into several smaller subclusters, and recursively partitions those clusters into smaller ones. The partitioning process continues until each cluster at the lowest level is coherent enough—either containing only one object, or the objects within a cluster are sufficiently similar to each other.

In either agglomerative or divisive hierarchical clustering, a user can specify the desired number of clusters as a termination condition.

Example 10.3 **Agglomerative versus divisive hierarchical clustering.** Figure 10.6 shows the application of **AGNES** (AGglomerative NESting), an agglomerative hierarchical clustering method, and **DIANA** (DIvisive ANAlysis), a divisive hierarchical clustering method, on a data set of five objects, $\{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{d}, \boldsymbol{e}\}$. Initially, AGNES, the agglomerative method, places each object into a cluster of its own. The clusters are then merged step-by-step according to some criterion. For example, clusters C_1 and C_2 may be merged if an object in C_1 and an object in C_2 form the minimum Euclidean distance between any two objects from

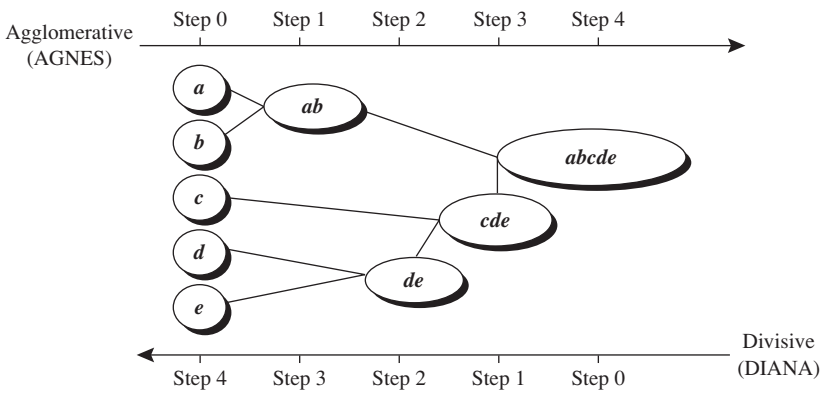


Figure 10.6 Agglomerative and divisive hierarchical clustering on data objects $\{a, b, c, d, e\}$.

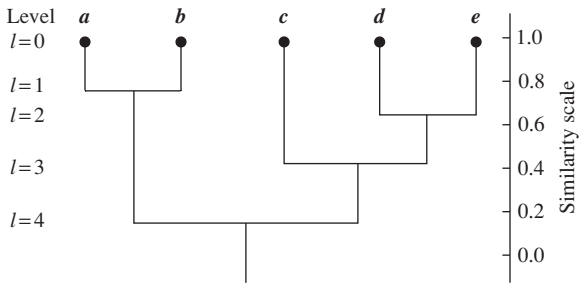


Figure 10.7 Dendrogram representation for hierarchical clustering of data objects $\{a, b, c, d, e\}$.

different clusters. This is a **single-linkage** approach in that each cluster is represented by all the objects in the cluster, and the similarity between two clusters is measured by the similarity of the *closest* pair of data points belonging to different clusters. The cluster-merging process repeats until all the objects are eventually merged to form one cluster.

DIANA, the divisive method, proceeds in the contrasting way. All the objects are used to form one initial cluster. The cluster is split according to some principle such as the maximum Euclidean distance between the closest neighboring objects in the cluster. The cluster-splitting process repeats until, eventually, each new cluster contains only a single object. ■

A tree structure called a **dendrogram** is commonly used to represent the process of hierarchical clustering. It shows how objects are grouped together (in an agglomerative method) or partitioned (in a divisive method) step-by-step. Figure 10.7 shows a dendrogram for the five objects presented in Figure 10.6, where $l = 0$ shows the five objects as singleton clusters at level 0. At $l = 1$, objects ***a*** and ***b*** are grouped together to form the

first cluster, and they stay together at all subsequent levels. We can also use a vertical axis to show the similarity scale between clusters. For example, when the similarity of two groups of objects, $\{\boldsymbol{a}, \boldsymbol{b}\}$ and $\{\boldsymbol{c}, \boldsymbol{d}, \boldsymbol{e}\}$, is roughly 0.16, they are merged together to form a single cluster.

A challenge with divisive methods is how to partition a large cluster into several smaller ones. For example, there are $2^{n-1} - 1$ possible ways to partition a set of n objects into two exclusive subsets, where n is the number of objects. When n is large, it is computationally prohibitive to examine all possibilities. Consequently, a divisive method typically uses heuristics in partitioning, which can lead to inaccurate results. For the sake of efficiency, divisive methods typically do not backtrack on partitioning decisions that have been made. Once a cluster is partitioned, any alternative partitioning of this cluster will not be considered again. Due to the challenges in divisive methods, there are many more agglomerative methods than divisive methods.

10.3.2 Distance Measures in Algorithmic Methods

Whether using an agglomerative method or a divisive method, a core need is to measure the distance between two clusters, where each cluster is generally a set of objects.

Four widely used measures for distance between clusters are as follows, where $|\boldsymbol{p} - \boldsymbol{p'}|$ is the distance between two objects or points, $\boldsymbol{p}$ and $\boldsymbol{p'}$; $\boldsymbol{m_i}$ is the mean for cluster, C_i; and n_i is the number of objects in C_i. They are also known as *linkage measures*.

$$\textbf{Minimum distance:} \quad dist_{min}(C_i, C_j) = \min_{\boldsymbol{p} \in C_i, \boldsymbol{p'} \in C_j} \{|\boldsymbol{p} - \boldsymbol{p'}|\} \tag{10.3}$$

$$\textbf{Maximum distance:} \quad dist_{max}(C_i, C_j) = \max_{\boldsymbol{p} \in C_i, \boldsymbol{p'} \in C_j} \{|\boldsymbol{p} - \boldsymbol{p'}|\} \tag{10.4}$$

$$\textbf{Mean distance:} \quad dist_{mean}(C_i, C_j) = |\boldsymbol{m_i} - \boldsymbol{m_j}| \tag{10.5}$$

$$\textbf{Average distance:} \quad dist_{avg}(C_i, C_j) = \frac{1}{n_i n_j} \sum_{\boldsymbol{p} \in C_i, \boldsymbol{p'} \in C_j} |\boldsymbol{p} - \boldsymbol{p'}| \tag{10.6}$$

When an algorithm uses the *minimum distance*, $d_{min}(C_i, C_j)$, to measure the distance between clusters, it is sometimes called a **nearest-neighbor clustering algorithm**. Moreover, if the clustering process is terminated when the distance between nearest clusters exceeds a user-defined threshold, it is called a **single-linkage algorithm**. If we view the data points as nodes of a graph, with edges forming a path between the nodes in a cluster, then the merging of two clusters, C_i and C_j, corresponds to adding an edge between the nearest pair of nodes in C_i and C_j. Because edges linking clusters always go between distinct clusters, the resulting graph will generate a tree. Thus, an agglomerative hierarchical clustering algorithm that uses the minimum distance measure is also called a

minimal spanning tree algorithm, where a spanning tree of a graph is a tree that connects all vertices, and a minimal spanning tree is the one with the least sum of edge weights.

When an algorithm uses the *maximum distance*, $d_{max}(C_i, C_j)$, to measure the distance between clusters, it is sometimes called a **farthest-neighbor clustering algorithm**. If the clustering process is terminated when the maximum distance between nearest clusters exceeds a user-defined threshold, it is called a **complete-linkage algorithm**. By viewing data points as nodes of a graph, with edges linking nodes, we can think of each cluster as a *complete* subgraph, that is, with edges connecting all the nodes in the clusters. The distance between two clusters is determined by the most distant nodes in the two clusters. Farthest-neighbor algorithms tend to minimize the increase in diameter of the clusters at each iteration. If the true clusters are rather compact and approximately equal size, the method will produce high-quality clusters. Otherwise, the clusters produced can be meaningless.

The previous minimum and maximum measures represent two extremes in measuring the distance between clusters. They tend to be overly sensitive to outliers or noisy data. The use of *mean* or *average distance* is a compromise between the minimum and maximum distances and overcomes the outlier sensitivity problem. Whereas the *mean distance* is the simplest to compute, the *average distance* is advantageous in that it can handle categoric as well as numeric data. The computation of the mean vector for categoric data can be difficult or impossible to define.

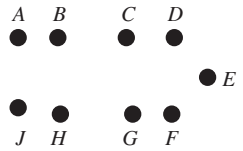
Example 10.4 **Single versus complete linkages.** Let us apply hierarchical clustering to the data set of Figure 10.8(a). Figure 10.8(b) shows the dendrogram using single linkage. Figure 10.8(c) shows the case using complete linkage, where the edges between clusters $\{A, B, J, H\}$ and $\{C, D, G, F, E\}$ are omitted for ease of presentation. This example shows that by using single linkages we can find hierarchical clusters defined by local proximity, whereas complete linkage tends to find clusters opting for global closeness. ■

There are variations of the four essential linkage measures just discussed. For example, we can measure the distance between two clusters by the distance between the centroids (i.e., the central objects) of the clusters.

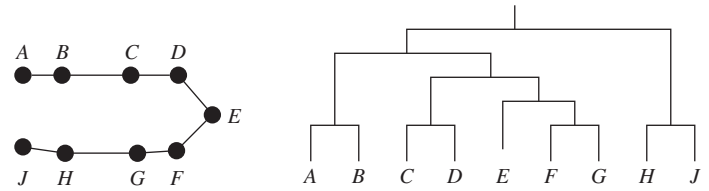
10.3.3 BIRCH: Multiphase Hierarchical Clustering Using Clustering Feature Trees

Balanced Iterative Reducing and Clustering using Hierarchies (BIRCH) is designed for clustering a large amount of numeric data by integrating hierarchical clustering (at the initial *microclustering* stage) and other clustering methods such as iterative partitioning (at the later *macroclustering* stage). It overcomes the two difficulties in agglomerative clustering methods: (1) scalability and (2) the inability to undo what was done in the previous step.

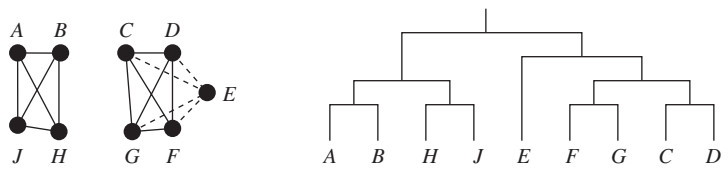
BIRCH uses the notions of *clustering feature* to summarize a cluster, and *clustering feature tree* (*CF-tree*) to represent a cluster hierarchy. These structures help



(a) Data set



(b) Clustering using single linkage



(c) Clustering using complete linkage

Figure 10.8 Hierarchical clustering using single and complete linkages.

the clustering method achieve good speed and scalability in large or even streaming databases, and also make it effective for incremental and dynamic clustering of incoming objects.

Consider a cluster of n d-dimensional data objects or points. The **clustering feature** (**CF**) of the cluster is a 3-D vector summarizing information about clusters of objects. It is defined as

$$CF = \langle n, LS, SS \rangle, \tag{10.7}$$

where LS is the linear sum of the n points (i.e., $\sum_{i=1}^{n} \boldsymbol{x_i}$), and SS is the square sum of the data points (i.e., $\sum_{i=1}^{n} \boldsymbol{x_i}^2$).

A clustering feature is essentially a summary of the statistics for the given cluster. Using a clustering feature, we can easily derive many useful statistics of a cluster. For example, the cluster's centroid, $\boldsymbol{x_0}$, radius, R, and diameter, D, are

$$\boldsymbol{x_0} = \frac{\sum_{i=1}^{n} \boldsymbol{x_i}}{n} = \frac{LS}{n}, \tag{10.8}$$

$$R = \sqrt{\frac{\sum_{i=1}^{n}(\boldsymbol{x_i} - \boldsymbol{x_0})^2}{n}} = \sqrt{\frac{nSS - 2LS^2 + nLS}{n^2}}, \tag{10.9}$$

$$D = \sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(\boldsymbol{x_i} - \boldsymbol{x_j})^2}{n(n-1)}} = \sqrt{\frac{2nSS - 2LS^2}{n(n-1)}}. \tag{10.10}$$

Here, R is the average distance from member objects to the centroid, and D is the average pairwise distance within a cluster. Both R and D reflect the tightness of the cluster around the centroid.

Summarizing a cluster using the clustering feature can avoid storing the detailed information about individual objects or points. Instead, we only need a constant size of space to store the clustering feature. This is the key to BIRCH efficiency in space. Moreover, clustering features are *additive*. That is, for two disjoint clusters, C_1 and C_2, with the clustering features $CF_1 = \langle n_1, LS_1, SS_1\rangle$ and $CF_2 = \langle n_2, LS_2, SS_2\rangle$, respectively, the clustering feature for the cluster that formed by merging C_1 and C_2 is simply

$$CF_1 + CF_2 = \langle n_1 + n_2, LS_1 + LS_2, SS_1 + SS_2\rangle. \tag{10.11}$$

Example 10.5 **Clustering feature.** Suppose there are three points, $(2,5), (3,2)$, and $(4,3)$, in a cluster, C_1. The clustering feature of C_1 is

$$CF_1 = \langle 3, (2+3+4, 5+2+3), (2^2+3^2+4^2, 5^2+2^2+3^2)\rangle = \langle 3, (9,10), (29,38)\rangle.$$

Suppose that C_1 is disjoint to a second cluster, C_2, where $CF_2 = \langle 3, (35,36), (417,440)\rangle$. The clustering feature of a new cluster, C_3, that is formed by merging C_1 and C_2, is derived by adding CF_1 and CF_2. That is,

$$CF_3 = \langle 3+3, (9+35, 10+36), (29+417, 38+440)\rangle = \langle 6, (44,46), (446,478)\rangle. \quad \blacksquare$$

A **CF-tree** is a height-balanced tree that stores the clustering features for a hierarchical clustering. An example is shown in Figure 10.9. By definition, a nonleaf node in a tree has descendants or "children." The nonleaf nodes store sums of the CFs of their children, and thus summarize clustering information about their children. A CF-tree has two parameters: *branching factor*, B, and *threshold*, T. The branching factor specifies the maximum number of children per nonleaf node. The threshold parameter specifies the maximum diameter of subclusters stored at the leaf nodes of the tree. These two parameters implicitly control the resulting tree's size.

Given a limited amount of main memory, an important consideration in BIRCH is to minimize the time required for input/output (I/O). BIRCH applies a *multiphase* clustering technique: A single scan of the data set yields a basic, good clustering, and

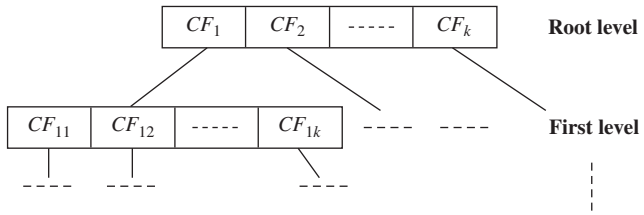


Figure 10.9 CF-tree structure.

one or more additional scans can optionally be used to further improve the quality. The primary phases are

- **Phase 1:** BIRCH scans the database to build an initial in-memory CF-tree, which can be viewed as a multilevel compression of the data that tries to preserve the data's inherent clustering structure.
- **Phase 2:** BIRCH applies a (selected) clustering algorithm to cluster the leaf nodes of the CF-tree, which removes sparse clusters as outliers and groups dense clusters into larger ones.

For Phase 1, the CF-tree is built dynamically as objects are inserted. Thus, the method is incremental. An object is inserted into the closest leaf entry (subcluster). If the diameter of the subcluster stored in the leaf node after insertion is larger than the threshold value, then the leaf node and possibly other nodes are split. After the insertion of the new object, information about the object is passed toward the root of the tree. The size of the CF-tree can be changed by modifying the threshold. If the size of the memory that is needed for storing the CF-tree is larger than the size of the main memory, then a larger threshold value can be specified and the CF-tree is rebuilt.

The rebuild process is performed by building a new tree from the leaf nodes of the old tree. Thus, the process of rebuilding the tree is done without the necessity of rereading all the objects or points. This is similar to the insertion and node split in the construction of B+-trees. Therefore, for building the tree, data has to be read just once. Some heuristics and methods have been introduced to deal with outliers and improve the quality of CF-trees by additional scans of the data. Once the CF-tree is built, any clustering algorithm, such as a typical partitioning algorithm, can be used with the CF-tree in Phase 2.

"*How effective is BIRCH?*" The time complexity of the algorithm is $O(n)$, where n is the number of objects to be clustered. Experiments have shown the linear scalability of the algorithm with respect to the number of objects, and good quality of clustering of the data. However, since each node in a CF-tree can hold only a limited number of entries due to its size, a CF-tree node does not always correspond to what a user may consider a natural cluster. Moreover, if the clusters are not spherical in shape, BIRCH does not perform well because it uses the notion of radius or diameter to control the boundary of a cluster.

The ideas of clustering features and CF-trees have been applied beyond BIRCH. The ideas have been borrowed by many others to tackle problems of clustering streaming and dynamic data.

10.3.4 Chameleon: Multiphase Hierarchical Clustering Using Dynamic Modeling

Chameleon is a hierarchical clustering algorithm that uses dynamic modeling to determine the similarity between pairs of clusters. In Chameleon, cluster similarity is assessed based on (1) how well connected objects are within a cluster and (2) the proximity of clusters. That is, two clusters are merged if their *interconnectivity* is high and they are *close together*. Thus, Chameleon does not depend on a static, user-supplied model and can automatically adapt to the internal characteristics of the clusters being merged. The merge process facilitates the discovery of natural and homogeneous clusters and applies to all data types as long as a similarity function can be specified.

Figure 10.10 illustrates how Chameleon works. Chameleon uses a k-nearest-neighbor graph approach to construct a sparse graph, where each vertex of the graph represents a data object, and there exists an edge between two vertices (objects) if one object is among the k-most similar objects to the other. The edges are weighted to reflect the similarity between objects. Chameleon uses a graph partitioning algorithm to partition the k-nearest-neighbor graph into a large number of relatively small subclusters such that it minimizes the **edge cut**. That is, a cluster C is partitioned into subclusters C_i and C_j so as to minimize the *weight of the edges* that would be cut should C be bisected into C_i and C_j. It assesses the *absolute* interconnectivity between clusters C_i and C_j.

Chameleon then uses an agglomerative hierarchical clustering algorithm that iteratively merges subclusters based on their similarity. To determine the pairs of most similar subclusters, it takes into account both the interconnectivity and the closeness of the clusters. Specifically, Chameleon determines the similarity between each pair of clusters C_i and C_j according to their *relative interconnectivity*, $RI(C_i, C_j)$, and their *relative closeness*, $RC(C_i, C_j)$.

- The **relative interconnectivity**, $RI(C_i, C_j)$, between two clusters, C_i and C_j, is defined as the absolute interconnectivity between C_i and C_j, normalized with respect to the

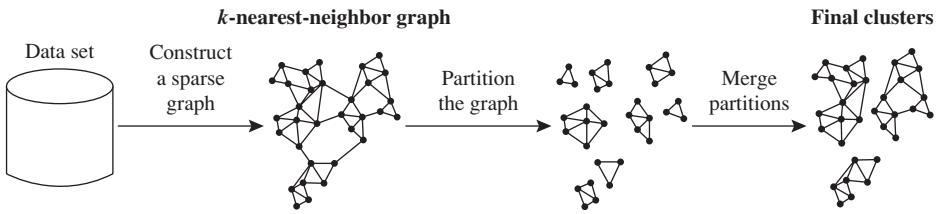


Figure 10.10 Chameleon: hierarchical clustering based on k-nearest neighbors and dynamic modeling. *Source:* Based on Karypis, Han, and Kumar [KHK99].

internal interconnectivity of the two clusters, C_i and C_j. That is,

$$RI(C_i, C_j) = \frac{|EC_{\{C_i,C_j\}}|}{\frac{1}{2}(|EC_{C_i}| + |EC_{C_j}|)}, \tag{10.12}$$

where $EC_{\{C_i,C_j\}}$ is the edge cut as previously defined for a cluster containing both C_i and C_j. Similarly, EC_{C_i} (or EC_{C_j}) is the minimum sum of the cut edges that partition C_i (or C_j) into two roughly equal parts.

- The **relative closeness**, $RC(C_i, C_j)$, between a pair of clusters, C_i and C_j, is the absolute closeness between C_i and C_j, normalized with respect to the internal closeness of the two clusters, C_i and C_j. It is defined as

$$RC(C_i, C_j) = \frac{\overline{S}_{EC_{\{C_i,C_j\}}}}{\frac{|C_i|}{|C_i|+|C_j|}\overline{S}_{EC_{C_i}} + \frac{|C_j|}{|C_i|+|C_j|}\overline{S}_{EC_{C_j}}}, \tag{10.13}$$

where $\overline{S}_{EC_{\{C_i,C_j\}}}$ is the average weight of the edges that connect vertices in C_i to vertices in C_j, and $\overline{S}_{EC_{C_i}}$ (or $\overline{S}_{EC_{C_j}}$) is the average weight of the edges that belong to the min-cut bisector of cluster C_i (or C_j).

Chameleon has been shown to have greater power at discovering arbitrarily shaped clusters of high quality than several well-known algorithms such as BIRCH and density-based DBSCAN (Section 10.4.1). However, the processing cost for high-dimensional data may require $O(n^2)$ time for n objects in the worst case.

10.3.5 Probabilistic Hierarchical Clustering

Algorithmic hierarchical clustering methods using linkage measures tend to be easy to understand and are often efficient in clustering. They are commonly used in many clustering analysis applications. However, algorithmic hierarchical clustering methods can suffer from several drawbacks. First, choosing a good distance measure for hierarchical clustering is often far from trivial. Second, to apply an algorithmic method, the data objects cannot have any missing attribute values. In the case of data that are partially observed (i.e., some attribute values of some objects are missing), it is not easy to apply an algorithmic hierarchical clustering method because the distance computation cannot be conducted. Third, most of the algorithmic hierarchical clustering methods are heuristic, and at each step locally search for a good merging/splitting decision. Consequently, the optimization goal of the resulting cluster hierarchy can be unclear.

Probabilistic hierarchical clustering aims to overcome some of these disadvantages by using probabilistic models to measure distances between clusters.

One way to look at the clustering problem is to regard the set of data objects to be clustered as a sample of the underlying data generation mechanism to be analyzed or, formally, the *generative model*. For example, when we conduct clustering analysis on a set of marketing surveys, we assume that the surveys collected are a sample of the opinions of all possible customers. Here, the data generation mechanism is a probability

distribution of opinions with respect to different customers, which cannot be obtained directly and completely. The task of clustering is to estimate the generative model as accurately as possible using the observed data objects to be clustered.

In practice, we can assume that the data generative models adopt common distribution functions, such as Gaussian distribution or Bernoulli distribution, which are governed by parameters. The task of learning a generative model is then reduced to finding the parameter values for which the model best fits the observed data set.

Example 10.6 **Generative model.** Suppose we are given a set of 1-D points $X = \{x_1, \ldots, x_n\}$ for clustering analysis. Let us assume that the data points are generated by a Gaussian distribution,

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{10.14}$$

where the parameters are μ (the mean) and σ^2 (the variance).

The probability that a point $x_i \in X$ is then generated by the model is

$$P(x_i|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}. \tag{10.15}$$

Consequently, the likelihood that X is generated by the model is

$$L(\mathcal{N}(\mu, \sigma^2) : X) = P(X|\mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}. \tag{10.16}$$

The task of learning the generative model is to find the parameters μ and σ^2 such that the likelihood $L(\mathcal{N}(\mu, \sigma^2) : X)$ is maximized, that is, finding

$$\mathcal{N}(\mu_0, \sigma_0^2) = \arg\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}, \tag{10.17}$$

where $\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}$ is called the *maximum likelihood*. ■

Given a set of objects, the quality of a cluster formed by all the objects can be measured by the maximum likelihood. For a set of objects partitioned into m clusters $C_1, \ldots, C_m$, the quality can be measured by

$$Q(\{C_1, \ldots, C_m\}) = \prod_{i=1}^{m} P(C_i), \tag{10.18}$$

where $P()$ is the maximum likelihood. If we merge two clusters, C_{j_1} and C_{j_2}, into a cluster, $C_{j_1} \cup C_{j_2}$, then, the change in quality of the overall clustering is

$$\begin{aligned} &Q((\{C_1, \ldots, C_m\} - \{C_{j_1}, C_{j_2}\}) \cup \{C_{j_1} \cup C_{j_2}\}) - Q(\{C_1, \ldots, C_m\}) \\ &= \frac{\prod_{i=1}^{m} P(C_i) \cdot P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - \prod_{i=1}^{m} P(C_i) \\ &= \prod_{i=1}^{m} P(C_i) \left(\frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - 1 \right). \end{aligned} \tag{10.19}$$

When choosing to merge two clusters in hierarchical clustering, $\prod_{i=1}^{m} P(C_i)$ is constant for any pair of clusters. Therefore, given clusters C_1 and C_2, the distance between them can be measured by

$$dist(C_i, C_j) = -\log \frac{P(C_1 \cup C_2)}{P(C_1)P(C_2)}. \tag{10.20}$$

A probabilistic hierarchical clustering method can adopt the agglomerative clustering framework, but use probabilistic models (Eq. 10.20) to measure the distance between clusters.

Upon close observation of Eq. (10.19), we see that merging two clusters may not always lead to an improvement in clustering quality, that is, $\frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})}$ may be less than 1. For example, assume that Gaussian distribution functions are used in the model of Figure 10.11. Although merging clusters C_1 and C_2 results in a cluster that better fits a Gaussian distribution, merging clusters C_3 and C_4 lowers the clustering quality because no Gaussian functions can fit the merged cluster well.

Based on this observation, a probabilistic hierarchical clustering scheme can start with one cluster per object, and merge two clusters, C_i and C_j, if the distance between them is negative. In each iteration, we try to find C_i and C_j so as to maximize $\log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)}$. The iteration continues as long as $\log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)} > 0$, that is, as long as there is an improvement in clustering quality. The pseudocode is given in Figure 10.12.

Probabilistic hierarchical clustering methods are easy to understand, and generally have the same efficiency as algorithmic agglomerative hierarchical clustering methods; in fact, they share the same framework. Probabilistic models are more interpretable, but sometimes less flexible than distance metrics. Probabilistic models can handle partially observed data. For example, given a multidimensional data set where some objects have missing values on some dimensions, we can learn a Gaussian model on each dimension independently using the observed values on the dimension. The resulting cluster hierarchy accomplishes the optimization goal of fitting data to the selected probabilistic models.

A drawback of using probabilistic hierarchical clustering is that it outputs only one hierarchy with respect to a chosen probabilistic model. It cannot handle the uncertainty of cluster hierarchies. Given a data set, there may exist multiple hierarchies that

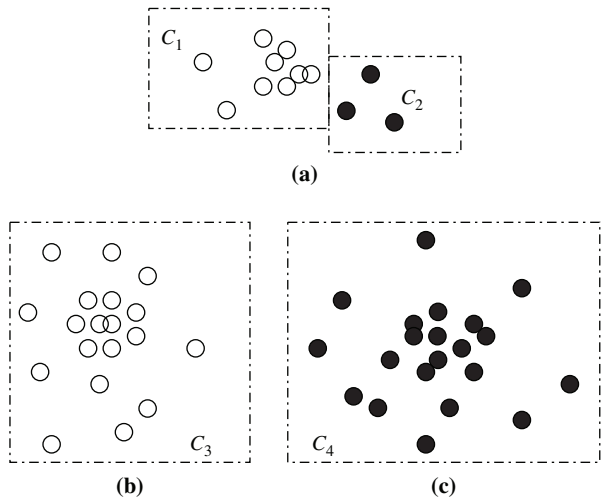


Figure 10.11 Merging clusters in probabilistic hierarchical clustering: (a) Merging clusters C_1 and C_2 leads to an increase in overall cluster quality, but merging clusters (b) C_3 and (c) C_4 does not.

Algorithm: A probabilistic hierarchical clustering algorithm.

Input:

- $D = \{\boldsymbol{o_1}, \ldots, \boldsymbol{o_n}\}$: a data set containing n objects;

Output: A hierarchy of clusters.

Method:

(1) **create** a cluster for each object $C_i = \{\boldsymbol{o_i}\}$, $1 \leq i \leq n$;
(2) **for** $i = 1$ to n
(3) **find** pair of clusters C_i and C_j such that $C_i, C_j = \arg\max_{i \neq j} \log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)}$;
(4) **if** $\log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)} > 0$ then merge C_i and C_j;
(5) **else** stop;

Figure 10.12 A probabilistic hierarchical clustering algorithm.

fit the observed data. Neither algorithmic approaches nor probabilistic approaches can find the distribution of such hierarchies. Recently, Bayesian tree-structured models have been developed to handle such problems. Bayesian and other sophisticated probabilistic clustering methods are considered advanced topics and are not covered in this book.

10.4 Density-Based Methods

Partitioning and hierarchical methods are designed to find spherical-shaped clusters. They have difficulty finding clusters of arbitrary shape such as the "S" shape and oval clusters in Figure 10.13. Given such data, they would likely inaccurately identify convex regions, where noise or outliers are included in the clusters.

To find clusters of arbitrary shape, alternatively, we can model clusters as dense regions in the data space, separated by sparse regions. This is the main strategy behind *density-based clustering methods*, which can discover clusters of nonspherical shape. In this section, you will learn the basic techniques of density-based clustering by studying three representative methods, namely, DBSCAN (Section 10.4.1), OPTICS (Section 10.4.2), and DENCLUE (Section 10.4.3).

10.4.1 DBSCAN: Density-Based Clustering Based on Connected Regions with High Density

"*How can we find dense regions in density-based clustering?*" The *density* of an object $\boldsymbol{o}$ can be measured by the number of objects close to $\boldsymbol{o}$. **DBSCAN** (Density-Based Spatial Clustering of Applications with Noise) finds *core objects*, that is, objects that have dense neighborhoods. It connects core objects and their neighborhoods to form dense regions as clusters.

"*How does* **DBSCAN** *quantify the neighborhood of an object?*" A user-specified parameter $\epsilon > 0$ is used to specify the radius of a neighborhood we consider for every object. The ϵ**-neighborhood** of an object $\boldsymbol{o}$ is the space within a radius ϵ centered at $\boldsymbol{o}$.

Due to the fixed neighborhood size parameterized by ϵ, the **density of a neighborhood** can be measured simply by the number of objects in the neighborhood. To determine whether a neighborhood is dense or not, DBSCAN uses another user-specified

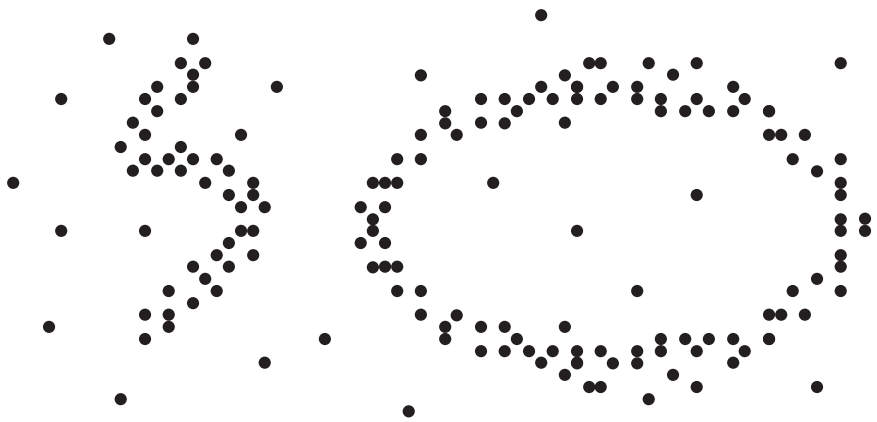


Figure 10.13 Clusters of arbitrary shape.

parameter, *MinPts*, which specifies the density threshold of dense regions. An object is a **core object** if the ϵ-neighborhood of the object contains at least *MinPts* objects. Core objects are the pillars of dense regions.

Given a set, D, of objects, we can identify all core objects with respect to the given parameters, ϵ and *MinPts*. The clustering task is therein reduced to using core objects and their neighborhoods to form dense regions, where the dense regions are clusters. For a core object $\boldsymbol{q}$ and an object $\boldsymbol{p}$, we say that $\boldsymbol{p}$ is **directly density-reachable** from $\boldsymbol{q}$ (with respect to ϵ and *MinPts*) if $\boldsymbol{p}$ is within the ϵ-neighborhood of $\boldsymbol{q}$. Clearly, an object $\boldsymbol{p}$ is directly density-reachable from another object $\boldsymbol{q}$ if and only if $\boldsymbol{q}$ is a core object and $\boldsymbol{p}$ is in the ϵ-neighborhood of $\boldsymbol{q}$. Using the directly density-reachable relation, a core object can "bring" all objects from its ϵ-neighborhood into a dense region.

"*How can we assemble a large dense region using small dense regions centered by core objects?*" In DBSCAN, $\boldsymbol{p}$ is **density-reachable** from $\boldsymbol{q}$ (with respect to ϵ and *MinPts* in D) if there is a chain of objects $\boldsymbol{p_1}, \ldots, \boldsymbol{p_n}$, such that $\boldsymbol{p_1} = \boldsymbol{q}$, $\boldsymbol{p_n} = \boldsymbol{p}$, and $\boldsymbol{p_{i+1}}$ is directly density-reachable from $\boldsymbol{p_i}$ with respect to ϵ and *MinPts*, for $1 \leq i \leq n$, $\boldsymbol{p_i} \in D$. Note that density-reachability is not an equivalence relation because it is not symmetric. If both $\boldsymbol{o_1}$ and $\boldsymbol{o_2}$ are core objects and $\boldsymbol{o_1}$ is density-reachable from $\boldsymbol{o_2}$, then $\boldsymbol{o_2}$ is density-reachable from $\boldsymbol{o_1}$. However, if $\boldsymbol{o_2}$ is a core object but $\boldsymbol{o_1}$ is not, then $\boldsymbol{o_1}$ may be density-reachable from $\boldsymbol{o_2}$, but not vice versa.

To connect core objects as well as their neighbors in a dense region, **DBSCAN** uses the notion of density-connectedness. Two objects $\boldsymbol{p_1}, \boldsymbol{p_2} \in D$ are **density-connected** with respect to ϵ and *MinPts* if there is an object $\boldsymbol{q} \in D$ such that both $\boldsymbol{p_1}$ and $\boldsymbol{p_2}$ are density-reachable from $\boldsymbol{q}$ with respect to ϵ and *MinPts*. Unlike density-reachability, density-connectedness is an equivalence relation. It is easy to show that, for objects $\boldsymbol{o_1}$, $\boldsymbol{o_2}$, and $\boldsymbol{o_3}$, if $\boldsymbol{o_1}$ and $\boldsymbol{o_2}$ are density-connected, and $\boldsymbol{o_2}$ and $\boldsymbol{o_3}$ are density-connected, then so are $\boldsymbol{o_1}$ and $\boldsymbol{o_3}$.

Example 10.7 **Density-reachability and density-connectivity.** Consider Figure 10.14 for a given ϵ represented by the radius of the circles, and, say, let $MinPts = 3$.

Of the labeled points, $\boldsymbol{m}, \boldsymbol{p}, \boldsymbol{o}, \boldsymbol{r}$ are core objects because each is in an ϵ-neighborhood containing at least three points. Object $\boldsymbol{q}$ is directly density-reachable from $\boldsymbol{m}$. Object $\boldsymbol{m}$ is directly density-reachable from $\boldsymbol{p}$ and vice versa.

Object $\boldsymbol{q}$ is (indirectly) density-reachable from $\boldsymbol{p}$ because $\boldsymbol{q}$ is directly density-reachable from $\boldsymbol{m}$ and $\boldsymbol{m}$ is directly density-reachable from $\boldsymbol{p}$. However, $\boldsymbol{p}$ is not density-reachable from $\boldsymbol{q}$ because $\boldsymbol{q}$ is not a core object. Similarly, $\boldsymbol{r}$ and $\boldsymbol{s}$ are density-reachable from $\boldsymbol{o}$ and $\boldsymbol{o}$ is density-reachable from $\boldsymbol{r}$. Thus, $\boldsymbol{o}$, $\boldsymbol{r}$, and $\boldsymbol{s}$ are all density-connected. ■

We can use the closure of density-connectedness to find connected dense regions as clusters. Each closed set is a **density-based cluster**. A subset $C \subseteq D$ is a cluster if (1) for any two objects $\boldsymbol{o_1}, \boldsymbol{o_2} \in C$, $\boldsymbol{o_1}$ and $\boldsymbol{o_2}$ are density-connected; and (2) there does not exist an object $\boldsymbol{o} \in C$ and another object $\boldsymbol{o'} \in (D - C)$ such that $\boldsymbol{o}$ and $\boldsymbol{o'}$ are density-connected.

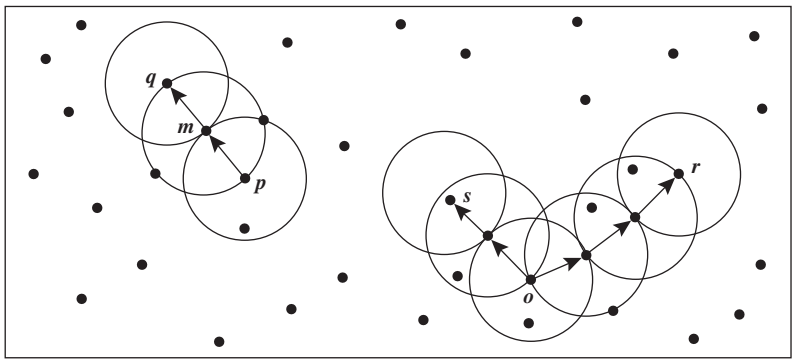


Figure 10.14 Density-reachability and density-connectivity in density-based clustering. *Source:* Based on Ester, Kriegel, Sander, and Xu [EKSX96].

"*How does DBSCAN find clusters?*" Initially, all objects in a given data set D are marked as "unvisited." DBSCAN randomly selects an unvisited object $\boldsymbol{p}$, marks $\boldsymbol{p}$ as "visited," and checks whether the ϵ-neighborhood of $\boldsymbol{p}$ contains at least *MinPts* objects. If not, $\boldsymbol{p}$ is marked as a noise point. Otherwise, a new cluster C is created for $\boldsymbol{p}$, and all the objects in the ϵ-neighborhood of $\boldsymbol{p}$ are added to a candidate set, N. DBSCAN iteratively adds to C those objects in N that do not belong to any cluster. In this process, for an object $\boldsymbol{p'}$ in N that carries the label "unvisited," DBSCAN marks it as "visited" and checks its ϵ-neighborhood. If the ϵ-neighborhood of $\boldsymbol{p'}$ has at least *MinPts* objects, those objects in the ϵ-neighborhood of $\boldsymbol{p'}$ are added to N. DBSCAN continues adding objects to C until C can no longer be expanded, that is, N is empty. At this time, cluster C is completed, and thus is output.

To find the next cluster, DBSCAN randomly selects an unvisited object from the remaining ones. The clustering process continues until all objects are visited. The pseudocode of the DBSCAN algorithm is given in Figure 10.15.

If a spatial index is used, the computational complexity of DBSCAN is $O(n \log n)$, where n is the number of database objects. Otherwise, the complexity is $O(n^2)$. With appropriate settings of the user-defined parameters, ϵ and *MinPts*, the algorithm is effective in finding arbitrary-shaped clusters.

10.4.2 OPTICS: Ordering Points to Identify the Clustering Structure

Although DBSCAN can cluster objects given input parameters such as ϵ (the maximum radius of a neighborhood) and *MinPts* (the minimum number of points required in the neighborhood of a core object), it encumbers users with the responsibility of selecting parameter values that will lead to the discovery of acceptable clusters. This is a problem associated with many other clustering algorithms. Such parameter settings

Algorithm: DBSCAN: a density-based clustering algorithm.

Input:

- D: a data set containing n objects,
- ϵ: the radius parameter, and
- *MinPts*: the neighborhood density threshold.

Output: A set of density-based clusters.

Method:

```
(1)  mark all objects as unvisited;
(2)  do
(3)      randomly select an unvisited object p;
(4)      mark p as visited;
(5)      if the ε-neighborhood of p has at least MinPts objects
(6)          create a new cluster C, and add p to C;
(7)          let N be the set of objects in the ε-neighborhood of p;
(8)          for each point p' in N
(9)              if p' is unvisited
(10)                 mark p' as visited;
(11)                 if the ε-neighborhood of p' has at least MinPts points,
                     add those points to N;
(12)             if p' is not yet a member of any cluster, add p' to C;
(13)         end for
(14)         output C;
(15)     else mark p as noise;
(16) until no object is unvisited;
```

Figure 10.15 DBSCAN algorithm.

are usually empirically set and difficult to determine, especially for real-world, high-dimensional data sets. Most algorithms are sensitive to these parameter values: Slightly different settings may lead to very different clusterings of the data. Moreover, real-world, high-dimensional data sets often have very skewed distributions such that their intrinsic clustering structure may not be well characterized by a single set of *global* density parameters.

Note that density-based clusters are monotonic with respect to the neighborhood threshold. That is, in DBSCAN, for a fixed *MinPts* value and two neighborhood thresholds, $\epsilon_1 < \epsilon_2$, a cluster C with respect to ϵ_1 and *MinPts* must be a subset of a cluster C' with respect to ϵ_2 and *MinPts*. This means that if two objects are in a density-based cluster, they must also be in a cluster with a lower density requirement.

To overcome the difficulty in using one set of global parameters in clustering analysis, a cluster analysis method called **OPTICS** was proposed. OPTICS does not explicitly produce a data set clustering. Instead, it outputs a **cluster ordering**. This is a linear list

of all objects under analysis and represents the *density-based clustering structure* of the data. Objects in a denser cluster are listed closer to each other in the cluster ordering. This ordering is equivalent to density-based clustering obtained from a wide range of parameter settings. Thus, OPTICS does not require the user to provide a specific density threshold. The cluster ordering can be used to extract basic clustering information (e.g., cluster centers, or arbitrary-shaped clusters), derive the intrinsic clustering structure, as well as provide a visualization of the clustering.

To construct the different clusterings simultaneously, the objects are processed in a specific order. This order selects an object that is density-reachable with respect to the lowest ϵ value so that clusters with higher density (lower ϵ) will be finished first. Based on this idea, OPTICS needs two important pieces of information per object:

- The **core-distance** of an object $\boldsymbol{p}$ is the smallest value ϵ' such that the ϵ'-neighborhood of $\boldsymbol{p}$ has at least *MinPts* objects. That is, ϵ' is the minimum distance threshold that makes $\boldsymbol{p}$ a core object. If $\boldsymbol{p}$ is not a core object with respect to ϵ and *MinPts*, the core-distance of $\boldsymbol{p}$ is undefined.
- The **reachability-distance** to object $\boldsymbol{p}$ from $\boldsymbol{q}$ is the minimum radius value that makes $\boldsymbol{p}$ density-reachable from $\boldsymbol{q}$. According to the definition of density-reachability, $\boldsymbol{q}$ has to be a core object and $\boldsymbol{p}$ must be in the neighborhood of $\boldsymbol{q}$. Therefore, the reachability-distance from $\boldsymbol{q}$ to $\boldsymbol{p}$ is $\max\{\textit{core-distance}(\boldsymbol{q}), \textit{dist}(\boldsymbol{p}, \boldsymbol{q})\}$. If $\boldsymbol{q}$ is not a core object with respect to ϵ and *MinPts*, the reachability-distance to $\boldsymbol{p}$ from $\boldsymbol{q}$ is undefined.

  An object $\boldsymbol{p}$ may be directly reachable from multiple core objects. Therefore, $\boldsymbol{p}$ may have multiple reachability-distances with respect to different core objects. The smallest reachability-distance of $\boldsymbol{p}$ is of particular interest because it gives the shortest path for which $\boldsymbol{p}$ is connected to a dense cluster.

Example 10.8 **Core-distance and reachability-distance.** Figure 10.16 illustrates the concepts of core-distance and reachability-distance. Suppose that $\epsilon = 6$ mm and $\textit{MinPts} = 5$. The core-distance of $\boldsymbol{p}$ is the distance, ϵ', between $\boldsymbol{p}$ and the fourth closest data object from $\boldsymbol{p}$. The reachability-distance of $\boldsymbol{q_1}$ from $\boldsymbol{p}$ is the core-distance of $\boldsymbol{p}$ (i.e., $\epsilon' = 3$ mm) because this is greater than the Euclidean distance from $\boldsymbol{p}$ to $\boldsymbol{q_1}$. The reachability-distance of $\boldsymbol{q_2}$ with respect to $\boldsymbol{p}$ is the Euclidean distance from $\boldsymbol{p}$ to $\boldsymbol{q_2}$ because this is greater than the core-distance of $\boldsymbol{p}$. ■

OPTICS computes an ordering of all objects in a given database and, for each object in the database, stores the core-distance and a suitable reachability-distance. OPTICS maintains a list called OrderSeeds to generate the output ordering. Objects in OrderSeeds are sorted by the reachability-distance from their respective closest core objects, that is, by the smallest reachability-distance of each object.

OPTICS begins with an arbitrary object from the input database as the current object, $\boldsymbol{p}$. It retrieves the ϵ-neighborhood of $\boldsymbol{p}$, determines the core-distance, and sets the reachability-distance to *undefined*. The current object, $\boldsymbol{p}$, is then written to output.

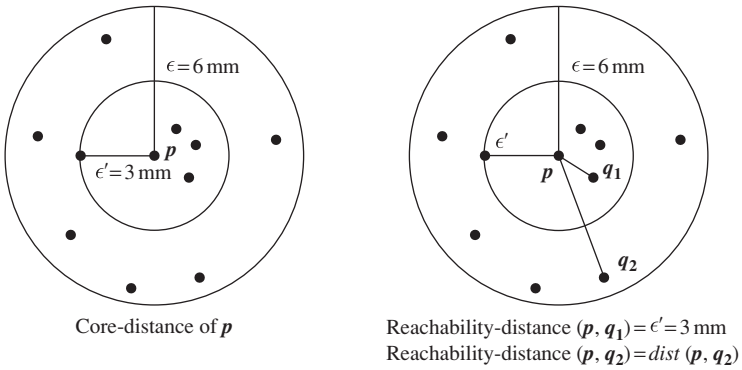


Figure 10.16 OPTICS terminology. *Source:* Based on Ankerst, Breunig, Kriegel, and Sander [ABKS99].

If $\boldsymbol{p}$ is not a core object, OPTICS simply moves on to the next object in the OrderSeeds list (or the input database if OrderSeeds is empty). If $\boldsymbol{p}$ is a core object, then for each object, $\boldsymbol{q}$, in the ϵ-neighborhood of $\boldsymbol{p}$, OPTICS updates its reachability-distance from $\boldsymbol{p}$ and inserts $\boldsymbol{q}$ into OrderSeeds if $\boldsymbol{q}$ has not yet been processed. The iteration continues until the input is fully consumed and OrderSeeds is empty.

A data set's cluster ordering can be represented graphically, which helps to visualize and understand the clustering structure in a data set. For example, Figure 10.17 is the reachability plot for a simple 2-D data set, which presents a general overview of how the data are structured and clustered. The data objects are plotted in the clustering order (horizontal axis) together with their respective reachability-distances (vertical axis). The three Gaussian "bumps" in the plot reflect three clusters in the data set. Methods have also been developed for viewing clustering structures of high-dimensional data at various levels of detail.

The structure of the OPTICS algorithm is very similar to that of DBSCAN. Consequently, the two algorithms have the same time complexity. The complexity is $O(n \log n)$ if a spatial index is used, and $O(n^2)$ otherwise, where n is the number of objects.

10.4.3 DENCLUE: Clustering Based on Density Distribution Functions

Density estimation is a core issue in density-based clustering methods. **DENCLUE** (DENsity-based CLUstEring) is a clustering method based on a set of density distribution functions. We first give some background on density estimation, and then describe the DENCLUE algorithm.

In probability and statistics, **density estimation** is the estimation of an unobservable underlying probability density function based on a set of observed data. In the context of density-based clustering, the unobservable underlying probability density function is the true distribution of the population of all possible objects to be analyzed. The observed data set is regarded as a random sample from that population.

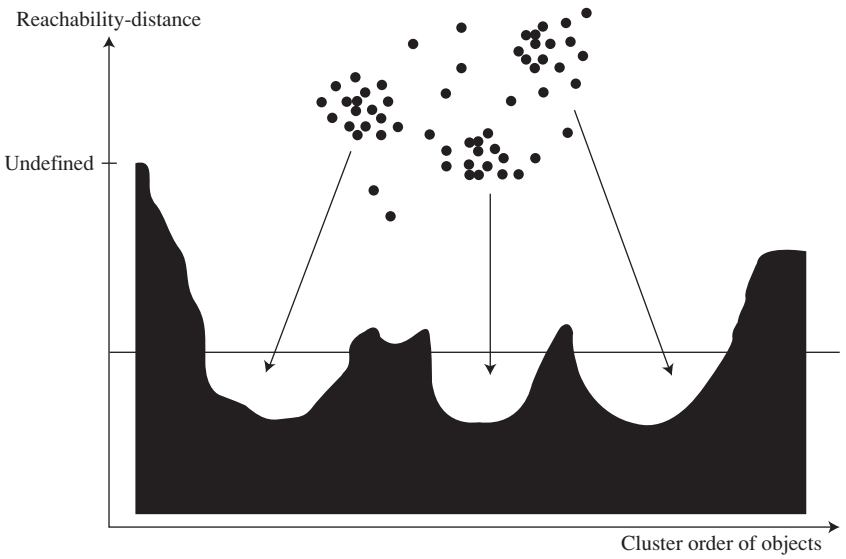


Figure 10.17 Cluster ordering in OPTICS. *Source:* Adapted from Ankerst, Breunig, Kriegel, and Sander [ABKS99].

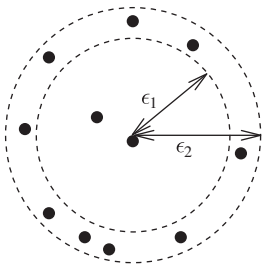


Figure 10.18 The subtlety in density estimation in DBSCAN and OPTICS: Increasing the neighborhood radius slightly from ϵ_1 to ϵ_2 results in a much higher density.

In DBSCAN and OPTICS, density is calculated by counting the number of objects in a neighborhood defined by a radius parameter, ϵ. Such density estimates can be highly sensitive to the radius value used. For example, in Figure 10.18, the density changes significantly as the radius increases by a small amount.

To overcome this problem, **kernel density estimation** can be used, which is a nonparametric density estimation approach from statistics. The general idea behind kernel density estimation is simple. We treat an observed object as an indicator of

high-probability density in the surrounding region. The probability density at a point depends on the distances from this point to the observed objects.

Formally, let $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}$ be an independent and identically distributed sample of a random variable f. The *kernel density approximation of the probability density function* is

$$\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{\boldsymbol{x} - \boldsymbol{x_i}}{h}\right), \tag{10.21}$$

where $K()$ is a kernel and h is the bandwidth serving as a smoothing parameter. A **kernel** can be regarded as a function modeling the influence of a sample point within its neighborhood. Technically, a kernel $K()$ is a non-negative real-valued integrable function that should satisfy two requirements: $\int_{-\infty}^{+\infty} K(u)du = 1$ and $K(-u) = K(u)$ for all values of u. A frequently used kernel is a standard Gaussian function with a mean of 0 and a variance of 1:

$$K\left(\frac{\boldsymbol{x} - \boldsymbol{x_i}}{h}\right) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(\boldsymbol{x} - \boldsymbol{x_i})^2}{2h^2}}. \tag{10.22}$$

DENCLUE uses a Gaussian kernel to estimate density based on the given set of objects to be clustered. A point $\boldsymbol{x^*}$ is called a **density attractor** if it is a local maximum of the estimated density function. To avoid trivial local maximum points, DENCLUE uses a noise threshold, ξ, and only considers those density attractors $\boldsymbol{x^*}$ such that $\hat{f}(\boldsymbol{x^*}) \geq \xi$. These nontrivial density attractors are the centers of clusters.

Objects under analysis are assigned to clusters through density attractors using a stepwise hill-climbing procedure. For an object, $\boldsymbol{x}$, the hill-climbing procedure starts from $\boldsymbol{x}$ and is guided by the gradient of the estimated density function. That is, the density attractor for $\boldsymbol{x}$ is computed as

$$\boldsymbol{x^0} = \boldsymbol{x}$$
$$\boldsymbol{x^{j+1}} = \boldsymbol{x^j} + \delta \frac{\nabla \hat{f}(\boldsymbol{x^j})}{|\nabla \hat{f}(\boldsymbol{x^j})|}, \tag{10.23}$$

where δ is a parameter to control the speed of convergence, and

$$\nabla \hat{f}(\boldsymbol{x}) = \frac{1}{h^{d+2} n \sum_{i=1}^{n} K\left(\frac{\boldsymbol{x} - \boldsymbol{x_i}}{h}\right)(\boldsymbol{x_i} - \boldsymbol{x})}. \tag{10.24}$$

The hill-climbing procedure stops at step $k > 0$ if $\hat{f}(\boldsymbol{x^{k+1}}) < \hat{f}(\boldsymbol{x^k})$, and assigns $\boldsymbol{x}$ to the density attractor $\boldsymbol{x^*} = \boldsymbol{x^k}$. An object $\boldsymbol{x}$ is an outlier or noise if it converges in the hill-climbing procedure to a local maximum $\boldsymbol{x^*}$ with $\hat{f}(\boldsymbol{x^*}) < \xi$.

A cluster in DENCLUE is a set of density attractors X and a set of input objects C such that each object in C is assigned to a density attractor in X, and there exists a path between every pair of density attractors where the density is above ξ. By using multiple density attractors connected by paths, DENCLUE can find clusters of arbitrary shape.

DENCLUE has several advantages. It can be regarded as a generalization of several well-known clustering methods such as single-linkage approaches and DBSCAN. Moreover, DENCLUE is invariant against noise. The kernel density estimation can effectively reduce the influence of noise by uniformly distributing noise into the input data.

10.5 Grid-Based Methods

The clustering methods discussed so far are data-driven—they partition the set of objects and adapt to the distribution of the objects in the embedding space. Alternatively, a **grid-based clustering** method takes a space-driven approach by partitioning the embedding space into *cells* independent of the distribution of the input objects.

The *grid-based clustering* approach uses a multiresolution grid data structure. It quantizes the object space into a finite number of cells that form a grid structure on which all of the operations for clustering are performed. The main advantage of the approach is its fast processing time, which is typically independent of the number of data objects, yet dependent on only the number of cells in each dimension in the quantized space.

In this section, we illustrate grid-based clustering using two typical examples. STING (Section 10.5.1) explores statistical information stored in the grid cells. CLIQUE (Section 10.5.2) represents a grid- and density-based approach for subspace clustering in a high-dimensional data space.

10.5.1 STING: STatistical INformation Grid

STING is a grid-based multiresolution clustering technique in which the embedding spatial area of the input objects is divided into rectangular cells. The space can be divided in a hierarchical and recursive way. Several levels of such rectangular cells correspond to different levels of resolution and form a hierarchical structure: Each cell at a high level is partitioned to form a number of cells at the next lower level. Statistical information regarding the attributes in each grid cell, such as the mean, maximum, and minimum values, is precomputed and stored as *statistical parameters*. These statistical parameters are useful for query processing and for other data analysis tasks.

Figure 10.19 shows a hierarchical structure for STING clustering. The statistical parameters of higher-level cells can easily be computed from the parameters of the lower-level cells. These parameters include the following: the attribute-independent parameter, *count*; and the attribute-dependent parameters, *mean*, *stdev* (standard deviation), *min* (minimum), *max* (maximum), and the type of *distribution* that the attribute value in the cell follows such as *normal*, *uniform*, *exponential*, or *none* (if the distribution is unknown). Here, the attribute is a selected measure for analysis such as *price* for house objects. When the data are loaded into the database, the parameters *count*, *mean*, *stdev*, *min*, and *max* of the bottom-level cells are calculated directly from the data. The value of *distribution* may either be assigned by the user if the distribution type is known

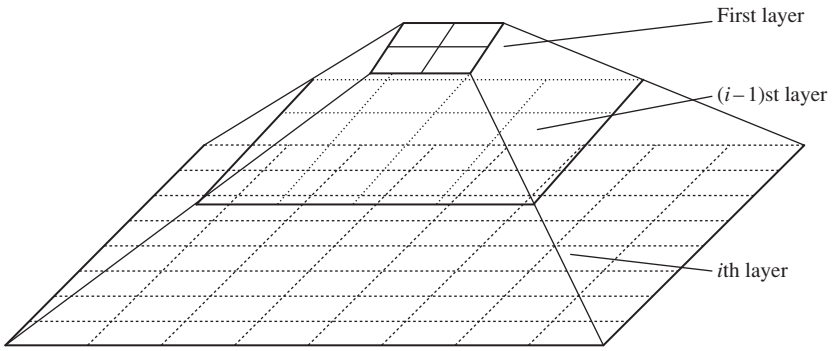


Figure 10.19 Hierarchical structure for STING clustering.

beforehand or obtained by hypothesis tests such as the χ^2 test. The type of distribution of a higher-level cell can be computed based on the majority of distribution types of its corresponding lower-level cells in conjunction with a threshold filtering process. If the distributions of the lower-level cells disagree with each other and fail the threshold test, the distribution type of the high-level cell is set to *none*.

"*How is this statistical information useful for query answering?*" The statistical parameters can be used in a top-down, grid-based manner as follows. First, a layer within the hierarchical structure is determined from which the query-answering process is to start. This layer typically contains a small number of cells. For each cell in the current layer, we compute the confidence interval (or estimated probability range) reflecting the cell's relevancy to the given query. The irrelevant cells are removed from further consideration. Processing of the next lower level examines only the remaining relevant cells. This process is repeated until the bottom layer is reached. At this time, if the query specification is met, the regions of relevant cells that satisfy the query are returned. Otherwise, the data that fall into the relevant cells are retrieved and further processed until they meet the query's requirements.

An interesting property of STING is that it approaches the clustering result of DBSCAN if the granularity approaches 0 (i.e., toward very low-level data). In other words, using the count and cell size information, dense clusters can be identified approximately using STING. Therefore, STING can also be regarded as a density-based clustering method.

"*What advantages does STING offer over other clustering methods?*" STING offers several advantages: (1) the grid-based computation is *query-independent* because the statistical information stored in each cell represents the summary information of the data in the grid cell, independent of the query; (2) the grid structure facilitates parallel processing and incremental updating; and (3) the method's efficiency is a major advantage: STING goes through the database once to compute the statistical parameters of the cells, and hence the time complexity of generating clusters is $O(n)$, where n is the total number of objects. After generating the hierarchical structure, the query processing time

is $O(g)$, where g is the total number of grid cells at the lowest level, which is usually much smaller than n.

Because STING uses a multiresolution approach to cluster analysis, the quality of STING clustering depends on the granularity of the lowest level of the grid structure. If the granularity is very fine, the cost of processing will increase substantially; however, if the bottom level of the grid structure is too coarse, it may reduce the quality of cluster analysis. Moreover, STING does not consider the spatial relationship between the children and their neighboring cells for construction of a parent cell. As a result, the shapes of the resulting clusters are isothetic, that is, all the cluster boundaries are either horizontal or vertical, and no diagonal boundary is detected. This may lower the quality and accuracy of the clusters despite the fast processing time of the technique.

10.5.2 CLIQUE: An Apriori-like Subspace Clustering Method

A data object often has tens of attributes, many of which may be irrelevant. The values of attributes may vary considerably. These factors can make it difficult to locate clusters that span the entire data space. It may be more meaningful to instead search for clusters within different *subspaces* of the data. For example, consider a health-informatics application where patient records contain extensive attributes describing personal information, numerous symptoms, conditions, and family history.

Finding a nontrivial group of patients for which all or even most of the attributes strongly agree is unlikely. In bird flu patients, for instance, the *age*, *gender*, and *job* attributes may vary dramatically within a wide range of values. Thus, it can be difficult to find such a cluster within the entire data space. Instead, by searching in subspaces, we may find a cluster of similar patients in a lower-dimensional space (e.g., patients who are similar to one other with respect to symptoms like high fever, cough but no runny nose, and aged between 3 and 16).

CLIQUE (CLustering In QUEst) is a simple grid-based method for finding density-based clusters in subspaces. CLIQUE partitions each dimension into nonoverlapping intervals, thereby partitioning the entire embedding space of the data objects into cells. It uses a density threshold to identify *dense* cells and *sparse* ones. A cell is dense if the number of objects mapped to it exceeds the density threshold.

The main strategy behind CLIQUE for identifying a candidate search space uses the monotonicity of dense cells with respect to dimensionality. This is based on the *Apriori property* used in frequent pattern and association rule mining (Chapter 6). In the context of clusters in subspaces, the monotonicity says the following. A k-dimensional cell c ($k > 1$) can have at least l points only if every $(k-1)$-dimensional projection of c, which is a cell in a $(k-1)$-dimensional subspace, has at least l points. Consider Figure 10.20, where the embedding data space contains three dimensions: *age, salary*, and *vacation*. A 2-D cell, say in the subspace formed by *age* and *salary*, contains l points only if the projection of this cell in every dimension, that is, *age* and *salary*, respectively, contains at least l points.

CLIQUE performs clustering in two steps. In the first step, CLIQUE partitions the d-dimensional data space into nonoverlapping rectangular units, identifying the dense units among these. CLIQUE finds dense cells in all of the subspaces. To do so,

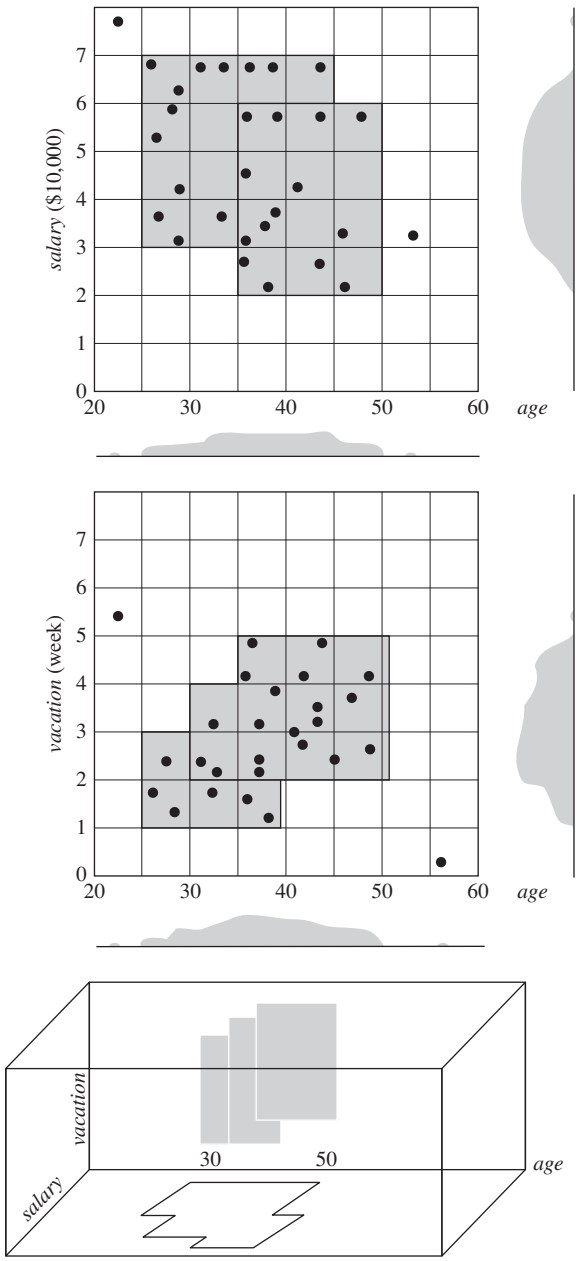


Figure 10.20 Dense units found with respect to *age* for the dimensions *salary* and *vacation* are intersected to provide a candidate search space for dense units of higher dimensionality.

CLIQUE partitions every dimension into intervals, and identifies intervals containing at least l points, where l is the density threshold. CLIQUE then iteratively joins two k-dimensional dense cells, c_1 and c_2, in subspaces $(D_{i_1}, \ldots, D_{i_k})$ and $(D_{j_1}, \ldots, D_{j_k})$, respectively, if $D_{i_1} = D_{j_1}, \ldots, D_{i_{k-1}} = D_{j_{k-1}}$, and c_1 and c_2 share the same intervals in those dimensions. The join operation generates a new $(k+1)$-dimensional candidate cell c in space $(D_{i_1}, \ldots, D_{i_{k-1}}, D_{i_k}, D_{j_k})$. CLIQUE checks whether the number of points in c passes the density threshold. The iteration terminates when no candidates can be generated or no candidate cells are dense.

In the second step, CLIQUE uses the dense cells in each subspace to assemble clusters, which can be of arbitrary shape. The idea is to apply the Minimum Description Length (MDL) principle (Chapter 8) to use the *maximal regions* to cover connected dense cells, where a maximal region is a hyperrectangle where every cell falling into this region is dense, and the region cannot be extended further in any dimension in the subspace. Finding the best description of a cluster in general is NP-Hard. Thus, CLIQUE adopts a simple greedy approach. It starts with an arbitrary dense cell, finds a maximal region covering the cell, and then works on the remaining dense cells that have not yet been covered. The greedy method terminates when all dense cells are covered.

"*How effective is CLIQUE?*" CLIQUE automatically finds subspaces of the highest dimensionality such that high-density clusters exist in those subspaces. It is insensitive to the order of input objects and does not presume any canonical data distribution. It scales linearly with the size of the input and has good scalability as the number of dimensions in the data is increased. However, obtaining a meaningful clustering is dependent on proper tuning of the grid size (which is a stable structure here) and the density threshold. This can be difficult in practice because the grid size and density threshold are used across all combinations of dimensions in the data set. Thus, the accuracy of the clustering results may be degraded at the expense of the method's simplicity. Moreover, for a given dense region, all projections of the region onto lower-dimensionality subspaces will also be dense. This can result in a large overlap among the reported dense regions. Furthermore, it is difficult to find clusters of rather different densities within different dimensional subspaces.

Several extensions to this approach follow a similar philosophy. For example, we can think of a grid as a set of fixed bins. Instead of using fixed bins for each of the dimensions, we can use an adaptive, data-driven strategy to dynamically determine the bins for each dimension based on data distribution statistics. Alternatively, instead of using a density threshold, we may use entropy (Chapter 8) as a measure of the quality of subspace clusters.

10.6 Evaluation of Clustering

By now you have learned what clustering is and know several popular clustering methods. You may ask, "*When I try out a clustering method on a data set, how can I evaluate whether the clustering results are good?*" In general, *cluster evaluation* assesses

the feasibility of clustering analysis on a data set and the quality of the results generated by a clustering method. The major tasks of clustering evaluation include the following:

- *Assessing clustering tendency*. In this task, for a given data set, we assess whether a nonrandom structure exists in the data. Blindly applying a clustering method on a data set will return clusters; however, the clusters mined may be misleading. Clustering analysis on a data set is meaningful only when there is a nonrandom structure in the data.
- *Determining the number of clusters in a data set*. A few algorithms, such as k-means, require the number of clusters in a data set as the parameter. Moreover, the number of clusters can be regarded as an interesting and important summary statistic of a data set. Therefore, it is desirable to estimate this number even before a clustering algorithm is used to derive detailed clusters.
- *Measuring clustering quality*. After applying a clustering method on a data set, we want to assess how good the resulting clusters are. A number of measures can be used. Some methods measure how well the clusters fit the data set, while others measure how well the clusters match the ground truth, if such truth is available. There are also measures that score clusterings and thus can compare two sets of clustering results on the same data set.

In the rest of this section, we discuss each of these three topics.

10.6.1 Assessing Clustering Tendency

Clustering tendency assessment determines whether a given data set has a non-random structure, which may lead to meaningful clusters. Consider a data set that does not have any non-random structure, such as a set of uniformly distributed points in a data space. Even though a clustering algorithm may return clusters for the data, those clusters are random and are not meaningful.

Example 10.9 **Clustering requires nonuniform distribution of data.** Figure 10.21 shows a data set that is uniformly distributed in 2-D data space. Although a clustering algorithm may still artificially partition the points into groups, the groups will unlikely mean anything significant to the application due to the uniform distribution of the data. ■

"*How can we assess the clustering tendency of a data set?*" Intuitively, we can try to measure the probability that the data set is generated by a uniform data distribution. This can be achieved using statistical tests for spatial randomness. To illustrate this idea, let's look at a simple yet effective statistic called the Hopkins Statistic.

The **Hopkins Statistic** is a spatial statistic that tests the spatial randomness of a variable as distributed in a space. Given a data set, D, which is regarded as a sample of

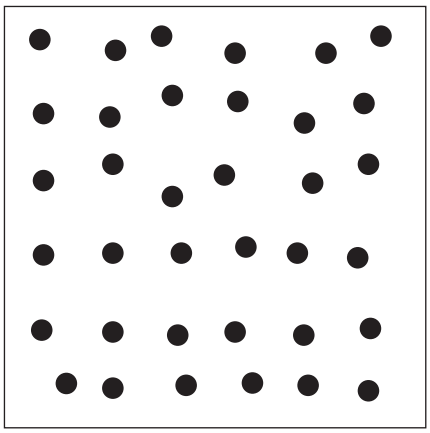


Figure 10.21 A data set that is uniformly distributed in the data space.

a random variable, o, we want to determine how far away o is from being uniformly distributed in the data space. We calculate the Hopkins Statistic as follows:

1. Sample n points, $\boldsymbol{p_1}, \ldots, \boldsymbol{p_n}$, uniformly from D. That is, each point in D has the same probability of being included in this sample. For each point, $\boldsymbol{p_i}$, we find the nearest neighbor of $\boldsymbol{p_i}$ ($1 \leq i \leq n$) in D, and let x_i be the distance between $\boldsymbol{p_i}$ and its nearest neighbor in D. That is,

$$x_i = \min_{\boldsymbol{v} \in D} \{dist(\boldsymbol{p_i}, \boldsymbol{v})\}. \tag{10.25}$$

2. Sample n points, $\boldsymbol{q_1}, \ldots, \boldsymbol{q_n}$, uniformly from D. For each $\boldsymbol{q_i}$ ($1 \leq i \leq n$), we find the nearest neighbor of $\boldsymbol{q_i}$ in $D - \{\boldsymbol{q_i}\}$, and let y_i be the distance between $\boldsymbol{q_i}$ and its nearest neighbor in $D - \{\boldsymbol{q_i}\}$. That is,

$$y_i = \min_{\boldsymbol{v} \in D, \boldsymbol{v} \neq \boldsymbol{q_i}} \{dist(\boldsymbol{q_i}, \boldsymbol{v})\}. \tag{10.26}$$

3. Calculate the Hopkins Statistic, H, as

$$H = \frac{\sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i}. \tag{10.27}$$

"*What does the Hopkins Statistic tell us about how likely data set* D *follows a uniform distribution in the data space?*" If D were uniformly distributed, then $\sum_{i=1}^{n} y_i$ and $\sum_{i=1}^{n} x_i$ would be close to each other, and thus H would be about 0.5. However, if D were highly skewed, then $\sum_{i=1}^{n} y_i$ would be substantially smaller than $\sum_{i=1}^{n} x_i$ in expectation, and thus H would be close to 0.

Our null hypothesis is the *homogeneous hypothesis*—that D is uniformly distributed and thus contains no meaningful clusters. The *nonhomogeneous hypothesis* (i.e., that D is not uniformly distributed and thus contains clusters) is the alternative hypothesis. We can conduct the Hopkins Statistic test iteratively, using 0.5 as the threshold to reject the alternative hypothesis. That is, if $H > 0.5$, then it is unlikely that D has statistically significant clusters.

10.6.2 Determining the Number of Clusters

Determining the "right" number of clusters in a data set is important, not only because some clustering algorithms like k-means require such a parameter, but also because the appropriate number of clusters controls the proper granularity of cluster analysis. It can be regarded as finding a good balance between *compressibility* and *accuracy* in cluster analysis. Consider two extreme cases. What if you were to treat the entire data set as a cluster? This would maximize the compression of the data, but such a cluster analysis has no value. On the other hand, treating each object in a data set as a cluster gives the finest clustering resolution (i.e., most accurate due to the zero distance between an object and the corresponding cluster center). In some methods like k-means, this even achieves the best cost. However, having one object per cluster does not enable any data summarization.

Determining the number of clusters is far from easy, often because the "right" number is ambiguous. Figuring out what the right number of clusters should be often depends on the distribution's shape and scale in the data set, as well as the clustering resolution required by the user. There are many possible ways to estimate the number of clusters. Here, we briefly introduce a few simple yet popular and effective methods.

A simple method is to set the number of clusters to about $\sqrt{\frac{n}{2}}$ for a data set of n points. In expectation, each cluster has $\sqrt{2n}$ points.

The **elbow method** is based on the observation that increasing the number of clusters can help to reduce the sum of within-cluster variance of each cluster. This is because having more clusters allows one to capture finer groups of data objects that are more similar to each other. However, the marginal effect of reducing the sum of within-cluster variances may drop if too many clusters are formed, because splitting a cohesive cluster into two gives only a small reduction. Consequently, a heuristic for selecting the right number of clusters is to use the turning point in the curve of the sum of within-cluster variances with respect to the number of clusters.

Technically, given a number, $k > 0$, we can form k clusters on the data set in question using a clustering algorithm like k-means, and calculate the sum of within-cluster variances, $var(k)$. We can then plot the curve of var with respect to k. The first (or most significant) turning point of the curve suggests the "right" number.

More advanced methods can determine the number of clusters using information criteria or information theoretic approaches. Please refer to the bibliographic notes for further information (Section 10.9).

The "right" number of clusters in a data set can also be determined by **cross-validation**, a technique often used in classification (Chapter 8). First, divide the given data set, D, into m parts. Next, use $m-1$ parts to build a clustering model, and use the remaining part to test the quality of the clustering. For example, for each point in the test set, we can find the closest centroid. Consequently, we can use the sum of the squared distances between all points in the test set and the closest centroids to measure how well the clustering model fits the test set. For any integer $k > 0$, we repeat this process m times to derive clusterings of k clusters by using each part in turn as the test set. The average of the quality measure is taken as the overall quality measure. We can then compare the overall quality measure with respect to different values of k, and find the number of clusters that best fits the data.

10.6.3 Measuring Clustering Quality

Suppose you have assessed the clustering tendency of a given data set. You may have also tried to predetermine the number of clusters in the set. You can now apply one or multiple clustering methods to obtain clusterings of the data set. "*How good is the clustering generated by a method, and how can we compare the clusterings generated by different methods?*"

We have a few methods to choose from for measuring the quality of a clustering. In general, these methods can be categorized into two groups according to whether ground truth is available. Here, *ground truth* is the ideal clustering that is often built using human experts.

If ground truth is available, it can be used by **extrinsic methods**, which compare the clustering against the group truth and measure. If the ground truth is unavailable, we can use **intrinsic methods**, which evaluate the goodness of a clustering by considering how well the clusters are separated. Ground truth can be considered as supervision in the form of "cluster labels." Hence, extrinsic methods are also known as *supervised methods*, while intrinsic methods are *unsupervised methods*.

Let's have a look at simple methods from each category.

Extrinsic Methods

When the ground truth is available, we can compare it with a clustering to assess the clustering. Thus, the core task in extrinsic methods is to assign a score, $Q(\mathcal{C}, \mathcal{C}_g)$, to a clustering, $\mathcal{C}$, given the ground truth, $\mathcal{C}_g$. Whether an extrinsic method is effective largely depends on the measure, Q, it uses.

In general, a measure Q on clustering quality is effective if it satisfies the following four essential criteria:

- **Cluster homogeneity.** This requires that the more pure the clusters in a clustering are, the better the clustering. Suppose that ground truth says that the objects in a data set, D, can belong to categories $L_1, \ldots, L_n$. Consider clustering, $\mathcal{C}_1$, wherein a cluster $C \in \mathcal{C}_1$ contains objects from two categories L_i, L_j $(1 \leq i < j \leq n)$. Also

consider clustering $\mathcal{C}_2$, which is identical to $\mathcal{C}_1$ except that C_2 is split into two clusters containing the objects in L_i and L_j, respectively. A clustering quality measure, Q, respecting cluster homogeneity should give a higher score to $\mathcal{C}_2$ than $\mathcal{C}_1$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.

- **Cluster completeness.** This is the counterpart of cluster homogeneity. Cluster completeness requires that for a clustering, if any two objects belong to the same category according to ground truth, then they should be assigned to the same cluster. Cluster completeness requires that a clustering should assign objects belonging to the same category (according to ground truth) to the same cluster. Consider clustering $\mathcal{C}_1$, which contains clusters C_1 and C_2, of which the members belong to the same category according to ground truth. Let clustering $\mathcal{C}_2$ be identical to $\mathcal{C}_1$ except that C_1 and C_2 are merged into one cluster in $\mathcal{C}_2$. Then, a clustering quality measure, Q, respecting cluster completeness should give a higher score to $\mathcal{C}_2$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.
- **Rag bag.** In many practical scenarios, there is often a "rag bag" category containing objects that cannot be merged with other objects. Such a category is often called "miscellaneous," "other," and so on. The rag bag criterion states that putting a heterogeneous object into a pure cluster should be penalized more than putting it into a rag bag. Consider a clustering $\mathcal{C}_1$ and a cluster $C \in \mathcal{C}_1$ such that all objects in C except for one, denoted by $\boldsymbol{o}$, belong to the same category according to ground truth. Consider a clustering $\mathcal{C}_2$ identical to $\mathcal{C}_1$ except that $\boldsymbol{o}$ is assigned to a cluster $C' \neq C$ in $\mathcal{C}_2$ such that C' contains objects from various categories according to ground truth, and thus is noisy. In other words, C' in $\mathcal{C}_2$ is a rag bag. Then, a clustering quality measure Q respecting the rag bag criterion should give a higher score to $\mathcal{C}_2$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.
- **Small cluster preservation.** If a small category is split into small pieces in a clustering, those small pieces may likely become noise and thus the small category cannot be discovered from the clustering. The small cluster preservation criterion states that splitting a small category into pieces is more harmful than splitting a large category into pieces. Consider an extreme case. Let D be a data set of $n+2$ objects such that, according to ground truth, n objects, denoted by $\boldsymbol{o_1}, \ldots, \boldsymbol{o_n}$, belong to one category and the other two objects, denoted by $\boldsymbol{o_{n+1}}, \boldsymbol{o_{n+2}}$, belong to another category. Suppose clustering $\mathcal{C}_1$ has three clusters, $C_1 = \{\boldsymbol{o_1}, \ldots, \boldsymbol{o_n}\}$, $C_2 = \{\boldsymbol{o_{n+1}}\}$, and $C_3 = \{\boldsymbol{o_{n+2}}\}$. Let clustering $\mathcal{C}_2$ have three clusters, too, namely $C_1 = \{\boldsymbol{o_1}, \ldots, \boldsymbol{o_{n-1}}\}$, $C_2 = \{\boldsymbol{o_n}\}$, and $C_3 = \{\boldsymbol{o_{n+1}}, \boldsymbol{o_{n+2}}\}$. In other words, C_1 splits the small category and C_2 splits the big category. A clustering quality measure Q preserving small clusters should give a higher score to $\mathcal{C}_2$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.

Many clustering quality measures satisfy some of these four criteria. Here, we introduce the *BCubed precision* and *recall* metrics, which satisfy all four criteria.

BCubed evaluates the precision and recall for every object in a clustering on a given data set according to ground truth. The precision of an object indicates how many other objects in the same cluster belong to the same category as the object. The recall

of an object reflects how many objects of the same category are assigned to the same cluster.

Formally, let $D = \{\boldsymbol{o_1}, \ldots, \boldsymbol{o_n}\}$ be a set of objects, and $\mathcal{C}$ be a clustering on D. Let $L(\boldsymbol{o_i})$ $(1 \leq i \leq n)$ be the category of $\boldsymbol{o_i}$ given by ground truth, and $C(o_i)$ be the *cluster_ID* of $\boldsymbol{o_i}$ in $\mathcal{C}$. Then, for two objects, $\boldsymbol{o_i}$ and $\boldsymbol{o_j}$, $(1 \leq i, j, \leq n, i \neq j)$, the *correctness* of the relation between $\boldsymbol{o_i}$ and $\boldsymbol{o_j}$ in clustering $\mathcal{C}$ is given by

$$\text{Correctness}(\boldsymbol{o_i}, \boldsymbol{o_j}) = \begin{cases} 1 & \text{if } L(\boldsymbol{o_i}) = L(\boldsymbol{o_j}) \Leftrightarrow C(\boldsymbol{o_i}) = C(\boldsymbol{o_j}) \\ 0 & \text{otherwise.} \end{cases} \tag{10.28}$$

BCubed precision is defined as

$$\text{Precision BCubed} = \frac{\sum_{i=1}^{n} \frac{\sum_{\boldsymbol{o_j}: i \neq j, C(\boldsymbol{o_i}) = C(\boldsymbol{o_j})} \text{Correctness}(\boldsymbol{o_i}, \boldsymbol{o_j})}{\|\{\boldsymbol{o_j} | i \neq j, C(\boldsymbol{o_i}) = C(\boldsymbol{o_j})\}\|}}{n}. \tag{10.29}$$

BCubed recall is defined as

$$\text{Recall BCubed} = \frac{\sum_{i=1}^{n} \frac{\sum_{\boldsymbol{o_j}: i \neq j, L(\boldsymbol{o_i}) = L(\boldsymbol{o_j})} \text{Correctness}(\boldsymbol{o_i}, \boldsymbol{o_j})}{\|\{\boldsymbol{o_j} | i \neq j, L(\boldsymbol{o_i}) = L(\boldsymbol{o_j})\}\|}}{n}. \tag{10.30}$$

Intrinsic Methods

When the ground truth of a data set is not available, we have to use an intrinsic method to assess the clustering quality. In general, intrinsic methods evaluate a clustering by examining how well the clusters are separated and how compact the clusters are. Many intrinsic methods have the advantage of a similarity metric between objects in the data set.

The **silhouette coefficient** is such a measure. For a data set, D, of n objects, suppose D is partitioned into k clusters, $C_1, \ldots, C_k$. For each object $\boldsymbol{o} \in D$, we calculate $a(\boldsymbol{o})$ as the average distance between $\boldsymbol{o}$ and all other objects in the cluster to which $\boldsymbol{o}$ belongs. Similarly, $b(\boldsymbol{o})$ is the minimum average distance from $\boldsymbol{o}$ to all clusters to which $\boldsymbol{o}$ does not belong. Formally, suppose $\boldsymbol{o} \in C_i$ $(1 \leq i \leq k)$; then

$$a(\boldsymbol{o}) = \frac{\sum_{\boldsymbol{o'} \in C_i, \boldsymbol{o} \neq \boldsymbol{o'}} dist(\boldsymbol{o}, \boldsymbol{o'})}{|C_i| - 1} \tag{10.31}$$

and

$$b(\boldsymbol{o}) = \min_{C_j:1\le j\le k, j\neq i} \left\{ \frac{\sum_{\boldsymbol{o}' \in C_j} dist(\boldsymbol{o}, \boldsymbol{o}')}{|C_j|} \right\}. \tag{10.32}$$

The **silhouette coefficient** of $\boldsymbol{o}$ is then defined as

$$s(\boldsymbol{o}) = \frac{b(\boldsymbol{o}) - a(\boldsymbol{o})}{\max\{a(\boldsymbol{o}), b(\boldsymbol{o})\}}. \tag{10.33}$$

The value of the silhouette coefficient is between -1 and 1. The value of $\boldsymbol{a(o)}$ reflects the compactness of the cluster to which $\boldsymbol{o}$ belongs. The smaller the value, the more compact the cluster. The value of $b(\boldsymbol{o})$ captures the degree to which $\boldsymbol{o}$ is separated from other clusters. The larger $b(\boldsymbol{o})$ is, the more separated $\boldsymbol{o}$ is from other clusters. Therefore, when the silhouette coefficient value of $\boldsymbol{o}$ approaches 1, the cluster containing $\boldsymbol{o}$ is compact and $\boldsymbol{o}$ is far away from other clusters, which is the preferable case. However, when the silhouette coefficient value is negative (i.e., $b(\boldsymbol{o}) < a(\boldsymbol{o})$), this means that, in expectation, $\boldsymbol{o}$ is closer to the objects in another cluster than to the objects in the same cluster as $\boldsymbol{o}$. In many cases, this is a bad situation and should be avoided.

To measure a cluster's fitness within a clustering, we can compute the average silhouette coefficient value of all objects in the cluster. To measure the quality of a clustering, we can use the average silhouette coefficient value of all objects in the data set. The silhouette coefficient and other intrinsic measures can also be used in the elbow method to heuristically derive the number of clusters in a data set by replacing the sum of within-cluster variances.

10.7 Summary

- A **cluster** is a collection of data objects that are *similar* to one another within the same cluster and are *dissimilar* to the objects in other clusters. The process of grouping a set of physical or abstract objects into classes of *similar* objects is called **clustering**.
- Cluster analysis has extensive **applications**, including business intelligence, image pattern recognition, Web search, biology, and security. Cluster analysis can be used as a standalone data mining tool to gain insight into the data distribution, or as a preprocessing step for other data mining algorithms operating on the detected clusters.
- Clustering is a dynamic field of research in data mining. It is related to **unsupervised learning** in machine learning.
- Clustering is a challenging field. Typical **requirements** of it include scalability, the ability to deal with different types of data and attributes, the discovery of clusters in arbitrary shape, minimal requirements for domain knowledge to determine input parameters, the ability to deal with noisy data, incremental clustering and

insensitivity to input order, the capability of clustering high-dimensionality data, constraint-based clustering, as well as interpretability and usability.

- Many clustering algorithms have been developed. These can be categorized from several **orthogonal aspects** such as those regarding partitioning criteria, separation of clusters, similarity measures used, and clustering space. This chapter discusses major fundamental clustering methods of the following categories: *partitioning methods, hierarchical methods, density-based methods*, and *grid-based methods*. Some algorithms may belong to more than one category.
- A **partitioning method** first creates an initial set of k partitions, where parameter k is the number of partitions to construct. It then uses an *iterative relocation technique* that attempts to improve the partitioning by moving objects from one group to another. Typical partitioning methods include k-means, k-medoids, and CLARANS.
- A **hierarchical method** creates a hierarchical decomposition of the given set of data objects. The method can be classified as being either *agglomerative* (*bottom-up*) or *divisive* (*top-down*), based on how the hierarchical decomposition is formed. To compensate for the rigidity of *merge* or *split*, the quality of hierarchical agglomeration can be improved by analyzing object linkages at each hierarchical partitioning (e.g., in Chameleon), or by first performing *microclustering* (that is, grouping objects into "microclusters") and then operating on the microclusters with other clustering techniques such as iterative relocation (as in BIRCH).
- A **density-based method** clusters objects based on the notion of density. It grows clusters either according to the density of neighborhood objects (e.g., in DBSCAN) or according to a density function (e.g., in DENCLUE). OPTICS is a density-based method that generates an augmented ordering of the data's clustering structure.
- A **grid-based method** first quantizes the object space into a finite number of cells that form a grid structure, and then performs clustering on the grid structure. STING is a typical example of a grid-based method based on statistical information stored in grid cells. CLIQUE is a grid-based and subspace clustering algorithm.
- **Clustering evaluation** assesses the feasibility of clustering analysis on a data set and the quality of the results generated by a clustering method. The tasks include assessing clustering tendency, determining the number of clusters, and measuring clustering quality.

10.8 Exercises

10.1 Briefly describe and give examples of each of the following approaches to clustering: *partitioning* methods, *hierarchical* methods, *density-based* methods, and *grid-based* methods.

10.2 Suppose that the data mining task is to cluster points (with (x, y) representing location) into three clusters, where the points are

$$A_1(2,10), A_2(2,5), A_3(8,4), B_1(5,8), B_2(7,5), B_3(6,4), C_1(1,2), C_2(4,9).$$

The distance function is Euclidean distance. Suppose initially we assign A_1, B_1, and C_1 as the center of each cluster, respectively. Use the *k-means* algorithm to show *only*

(a) The three cluster centers after the first round of execution.

(b) The final three clusters.

10.3 Use an example to show why the *k*-means algorithm may not find the global optimum, that is, optimizing the within-cluster variation.

10.4 For the *k*-means algorithm, it is interesting to note that by choosing the initial cluster centers carefully, we may be able to not only speed up the algorithm's convergence, but also guarantee the quality of the final clustering. The ***k*-means++** algorithm is a variant of *k*-means, which chooses the initial centers as follows. First, it selects one center uniformly at random from the objects in the data set. Iteratively, for each object $\boldsymbol{p}$ other than the chosen center, it chooses an object as the new center. This object is chosen at random with probability proportional to $dist(\boldsymbol{p})^2$, where $dist(\boldsymbol{p})$ is the distance from $\boldsymbol{p}$ to the closest center that has already been chosen. The iteration continues until k centers are selected.

Explain why this method will not only speed up the convergence of the *k*-means algorithm, but also guarantee the quality of the final clustering results.

10.5 Provide the pseudocode of the object reassignment step of the PAM algorithm.

10.6 Both *k-means* and *k-medoids* algorithms can perform effective clustering.

(a) Illustrate the strength and weakness of *k-means* in comparison with *k-medoids*.

(b) Illustrate the strength and weakness of these schemes in comparison with a hierarchical clustering scheme (e.g., AGNES).

10.7 Prove that in DBSCAN, the density-connectedness is an equivalence relation.

10.8 Prove that in DBSCAN, for a fixed *MinPts* value and two neighborhood thresholds, $\epsilon_1 < \epsilon_2$, a cluster C with respect to ϵ_1 and *MinPts* must be a subset of a cluster C' with respect to ϵ_2 and *MinPts*.

10.9 Provide the pseudocode of the OPTICS algorithm.

10.10 Why is it that BIRCH encounters difficulties in finding clusters of arbitrary shape but OPTICS does not? Propose modifications to BIRCH to help it find clusters of arbitrary shape.

10.11 Provide the pseudocode of the step in CLIQUE that finds dense cells in all subspaces.

10.12 Present conditions under which density-based clustering is more suitable than partitioning-based clustering and hierarchical clustering. Give application examples to support your argument.

10.13 Give an example of how specific clustering methods can be *integrated*, for example, where one clustering algorithm is used as a preprocessing step for another. In addition, provide reasoning as to why the integration of two methods may sometimes lead to improved clustering quality and efficiency.

10.14 Clustering is recognized as an important data mining task with broad applications. Give one application example for each of the following cases:

(a) An application that uses clustering as a major data mining function.

(b) An application that uses clustering as a preprocessing tool for data preparation for other data mining tasks.

10.15 Data cubes and multidimensional databases contain nominal, ordinal, and numeric data in hierarchical or aggregate forms. Based on what you have learned about the clustering methods, design a clustering method that finds clusters in large data cubes effectively and efficiently.

10.16 Describe each of the following clustering algorithms in terms of the following criteria: (1) shapes of clusters that can be determined; (2) input parameters that must be specified; and (3) limitations.

(a) *k*-means

(b) *k*-medoids

(c) CLARA

(d) BIRCH

(e) CHAMELEON

(f) DBSCAN

10.17 Human eyes are fast and effective at judging the quality of clustering methods for 2-D data. Can you design a data visualization method that may help humans visualize data clusters and judge the clustering quality for 3-D data? What about for even higher-dimensional data?

10.18 Suppose that you are to allocate a number of automatic teller machines (ATMs) in a given region so as to satisfy a number of constraints. Households or workplaces may be clustered so that typically one ATM is assigned per cluster. The clustering, however, may be constrained by two factors: (1) obstacle objects (i.e., there are bridges, rivers, and highways that can affect ATM accessibility), and (2) additional user-specified constraints such as that each ATM should serve at least 10,000 households. How can a clustering algorithm such as *k*-means be modified for quality clustering under *both* constraints?

10.19 For *constraint-based clustering*, aside from having the minimum number of customers in each cluster (for ATM allocation) as a constraint, there can be many other kinds of

constraints. For example, a constraint could be in the form of the maximum number of customers per cluster, average income of customers per cluster, maximum distance between every two clusters, and so on. Categorize the kinds of constraints that can be imposed on the clusters produced and discuss how to perform clustering efficiently under such kinds of constraints.

10.20 Design a *privacy-preserving clustering* method so that a data owner would be able to ask a third party to mine the data for quality clustering without worrying about the potential inappropriate disclosure of certain private or sensitive information stored in the data.

10.21 Show that BCubed metrics satisfy the four essential requirements for extrinsic clustering evaluation methods.

10.9 Bibliographic Notes

Clustering has been extensively studied for over 40 years and across many disciplines due to its broad applications. Most books on pattern classification and machine learning contain chapters on cluster analysis or unsupervised learning. Several textbooks are dedicated to the methods of cluster analysis, including Hartigan [Har75]; Jain and Dubes [JD88]; Kaufman and Rousseeuw [KR90]; and Arabie, Hubert, and De Sorte [AHS96]. There are also many survey articles on different aspects of clustering methods. Recent ones include Jain, Murty, and Flynn [JMF99]; Parsons, Haque, and Liu [PHL04]; and Jain [Jai10].

For partitioning methods, the k-means algorithm was first introduced by Lloyd [Llo57], and then by MacQueen [Mac67]. Arthur and Vassilvitskii [AV07] presented the k-means++ algorithm. A filtering algorithm, which uses a spatial hierarchical data index to speed up the computation of cluster means, is given in Kanungo, Mount, Netanyahu, et al. [KMN+02].

The k-medoids algorithms of PAM and CLARA were proposed by Kaufman and Rousseeuw [KR90]. The k-modes (for clustering nominal data) and k-prototypes (for clustering hybrid data) algorithms were proposed by Huang [Hua98]. The k-modes clustering algorithm was also proposed independently by Chaturvedi, Green, and Carroll [CGC94, CGC01]. The CLARANS algorithm was proposed by Ng and Han [NH94]. Ester, Kriegel, and Xu [EKX95] proposed techniques for further improvement of the performance of CLARANS using efficient spatial access methods such as R*-tree and focusing techniques. A k-means-based scalable clustering algorithm was proposed by Bradley, Fayyad, and Reina [BFR98].

An early survey of agglomerative hierarchical clustering algorithms was conducted by Day and Edelsbrunner [DE84]. Agglomerative hierarchical clustering, such as AGNES, and divisive hierarchical clustering, such as DIANA, were introduced by Kaufman and Rousseeuw [KR90]. An interesting direction for improving the clustering quality of hierarchical clustering methods is to integrate hierarchical clustering with distance-based iterative relocation or other nonhierarchical clustering methods. For example, BIRCH, by Zhang, Ramakrishnan, and Livny [ZRL96], first performs hierarchical clustering with

a CF-tree before applying other techniques. Hierarchical clustering can also be performed by sophisticated linkage analysis, transformation, or nearest-neighbor analysis, such as CURE by Guha, Rastogi, and Shim [GRS98]; ROCK (for clustering nominal attributes) by Guha, Rastogi, and Shim [GRS99]; and Chameleon by Karypis, Han, and Kumar [KHK99].

A probabilistic hierarchical clustering framework following normal linkage algorithms and using probabilistic models to define cluster similarity was developed by Friedman [Fri03] and Heller and Ghahramani [HG05].

For density-based clustering methods, DBSCAN was proposed by Ester, Kriegel, Sander, and Xu [EKSX96]. Ankerst, Breunig, Kriegel, and Sander [ABKS99] developed OPTICS, a cluster-ordering method that facilitates density-based clustering without worrying about parameter specification. The DENCLUE algorithm, based on a set of density distribution functions, was proposed by Hinneburg and Keim [HK98]. Hinneburg and Gabriel [HG07] developed DENCLUE 2.0, which includes a new hill-climbing procedure for Gaussian kernels that adjusts the step size automatically.

STING, a grid-based multiresolution approach that collects statistical information in grid cells, was proposed by Wang, Yang, and Muntz [WYM97]. WaveCluster, developed by Sheikholeslami, Chatterjee, and Zhang [SCZ98], is a multiresolution clustering approach that transforms the original feature space by wavelet transform.

Scalable methods for clustering nominal data were studied by Gibson, Kleinberg, and Raghavan [GKR98]; Guha, Rastogi, and Shim [GRS99]; and Ganti, Gehrke, and Ramakrishnan [GGR99]. There are also many other clustering paradigms. For example, fuzzy clustering methods are discussed in Kaufman and Rousseeuw [KR90], Bezdek [Bez81], and Bezdek and Pal [BP92].

For high-dimensional clustering, an Apriori-based dimension-growth subspace clustering algorithm called CLIQUE was proposed by Agrawal, Gehrke, Gunopulos, and Raghavan [AGGR98]. It integrates density-based and grid-based clustering methods.

Recent studies have proceeded to clustering stream data Babcock, Badu, Datar, et al. [BBD+02]. A *k*-median-based data stream clustering algorithm was proposed by Guha, Mishra, Motwani, and O'Callaghan [GMMO00] and by O'Callaghan et al. [OMM+02]. A method for clustering evolving data streams was proposed by Aggarwal, Han, Wang, and Yu [AHWY03]. A framework for projected clustering of high-dimensional data streams was proposed by Aggarwal, Han, Wang, and Yu [AHWY04a].

Clustering evaluation is discussed in a few monographs and survey articles such as Jain and Dubes [JD88] and Halkidi, Batistakis, and Vazirgiannis [HBV01]. The extrinsic methods for clustering quality evaluation are extensively explored. Some recent studies include Meilă [Mei03, Mei05] and Amigó, Gonzalo, Artiles, and Verdejo [AGAV09]. The four essential criteria introduced in this chapter are formulated in Amigó, Gonzalo, Artiles, and Verdejo [AGAV09], while some individual criteria were also mentioned earlier, for example, in Meilă [Mei03] and Rosenberg and Hirschberg [RH07]. Bagga and Baldwin [BB98] introduced the BCubed metrics. The silhouette coefficient is described in Kaufman and Rousseeuw [KR90].

Advanced Cluster Analysis

You learned the fundamentals of cluster analysis in Chapter 10. In this chapter, we discuss advanced topics of cluster analysis. Specifically, we investigate four major perspectives:

- **Probabilistic model-based clustering**: Section 11.1 introduces a general framework and a method for deriving clusters where each object is assigned a probability of belonging to a cluster. Probabilistic model-based clustering is widely used in many data mining applications such as text mining.
- **Clustering high-dimensional data**: When the dimensionality is high, conventional distance measures can be dominated by noise. Section 11.2 introduces fundamental methods for cluster analysis on high-dimensional data.
- **Clustering graph and network data**: Graph and network data are increasingly popular in applications such as online social networks, the World Wide Web, and digital libraries. In Section 11.3, you will study the key issues in clustering graph and network data, including similarity measurement and clustering methods.
- **Clustering with constraints**: In our discussion so far, we do not assume any constraints in clustering. In some applications, however, various constraints may exist. These constraints may rise from background knowledge or spatial distribution of the objects. You will learn how to conduct cluster analysis with different kinds of constraints in Section 11.4.

By the end of this chapter, you will have a good grasp of the issues and techniques regarding advanced cluster analysis.

11.1 Probabilistic Model-Based Clustering

In all the cluster analysis methods we have discussed so far, each data object can be assigned to only one of a number of clusters. This cluster assignment rule is required in some applications such as assigning customers to marketing managers. However,

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in other applications, this rigid requirement may not be desirable. In this section, we demonstrate the need for fuzzy or flexible cluster assignment in some applications, and introduce a general method to compute probabilistic clusters and assignments.

"*In what situations may a data object belong to more than one cluster?*" Consider Example 11.1.

Example 11.1 **Clustering product reviews.** *AllElectronics* has an online store, where customers not only purchase online, but also create reviews of products. Not every product receives reviews; instead, some products may have many reviews, while many others have none or only a few. Moreover, a review may involve multiple products. Thus, as the review editor of *AllElectronics*, your task is to cluster the reviews.

Ideally, a cluster is about a *topic*, for example, a group of products, services, or issues that are highly related. Assigning a review to one cluster exclusively would not work well for your task. Suppose there is a cluster for "cameras and camcorders" and another for "computers." What if a review talks about the compatibility between a camcorder and a computer? The review relates to both clusters; however, it does not exclusively belong to either cluster.

You would like to use a clustering method that allows a review to belong to more than one cluster if the review indeed involves more than one topic. To reflect the strength that a review belongs to a cluster, you want the assignment of a review to a cluster to carry a weight representing the partial membership. ■

The scenario where an object may belong to multiple clusters occurs often in many applications. This is illustrated in Example 11.2.

Example 11.2 **Clustering to study user search intent**. The *AllElectronics* online store records all customer browsing and purchasing behavior in a log. An important data mining task is to use the log data to categorize and understand *user search intent*. For example, consider a user *session* (a short period in which a user interacts with the online store). Is the user searching for a product, making comparisons among different products, or looking for customer support information? Clustering analysis helps here because it is difficult to predefine user behavior patterns thoroughly. A cluster that contains similar user browsing trajectories may represent similar user behavior.

However, not every session belongs to only one cluster. For example, suppose user sessions involving the purchase of digital cameras form one cluster, and user sessions that compare laptop computers form another cluster. What if a user in one session makes an order for a digital camera, and at the same time compares several laptop computers? Such a session should belong to both clusters to some extent. ■

In this section, we systematically study the theme of clustering that allows an object to belong to more than one cluster. We start with the notion of fuzzy clusters in Section 11.1.1. We then generalize the concept to probabilistic model-based clusters in Section 11.1.2. In Section 11.1.3, we introduce the expectation-maximization algorithm, a general framework for mining such clusters.

11.1.1 Fuzzy Clusters

Given a set of objects, $X = \{x_1, \ldots, x_n\}$, a **fuzzy set** S is a subset of X that allows each object in X to have a membership degree between 0 and 1. Formally, a fuzzy set, S, can be modeled as a function, $F_S{:}X \rightarrow [0,1]$.

Example 11.3 **Fuzzy set**. The more digital camera units that are sold, the more popular the camera is. In *AllElectronics*, we can use the following formula to compute the degree of popularity of a digital camera, o, given the sales of o:

$$pop(o) = \begin{cases} 1 & \text{if 1000 or more units of } o \text{ are sold} \\ \frac{i}{1000} & \text{if } i \ (i < 1000) \text{ units of } o \text{ are sold.} \end{cases} \tag{11.1}$$

Function $pop()$ defines a fuzzy set of popular digital cameras. For example, suppose the sales of digital cameras at *AllElectronics* are as shown in Table 11.1. The fuzzy set of popular digital cameras is $\{A(0.05), B(1), C(0.86), D(0.27)\}$, where the degrees of membership are written in parentheses. ■

We can apply the fuzzy set idea on clusters. That is, given a set of objects, a cluster is a fuzzy set of objects. Such a cluster is called a fuzzy cluster. Consequently, a clustering contains multiple *fuzzy clusters*.

Formally, given a set of objects, $o_1, \ldots, o_n$, a **fuzzy clustering** of k **fuzzy clusters**, $C_1, \ldots, C_k$, can be represented using a **partition matrix**, $M = [w_{ij}]$ $(1 \leq i \leq n, 1 \leq j \leq k)$, where w_{ij} is the membership degree of o_i in fuzzy cluster C_j. The partition matrix should satisfy the following three requirements:

- For each object, o_i, and cluster, C_j, $0 \leq w_{ij} \leq 1$. This requirement enforces that a fuzzy cluster is a fuzzy set.
- For each object, o_i, $\sum_{j=1}^{k} w_{ij} = 1$. This requirement ensures that every object participates in the clustering equivalently.

Table 11.1 Set of Digital Cameras and Their Sales at *AllElectronics*

Camera	*Sales (units)*
A	50
B	1320
C	860
D	270

- For each cluster, C_j, $0 < \sum_{i=1}^{n} w_{ij} < n$. This requirement ensures that for every cluster, there is at least one object for which the membership value is nonzero.

Example 11.4 **Fuzzy clusters**. Suppose the *AllElectronics* online store has six reviews. The keywords contained in these reviews are listed in Table 11.2.

We can group the reviews into two fuzzy clusters, C_1 and C_2. C_1 is for "digital camera" and "lens," and C_2 is for "computer." The partition matrix is

$$M = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ \frac{2}{3} & \frac{1}{3} \\ 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

Here, we use the keywords "digital camera" and "lens" as the features of cluster C_1, and "computer" as the feature of cluster C_2. For review, R_i, and cluster, C_j ($1 \le i \le 6, 1 \le j \le 2$), w_{ij} is defined as

$$w_{ij} = \frac{|R_i \cap C_j|}{|R_i \cap (C_1 \cup C_2)|} = \frac{|R_i \cap C_j|}{|R_i \cap \{digital\ camera, lens, computer\}|}.$$

In this fuzzy clustering, review R_4 belongs to clusters C_1 and C_2 with membership degrees $\frac{2}{3}$ and $\frac{1}{3}$, respectively. ■

"How can we evaluate how well a fuzzy clustering describes a data set?" Consider a set of objects, $o_1, \ldots, o_n$, and a fuzzy clustering $\mathcal{C}$ of k clusters, $C_1, \ldots, C_k$. Let $M = [w_{ij}]$ ($1 \le i \le n, 1 \le j \le k$) be the partition matrix. Let $c_1, \ldots, c_k$ be the *centers* of clusters $C_1, \ldots, C_k$, respectively. Here, a center can be defined either as the mean or the medoid, or in other ways specific to the application.

As discussed in Chapter 10, the distance or similarity between an object and the center of the cluster to which the object is assigned can be used to measure how well the

Table 11.2 Set of Reviews and the Keywords Used

Review_ID	*Keywords*
R_1	digital camera, lens
R_2	digital camera
R_3	lens
R_4	digital camera, lens, computer
R_5	computer, CPU
R_6	computer, computer game

object belongs to the cluster. This idea can be extended to fuzzy clustering. For any object, o_i, and cluster, C_j, if $w_{ij} > 0$, then $dist(o_i, c_j)$ measures how well o_i is represented by c_j, and thus belongs to cluster C_j. Because an object can participate in more than one cluster, the sum of distances to the corresponding cluster centers weighted by the degrees of membership captures how well the object fits the clustering.

Formally, for an object o_i, the **sum of the squared error** (SSE) is given by

$$\text{SSE}(o_i) = \sum_{j=1}^{k} w_{ij}^{p} dist(o_i, c_j)^2, \tag{11.2}$$

where the parameter $p (p \geq 1)$ controls the influence of the degrees of membership. The larger the value of p, the larger the influence of the degrees of membership. Orthogonally, the SSE for a cluster, C_j, is

$$\text{SSE}(C_j) = \sum_{i=1}^{n} w_{ij}^{p} dist(o_i, c_j)^2. \tag{11.3}$$

Finally, the SSE of the clustering is defined as

$$\text{SSE}(\mathcal{C}) = \sum_{i=1}^{n} \sum_{j=1}^{k} w_{ij}^{p} dist(o_i, c_j)^2. \tag{11.4}$$

The SSE can be used to measure how well a fuzzy clustering fits a data set.

Fuzzy clustering is also called *soft clustering* because it allows an object to belong to more than one cluster. It is easy to see that traditional (rigid) clustering, which enforces each object to belong to only one cluster exclusively, is a special case of fuzzy clustering. We defer the discussion of how to compute fuzzy clustering to Section 11.1.3.

11.1.2 Probabilistic Model-Based Clusters

"*Fuzzy clusters (Section 11.1.1) provide the flexibility of allowing an object to participate in multiple clusters. Is there a general framework to specify clusterings where objects may participate in multiple clusters in a probabilistic way?*" In this section, we introduce the general notion of probabilistic model-based clusters to answer this question.

As discussed in Chapter 10, we conduct cluster analysis on a data set because we assume that the objects in the data set in fact belong to different inherent categories. Recall that clustering tendency analysis (Section 10.6.1) can be used to examine whether a data set contains objects that may lead to meaningful clusters. Here, the inherent categories hidden in the data are *latent*, which means they cannot be directly observed. Instead, we have to infer them using the data observed. For example, the topics hidden in a set of reviews in the *AllElectronics* online store are latent because one cannot read the topics directly. However, the topics can be inferred from the reviews because each review is about one or multiple topics.

Therefore, the goal of cluster analysis is to find hidden categories. A data set that is the subject of cluster analysis can be regarded as a sample of the possible instances of the hidden categories, but without any category labels. The clusters derived from cluster analysis are inferred using the data set, and are designed to approach the hidden categories.

Statistically, we can assume that a hidden category is a distribution over the data space, which can be mathematically represented using a probability density function (or distribution function). We call such a hidden category a *probabilistic cluster*. For a probabilistic cluster, C, its probability density function, f, and a point, o, in the data space, $f(o)$ is the relative likelihood that an instance of C appears at o.

Example 11.5 **Probabilistic clusters**. Suppose the digital cameras sold by *AllElectronics* can be divided into two categories: C_1, a consumer line (e.g., point-and-shoot cameras), and C_2, a professional line (e.g., single-lens reflex cameras). Their respective probability density functions, f_1 and f_2, are shown in Figure 11.1 with respect to the attribute *price*.

For a price value of, say, \$1000, $f_1(1000)$ is the relative likelihood that the price of a consumer-line camera is \$1000. Similarly, $f_2(1000)$ is the relative likelihood that the price of a professional-line camera is \$1000.

The probability density functions, f_1 and f_2, cannot be observed directly. Instead, *AllElectronics* can only infer these distributions by analyzing the prices of the digital cameras it sells. Moreover, a camera often does not come with a well-determined category (e.g., "consumer line" or "professional line"). Instead, such categories are typically based on user background knowledge and can vary. For example, a camera in the *prosumer* segment may be regarded at the high end of the consumer line by some customers, and the low end of the professional line by others.

As an analyst at *AllElectronics*, you can consider each category as a probabilistic cluster, and conduct cluster analysis on the price of cameras to approach these categories. ■

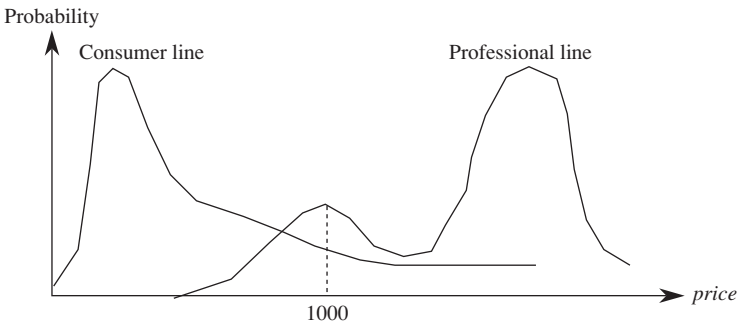

Figure 11.1 The probability density functions of two probabilistic clusters.

Suppose we want to find k probabilistic clusters, $C_1, \ldots, C_k$, through cluster analysis. For a data set, D, of n objects, we can regard D as a finite sample of the possible instances of the clusters. Conceptually, we can assume that D is formed as follows. Each cluster, C_j $(1 \leq j \leq k)$, is associated with a probability, ω_j, that some instance is sampled from the cluster. It is often assumed that $\omega_1, \ldots, \omega_k$ are given as part of the problem setting, and that $\sum_{j=1}^{k} \omega_j = 1$, which ensures that all objects are generated by the k clusters. Here, parameter ω_j captures background knowledge about the relative population of cluster C_j.

We then run the following two steps to generate an object in D. The steps are executed n times in total to generate n objects, $o_1, \ldots, o_n$, in D.

1. Choose a cluster, C_j, according to probabilities $\omega_1, \ldots, \omega_k$.

2. Choose an instance of C_j according to its probability density function, f_j.

The data generation process here is the basic assumption in mixture models. Formally, a **mixture model** assumes that a set of observed objects is a mixture of instances from multiple probabilistic clusters. Conceptually, each observed object is generated independently by two steps: first choosing a probabilistic cluster according to the probabilities of the clusters, and then choosing a sample according to the probability density function of the chosen cluster.

Given data set, D, and k, the number of clusters required, the task of *probabilistic model-based cluster analysis* is to infer a set of k probabilistic clusters that is most likely to generate D using this data generation process. An important question remaining is how we can measure the likelihood that a set of k probabilistic clusters and their probabilities will generate an observed data set.

Consider a set, $\boldsymbol{C}$, of k probabilistic clusters, $C_1, \ldots, C_k$, with probability density functions $f_1, \ldots, f_k$, respectively, and their probabilities, $\omega_1, \ldots, \omega_k$. For an object, o, the probability that o is generated by cluster C_j $(1 \leq j \leq k)$ is given by $P(o|C_j) = \omega_j f_j(o)$. Therefore, the probability that o is generated by the set $\boldsymbol{C}$ of clusters is

$$P(o|\boldsymbol{C}) = \sum_{j=1}^{k} \omega_j f_j(o). \tag{11.5}$$

Since the objects are assumed to have been generated independently, for a data set, $D = \{o_1, \ldots, o_n\}$, of n objects, we have

$$P(D|\boldsymbol{C}) = \prod_{i=1}^{n} P(o_i|\boldsymbol{C}) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j f_j(o_i). \tag{11.6}$$

Now, it is clear that the task of probabilistic model-based cluster analysis on a data set, D, is to find a set $\boldsymbol{C}$ of k probabilistic clusters such that $P(D|\boldsymbol{C})$ is maximized. Maximizing $P(D|\boldsymbol{C})$ is often intractable because, in general, the probability density function

of a cluster can take an arbitrarily complicated form. To make probabilistic model-based clusters computationally feasible, we often compromise by assuming that the probability density functions are parameterized distributions.

Formally, let $o_1, \ldots, o_n$ be the n observed objects, and $\Theta_1, \ldots, \Theta_k$ be the parameters of the k distributions, denoted by $\mathbf{O} = \{o_1, \ldots, o_n\}$ and $\Theta = \{\Theta_1, \ldots, \Theta_k\}$, respectively. Then, for any object, $o_i \in \mathbf{O}$ $(1 \leq i \leq n)$, Eq. (11.5) can be rewritten as

$$P(o_i|\Theta) = \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j), \tag{11.7}$$

where $P_j(o_i|\Theta_j)$ is the probability that o_i is generated from the jth distribution using parameter Θ_j. Consequently, Eq. (11.6) can be rewritten as

$$P(\mathbf{O}|\Theta) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j). \tag{11.8}$$

Using the parameterized probability distribution models, the task of probabilistic model-based cluster analysis is to infer a set of parameters, Θ, that maximizes Eq. (11.8).

Example 11.6 **Univariate Gaussian mixture model.** Let's use univariate Gaussian distributions as an example. That is, we assume that the probability density function of each cluster follows a 1-D Gaussian distribution. Suppose there are k clusters. The two parameters for the probability density function of each cluster are center, μ_j, and standard deviation, σ_j $(1 \leq j \leq k)$. We denote the parameters as $\Theta_j = (\mu_j, \sigma_j)$ and $\Theta = \{\Theta_1, \ldots, \Theta_k\}$. Let the data set be $\mathbf{O} = \{o_1, \ldots, o_n\}$, where o_i $(1 \leq i \leq n)$ is a real number. For any point, $o_i \in \mathbf{O}$, we have

$$P(o_i|\Theta_j) = \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i - \mu_j)^2}{2\sigma^2}}. \tag{11.9}$$

Assuming that each cluster has the same probability, that is $\omega_1 = \omega_2 = \cdots = \omega_k = \frac{1}{k}$, and plugging Eq. (11.9) into Eq. (11.7), we have

$$P(o_i|\Theta) = \frac{1}{k} \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i - \mu_j)^2}{2\sigma^2}}. \tag{11.10}$$

Applying Eq. (11.8), we have

$$P(\mathbf{O}|\Theta) = \frac{1}{k} \prod_{i=1}^{n} \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i - \mu_j)^2}{2\sigma^2}}. \tag{11.11}$$

The task of probabilistic model-based cluster analysis using a univariate Gaussian mixture model is to infer Θ such that Eq. (11.11) is maximized. ■

11.1.3 Expectation-Maximization Algorithm

"How can we compute fuzzy clusterings and probabilistic model-based clusterings?" In this section, we introduce a principled approach. Let's start with a review of the k-means clustering problem and the k-means algorithm studied in Chapter 10.

It can easily be shown that k-means clustering is a special case of fuzzy clustering (Exercise 11.1). The k-means algorithm iterates until the clustering cannot be improved. Each iteration consists of two steps:

The expectation step (E-step): Given the current cluster centers, each object is assigned to the cluster with a center that is closest to the object. Here, an object is expected to belong to the closest cluster.

The maximization step (M-step): Given the cluster assignment, for each cluster, the algorithm adjusts the center so that the sum of the distances from the objects assigned to this cluster and the new center is minimized. That is, the similarity of objects assigned to a cluster is maximized.

We can generalize this two-step method to tackle fuzzy clustering and probabilistic model-based clustering. In general, an **expectation-maximization (EM) algorithm** is a framework that approaches maximum likelihood or maximum a posteriori estimates of parameters in statistical models. In the context of fuzzy or probabilistic model-based clustering, an EM algorithm starts with an initial set of parameters and iterates until the clustering cannot be improved, that is, until the clustering converges or the change is sufficiently small (less than a preset threshold). Each iteration also consists of two steps:

- The **expectation step** assigns objects to clusters according to the current fuzzy clustering or parameters of probabilistic clusters.
- The **maximization step** finds the new clustering or parameters that maximize the SSE in fuzzy clustering (Eq. 11.4) or the expected likelihood in probabilistic model-based clustering.

Example 11.7 **Fuzzy clustering using the EM algorithm.** Consider the six points in Figure 11.2, where the coordinates of the points are also shown. Let's compute two fuzzy clusters using the EM algorithm.

We randomly select two points, say $c_1 = a$ and $c_2 = b$, as the initial centers of the two clusters. The first iteration conducts the expectation step and the maximization step as follows.

In the **E-step**, for each point we calculate its membership degree in each cluster. For any point, o, we assign o to c_1 and c_2 with membership weights

$$\frac{\frac{1}{dist(o,c_1)^2}}{\frac{1}{dist(o,c_1)^2}+\frac{1}{dist(o,c_2)^2}} = \frac{dist(o,c_2)^2}{dist(o,c_1)^2+dist(o,c_2)^2} \text{ and } \frac{dist(o,c_1)^2}{dist(o,c_1)^2+dist(o,c_2)^2},$$

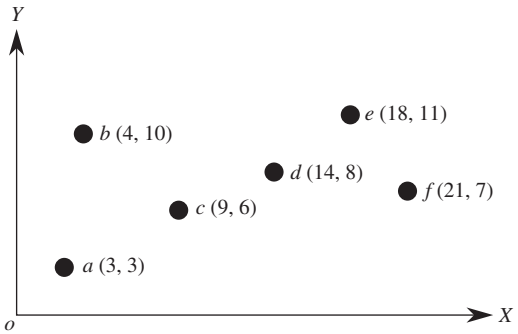

Figure 11.2 Data set for fuzzy clustering.

Table 11.3 Intermediate Results from the First Three Iterations of Example 11.7's EM Algorithm

Iteration	*E-Step*	*M-Step*
1	$M^T = \begin{bmatrix} 1 & 0 & 0.48 & 0.42 & 0.41 & 0.47 \\ 0 & 1 & 0.52 & 0.58 & 0.59 & 0.53 \end{bmatrix}$	$c_1 = (8.47, 5.12)$ $c_2 = (10.42, 8.99)$
2	$M^T = \begin{bmatrix} 0.73 & 0.49 & 0.91 & 0.26 & 0.33 & 0.42 \\ 0.27 & 0.51 & 0.09 & 0.74 & 0.67 & 0.58 \end{bmatrix}$	$c_1 = (8.51, 6.11)$ $c_2 = (14.42, 8.69)$
3	$M^T = \begin{bmatrix} 0.80 & 0.76 & 0.99 & 0.02 & 0.14 & 0.23 \\ 0.20 & 0.24 & 0.01 & 0.98 & 0.86 & 0.77 \end{bmatrix}$	$c_1 = (6.40, 6.24)$ $c_2 = (16.55, 8.64)$

respectively, where $dist(,)$ is the Euclidean distance. The rationale is that, if o is close to c_1 and $dist(o, c_1)$ is small, the membership degree of o with respect to c_1 should be high. We also normalize the membership degrees so that the sum of degrees for an object is equal to 1.

For point a, we have $w_{a,c_1} = 1$ and $w_{a,c_2} = 0$. That is, a exclusively belongs to c_1. For point b, we have $w_{b,c_1} = 0$ and $w_{b,c_2} = 1$. For point c, we have $w_{c,c_1} = \frac{41}{45+41} = 0.48$ and $w_{c,c_2} = \frac{45}{45+41} = 0.52$. The degrees of membership of the other points are shown in the partition matrix in Table 11.3. ■

In the **M-step**, we recalculate the centroids according to the partition matrix, minimizing the SSE given in Eq. (11.4). The new centroid should be adjusted to

$$c_j = \frac{\sum_{\text{each point } o} w_{o,c_j}^2 o}{\sum_{\text{each point } o} w_{o,c_j}^2}, \tag{11.12}$$

where $j = 1, 2$.

In this example,

$$c_1 = \left(\frac{1^2 \times 3 + 0^2 \times 4 + 0.48^2 \times 9 + 0.42^2 \times 14 + 0.41^2 \times 18 + 0.47^2 \times 21}{1^2 + 0^2 + 0.48^2 + 0.42^2 + 0.41^2 + 0.47^2}, \right.$$
$$\left. \frac{1^2 \times 3 + 0^2 \times 10 + 0.48^2 \times 6 + 0.42^2 \times 8 + 0.41^2 \times 11 + 0.47^2 \times 7}{1^2 + 0^2 + 0.48^2 + 0.42^2 + 0.41^2 + 0.47^2} \right)$$
$$= (8.47, 5.12)$$

and

$$c_2 = \left(\frac{0^2 \times 3 + 1^2 \times 4 + 0.52^2 \times 9 + 0.58^2 \times 14 + 0.59^2 \times 18 + 0.53^2 \times 21}{0^2 + 1^2 + 0.52^2 + 0.58^2 + 0.59^2 + 0.53^2}, \right.$$
$$\left. \frac{0^2 \times 3 + 1^2 \times 10 + 0.52^2 \times 6 + 0.58^2 \times 8 + 0.59^2 \times 11 + 0.53^2 \times 7}{0^2 + 1^2 + 0.52^2 + 0.58^2 + 0.59^2 + 0.53^2} \right)$$
$$= (10.42, 8.99).$$

We repeat the iterations, where each iteration contains an E-step and an M-step. Table 11.3 shows the results from the first three iterations. The algorithm stops when the cluster centers converge or the change is small enough.

"*How can we apply the EM algorithm to compute probabilistic model-based clustering?*" Let's use a univariate Gaussian mixture model (Example 11.6) to illustrate.

Example 11.8 **Using the EM algorithm for mixture models.** Given a set of objects, $\mathbf{O} = \{o_1, \ldots, o_n\}$, we want to mine a set of parameters, $\Theta = \{\Theta_1, \ldots, \Theta_k\}$, such that $P(\mathbf{O}|\Theta)$ in Eq. (11.11) is maximized, where $\Theta_j = (\mu_j, \sigma_j)$ are the mean and standard deviation, respectively, of the jth univariate Gaussian distribution, $(1 \leq j \leq k)$.

We can apply the EM algorithm. We assign random values to parameters Θ as the initial values. We then iteratively conduct the E-step and the M-step as follows until the parameters converge or the change is sufficiently small.

In the **E-step**, for each object, $o_i \in \mathbf{O}$ $(1 \leq i \leq n)$, we calculate the probability that o_i belongs to each distribution, that is,

$$P(\Theta_j|o_i, \Theta) = \frac{P(o_i|\Theta_j)}{\sum_{l=1}^{k} P(o_i|\Theta_l)}. \tag{11.13}$$

In the **M-step**, we adjust the parameters Θ so that the expected likelihood $P(\mathbf{O}|\Theta)$ in Eq. (11.11) is maximized. This can be achieved by setting

$$\mu_j = \frac{1}{k} \sum_{i=1}^{n} o_i \frac{P(\Theta_j|o_i, \Theta)}{\sum_{l=1}^{n} P(\Theta_j|o_l, \Theta)} = \frac{1}{k} \frac{\sum_{i=1}^{n} o_i P(\Theta_j|o_i, \Theta)}{\sum_{i=1}^{n} P(\Theta_j|o_i, \Theta)} \tag{11.14}$$

and

$$\sigma_j = \sqrt{\frac{\sum_{i=1}^{n} P(\Theta_j|o_i,\Theta)(o_i - u_j)^2}{\sum_{i=1}^{n} P(\Theta_j|o_i,\Theta)}}. \tag{11.15}$$

■

In many applications, probabilistic model-based clustering has been shown to be effective because it is more general than partitioning methods and fuzzy clustering methods. A distinct advantage is that appropriate statistical models can be used to capture latent clusters. The EM algorithm is commonly used to handle many learning problems in data mining and statistics due to its simplicity. Note that, in general, the EM algorithm may not converge to the optimal solution. It may instead converge to a local maximum. Many heuristics have been explored to avoid this. For example, we could run the EM process multiple times using different random initial values. Furthermore, the EM algorithm can be very costly if the number of distributions is large or the data set contains very few observed data points.

11.2 Clustering High-Dimensional Data

The clustering methods we have studied so far work well when the dimensionality is not high, that is, having less than 10 attributes. There are, however, important applications of high dimensionality. "*How can we conduct cluster analysis on high-dimensional data?*"

In this section, we study approaches to clustering high-dimensional data. Section 11.2.1 starts with an overview of the major challenges and the approaches used. Methods for high-dimensional data clustering can be divided into two categories: subspace clustering methods (Section 11.2.2) and dimensionality reduction methods (Section 11.2.3).

11.2.1 Clustering High-Dimensional Data: Problems, Challenges, and Major Methodologies

Before we present any specific methods for clustering high-dimensional data, let's first demonstrate the needs of cluster analysis on high-dimensional data using examples. We examine the challenges that call for new methods. We then categorize the major methods according to whether they search for clusters in subspaces of the original space, or whether they create a new lower-dimensionality space and search for clusters there.

In some applications, a data object may be described by 10 or more attributes. Such objects are referred to as a high-dimensional data space.

Example 11.9 High-dimensional data and clustering. *AllElectronics* keeps track of the products purchased by every customer. As a customer-relationship manager, you want to cluster customers into groups according to what they purchased from *AllElectronics*.

Table 11.4 Customer Purchase Data

Customer	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}
Ada	1	0	0	0	0	0	0	0	0	0
Bob	0	0	0	0	0	0	0	0	0	1
Cathy	1	0	0	0	1	0	0	0	0	1

The customer purchase data are of very high dimensionality. *AllElectronics* carries tens of thousands of products. Therefore, a customer's purchase profile, which is a vector of the products carried by the company, has tens of thousands of dimensions.

"Are the traditional distance measures, which are frequently used in low-dimensional cluster analysis, also effective on high-dimensional data?" Consider the customers in Table 11.4, where 10 products, $P_1, \ldots, P_{10}$, are used in demonstration. If a customer purchases a product, a 1 is set at the corresponding bit; otherwise, a 0 appears. Let's calculate the Euclidean distances (Eq. 2.16) among Ada, Bob, and Cathy. It is easy to see that

$$dist(\text{Ada}, \text{Bob}) = dist(\text{Bob}, \text{Cathy}) = dist(\text{Ada}, \text{Cathy}) = \sqrt{2}.$$

According to Euclidean distance, the three customers are equivalently similar (or dissimilar) to each other. However, a close look tells us that Ada should be more similar to Cathy than to Bob because Ada and Cathy share one common purchased item, P_1. ■

As shown in Example 11.9, the traditional distance measures can be ineffective on high-dimensional data. Such distance measures may be dominated by the noise in many dimensions. Therefore, clusters in the full, high-dimensional space can be unreliable, and finding such clusters may not be meaningful.

"*Then what kinds of clusters are meaningful on high-dimensional data?*" For cluster analysis of high-dimensional data, we still want to group similar objects together. However, the data space is often too big and too messy. An additional challenge is that we need to find not only clusters, but, for each cluster, a set of attributes that manifest the cluster. In other words, a cluster on high-dimensional data often is defined using a small set of attributes instead of the full data space. Essentially, clustering high-dimensional data should return groups of objects as clusters (as conventional cluster analysis does), *in addition to*, for each cluster, the set of attributes that characterize the cluster. For example, in Table 11.4, to characterize the similarity between Ada and Cathy, P_1 may be returned as the attribute because Ada and Cathy both purchased P_1.

Clustering high-dimensional data is the search for clusters and the space in which they exist. Thus, there are two major kinds of methods:

- *Subspace clustering approaches* search for clusters existing in subspaces of the given high-dimensional data space, where a subspace is defined using a subset of attributes in the full space. Subspace clustering approaches are discussed in Section 11.2.2.

- *Dimensionality reduction approaches* try to construct a much lower-dimensional space and search for clusters in such a space. Often, a method may construct new dimensions by combining some dimensions from the original data. Dimensionality reduction methods are the topic of Section 11.2.4.

In general, clustering high-dimensional data raises several new challenges in addition to those of conventional clustering:

- A major issue is how to create appropriate models for clusters in high-dimensional data. Unlike conventional clusters in low-dimensional spaces, clusters hidden in high-dimensional data are often significantly smaller. For example, when clustering customer-purchase data, we would not expect many users to have similar purchase patterns. Searching for such small but meaningful clusters is like finding needles in a haystack. As shown before, the conventional distance measures can be ineffective. Instead, we often have to consider various more sophisticated techniques that can model correlations and consistency among objects in subspaces.
- There are typically an exponential number of possible subspaces or dimensionality reduction options, and thus the optimal solutions are often computationally prohibitive. For example, if the original data space has 1000 dimensions, and we want to find clusters of dimensionality 10, then there are $\binom{1000}{10} = 2.63 \times 10^{23}$ possible subspaces.

11.2.2 Subspace Clustering Methods

"How can we find subspace clusters from high-dimensional data?" Many methods have been proposed. They generally can be categorized into three major groups: *subspace search methods*, *correlation-based clustering methods*, and *biclustering methods*.

Subspace Search Methods

A subspace search method searches various subspaces for clusters. Here, a cluster is a subset of objects that are similar to each other in a subspace. The similarity is often captured by conventional measures such as distance or density. For example, the CLIQUE algorithm introduced in Section 10.5.2 is a subspace clustering method. It enumerates subspaces and the clusters in those subspaces in a dimensionality-increasing order, and applies antimonotonicity to prune subspaces in which no cluster may exist.

A major challenge that subspace search methods face is how to search a series of subspaces effectively and efficiently. Generally there are two kinds of strategies:

- *Bottom-up approaches* start from low-dimensional subspaces and search higher-dimensional subspaces only when there may be clusters in those higher-dimensional

subspaces. Various pruning techniques are explored to reduce the number of higher-dimensional subspaces that need to be searched. CLIQUE is an example of a bottom-up approach.

- *Top-down approaches* start from the full space and search smaller and smaller subspaces recursively. Top-down approaches are effective only if the *locality assumption* holds, which require that the subspace of a cluster can be determined by the local neighborhood.

Example 11.10 **PROCLUS, a top-down subspace approach.** PROCLUS is a k-medoid-like method that first generates k potential cluster centers for a high-dimensional data set using a sample of the data set. It then refines the subspace clusters iteratively. In each iteration, for each of the current k-medoids, PROCLUS considers the local neighborhood of the medoid in the whole data set, and identifies a subspace for the cluster by minimizing the standard deviation of the distances of the points in the neighborhood to the medoid on each dimension. Once all the subspaces for the medoids are determined, each point in the data set is assigned to the closest medoid according to the corresponding subspace. Clusters and possible outliers are identified. In the next iteration, new medoids replace existing ones if doing so improves the clustering quality. ■

Correlation-Based Clustering Methods

While subspace search methods search for clusters with a similarity that is measured using conventional metrics like distance or density, *correlation-based approaches* can further discover clusters that are defined by advanced correlation models.

Example 11.11 **A correlation-based approach using PCA.** As an example, a *PCA-based approach* first applies PCA (Principal Components Analysis; see Chapter 3) to derive a set of new, uncorrelated dimensions, and then mine clusters in the new space or its subspaces. In addition to PCA, other space transformations may be used, such as the Hough transform or fractal dimensions. ■

For additional details on subspace search methods and correlation-based clustering methods, please refer to the bibliographic notes (Section 11.7).

Biclustering Methods

In some applications, we want to cluster both objects and attributes simultaneously. The resulting clusters are known as *biclusters* and meet four requirements: (1) only a small set of objects participate in a cluster; (2) a cluster only involves a small number of attributes; (3) an object may participate in multiple clusters, or does not participate in any cluster; and (4) an attribute may be involved in multiple clusters, or is not involved in any cluster. Section 11.2.3 discusses biclustering in detail.

11.2.3 Biclustering

In the cluster analysis discussed so far, we cluster objects according to their attribute values. Objects and attributes are not treated in the same way. However, in some applications, objects and attributes are defined in a symmetric way, where data analysis involves searching data matrices for submatrices that show unique patterns as clusters. This kind of clustering technique belongs to the category of biclustering.

This section first introduces two motivating application examples of biclustering—gene expression and recommender systems. You will then learn about the different types of biclusters. Last, we present biclustering methods.

Application Examples

Biclustering techniques were first proposed to address the needs for analyzing gene expression data. A *gene* is a unit of the passing-on of traits from a living organism to its offspring. Typically, a gene resides on a segment of DNA. Genes are critical for all living things because they specify all proteins and functional RNA chains. They hold the information to build and maintain a living organism's cells and pass genetic traits to offspring. Synthesis of a functional gene product, either RNA or protein, relies on the process of gene expression. A *genotype* is the genetic makeup of a cell, an organism, or an individual. *Phenotypes* are observable characteristics of an organism. *Gene expression* is the most fundamental level in genetics in that genotypes cause phenotypes.

Using *DNA chips* (also known as *DNA microarrays*) and other biological engineering techniques, we can measure the expression level of a large number (possibly all) of an organism's genes, in a number of different experimental conditions. Such conditions may correspond to different time points in an experiment or samples from different organs. Roughly speaking, the *gene expression data* or *DNA microarray data* are conceptually a gene-sample/condition matrix, where each row corresponds to one gene, and each column corresponds to one sample or condition. Each element in the matrix is a real number and records the expression level of a gene under a specific condition. Figure 11.3 shows an illustration.

From the clustering viewpoint, an interesting issue is that a gene expression data matrix can be analyzed in two dimensions—the gene dimension and the sample/condition dimension.

- When analyzing in the *gene dimension*, we treat each gene as an object and treat the samples/conditions as attributes. By mining in the gene dimension, we may find patterns shared by multiple genes, or cluster genes into groups. For example, we may find a group of genes that express themselves similarly, which is highly interesting in bioinformatics, such as in finding pathways.
- When analyzing in the *sample/condition dimension*, we treat each sample/condition as an object and treat the genes as attributes. In this way, we may find patterns of samples/conditions, or cluster samples/conditions into groups. For example, we may find the differences in gene expression by comparing a group of tumor samples and nontumor samples.

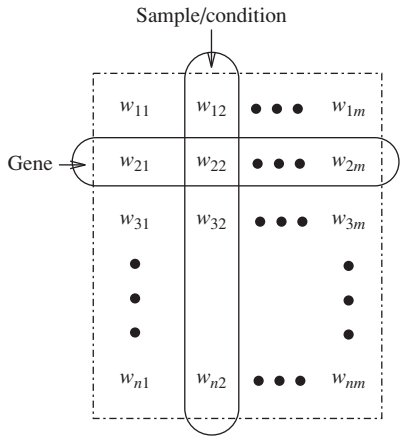

Figure 11.3 Microarrary data matrix.

Example 11.12 **Gene expression.** Gene expression matrices are popular in bioinformatics research and development. For example, an important task is to classify a new gene using the expression data of the gene and that of other genes in known classes. Symmetrically, we may classify a new sample (e.g., a new patient) using the expression data of the sample and that of samples in known classes (e.g., tumor and nontumor). Such tasks are invaluable in understanding the mechanisms of diseases and in clinical treatment. ■

As can be seen, many gene expression data mining problems are highly related to cluster analysis. However, a challenge here is that, instead of clustering in one dimension (e.g., gene or sample/condition), in many cases we need to cluster in two dimensions simultaneously (e.g., both gene and sample/condition). Moreover, unlike the clustering models we have discussed so far, a cluster in a gene expression data matrix is a *submatrix* and usually has the following characteristics:

- Only a small set of genes participate in the cluster.
- The cluster involves only a small subset of samples/conditions.
- A gene may participate in multiple clusters, or may not participate in any cluster.
- A sample/condition may be involved in multiple clusters, or may not be involved in any cluster.

To find clusters in gene-sample/condition matrices, we need new clustering techniques that meet the following requirements for *biclustering*:

- A cluster of genes is defined using only a subset of samples/conditions.
- A cluster of samples/conditions is defined using only a subset of genes.

- The clusters are neither *exclusive* (e.g., where one gene can participate in multiple clusters) nor *exhaustive* (e.g., where a gene may not participate in any cluster).

Biclustering is useful not only in bioinformatics, but also in other applications as well. Consider recommender systems as an example.

Example 11.13 Using biclustering for a recommender system. *AllElectronics* collects data from customers' evaluations of products and uses the data to recommend products to customers. The data can be modeled as a customer-product matrix, where each row represents a customer, and each column represents a product. Each element in the matrix represents a customer's evaluation of a product, which may be a score (e.g., like, like somewhat, not like) or purchase behavior (e.g., buy or not). Figure 11.4 illustrates the structure.

The customer-product matrix can be analyzed in two dimensions: the *customer* dimension and the *product* dimension. Treating each customer as an object and products as attributes, *AllElectronics* can find customer groups that have similar preferences or purchase patterns. Using products as objects and customers as attributes, *AllElectronics* can mine product groups that are similar in customer interest.

Moreover, *AllElectronics* can mine clusters in both customers and products simultaneously. Such a cluster contains a subset of customers and involves a subset of products. For example, *AllElectronics* is highly interested in finding a group of customers who all like the same group of products. Such a cluster is a submatrix in the customer-product matrix, where all elements have a high value. Using such a cluster, *AllElectronics* can make recommendations in two directions. First, the company can recommend products to new customers who are similar to the customers in the cluster. Second, the company can recommend to customers new products that are similar to those involved in the cluster. ■

As with biclusters in a gene expression data matrix, the biclusters in a customer-product matrix usually have the following characteristics:

- Only a small set of customers participate in a cluster.
- A cluster involves only a small subset of products.
- A customer can participate in multiple clusters, or may not participate in any cluster.

	Products			
Customers	w_{11}	w_{12}	$\cdots$	w_{1m}
	w_{21}	w_{22}	$\cdots$	w_{2m}
	$\cdots$	$\cdots$	$\cdots$	$\cdots$
	w_{n1}	w_{n2}	$\cdots$	w_{nm}

Figure 11.4 Customer–product matrix.

- A product may be involved in multiple clusters, or may not be involved in any cluster.

Biclustering can be applied to customer-product matrices to mine clusters satisfying these requirements.

Types of Biclusters

"How can we model biclusters and mine them?" Let's start with some basic notation. For the sake of simplicity, we will use "genes" and "conditions" to refer to the two dimensions in our discussion. Our discussion can easily be extended to other applications. For example, we can simply replace "genes" and "conditions" by "customers" and "products" to tackle the customer-product biclustering problem.

Let $A = \{a_1, \ldots, a_n\}$ be a set of genes and $B = \{b_1, \ldots, b_m\}$ be a set of conditions. Let $E = [e_{ij}]$ be a gene expression data matrix, that is, a gene-condition matrix, where $1 \leq i \leq n$ and $1 \leq j \leq m$. A submatrix $I \times J$ is defined by a subset $I \subseteq A$ of genes and a subset $J \subseteq B$ of conditions. For example, in the matrix shown in Figure 11.5, $\{a_1, a_{33}, a_{86}\} \times \{b_6, b_{12}, b_{36}, b_{99}\}$ is a submatrix.

A bicluster is a submatrix where genes and conditions follow consistent patterns. We can define different types of biclusters based on such patterns.

- As the simplest case, a submatrix $I \times J$ ($I \subseteq A, J \subseteq B$) is a **bicluster with constant values** if for any $i \in I$ and $j \in J$, $e_{ij} = c$, where c is a constant. For example, the submatrix $\{a_1, a_{33}, a_{86}\} \times \{b_6, b_{12}, b_{36}, b_{99}\}$ in Figure 11.5 is a bicluster with constant values.
- A bicluster is interesting if each row has a constant value, though different rows may have different values. A **bicluster with constant values on rows** is a submatrix $I \times J$ such that for any $i \in I$ and $j \in J$, $e_{ij} = c + \alpha_i$, where α_i is the adjustment for row i. For example, Figure 11.6 shows a bicluster with constant values on rows.

  Symmetrically, a **bicluster with constant values on columns** is a submatrix $I \times J$ such that for any $i \in I$ and $j \in J$, $e_{ij} = c + \beta_j$, where β_j is the adjustment for column j.

	$\cdots$	b_6	$\cdots$	b_{12}	$\cdots$	b_{36}	$\cdots$	b_{99} $\cdots$
a_1	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$	60 $\cdots$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$ $\cdots$
a_{33}	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$	60 $\cdots$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$ $\cdots$
a_{86}	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$	60 $\cdots$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$ $\cdots$

Figure 11.5 Gene-condition matrix, a submatrix, and a bicluster.

- More generally, a bicluster is interesting if the rows change in a synchronized way with respect to the columns and vice versa. Mathematically, a **bicluster with coherent values** (also known as **a pattern-based cluster**) is a submatrix $I \times J$ such that for any $i \in I$ and $j \in J$, $e_{ij} = c + \alpha_i + \beta_j$, where α_i and β_j are the adjustment for row i and column j, respectively. For example, Figure 11.7 shows a bicluster with coherent values.

  It can be shown that $I \times J$ is a bicluster with coherent values if and only if for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, then $e_{i_1 j_1} - e_{i_2 j_1} = e_{i_1 j_2} - e_{i_2 j_2}$. Moreover, instead of using addition, we can define a bicluster with coherent values using multiplication, that is, $e_{ij} = c \cdot (\alpha_i \cdot \beta_j)$. Clearly, biclusters with constant values on rows or columns are special cases of biclusters with coherent values.

- In some applications, we may only be interested in the up- or down-regulated changes across genes or conditions without constraining the exact values. A **bicluster with coherent evolutions on rows** is a submatrix $I \times J$ such that for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, $(e_{i_1 j_1} - e_{i_1 j_2})(e_{i_2 j_1} - e_{i_2 j_2}) \geq 0$. For example, Figure 11.8 shows a bicluster with coherent evolutions on rows. Symmetrically, we can define biclusters with coherent evolutions on columns.

Next, we study how to mine biclusters.

10	10	10	10	10
20	20	20	20	20
50	50	50	50	50
0	0	0	0	0

Figure 11.6 Bicluster with constant values on rows.

10	50	30	70	20
20	60	40	80	30
50	90	70	110	60
0	40	20	60	10

Figure 11.7 Bicluster with coherent values.

10	50	30	70	20
20	100	50	1000	30
50	100	90	120	80
0	80	20	100	10

Figure 11.8 Bicluster with coherent evolutions on rows.

Biclustering Methods

The previous specification of the types of biclusters only considers ideal cases. In real data sets, such perfect biclusters rarely exist. When they do exist, they are usually very small. Instead, random noise can affect the readings of e_{ij} and thus prevent a bicluster in nature from appearing in a perfect shape.

There are two major types of methods for discovering biclusters in data that may come with noise. **Optimization-based methods** conduct an iterative search. At each iteration, the submatrix with the highest significance score is identified as a bicluster. The process terminates when a user-specified condition is met. Due to cost concerns in computation, greedy search is often employed to find local optimal biclusters. **Enumeration methods** use a tolerance threshold to specify the degree of noise allowed in the biclusters to be mined, and then tries to enumerate all submatrices of biclusters that satisfy the requirements. We use the δ-Cluster and MaPle algorithms as examples to illustrate these ideas.

Optimization Using the δ-Cluster Algorithm

For a submatrix, $I \times J$, the mean of the ith row is

$$e_{iJ} = \frac{1}{|J|} \sum_{j \in J} e_{ij}. \tag{11.16}$$

Symmetrically, the mean of the jth column is

$$e_{Ij} = \frac{1}{|I|} \sum_{i \in I} e_{ij}. \tag{11.17}$$

The mean of all elements in the submatrix is

$$e_{IJ} = \frac{1}{|I||J|} \sum_{i \in I, j \in J} e_{ij} = \frac{1}{|I|} \sum_{i \in I} e_{iJ} = \frac{1}{|J|} \sum_{j \in J} e_{Ij}. \tag{11.18}$$

The quality of the submatrix as a bicluster can be measured by the *mean-squared residue* value as

$$H(I \times J) = \frac{1}{|I||J|} \sum_{i \in I, j \in J} (e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2. \tag{11.19}$$

Submatrix $I \times J$ is a δ-**bicluster** if $H(I \times J) \leq \delta$, where $\delta \geq 0$ is a threshold. When $\delta = 0$, $I \times J$ is a perfect bicluster with coherent values. By setting $\delta > 0$, a user can specify the tolerance of average noise per element against a perfect bicluster, because in Eq. (11.19) the residue on each element is

$$\text{residue}(e_{ij}) = e_{ij} - e_{iJ} - e_{Ij} + e_{IJ}. \tag{11.20}$$

A *maximal δ-bicluster* is a δ-bicluster $I \times J$ such that there does not exist another δ-bicluster $I' \times J'$, and $I \subseteq I'$, $J \subseteq J'$, and at least one inequality holds. Finding the

maximal δ-bicluster of the largest size is computationally costly. Therefore, we can use a heuristic greedy search method to obtain a local optimal cluster. The algorithm works in two phases.

- In the *deletion phase*, we start from the whole matrix. While the mean-squared residue of the matrix is over δ, we iteratively remove rows and columns. At each iteration, for each row i, we compute the *mean-squared residue* as

$$d(i) = \frac{1}{|J|}\sum_{j\in J}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2. \tag{11.21}$$

  Moreover, for each column j, we compute the *mean-squared residue* as

$$d(j) = \frac{1}{|I|}\sum_{i\in I}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2. \tag{11.22}$$

  We remove the row or column of the largest mean-squared residue. At the end of this phase, we obtain a submatrix $I \times J$ that is a δ-bicluster. However, the submatrix may not be maximal.

- In the *addition phase*, we iteratively expand the δ-bicluster $I \times J$ obtained in the deletion phase as long as the δ-bicluster requirement is maintained. At each iteration, we consider rows and columns that are not involved in the current bicluster $I \times J$ by calculating their mean-squared residues. A row or column of the smallest mean-squared residue is added into the current δ-bicluster.

This greedy algorithm can find one δ-bicluster only. To find multiple biclusters that do not have heavy overlaps, we can run the algorithm multiple times. After each execution where a δ-bicluster is output, we can replace the elements in the output bicluster by random numbers. Although the greedy algorithm may find neither the optimal biclusters nor all biclusters, it is very fast even on large matrices.

Enumerating All Biclusters Using MaPle

As mentioned, a submatrix $I \times J$ is a bicluster with coherent values if and only if for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, $e_{i_1 j_1} - e_{i_2 j_1} = e_{i_1 j_2} - e_{i_2 j_2}$. For any 2×2 submatrix of $I \times J$, we can define a *p-score* as

$$p\text{-score}\begin{pmatrix} e_{i_1 j_1} & e_{i_1 j_2} \\ e_{i_2 j_1} & e_{i_2 j_2} \end{pmatrix} = |(e_{i_1 j_1} - e_{i_2 j_1}) - (e_{i_1 j_2} - e_{i_2 j_2})|. \tag{11.23}$$

A submatrix $I \times J$ is a δ-**pCluster** (for *p*attern-based *cluster*) if the p-score of every 2×2 submatrix of $I \times J$ is at most δ, where $\delta \geq 0$ is a threshold specifying a user's tolerance of noise against a perfect bicluster. Here, the p-score controls the noise on every element in a bicluster, while the mean-squared residue captures the average noise.

An interesting property of δ-pCluster is that if $I \times J$ is a δ-pCluster, then every $x \times y$ $(x, y \geq 2)$ submatrix of $I \times J$ is also a δ-pCluster. This monotonicity enables

us to obtain a succinct representation of nonredundant δ-pClusters. A δ-pCluster is maximal if no more rows or columns can be added into the cluster while maintaining the δ-pCluster property. To avoid redundancy, instead of finding all δ-pClusters, we only need to compute all maximal δ-pClusters.

MaPle is an algorithm that enumerates all maximal δ-pClusters. It systematically enumerates every combination of conditions using a set enumeration tree and a depth-first search. This enumeration framework is the same as the pattern-growth methods for frequent pattern mining (Chapter 6). Consider gene expression data. For each condition combination, J, MaPle finds the maximal subsets of genes, I, such that $I \times J$ is a δ-pCluster. If $I \times J$ is not a submatrix of another δ-pCluster, then $I \times J$ is a maximal δ-pCluster.

There may be a huge number of condition combinations. MaPle prunes many unfruitful combinations using the monotonicity of δ-pClusters. For a condition combination, J, if there does not exist a set of genes, I, such that $I \times J$ is a δ-pCluster, then we do not need to consider any superset of J. Moreover, we should consider $I \times J$ as a candidate of a δ-pCluster only if for every $(|J| - 1)$-subset J' of J, $I \times J'$ is a δ-pCluster. MaPle also employs several pruning techniques to speed up the search while retaining the completeness of returning all maximal δ-pClusters. For example, when examining a current δ-pCluster, $I \times J$, MaPle collects all the genes and conditions that may be added to expand the cluster. If these candidate genes and conditions together with I and J form a submatrix of a δ-pCluster that has already been found, then the search of $I \times J$ and any superset of J can be pruned. Interested readers may refer to the bibliographic notes for additional information on the MaPle algorithm (Section 11.7).

An interesting observation here is that the search for maximal δ-pClusters in MaPle is somewhat similar to mining frequent closed itemsets. Consequently, MaPle borrows the depth-first search framework and ideas from the pruning techniques of pattern-growth methods for frequent pattern mining. This is an example where frequent pattern mining and cluster analysis may share similar techniques and ideas.

An advantage of MaPle and the other algorithms that enumerate all biclusters is that they guarantee the completeness of the results and do not miss any overlapping biclusters. However, a challenge for such enumeration algorithms is that they may become very time consuming if a matrix becomes very large, such as a customer-purchase matrix of hundreds of thousands of customers and millions of products.

11.2.4 Dimensionality Reduction Methods and Spectral Clustering

Subspace clustering methods try to find clusters in subspaces of the original data space. In some situations, it is more effective to construct a new space instead of using subspaces of the original data. This is the motivation behind dimensionality reduction methods for clustering high-dimensional data.

Example 11.14 Clustering in a derived space. Consider the three clusters of points in Figure 11.9. It is not possible to cluster these points in any subspace of the original space, $X \times Y$, because

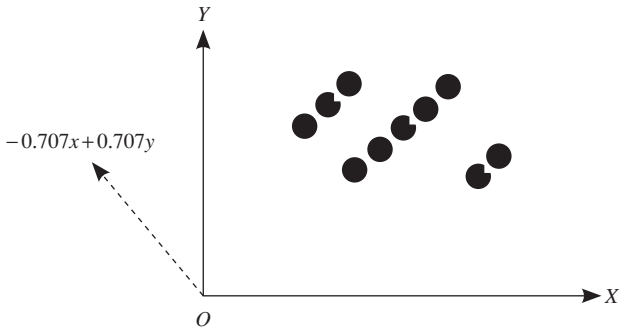

Figure 11.9 Clustering in a derived space may be more effective.

all three clusters would end up being projected onto overlapping areas in the x and y axes. What if, instead, we construct a new dimension, $-\frac{\sqrt{2}}{2}x + \frac{\sqrt{2}}{2}y$ (shown as a dashed line in the figure)? By projecting the points onto this new dimension, the three clusters become apparent. ■

Although Example 11.14 involves only two dimensions, the idea of constructing a new space (so that any clustering structure that is hidden in the data becomes well manifested) can be extended to high-dimensional data. Preferably, the newly constructed space should have low dimensionality.

There are many dimensionality reduction methods. A straightforward approach is to apply feature selection and extraction methods to the data set such as those discussed in Chapter 3. However, such methods may not be able to detect the clustering structure. Therefore, methods that combine feature extraction and clustering are preferred. In this section, we introduce *spectral clustering*, a group of methods that are effective in high-dimensional data applications.

Figure 11.10 shows the general framework for spectral clustering approaches. The Ng-Jordan-Weiss algorithm is a spectral clustering method. Let's have a look at each step of the framework. In doing so, we also note special conditions that apply to the Ng-Jordan-Weiss algorithm as an example.

Given a set of objects, $o_1, \ldots, o_n$, the distance between each pair of objects, $dist(o_i, o_j)$ $(1 \leq i, j \leq n)$, and the desired number k of clusters, a spectral clustering approach works as follows.

1. Using the distance measure, calculate an *affinity matrix*, W, such that

$$W_{ij} = e^{-\frac{dist(o_i,o_j)}{\sigma^2}},$$

where σ is a scaling parameter that controls how fast the affinity W_{ij} decreases as $dist(o_i, o_j)$ increases. In the Ng-Jordan-Weiss algorithm, W_{ii} is set to 0.

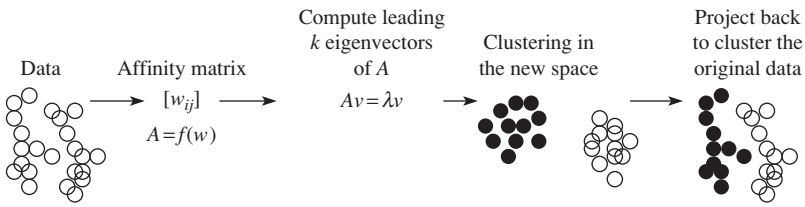

Figure 11.10 The framework of spectral clustering approaches. *Source:* Adapted from Slide 8 at *http://videolectures.net/micued08_azran_mcl/*.

2. Using the affinity matrix W, derive a matrix $A = f(W)$. The way in which this is done can vary. The Ng-Jordan-Weiss algorithm defines a matrix, D, as a diagonal matrix such that D_{ii} is the sum of the ith row of W, that is,

$$D_{ii} = \sum_{j=1}^{n} W_{ij}. \tag{11.24}$$

A is then set to

$$A = D^{-\frac{1}{2}} W D^{-\frac{1}{2}}. \tag{11.25}$$

3. Find the k leading eigenvectors of A. Recall that the *eigenvectors* of a square matrix are the nonzero vectors that remain proportional to the original vector after being multiplied by the matrix. Mathematically, a vector $\boldsymbol{v}$ is an eigenvector of matrix A if $A\boldsymbol{v} = \lambda \boldsymbol{v}$, where λ is called the corresponding *eigenvalue*. This step derives k new dimensions from A, which are based on the affinity matrix W. Typically, k should be much smaller than the dimensionality of the original data.

The Ng-Jordan-Weiss algorithm computes the k eigenvectors with the largest eigenvalues $x_1, \ldots, x_k$ of A.

4. Using the k leading eigenvectors, project the original data into the new space defined by the k leading eigenvectors, and run a clustering algorithm such as k-means to find k clusters.

The Ng-Jordan-Weiss algorithm stacks the k largest eigenvectors in columns to form a matrix $X = [x_1 x_2 \cdots x_k] \in \mathbb{R}^{n \times k}$. The algorithm forms a matrix Y by renormalizing each row in X to have unit length, that is,

$$Y_{ij} = \frac{X_{ij}}{\sqrt{\sum_{j=1}^{k} X_{ij}^2}}. \tag{11.26}$$

The algorithm then treats each row in Y as a point in the k-dimensional space $\mathbb{R}^k$, and runs k-means (or any other algorithm serving the partitioning purpose) to cluster the points into k clusters.

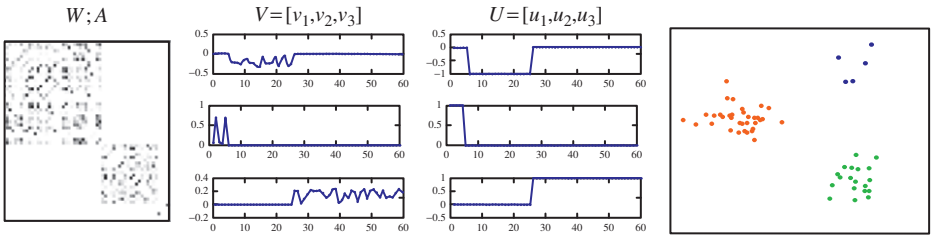

Figure 11.11 The new dimensions and the clustering results of the Ng-Jordan-Weiss algorithm. *Source:* Adapted from Slide 9 at *http://videolectures.net/micued08_azran_mcl/*.

5. Assign the original data points to clusters according to how the transformed points are assigned in the clusters obtained in step 4.

   In the Ng-Jordan-Weiss algorithm, the original object o_i is assigned to the jth cluster if and only if matrix Y's row i is assigned to the jth cluster as a result of step 4.

In spectral clustering methods, the dimensionality of the new space is set to the desired number of clusters. This setting expects that each new dimension should be able to manifest a cluster.

Example 11.15 The Ng-Jordan-Weiss algorithm. Consider the set of points in Figure 11.11. The data set, the affinity matrix, the three largest eigenvectors, and the normalized vectors are shown. Note that with the three new dimensions (formed by the three largest eigenvectors), the clusters are easily detected. ■

Spectral clustering is effective in high-dimensional applications such as image processing. Theoretically, it works well when certain conditions apply. Scalability, however, is a challenge. Computing eigenvectors on a large matrix is costly. Spectral clustering can be combined with other clustering methods, such as biclustering. Additional information on other dimensionality reduction clustering methods, such as kernel PCA, can be found in the bibliographic notes (Section 11.7).

11.3 Clustering Graph and Network Data

Cluster analysis on graph and network data extracts valuable knowledge and information. Such data are increasingly popular in many applications. We discuss applications and challenges of clustering graph and network data in Section 11.3.1. Similarity measures for this form of clustering are given in Section 11.3.2. You will learn about graph clustering methods in Section 11.3.3.

In general, the terms *graph* and *network* can be used interchangeably. In the rest of this section, we mainly use the term *graph*.

11.3.1 Applications and Challenges

As a customer relationship manager at *AllElectronics*, you notice that a lot of data relating to customers and their purchase behavior can be preferably modeled using graphs.

Example 11.16 **Bipartite graph.** The customer purchase behavior at *AllElectronics* can be represented in a *bipartite graph*. In a bipartite graph, vertices can be divided into two disjoint sets so that each edge connects a vertex in one set to a vertex in the other set. For the *AllElectronics* customer purchase data, one set of vertices represents customers, with one customer per vertex. The other set represents products, with one product per vertex. An edge connects a customer to a product, representing the purchase of the product by the customer. Figure 11.12 shows an illustration.

"*What kind of knowledge can we obtain by a cluster analysis of the customer-product bipartite graph?*" By clustering the customers such that those customers buying similar sets of products are placed into one group, a customer relationship manager can make product recommendations. For example, suppose Ada belongs to a customer cluster in which most of the customers purchased a digital camera in the last 12 months, but Ada has yet to purchase one. As manager, you decide to recommend a digital camera to her.

Alternatively, we can cluster products such that those products purchased by similar sets of customers are grouped together. This clustering information can also be used for product recommendations. For example, if a digital camera and a high-speed flash memory card belong to the same product cluster, then when a customer purchases a digital camera, we can recommend the high-speed flash memory card. ■

Bipartite graphs are widely used in many applications. Consider another example.

Example 11.17 **Web search engines.** In web search engines, search logs are archived to record user queries and the corresponding *click-through information*. (The click-through information tells us on which pages, given as a result of a search, the user clicked.) The query and click-through information can be represented using a bipartite graph, where the two sets

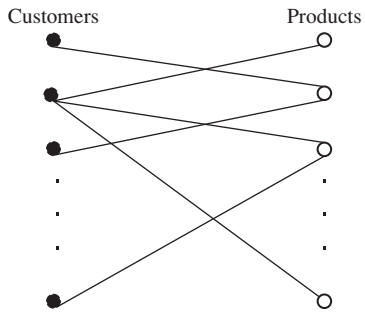

Figure 11.12 Bipartite graph representing customer-purchase data.

of vertices correspond to queries and web pages, respectively. An edge links a query to a web page if a user clicks the web page when asking the query. Valuable information can be obtained by cluster analyses on the query–web page bipartite graph. For instance, we may identify queries posed in different languages, but that mean the same thing, if the click-through information for each query is similar.

As another example, all the web pages on the Web form a directed graph, also known as the *web graph*, where each web page is a vertex, and each hyperlink is an edge pointing from a source page to a destination page. Cluster analysis on the web graph can disclose communities, find hubs and authoritative web pages, and detect web spams. ■

In addition to bipartite graphs, cluster analysis can also be applied to other types of graphs, including general graphs, as elaborated Example 11.18.

Example 11.18 **Social network.** A *social network* is a social structure. It can be represented as a graph, where the vertices are individuals or organizations, and the links are interdependencies between the vertices, representing friendship, common interests, or collaborative activities. *AllElectronics*' customers form a social network, where each customer is a vertex, and an edge links two customers if they know each other.

As customer relationship manager, you are interested in finding useful information that can be derived from *AllElectronics*' social network through cluster analysis. You obtain clusters from the network, where customers in a cluster know each other or have friends in common. Customers within a cluster may influence one another regarding purchase decision making. Moreover, communication channels can be designed to inform the "heads" of clusters (i.e., the "best" connected people in the clusters), so that promotional information can be spread out quickly. Thus, you may use customer clustering to promote sales at *AllElectronics*.

As another example, the authors of scientific publications form a social network, where the authors are vertices and two authors are connected by an edge if they coauthored a publication. The network is, in general, a weighted graph because an edge between two authors can carry a weight representing the strength of the collaboration such as how many publications the two authors (as the end vertices) coauthored. Clustering the coauthor network provides insight as to communities of authors and patterns of collaboration. ■

"Are there any challenges specific to cluster analysis on graph and network data?" In most of the clustering methods discussed so far, objects are represented using a set of attributes. A unique feature of graph and network data is that only objects (as vertices) and relationships between them (as edges) are given. No dimensions or attributes are explicitly defined. To conduct cluster analysis on graph and network data, there are two major new challenges.

- *"How can we measure the similarity between two objects on a graph accordingly?"* Typically, we cannot use conventional distance measures, such as Euclidean distance. Instead, we need to develop new measures to quantify the similarity. Such

measures often are not metric, and thus raise new challenges regarding the development of efficient clustering methods. Similarity measures for graphs are discussed in Section 11.3.2.

- *"How can we design clustering models and methods that are effective on graph and network data?"* Graph and network data are often complicated, carrying topological structures that are more sophisticated than traditional cluster analysis applications. Many graph data sets are large, such as the web graph containing at least tens of billions of web pages in the publicly indexable Web. Graphs can also be sparse where, on average, a vertex is connected to only a small number of other vertices in the graph. To discover accurate and useful knowledge hidden deep in the data, a good clustering method has to accommodate these factors. Clustering methods for graph and network data are introduced in Section 11.3.3.

11.3.2 Similarity Measures

"How can we measure the similarity or distance between two vertices in a graph?" In our discussion, we examine two types of measures: *geodesic distance* and *distance based on random walk*.

Geodesic Distance

A simple measure of the distance between two vertices in a graph is the shortest path between the vertices. Formally, the **geodesic distance** between two vertices is the length in terms of the number of edges of the shortest path between the vertices. For two vertices that are not connected in a graph, the geodesic distance is defined as infinite.

Using geodesic distance, we can define several other useful measurements for graph analysis and clustering. Given a graph $G = (V, E)$, where V is the set of vertices and E is the set of edges, we define the following:

- For a vertext $v \in V$, the **eccentricity** of v, denoted $eccen(v)$, is the largest geodesic distance between v and any other vertex $u \in V - \{v\}$. The eccentricity of v captures how far away v is from its remotest vertex in the graph.
- The **radius** of graph G is the minimum eccentricity of all vertices. That is,

$$r = \min_{v \in V} eccen(v). \tag{11.27}$$

  The radius captures the distance between the "most central point" and the "farthest border" of the graph.
- The **diameter** of graph G is the maximum eccentricity of all vertices. That is,

$$d = \max_{v \in V} eccen(v). \tag{11.28}$$

  The diameter represents the largest distance between any pair of vertices.
- A **peripheral vertex** is a vertex that achieves the diameter.

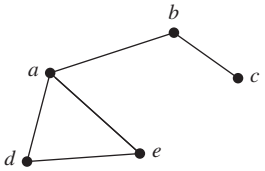

Figure 11.13 A graph, G, where vertices c, d, and e are peripheral.

Example 11.19 **Measurements based on geodesic distance.** Consider graph G in Figure 11.13. The eccentricity of a is 2, that is, $eccen(a) = 2$, $eccen(b) = 2$, and $eccen(c) = eccen(d) = eccen(e) = 3$. Thus, the radius of G is 2, and the diameter is 3. Note that it is not necessary that $d = 2 \times r$. Vertices c, d, and e are peripheral vertices. ■

SimRank: Similarity Based on Random Walk and Structural Context

For some applications, geodesic distance may be inappropriate in measuring the similarity between vertices in a graph. Here we introduce SimRank, a similarity measure based on random walk and on the structural context of the graph. In mathematics, a *random walk* is a trajectory that consists of taking successive random steps.

Example 11.20 **Similarity between people in a social network.** Let's consider measuring the similarity between two vertices in the *AllElectronics* customer social network of Example 11.18. Here, similarity can be explained as the closeness between two participants in the network, that is, how close two people are in terms of the relationship represented by the social network.

"*How well can the geodesic distance measure similarity and closeness in such a network?*" Suppose Ada and Bob are two customers in the network, and the network is undirected. The geodesic distance (i.e., the length of the shortest path between Ada and Bob) is the shortest path that a message can be passed from Ada to Bob and vice versa. However, this information is not useful for *AllElectronics*' customer relationship management because the company typically does not want to send a specific message from one customer to another. Therefore, geodesic distance does not suit the application.

"*What does similarity mean in a social network?*" We consider two ways to define similarity:

- Two customers are considered similar to one another if they have similar neighbors in the social network. This heuristic is intuitive because, in practice, two people receiving recommendations from a good number of common friends often make similar decisions. This kind of similarity is based on the local structure (i.e., the *neighborhoods*) of the vertices, and thus is called *structural context–based similarity*.

- Suppose *AllElectronics* sends promotional information to both Ada and Bob in the social network. Ada and Bob may randomly forward such information to their friends (or *neighbors*) in the network. The closeness between Ada and Bob can then be measured by the likelihood that other customers simultaneously receive the promotional information that was originally sent to Ada and Bob. This kind of similarity is based on the random walk reachability over the network, and thus is referred to as *similarity based on random walk*. ■

Let's have a closer look at what is meant by similarity based on structural context, and similarity based on random walk.

The intuition behind similarity based on structural context is that two vertices in a graph are similar if they are connected to similar vertices. To measure such similarity, we need to define the notion of individual neighborhood. In a directed graph $G = (V, E)$, where V is the set of vertices and $E \subseteq V \times V$ is the set of edges, for a vertex $v \in V$, the *individual in-neighborhood* of v is defined as

$$I(v) = \{u | (u, v) \in E\}. \tag{11.29}$$

Symmetrically, we define the *individual out-neighborhood* of v as

$$O(v) = \{w | (v, w) \in E\}. \tag{11.30}$$

Following the intuition illustrated in Example 11.20, we define SimRank, a structural-context similarity, with a value that is between 0 and 1 for any pair of vertices. For any vertex, $v \in V$, the similarity between the vertex and itself is $s(v, v) = 1$ because the neighborhoods are identical. For vertices $u, v \in V$ such that $u \neq v$, we can define

$$s(u, v) = \frac{C}{|I(u)||I(v)|} \sum_{x \in I(u)} \sum_{y \in I(v)} s(x, y), \tag{11.31}$$

where C is a constant between 0 and 1. A vertex may not have any in-neighbors. Thus, we define Eq. (11.31) to be 0 when either $I(u)$ or $I(v)$ is $\emptyset$. Parameter C specifies the rate of decay as similarity is propagated across edges.

"*How can we compute SimRank?*" A straightforward method iteratively evaluates Eq. (11.31) until a fixed point is reached. Let $s_i(u, v)$ be the SimRank score calculated at the ith round. To begin, we set

$$s_0(u, v) = \begin{cases} 0 & \text{if } u \neq v \\ 1 & \text{if } u = v. \end{cases} \tag{11.32}$$

We use Eq. (11.31) to compute s_{i+1} from s_i as

$$s_{i+1}(u, v) = \frac{C}{|I(u)||I(v)|} \sum_{x \in I(u)} \sum_{y \in I(v)} s_i(x, y). \tag{11.33}$$

It can be shown that $\lim_{i \to \infty} s_i(u, v) = s(u, v)$. Additional methods for approximating SimRank are given in the bibliographic notes (Section 11.7).

Now, let's consider similarity based on random walk. A directed graph is *strongly connected* if, for any two nodes u and v, there is a path from u to v and another path from v to u. In a strongly connected graph, $G = (V, E)$, for any two vertices, $u, v \in V$, we can define the *expected distance* from u to v as

$$d(u, v) = \sum_{t: u \rightsquigarrow v} P[t] l(t), \tag{11.34}$$

where $u \rightsquigarrow v$ is a path starting from u and ending at v that may contain cycles but does not reach v until the end. For a *traveling tour*, $t = w_1 \to w_2 \to \cdots \to w_k$, its length is $l(t) = k - 1$. The probability of the tour is defined as

$$P[t] = \begin{cases} \prod_{i=1}^{k-1} \frac{1}{|O(w_i)|} & \text{if } l(t) > 0 \\ 0 & \text{if } l(t) = 0. \end{cases} \tag{11.35}$$

To measure the probability that a vertex w receives a message that originated simultaneously from u and v, we extend the expected distance to the notion of *expected meeting distance*, that is,

$$m(u, v) = \sum_{t: (u,v) \rightsquigarrow (x,x)} P[t] l(t), \tag{11.36}$$

where $(u, v) \rightsquigarrow (x, x)$ is a pair of tours $u \rightsquigarrow x$ and $v \rightsquigarrow x$ of the same length. Using a constant C between 0 and 1, we define the *expected meeting probability* as

$$p(u, v) = \sum_{t: (u,v) \rightsquigarrow (x,x)} P[t] C^{l(t)}, \tag{11.37}$$

which is a similarity measure based on random walk. Here, the parameter C specifies the probability of continuing the walk at each step of the trajectory.

It has been shown that $s(u, v) = p(u, v)$ for any two vertices, u and v. That is, SimRank is based on both structural context and random walk.

11.3.3 Graph Clustering Methods

Let's consider how to conduct clustering on a graph. We first describe the intuition behind graph clustering. We then discuss two general categories of graph clustering methods.

To find clusters in a graph, imagine cutting the graph into pieces, each piece being a cluster, such that the vertices within a cluster are well connected and the vertices in different clusters are connected in a much weaker way. Formally, for a graph, $G = (V, E)$,

a **cut**, $C = (S, T)$, is a partitioning of the set of vertices V in G, that is, $V = S \cup T$ and $S \cap T = \emptyset$. The *cut set* of a cut is the set of edges, $\{(u, v) \in E | u \in S, v \in T\}$. The *size* of the cut is the number of edges in the cut set. For weighted graphs, the size of a cut is the sum of the weights of the edges in the cut set.

"What kinds of cuts are good for deriving clusters in graphs?" In graph theory and some network applications, a minimum cut is of importance. A cut is *minimum* if the cut's size is not greater than any other cut's size. There are polynomial time algorithms to compute minimum cuts of graphs. Can we use these algorithms in graph clustering?

Example 11.21 **Cuts and clusters.** Consider graph G in Figure 11.14. The graph has two clusters: $\{a, b, c, d, e, f\}$ and $\{g, h, i, j, k\}$, and one outlier vertex, l.

Consider cut $C_1 = (\{a, b, c, d, e, f, g, h, i, j, k\}, \{l\})$. Only one edge, namely, (e, l), crosses the two partitions created by C_1. Therefore, the cut set of C_1 is $\{(e, l)\}$ and the size of C_1 is 1. (Note that the size of any cut in a connected graph cannot be smaller than 1.) As a minimum cut, C_1 does not lead to a good clustering because it only separates the outlier vertex, l, from the rest of the graph.

Cut $C_2 = (\{a, b, c, d, e, f, l\}, \{g, h, i, j, k\})$ leads to a much better clustering than C_1. The edges in the cut set of C_2 are those connecting the two "natural clusters" in the graph. Specifically, for edges (d, h) and (e, k) that are in the cut set, most of the edges connecting d, h, e, and k belong to one cluster. ■

Example 11.21 indicates that using a minimum cut is unlikely to lead to a good clustering. We are better off choosing a cut where, for each vertex u that is involved in an edge in the cut set, most of the edges connecting to u belong to one cluster. Formally, let $deg(u)$ be the degree of u, that is, the number of edges connecting to u. The *sparsity* of a cut $C = (S, T)$ is defined as

$$\Phi = \frac{\text{cut size}}{\min\{|S|, |T|\}}. \tag{11.38}$$

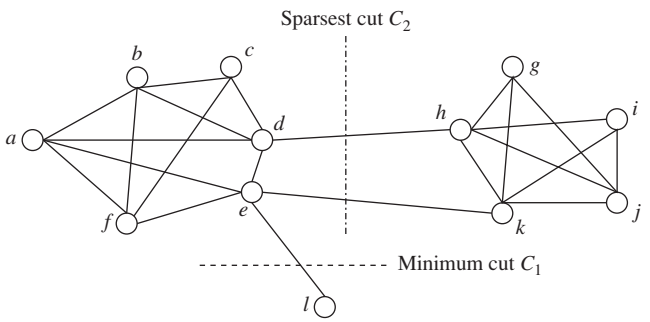

Figure 11.14 A graph G and two cuts.

A cut is *sparsest* if its sparsity is not greater than the sparsity of any other cut. There may be more than one sparsest cut.

In Example 11.21 and Figure 11.14, C_2 is a sparsest cut. Using sparsity as the objective function, a sparsest cut tries to minimize the number of edges crossing the partitions and balance the partitions in size.

Consider a clustering on a graph $G = (V, E)$ that partitions the graph into k clusters. The **modularity** of a clustering assesses the quality of the clustering and is defined as

$$Q = \sum_{i=1}^{k} \left(\frac{l_i}{|E|} - \left(\frac{d_i}{2|E|} \right)^2 \right), \tag{11.39}$$

where l_i is the number of edges between vertices in the ith cluster, and d_i is the sum of the degrees of the vertices in the ith cluster. The modularity of a clustering of a graph is the difference between the fraction of all edges that fall into individual clusters and the fraction that would do so if the graph vertices were randomly connected. The optimal clustering of graphs maximizes the modularity.

Theoretically, many graph clustering problems can be regarded as finding good cuts, such as the sparsest cuts, on the graph. In practice, however, a number of challenges exist:

- **High computational cost:** Many graph cut problems are computationally expensive. The sparsest cut problem, for example, is NP-hard. Therefore, finding the optimal solutions on large graphs is often impossible. A good trade-off between efficiency/scalability and quality has to be achieved.
- **Sophisticated graphs:** Graphs can be more sophisticated than the ones described here, involving weights and/or cycles.
- **High dimensionality:** A graph can have many vertices. In a similarity matrix, a vertex is represented as a vector (a row in the matrix) with a dimensionality that is the number of vertices in the graph. Therefore, graph clustering methods must handle high dimensionality.
- **Sparsity:** A large graph is often sparse, meaning each vertex on average connects to only a small number of other vertices. A similarity matrix from a large sparse graph can also be sparse.

There are two kinds of methods for clustering graph data, which address these challenges. One uses clustering methods for high-dimensional data, while the other is designed specifically for clustering graphs.

The first group of methods is based on generic clustering methods for high-dimensional data. They extract a similarity matrix from a graph using a similarity measure such as those discussed in Section 11.3.2. A generic clustering method can then be applied on the similarity matrix to discover clusters. Clustering methods for

high-dimensional data are typically employed. For example, in many scenarios, once a similarity matrix is obtained, spectral clustering methods (Section 11.2.4) can be applied. Spectral clustering can approximate optimal graph cut solutions. For additional information, please refer to the bibliographic notes (Section 11.7).

The second group of methods is specific to graphs. They search the graph to find well-connected components as clusters. Let's look at a method called **SCAN** (Structural Clustering Algorithm for Networks) as an example.

Given an undirected graph, $G = (V, E)$, for a vertex, $u \in V$, the neighborhood of u is $\Gamma(u) = \{v | (u, v) \in E\} \cup \{u\}$. Using the idea of structural-context similarity, SCAN measures the similarity between two vertices, $u, v \in V$, by the normalized common neighborhood size, that is,

$$\sigma(u, v) = \frac{|\Gamma(u) \cap \Gamma(v)|}{\sqrt{|\Gamma(u)||\Gamma(v)|}}. \tag{11.40}$$

The larger the value computed, the more similar the two vertices. SCAN uses a similarity threshold ε to define the cluster membership. For a vertex, $u \in V$, the *ε-neighborhood* of u is defined as $N_\varepsilon(u) = \{v \in \Gamma(u) | \sigma(u, v) \geq \varepsilon\}$. The ε-neighborhood of u contains all neighbors of u with a structural-context similarity to u that is at least ε.

In SCAN, a *core vertex* is a vertex inside of a cluster. That is, $u \in V$ is a core vertex if $|N_\varepsilon(u)| \geq \mu$, where μ is a popularity threshold. SCAN grows clusters from core vertices. If a vertex v is in the ε-neighborhood of a core u, then v is assigned to the same cluster as u. This process of growing clusters continues until no cluster can be further grown. The process is similar to the density-based clustering method, DBSCAN (Chapter 10).

Formally, a vertex v can be *directly reached* from a core u if $v \in N_\varepsilon(u)$. Transitively, a vertex v can be *reached* from a core u if there exist vertices $w_1, \ldots, w_n$ such that w_1 can be reached from u, w_i can be reached from w_{i-1} for $1 < i \leq n$, and v can be reached from w_n. Moreover, two vertices, $u, v \in V$, which may or may not be cores, are said to be *connected* if there exists a core w such that both u and v can be reached from w. All vertices in a cluster are connected. A cluster is a maximum set of vertices such that every pair in the set is connected.

Some vertices may not belong to any cluster. Such a vertex u is a *hub* if the neighborhood $\Gamma(u)$ of u contains vertices from more than one cluster. If a vertex does not belong to any cluster, and is not a hub, it is an *outlier*.

The SCAN algorithm is shown in Figure 11.15. The search framework closely resembles the cluster-finding process in DBSCAN. SCAN finds a cut of the graph, where each cluster is a set of vertices that are connected based on the transitive similarity in a structural context.

An advantage of SCAN is that its time complexity is linear with respect to the number of edges. In very large and sparse graphs, the number of edges is in the same scale of the number of vertices. Therefore, SCAN is expected to have good scalability on clustering large graphs.

```
Algorithm: SCAN for clusters on graph data.
Input: a graph G = (V, E), a similarity threshold ε, and a
  population threshold μ
Output: a set of clusters
Method: set all vertices in V unlabeled
  for all unlabeled vertex u do
    if u is a core then
      generate a new cluster-id c
      insert all v ∈ N_ε(u) into a queue Q
      while Q ≠ do
        w ← the first vertex in Q
        R ← the set of vertices that can be directly reached from w
        for all s ∈ R do
          if s is not unlabeled or labeled as nonmember then
            assign the current cluster-id c to s
          endif
          if s is unlabeled then
            insert s into queue Q
          endif
        endfor
        remove w from Q
      end while
    else
      label u as nonmember
    endif
  endfor
  for all vertex u labeled nonmember do
    if ∃x, y ∈ Γ(u) : x and y have different cluster-ids then
      label u as hub
    else
      label u as outlier
    endif
  endfor
```

Figure 11.15 SCAN algorithm for cluster analysis on graph data.

11.4 Clustering with Constraints

Users often have background knowledge that they want to integrate into cluster analysis. There may also be application-specific requirements. Such information can be modeled as clustering constraints. We approach the topic of clustering with constraints in two steps. Section 11.4.1 categorizes the types of constraints for clustering graph data. Methods for clustering with constraints are introduced in Section 11.4.2.

11.4.1 Categorization of Constraints

This section studies how to categorize the constraints used in cluster analysis. Specifically, we can categorize constraints according to the subjects on which they are set, or on how strongly the constraints are to be enforced.

As discussed in Chapter 10, cluster analysis involves three essential aspects: objects as instances of clusters, clusters as groups of objects, and the similarity among objects. Therefore, the first method we discuss categorizes constraints according to what they are applied to. We thus have three types: *constraints on instances*, *constraints on clusters*, and *constraints on similarity measurement*.

Constraints on instances: A *constraint on instances* specifies how a pair or a set of instances should be grouped in the cluster analysis. Two common types of constraints from this category include:

- **Must-link constraints.** If a must-link constraint is specified on two objects x and y, then x and y should be grouped into one cluster in the output of the cluster analysis. These must-link constraints are transitive. That is, if must-link(x, y) and must-link(y, z), then must-link(x, z).
- **Cannot-link constraints.** Cannot-link constraints are the opposite of must-link constraints. If a cannot-link constraint is specified on two objects, x and y, then in the output of the cluster analysis, x and y should belong to different clusters. Cannot-link constraints can be entailed. That is, if cannot-link(x, y), must-link(x, x'), and must-link(y, y'), then cannot-link(x', y').

A constraint on instances can be defined using specific instances. Alternatively, it can also be defined using instance variables or attributes of instances. For example, a constraint,

$$Constraint(x, y) : \text{must-link}(x, y) \text{ if } dist(x, y) \leq \epsilon,$$

uses the distance between objects to specify a must-link constraint.

Constraints on clusters: A *constraint on clusters* specifies a requirement on the clusters, possibly using attributes of the clusters. For example, a constraint may specify the minimum number of objects in a cluster, the maximum diameter of a cluster, or the shape of a cluster (e.g., a convex). The number of clusters specified for partitioning clustering methods can be regarded as a constraint on clusters.

Constraints on similarity measurement: Often, a similarity measure, such as Euclidean distance, is used to measure the similarity between objects in a cluster analysis. In some applications, exceptions apply. A *constraint on similarity measurement* specifies a requirement that the similarity calculation must respect. For example, to cluster people as moving objects in a plaza, while Euclidean distance is used to give

the walking distance between two points, a constraint on similarity measurement is that the trajectory implementing the shortest distance cannot cross a wall.

There can be more than one way to express a constraint, depending on the category. For example, we can specify a constraint on clusters as

$$Constraint_1\text{: the diameter of a cluster cannot be larger than } d.$$

The requirement can also be expressed using a constraint on instances as

$$Constraint_1'\text{: cannot-link}(x, y) \text{ if } dist(x, y) > d. \tag{11.41}$$

Example 11.22 **Constraints on instances, clusters, and similarity measurement.** *AllElectronics* clusters its customers so that each group of customers can be assigned to a customer relationship manager. Suppose we want to specify that all customers at the same address are to be placed in the same group, which would allow more comprehensive service to families. This can be expressed using a must-link constraint on instances:

$$Constraint_{family}(x, y) : \text{must-link}(x, y) \text{ if } x.address = y.address.$$

AllElectronics has eight customer relationship managers. To ensure that they each have a similar workload, we place a constraint on clusters such that there should be eight clusters, and each cluster should have at least 10% of the customers and no more than 15% of the customers. We can calculate the spatial distance between two customers using the driving distance between the two. However, if two customers live in different countries, we have to use the flight distance instead. This is a constraint on similarity measurement. ■

Another way to categorize clustering constraints considers how firmly the constraints have to be respected. A constraint is **hard** if a clustering that violates the constraint is unacceptable. A constraint is **soft** if a clustering that violates the constraint is not preferable but acceptable when no better solution can be found. Soft constraints are also called *preferences*.

Example 11.23 **Hard and soft constraints.** For *AllElectronics*, $Constraint_{family}$ in Example 11.22 is a hard constraint because splitting a family into different clusters could prevent the company from providing comprehensive services to the family, leading to poor customer satisfaction. The constraint on the number of clusters (which corresponds to the number of customer relationship managers in the company) is also hard. Example 11.22 also has a constraint to balance the size of clusters. While satisfying this constraint is strongly preferred, the company is flexible in that it is willing to assign a senior and more capable customer relationship manager to oversee a larger cluster. Therefore, the constraint is soft. ■

Ideally, for a specific data set and a set of constraints, all clusterings satisfy the constraints. However, it is possible that there may be no clustering of the data set that

satisfies all the constraints. Trivially, if two constraints in the set conflict, then no clustering can satisfy them at the same time.

Example 11.24 Conflicting constraints. Consider these constraints:

$$\text{must-link}(x, y) \text{ if } dist(x, y) < 5$$
$$\text{cannot-link}(x, y) \text{ if } dist(x, y) > 3.$$

If a data set has two objects, x, y, such that $dist(x, y) = 4$, then no clustering can satisfy both constraints simultaneously.

Consider these two constraints:

$$\text{must-link}(x, y) \text{ if } dist(x, y) < 5$$
$$\text{must-link}(x, y) \text{ if } dist(x, y) < 3.$$

The second constraint is redundant given the first. Moreover, for a data set where the distance between any two objects is at least 5, every possible clustering of the objects satisfies the constraints. ■

"How can we measure the quality and the usefulness of a set of constraints?" In general, we consider either their informativeness, or their coherence. The **informativeness** is the amount of information carried by the constraints that is beyond the clustering model. Given a data set, D, a clustering method, $\mathcal{A}$, and a set of constraints, $\mathcal{C}$, the informativeness of $\mathcal{C}$ with respect to $\mathcal{A}$ on D can be measured by the fraction of constraints in $\mathcal{C}$ that are unsatisfied by the clustering computed by $\mathcal{A}$ on D. The higher the informativeness, the more specific the requirements and background knowledge that the constraints carry. The **coherence** of a set of constraints is the degree of agreement among the constraints themselves, which can be measured by the redundancy among the constraints.

11.4.2 Methods for Clustering with Constraints

Although we can categorize clustering constraints, applications may have very different constraints of specific forms. Consequently, various techniques are needed to handle specific constraints. In this section, we discuss the general principles of handling hard and soft constraints.

Handling Hard Constraints

A general strategy for handling hard constraints is to strictly respect the constraints in the cluster assignment process. To illustrate this idea, we will use partitioning clustering as an example.

Given a data set and a set of constraints on instances (i.e., must-link or cannot-link constraints), how can we extend the k-means method to satisfy such constraints? The **COP-k-means algorithm** works as follows:

1. **Generate superinstances for must-link constraints**. Compute the transitive closure of the must-link constraints. Here, all must-link constraints are treated as an equivalence relation. The closure gives one or multiple subsets of objects where all objects in a subset must be assigned to one cluster. To represent such a subset, we replace all those objects in the subset by the mean. The superinstance also carries a weight, which is the number of objects it represents.

   After this step, the must-link constraints are always satisfied.

2. **Conduct modified k-means clustering.** Recall that, in k-means, an object is assigned to the closest center. What if a nearest-center assignment violates a cannot-link constraint? To respect cannot-link constraints, we modify the center assignment process in k-means to a *nearest feasible center assignment*. That is, when the objects are assigned to centers in sequence, at each step we make sure the assignments so far do not violate any cannot-link constraints. An object is assigned to the nearest center so that the assignment respects all cannot-link constraints.

Because COP-k-means ensures that no constraints are violated at every step, it does not require any backtracking. It is a greedy algorithm for generating a clustering that satisfies all constraints, provided that no conflicts exist among the constraints.

Handling Soft Constraints

Clustering with soft constraints is an optimization problem. When a clustering violates a soft constraint, a penalty is imposed on the clustering. Therefore, the optimization goal of the clustering contains two parts: optimizing the clustering quality and minimizing the constraint violation penalty. The overall objective function is a combination of the clustering quality score and the penalty score.

To illustrate, we again use partitioning clustering as an example. Given a data set and a set of soft constraints on instances, the **CVQE** (**Constrained Vector Quantization Error**) **algorithm** conducts k-means clustering while enforcing constraint violation penalties. The objective function used in CVQE is the sum of the distance used in k-means, adjusted by the constraint violation penalties, which are calculated as follows.

- **Penalty of a must-link violation.** If there is a must-link constraint on objects x and y, but they are assigned to two different centers, c_1 and c_2, respectively, then the constraint is violated. As a result, $dist(c_1, c_2)$, the distance between c_1 and c_2, is added to the objective function as the penalty.
- **Penalty of a cannot-link violation.** If there is a cannot-link constraint on objects x and y, but they are assigned to a common center, c, then the constraint is violated.

The distance, $dist(c, c')$, between c and c' is added to the objective function as the penalty.

Speeding up Constrained Clustering

Constraints, such as on similarity measurements, can lead to heavy costs in clustering. Consider the following **clustering with obstacles** problem: To cluster people as moving objects in a plaza, Euclidean distance is used to measure the walking distance between two points. However, a constraint on similarity measurement is that the trajectory implementing the shortest distance cannot cross a wall (Section 11.4.1). Because obstacles may occur between objects, the distance between two objects may have to be derived by geometric computations (e.g., involving triangulation). The computational cost is high if a large number of objects and obstacles are involved.

The clustering with obstacles problem can be represented using a graphical notation. First, a point, $\boldsymbol{p}$, is **visible** from another point, $\boldsymbol{q}$, in the region R if the straight line joining $\boldsymbol{p}$ and $\boldsymbol{q}$ does not intersect any obstacles. A **visibility graph** is the graph, $VG = (V, E)$, such that each vertex of the obstacles has a corresponding node in V and two nodes, $\boldsymbol{v_1}$ and $\boldsymbol{v_2}$, in V are joined by an edge in E if and only if the corresponding vertices they represent are visible to each other. Let $VG' = (V', E')$ be a visibility graph created from VG by adding two additional points, $\boldsymbol{p}$ and $\boldsymbol{q}$, in V'. E' contains an edge joining two points in V' if the two points are mutually visible. The shortest path between two points, $\boldsymbol{p}$ and $\boldsymbol{q}$, will be a subpath of VG', as shown in Figure 11.16(a). We see that it begins with an edge from $\boldsymbol{p}$ to either $\boldsymbol{v_1}$, $\boldsymbol{v_2}$, or $\boldsymbol{v_3}$, goes through a path in VG, and then ends with an edge from either $\boldsymbol{v_4}$ or $\boldsymbol{v_5}$ to $\boldsymbol{q}$.

To reduce the cost of distance computation between any two pairs of objects or points, several preprocessing and optimization techniques can be used. One method groups points that are close together into microclusters. This can be done by first triangulating the region R into triangles, and then grouping nearby points in the same triangle into microclusters, using a method similar to BIRCH or DBSCAN, as shown in Figure 11.16(b). By processing microclusters rather than individual points, the overall computation is reduced. After that, precomputation can be performed to build two

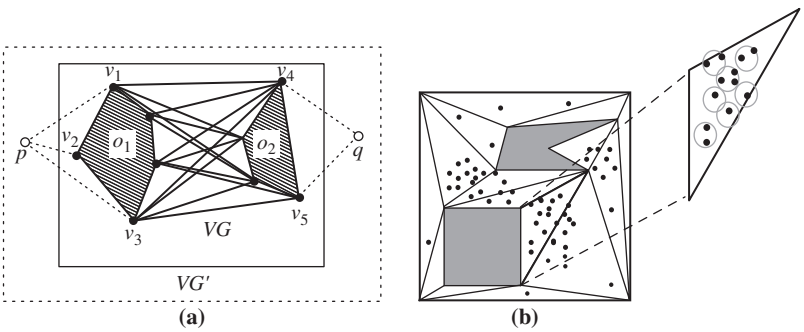

Figure 11.16 Clustering with obstacle objects (o_1 and o_2): (a) a visibility graph and (b) triangulation of regions with microclusters. *Source:* Adapted from Tung, Hou, and Han [THH01].

kinds of join indices based on the computation of the shortest paths: (1) *VV indices*, for any pair of obstacle vertices, and (2) *MV indices*, for any pair of microcluster and obstacle vertex. Use of the indices helps further optimize the overall performance.

Using such precomputation and optimization strategies, the distance between any two points (at the granularity level of a microcluster) can be computed efficiently. Thus, the clustering process can be performed in a manner similar to a typical efficient k-medoids algorithm, such as CLARANS, and achieve good clustering quality for large data sets.

11.5 Summary

- In conventional cluster analysis, an object is assigned to one cluster exclusively. However, in some applications, there is a need to assign an object to one or more clusters in a fuzzy or probabilistic way. **Fuzzy clustering** and **probabilistic model-based clustering** allow an object to belong to one or more clusters. A **partition matrix** records the membership degree of objects belonging to clusters.
- **Probabilistic model-based clustering** assumes that a cluster is a parameterized distribution. Using the data to be clustered as the observed samples, we can estimate the parameters of the clusters.
- A **mixture model** assumes that a set of observed objects is a mixture of instances from multiple probabilistic clusters. Conceptually, each observed object is generated independently by first choosing a probabilistic cluster according to the probabilities of the clusters, and then choosing a sample according to the probability density function of the chosen cluster.
- An **expectation-maximization algorithm** is a framework for approaching maximum likelihood or maximum a posteriori estimates of parameters in statistical models. Expectation-maximization algorithms can be used to compute fuzzy clustering and probabilistic model-based clustering.
- **High-dimensional data** pose several challenges for cluster analysis, including how to model high-dimensional clusters and how to search for such clusters.
- There are two major categories of clustering methods for high-dimensional data: subspace clustering methods and dimensionality reduction methods. **Subspace clustering methods** search for clusters in subspaces of the original space. Examples include **subspace search methods**, **correlation-based clustering methods**, and **biclustering methods**. **Dimensionality reduction methods** create a new space of lower dimensionality and search for clusters there.
- **Biclustering methods** cluster objects and attributes simultaneously. Types of biclusters include biclusters with **constant values**, **constant values on rows/columns**, **coherent values**, and **coherent evolutions on rows/columns**. Two major types of biclustering methods are **optimization-based methods** and **enumeration methods**.

- **Spectral clustering** is a **dimensionality reduction method**. The general idea is to construct new dimensions using an affinity matrix.
- **Clustering graph and network data** has many applications such as social network analysis. Challenges include how to measure the similarity between objects in a graph, and how to design clustering models and methods for graph and network data.
- **Geodesic distance** is the number of edges between two vertices on a graph. It can be used to measure similarity. Alternatively, similarity in graphs, such as social networks, can be measured using structural context and random walk. **SimRank** is a similarity measure that is based on both structural context and random walk.
- Graph clustering can be modeled as computing **graph cuts**. A **sparsest cut** may lead to a good clustering, while **modularity** can be used to measure the clustering quality.
- **SCAN** is a graph clustering algorithm that searches graphs to identify well-connected components as clusters.
- **Constraints** can be used to express application-specific requirements or background knowledge for cluster analysis. Constraints for clustering can be categorized as constraints on **instances**, on **clusters**, or on **similarity measurement**. Constraints on instances include **must-link** and **cannot-link** constraints. A constraint can be **hard** or **soft**.
- **Hard constraints for clustering** can be enforced by strictly respecting the constraints in the cluster assignment process. **Clustering with soft constraints** can be considered an optimization problem. Heuristics can be used to speed up constrained clustering.

11.6 Exercises

11.1 Traditional clustering methods are rigid in that they require each object to belong exclusively to only one cluster. Explain why this is a special case of fuzzy clustering. You may use k-means as an example.

11.2 *AllElectronics* carries 1000 products, $P_1, \ldots, P_{1000}$. Consider customers Ada, Bob, and Cathy such that Ada and Bob purchase three products in common, P_1, P_2, and P_3. For the other 997 products, Ada and Bob independently purchase seven of them randomly. Cathy purchases 10 products, randomly selected from the 1000 products. In Euclidean distance, what is the probability that $dist(\text{Ada}, \text{Bob}) > dist(\text{Ada}, \text{Cathy})$? What if Jaccard similarity (Chapter 2) is used? What can you learn from this example?

11.3 Show that $I \times J$ is a bicluster with coherent values if and only if, for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, $e_{i_1 j_1} - e_{i_2 j_1} = e_{i_1 j_2} - e_{i_2 j_2}$.

11.4 Compare the MaPle algorithm (Section 11.2.3) with the frequent closed itemset mining algorithm, CLOSET (Pei, Han, and Mao [PHM00]). What are the major similarities and differences?

11.5 SimRank is a similarity measure for clustering graph and network data.

(a) Prove $\lim_{i \to \infty} s_i(u, v) = s(u, v)$ for SimRank computation.

(b) Show $s(u, v) = p(u, v)$ for SimRank.

11.6 In a large sparse graph where on average each node has a low degree, is the similarity matrix using SimRank still sparse? If so, in what sense? If not, why? Deliberate on your answer.

11.7 Compare the SCAN algorithm (Section 11.3.3) with DBSCAN (Section 10.4.1). What are their similarities and differences?

11.8 Consider partitioning clustering and the following constraint on clusters: The number of objects in each cluster must be between $\frac{n}{k}(1-\delta)$ and $\frac{n}{k}(1+\delta)$, where n is the total number of objects in the data set, k is the number of clusters desired, and δ in $[0, 1)$ is a parameter. Can you extend the k-means method to handle this constraint? Discuss situations where the constraint is hard and soft.

11.7 Bibliographic Notes

Höppner Klawonn, Kruse, and Runkler [HKKR99] provide a thorough discussion of fuzzy clustering. The fuzzy c-means algorithm (on which Example 11.7 is based) was proposed by Bezdek [Bez81]. Fraley and Raftery [FR02] give a comprehensive overview of model-based cluster analysis and probabilistic models. McLachlan and Basford [MB88] present a systematic introduction to mixture models and applications in cluster analysis.

Dempster, Laird, and Rubin [DLR77] are recognized as the first to introduce the EM algorithm and give it its name. However, the idea of the EM algorithm had been "proposed many times in special circumstances" before, as admitted in Dempster, Laird, and Rubin [DLR77]. Wu [Wu83] gives the correct analysis of the EM algorithm.

Mixture models and EM algorithms are used extensively in many data mining applications. Introductions to model-based clustering, mixture models, and EM algorithms can be found in recent textbooks on machine learning and statistical learning—for example, Bishop [Bis06], Marsland [Mar09], and Alpaydin [Alp11].

The increase of dimensionality has severe effects on distance functions, as indicated by Beyer et al. [BGRS99]. It also has had a dramatic impact on various techniques for classification, clustering, and semisupervised learning (Radovanović, Nanopoulos, and Ivanović [RNI09]).

Kriegel, Kröger, and Zimek [KKZ09] present a comprehensive survey on methods for clustering high-dimensional data. The CLIQUE algorithm was developed by Agrawal, Gehrke, Gunopulos, and Raghavan [AGGR98]. The PROCLUS algorithm was proposed by Aggawal, Procopiuc, Wolf, et al. [APW+99].

The technique of biclustering was initially proposed by Hartigan [Har72]. The term *biclustering* was coined by Mirkin [Mir98]. Cheng and Church [CC00] introduced

biclustering into gene expression data analysis. There are many studies on biclustering models and methods. The notion of δ-pCluster was introduced by Wang, Wang, Yang, and Yu [WWYY02]. For informative surveys, see Madeira and Oliveira [MO04] and Tanay, Sharan, and Shamir [TSS04]. In this chapter, we introduced the δ-cluster algorithm by Cheng and Church [CC00] and MaPle by Pei, Zhang, Cho, et al. [PZC+03] as examples of optimization-based methods and enumeration methods for biclustering, respectively.

Donath and Hoffman [DH73] and Fiedler [Fie73] pioneered spectral clustering. In this chapter, we use an algorithm proposed by Ng, Jordan, and Weiss [NJW01] as an example. For a thorough tutorial on spectral clustering, see Luxburg [Lux07].

Clustering graph and network data is an important and fast-growing topic. Schaeffer [Sch07] provides a survey. The SimRank measure of similarity was developed by Jeh and Widom [JW02a]. Xu et al. [XYFS07] proposed the SCAN algorithm. Arora, Rao, and Vazirani [ARV09] discuss the sparsest cuts and approximation algorithms.

Clustering with constraints has been extensively studied. Davidson, Wagstaff, and Basu [DWB06] proposed the measures of informativeness and coherence. The COP-k-means algorithm is given by Wagstaff et al. [WCRS01]. The CVQE algorithm was proposed by Davidson and Ravi [DR05]. Tung, Han, Lakshmanan, and Ng [THLN01] presented a framework for constraint-based clustering based on user-specified constraints. An efficient method for constraint-based spatial clustering in the existence of physical obstacle constraints was proposed by Tung, Hou, and Han [THH01].

13 Data Mining Trends and Research Frontiers

As a young research field, data mining has made significant progress and covered a broad spectrum of applications since the 1980s. Today, data mining is used in a vast array of areas. Numerous commercial data mining systems and services are available. Many challenges, however, still remain. In this final chapter, we introduce the mining of complex data types as a prelude to further in-depth study readers may choose to do. In addition, we focus on trends and research frontiers in data mining. Section 13.1 presents an overview of methodologies for mining complex data types, which extend the concepts and tasks introduced in this book. Such mining includes mining time-series, sequential patterns, and biological sequences; graphs and networks; spatiotemporal data, including geospatial data, moving-object data, and cyber-physical system data; multimedia data; text data; web data; and data streams. Section 13.2 briefly introduces other approaches to data mining, including statistical methods, theoretical foundations, and visual and audio data mining.

In Section 13.3, you will learn more about data mining applications in business and in science, including the financial retail, and telecommunication industries, science and engineering, and recommender systems. The social impacts of data mining are discussed in Section 13.4, including ubiquitous and invisible data mining, and privacy-preserving data mining. Finally, in Section 13.5 we speculate on current and expected data mining trends that arise in response to new challenges in the field.

13.1 Mining Complex Data Types

In this section, we outline the major developments and research efforts in mining complex data types. Complex data types are summarized in Figure 13.1. Section 13.1.1 covers mining sequence data such as time-series, symbolic sequences, and biological sequences. Section 13.1.2 discusses mining graphs and social and information networks. Section 13.1.3 addresses mining other kinds of data, including spatial data, spatiotemporal data, moving-object data, cyber-physical system data, multimedia data, text data,

Data Mining: Concepts and Techniques. DOI: 10.1016/B978-0-12-381479-1.00013-7

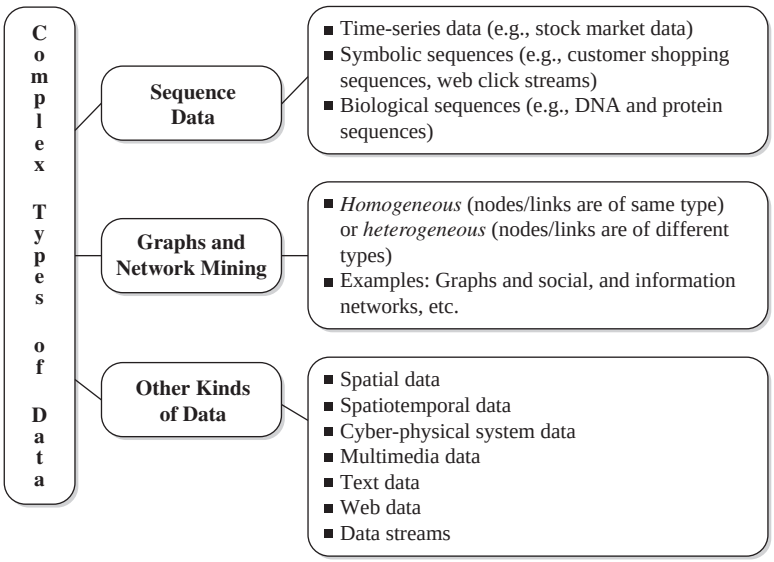

Figure 13.1 Complex data types for mining.

web data, and data streams. Due to the broad scope of these themes, this section presents only a high-level overview; these topics are not discussed in-depth in this book.

13.1.1 Mining Sequence Data: Time-Series, Symbolic Sequences, and Biological Sequences

A **sequence** is an ordered list of events. Sequences may be categorized into three groups, based on the characteristics of the events they describe: (1) *time-series data*, (2) *symbolic sequence data*, and (3) *biological sequences*. Let's consider each type.

In **time-series data**, sequence data consist of long sequences of numeric data, recorded at equal time intervals (e.g., per minute, per hour, or per day). Time-series data can be generated by many natural and economic processes such as stock markets, and scientific, medical, or natural observations.

Symbolic sequence data consist of long sequences of event or nominal data, which typically are not observed at equal time intervals. For many such sequences, *gaps* (i.e., lapses between recorded events) do not matter much. Examples include customer shopping sequences and web click streams, as well as sequences of events in science and engineering and in natural and social developments.

Biological sequences include DNA and protein sequences. Such sequences are typically very long, and carry important, complicated, but hidden semantic meaning. Here, gaps are usually important.

Let's look into data mining for each of these sequence data types.

Similarity Search in Time-Series Data

A **time-series data set** consists of sequences of numeric values obtained over repeated measurements of time. The values are typically measured at equal time intervals (e.g., every minute, hour, or day). Time-series databases are popular in many applications such as stock market analysis, economic and sales forecasting, budgetary analysis, utility studies, inventory studies, yield projections, workload projections, and process and quality control. They are also useful for studying natural phenomena (e.g., atmosphere, temperature, wind, earthquake), scientific and engineering experiments, and medical treatments.

Unlike normal database queries, which find data that match a given query *exactly*, a **similarity search** finds data sequences that *differ only slightly* from the given query sequence. Many time-series similarity queries require **subsequence matching**, that is, finding a set of sequences that contain subsequences that are similar to a given query sequence.

For similarity search, it is often necessary to first perform *data or dimensionality reduction and transformation* of time-series data. Typical *dimensionality reduction* techniques include (1) the *discrete Fourier transform* (*DFT*), (2) *discrete wavelet transforms (DWT)*, and (3) *singular value decomposition* (*SVD*) based on *principle components analysis* (*PCA*). Because we touched on these concepts in Chapter 3, and because a thorough explanation is beyond the scope of this book, we will not go into great detail here. With such techniques, the data or signal is mapped to a signal in a *transformed space*. A small subset of the "strongest" transformed coefficients are saved as features.

These features form a *feature space*, which is a projection of the transformed space. Indices can be constructed on the original or transformed time-series data to speed up a search. For a query-based similarity search, techniques include normalization transformation, atomic matching (i.e., finding pairs of gap-free windows of a small length that are similar), window stitching (i.e., stitching similar windows to form pairs of large similar subsequences, allowing gaps between atomic matches), and subsequence ordering (i.e., linearly ordering the subsequence matches to determine whether enough similar pieces exist). Numerous software packages exist for a similarity search in time-series data.

Recently, researchers have proposed transforming time-series data into piecewise aggregate approximations so that the data can be viewed as a sequence of symbolic representations. The problem of similarity search is then transformed into one of matching subsequences in symbolic sequence data. We can identify *motifs* (i.e., frequently occurring sequential patterns) and build index or hashing mechanisms for an efficient search based on such motifs. Experiments show this approach is fast and simple, and has comparable search quality to that of DFT, DWT, and other dimensionality reduction methods.

Regression and Trend Analysis in Time-Series Data

Regression analysis of time-series data has been studied substantially in the fields of statistics and signal analysis. However, one may often need to go beyond pure regression

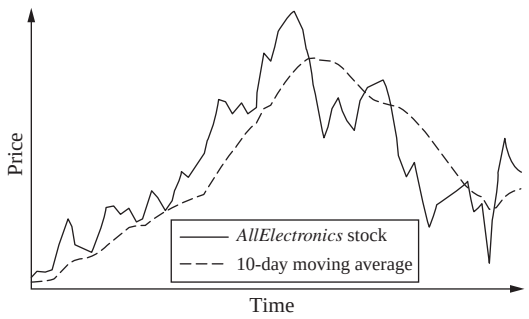

Figure 13.2 Time-series data for the stock price of *AllElectronics* over time. The *trend* is shown with a dashed curve, calculated by a moving average.

analysis and perform *trend analysis* for many practical applications. Trend analysis builds an integrated model using the following four major *components* or *movements* to characterize time-series data:

1. **Trend or long-term movements**: These indicate the general direction in which a time-series graph is moving over time, for example, using *weighted moving average* and the *least squares* methods to find *trend curves* such as the dashed curve indicated in Figure 13.2.
2. **Cyclic movements**: These are the long-term oscillations about a trend line or curve.
3. **Seasonal variations**: These are nearly identical patterns that a time series appears to follow during corresponding seasons of successive years such as holiday shopping seasons. For effective trend analysis, the data often need to be "deseasonalized" based on a **seasonal index** computed by autocorrelation.
4. **Random movements**: These characterize sporadic changes due to chance events such as labor disputes or announced personnel changes within companies.

Trend analysis can also be used for **time-series forecasting**, that is, finding a mathematical function that will approximately generate the historic patterns in a time series, and using it to make long-term or short-term predictions of future values. *ARIMA (auto-regressive integrated moving average)*, *long-memory time-series modeling*, and *autoregression* are popular methods for such analysis.

Sequential Pattern Mining in Symbolic Sequences

A **symbolic sequence** consists of an ordered set of elements or events, recorded with or without a concrete notion of time. There are many applications involving data of

symbolic sequences such as customer shopping sequences, web click streams, program execution sequences, biological sequences, and sequences of events in science and engineering and in natural and social developments. Because biological sequences carry very complicated semantic meaning and pose many challenging research issues, most investigations are conducted in the field of bioinformatics.

Sequential pattern mining has focused extensively on mining symbolic sequences. A sequential pattern is a frequent subsequence existing in a single sequence or a set of sequences. A sequence $\alpha = \langle a_1 a_2 \cdots a_n \rangle$ is a **subsequence** of another sequence $\beta = \langle b_1 b_2 \cdots b_m \rangle$ if there exist integers $1 \leq j_1 < j_2 < \cdots < j_n \leq m$ such that $a_1 \subseteq b_{j_1}$, $a_2 \subseteq b_{j_2}, \ldots, a_n \subseteq b_{j_n}$. For example, if $\alpha = \langle \{ab\}, d \rangle$ and $\beta = \langle \{abc\}, \{be\}, \{de\}, a \rangle$, where a, b, c, d, and e are items, then α is a subsequence of β. Mining of sequential patterns consists of mining the set of subsequences that are frequent in one sequence or a set of sequences. Many scalable algorithms have been developed as a result of extensive studies in this area. Alternatively, we can mine only the *set of closed* sequential patterns, where a sequential pattern s is **closed** if there exists no sequential pattern s', where s is a *proper* subsequence of s', and s' has the same (frequency) support as s. Similar to its frequent pattern mining counterpart, there are also studies on efficient mining of **multidimensional, multilevel sequential patterns**.

As with constraint-based frequent pattern mining, user-specified constraints can be used to reduce the search space in sequential pattern mining and derive only the patterns that are of interest to the user. This is referred to as **constraint-based sequential pattern mining**. Moreover, we may relax constraints or enforce additional constraints on the problem of sequential pattern mining to derive different kinds of patterns from sequence data. For example, we can enforce gap constraints so that the patterns derived contain only consecutive subsequences or subsequences with very small gaps. Alternatively, we may derive periodic sequential patterns by folding events into proper-size windows and finding recurring subsequences in these windows. Another approach derives *partial order patterns* by relaxing the requirement of strict sequential ordering in the mining of subsequence patterns. Besides mining partial order patterns, sequential pattern mining methodology can also be extended to mining trees, lattices, episodes, and some other ordered patterns.

Sequence Classification

Most classification methods perform model construction based on feature vectors. However, sequences do not have explicit features. Even with sophisticated feature selection techniques, the dimensionality of potential features can still be very high and the sequential nature of features is difficult to capture. This makes sequence classification a challenging task.

Sequence classification methods can be organized into three categories: (1) feature-based classification, which transforms a sequence into a feature vector and then applies conventional classification methods; (2) sequence distance–based classification, where the distance function that measures the similarity between sequences determines the

quality of the classification significantly; and (3) model-based classification such as using hidden Markov model (HMM) or other statistical models to classify sequences.

For time-series or other numeric-valued data, the feature selection techniques for symbolic sequences cannot be easily applied to time-series data without discretization. However, discretization can cause information loss. A recently proposed time-series *shapelets method* uses the time-series subsequences that can maximally represent a class as the features. It achieves quality classification results.

Alignment of Biological Sequences

Biological sequences generally refer to sequences of nucleotides or amino acids. **Biological sequence analysis** compares, aligns, indexes, and analyzes biological sequences and thus plays a crucial role in bioinformatics and modern biology.

Sequence alignment is based on the fact that all living organisms are related by evolution. This implies that the nucleotide (DNA, RNA) and protein sequences of species that are closer to each other in evolution should exhibit more similarities. An **alignment** is the process of lining up sequences to achieve a maximal identity level, which also expresses the degree of similarity between sequences. Two sequences are **homologous** if they share a common ancestor. The degree of similarity obtained by sequence alignment can be useful in determining the possibility of homology between two sequences. Such an alignment also helps determine the relative positions of multiple species in an evolution tree, which is called a **phylogenetic tree**.

The problem of alignment of biological sequences can be described as follows: *Given two or more input biological sequences, identify similar sequences with long conserved subsequences.* If the number of sequences to be aligned is exactly two, the problem is known as **pairwise sequence alignment**; otherwise, it is **multiple sequence alignment**. The sequences to be compared and aligned can be either nucleotides (DNA/RNA) or amino acids (proteins). For nucleotides, two symbols align if they are identical. However, for amino acids, two symbols align if they are identical, or if one can be derived from the other by substitutions that are likely to occur in nature. There are two kinds of alignments: *local alignments* and *global alignments*. The former means that only portions of the sequences are aligned, whereas the latter requires alignment over the entire length of the sequences.

For either nucleotides or amino acids, insertions, deletions, and substitutions occur in nature with different probabilities. **Substitution matrices** are used to represent the probabilities of substitutions of nucleotides or amino acids and probabilities of insertions and deletions. Usually, we use the gap character, −, to indicate positions where it is preferable not to align two symbols. To evaluate the quality of alignments, a *scoring* mechanism is typically defined, which usually counts identical or similar symbols as positive scores and gaps as negative ones. The algebraic sum of the scores is taken as the alignment measure. The goal of alignment is to achieve the maximal score among all the possible alignments. However, it is very expensive (more exactly, an NP-hard problem) to find optimal alignment. Therefore, various heuristic methods have been developed to find suboptimal alignments.

The dynamic programming approach is commonly used for sequence alignments. Among many available analysis packages, BLAST (Basic Local Alignment Search Tool) is one of the most popular tools in biosequence analysis.

Hidden Markov Model for Biological Sequence Analysis

Given a biological sequence, biologists would like to analyze what that sequence represents. To represent the structure or statistical regularities of sequence classes, biologists construct various probabilistic models such as *Markov chains* and *hidden Markov models*. In both models, the probability of a state depends only on that of the previous state; therefore, they are particularly useful for the analysis of biological sequence data. The most common methods for constructing hidden Markov models are the forward algorithm, the Viterbi algorithm, and the Baum-Welch algorithm. Given a sequence of symbols, x, the *forward algorithm* finds the probability of obtaining x in the model; the *Viterbi algorithm* finds the most probable path (corresponding to x) through the model, whereas the *Baum-Welch algorithm* learns or adjusts the model parameters so as to best explain a set of training sequences.

13.1.2 Mining Graphs and Networks

Graphs represents a more general class of structures than sets, sequences, lattices, and trees. There is a broad range of graph applications on the Web and in social networks, information networks, biological networks, bioinformatics, chemical informatics, computer vision, and multimedia and text retrieval. Hence, graph and network mining have become increasingly important and heavily researched. We overview the following major themes: (1) graph pattern mining; (2) statistical modeling of networks; (3) data cleaning, integration, and validation by network analysis; (4) clustering and classification of graphs and homogeneous networks; (5) clustering, ranking, and classification of heterogeneous networks; (6) role discovery and link prediction in information networks; (7) similarity search and OLAP in information networks; and (8) evolution of information networks.

Graph Pattern Mining

Graph pattern mining is the mining of *frequent subgraphs* (also called **(sub)graph patterns**) in one or a set of graphs. Methods for mining graph patterns can be categorized into Apriori-based and pattern growth–based approaches. Alternatively, we can mine the set of *closed graphs* where a graph g is *closed* if there exists no proper supergraph g' that carries the same support count as g. Moreover, there are many *variant graph patterns*, including approximate frequent graphs, coherent graphs, and dense graphs. User-specified constraints can be pushed deep into the graph pattern mining process to improve mining efficiency.

Graph pattern mining has many interesting applications. For example, it can be used to generate compact and effective *graph index structures* based on the concept of

frequent and discriminative graph patterns. Approximate *structure similarity search* can be achieved by exploring graph index structures and multiple graph features. Moreover, classification of graphs can also be performed effectively using frequent and discriminative subgraphs as features.

Statistical Modeling of Networks

A **network** consists of a set of *nodes*, each corresponding to an *object* associated with a set of properties, and a set of *edges* (or *links*) connecting those nodes, representing relationships between objects. A network is **homogeneous** if all the nodes and links are of the same type, such as a friend network, a coauthor network, or a web page network. A network is **heterogeneous** if the nodes and links are of different types, such as publication networks (linking together authors, conferences, papers, and contents), and health-care networks (linking together doctors, nurses, patients, diseases, and treatments).

Researchers have proposed multiple statistical models for modeling homogeneous networks. The most well-known generative models are the random graph model (i.e., the Erdös-Rényi model), the Watts-Strogatz model, and the scale-free model. The scale-free model assumes that the network follows the *power law distribution* (also known as the *Pareto distribution* or the *heavy-tailed distribution*). In most large-scale social networks, a **small-world phenomenon** is observed, that is, the network can be characterized as having a high degree of local clustering for a small fraction of the nodes (i.e., these nodes are interconnected with one another), while being no more than a few degrees of separation from the remaining nodes.

Social networks exhibit certain evolutionary characteristics. They tend to follow the **densification power law**, which states that networks become increasingly *dense* over time. **Shrinking diameter** is another characteristic, where the effective diameter often *decreases* as the network grows. Node *out-degrees* and *in-degrees* typically follow a heavy-tailed distribution.

Data Cleaning, Integration, and Validation by Information Network Analysis

Real-world data are often incomplete, noisy, uncertain, and unreliable. Information redundancy may exist among the multiple pieces of data that are interconnected in a large network. Information redundancy can be explored in such networks to perform quality data cleaning, data integration, information validation, and trustability analysis by network analysis. For example, we can distinguish authors who share the same names by examining the networked connections with other heterogeneous objects such as coauthors, publication venues, and terms. In addition, we can identify inaccurate author information presented by booksellers by exploring a network built based on author information provided by multiple booksellers.

Sophisticated information network analysis methods have been developed in this direction, and in many cases, portions of the data serve as the "training set." That is, relatively clean and reliable data or a consensus of data from multiple information

providers can be used to help consolidate the remaining, unreliable portions of the data. This reduces the costly efforts of labeling the data by hand and of training on massive, dynamic, real-world data sets.

Clustering and Classification of Graphs and Homogeneous Networks

Large graphs and networks have cohesive structures, which are often hidden among their massive, interconnected nodes and links. Cluster analysis methods have been developed on large networks to uncover network structures, discover hidden communities, hubs, and outliers based on network topological structures and their associated properties. Various kinds of network clustering methods have been developed and can be categorized as either partitioning, hierarchical, or density-based algorithms. Moreover, given human-labeled training data, the discovery of network structures can be guided by human-specified heuristic constraints. Supervised classification and semi-supervised classification of networks are recent hot topics in the data mining research community.

Clustering, Ranking, and Classification of Heterogeneous Networks

A heterogeneous network contains interconnected nodes and links of different types. Such interconnected structures contain rich information, which can be used to mutually enhance nodes and links, and propagate knowledge from one type to another. Clustering and ranking of such heterogeneous networks can be performed hand-in-hand in the context that highly ranked nodes/links in a cluster may contribute more than their lower-ranked counterparts in the evaluation of the cohesiveness of a cluster. Clustering may help consolidate the high ranking of objects/links dedicated to the cluster. Such mutual enhancement of ranking and clustering prompted the development of an algorithm called RankClus. Moreover, users may specify different ranking rules or present labeled nodes/links for certain data types. Knowledge of one type can be propagated to other types. Such propagation reaches the nodes/links of the same type via heterogeneous-type connections. Algorithms have been developed for supervised learning and semi-supervised learning in heterogeneous networks.

Role Discovery and Link Prediction in Information Networks

There exist many hidden roles or relationships among different nodes/links in a heterogeneous network. Examples include advisor–advisee and leader–follower relationships in a research publication network. To discover such hidden roles or relationships, experts can specify constraints based on their background knowledge. Enforcing such constraints may help cross-checking and validation in large interconnected networks. Information redundancy in a network can often be used to help weed out objects/links that do not follow such constraints.

Similarly, *link prediction* can be performed based on the assessment of the ranking of the expected relationships among the candidate nodes/links. For example, we may predict which papers an author may write, read, or cite, based on the author's recent publication history and the trend of research on similar topics. Such studies often require analyzing the proximity of network nodes/links and the trends and connections of their similar neighbors. Roughly speaking, people refer to link prediction as **link mining**; however, link mining covers additional tasks including *link-based object classification*, *object type prediction*, *link type prediction, link existence prediction*, *link cardinality estimation*, and *object reconciliation* (which predicts whether two objects are, in fact, the same). It also includes *group detection* (which clusters objects), as well as *subgraph identification* (which finds characteristic subgraphs within networks) and *metadata mining* (which uncovers schema-type information regarding unstructured data).

Similarity Search and OLAP in Information Networks

Similarity search is a primitive operation in database and web search engines. A heterogeneous information network consists of multityped, interconnected objects. Examples include bibliographic networks and social media networks, where two objects are considered similar if they are linked in a similar way with multityped objects. In general, object similarity within a network can be determined based on network structures and object properties, and with similarity measures. Moreover, network clusters and hierarchical network structures help organize objects in a network and identify subcommunities, as well as facilitate similarity search. Furthermore, similarity can be defined differently per user. By considering different linkage paths, we can derive various similarity semantics in a network, which is known as *path-based similarity*.

By organizing networks based on the notion of similarity and clusters, we can generate multiple hierarchies within a network. Online analytical processing (OLAP) can then be performed. For example, we can drill down or dice information networks based on different levels of abstraction and different angles of views. OLAP operations may generate multiple, interrelated networks. The relationships among such networks may disclose interesting hidden semantics.

Evolution of Social and Information Networks

Networks are dynamic and constantly evolving. Detecting evolving communities and evolving regularities or anomalies in homogeneous or heterogeneous networks can help people better understand the structural evolution of networks and predict trends and irregularities in evolving networks. For homogeneous networks, the evolving communities discovered are subnetworks consisting of objects of the same type such as a set of friends or coauthors. However, for heterogeneous networks, the communities discovered are subnetworks consisting of objects of different types, such as a connected set of papers, authors, venues, and terms, from which we can also derive a set of evolving objects for each type, like evolving authors and themes.

13.1.3 Mining Other Kinds of Data

In addition to sequences and graphs, there are many other kinds of semi-structured or unstructured data, such as spatiotemporal, multimedia, and hypertext data, which have interesting applications. Such data carry various kinds of semantics, are either stored in or dynamically streamed through a system, and call for specialized data mining methodologies. Thus, mining multiple kinds of data, including *spatial data, spatiotemporal data, cyber-physical system data, multimedia data, text data*, *web data*, and *data streams*, are increasingly important tasks in data mining. In this subsection, we overview the methodologies for mining these kinds of data.

Mining Spatial Data

Spatial data mining discovers patterns and knowledge from spatial data. Spatial data, in many cases, refer to geospace-related data stored in geospatial data repositories. The data can be in "vector" or "raster" formats, or in the form of imagery and geo-referenced multimedia. Recently, large *geographic data warehouses* have been constructed by integrating thematic and geographically referenced data from multiple sources. From these, we can construct *spatial data cubes* that contain spatial dimensions and measures, and support *spatial OLAP* for *multidimensional spatial data analysis*. Spatial data mining can be performed on spatial data warehouses, spatial databases, and other geospatial data repositories. Popular topics on geographic knowledge discovery and spatial data mining include *mining spatial associations and co-location patterns*, *spatial clustering*, *spatial classification*, *spatial modeling*, and *spatial trend and outlier analysis*.

Mining Spatiotemporal Data and Moving Objects

Spatiotemporal data are data that relate to both space and time. **Spatiotemporal data mining** refers to the process of discovering patterns and knowledge from spatiotemporal data. Typical examples of spatiotemporal data mining include discovering the evolutionary history of cities and lands, uncovering weather patterns, predicting earthquakes and hurricanes, and determining global warming trends. Spatiotemporal data mining has become increasingly important and has far-reaching implications, given the popularity of mobile phones, GPS devices, Internet-based map services, weather services, and digital Earth, as well as satellite, RFID, sensor, wireless, and video technologies.

Among many kinds of spatiotemporal data, *moving-object data* (i.e., data about moving objects) are especially important. For example, animal scientists attach telemetry equipment on wildlife to analyze ecological behavior, mobility managers embed GPS in cars to better monitor and guide vehicles, and meteorologists use weather satellites and radars to observe hurricanes. Massive-scale moving-object data are becoming rich, complex, and ubiquitous. Examples of **moving-object data mining** include mining *movement patterns of multiple moving objects* (i.e., the discovery of relationships among multiple moving objects such as moving clusters, leaders and followers, merge, convoy, swarm, and pincer, as well as other collective movement patterns). Other examples of

moving-object data mining include mining *periodic patterns* for one or a set of moving objects, and mining *trajectory patterns, clusters, models*, and *outliers*.

Mining Cyber-Physical System Data

A **cyber-physical system** (CPS) typically consists of a large number of interacting physical and information components. CPS systems may be interconnected so as to form large heterogeneous *cyber-physical networks*. Examples of cyber-physical networks include a patient care system that links a patient monitoring system with a network of patient/medical information and an emergency handling system; a transportation system that links a transportation monitoring network, consisting of many sensors and video cameras, with a traffic information and control system; and a battlefield commander system that links a sensor/reconnaissance network with a battlefield information analysis system. Clearly, cyber-physical systems and networks will be ubiquitous and form a critical component of modern information infrastructure.

Data generated in cyber-physical systems are dynamic, volatile, noisy, inconsistent, and interdependent, containing rich spatiotemporal information, and they are critically important for real-time decision making. In comparison with typical spatiotemporal data mining, mining cyber-physical data requires linking the current situation with a large information base, performing real-time calculations, and returning prompt responses. Research in the area includes rare-event detection and anomaly analysis in cyber-physical data streams, reliability and trustworthiness in cyber-physical data analysis, effective spatiotemporal data analysis in cyber-physical networks, and the integration of stream data mining with real-time automated control processes.

Mining Multimedia Data

Multimedia data mining is the discovery of interesting patterns from multimedia databases that store and manage large collections of multimedia objects, including image data, video data, audio data, as well as sequence data and hypertext data containing text, text markups, and linkages. Multimedia data mining is an interdisciplinary field that integrates image processing and understanding, computer vision, data mining, and pattern recognition. Issues in multimedia data mining include *content-based retrieval and similarity search*, and *generalization and multidimensional analysis*. Multimedia data cubes contain additional dimensions and measures for multimedia information. Other topics in multimedia mining include *classification and prediction analysis*, *mining associations*, and *video and audio data mining* (Section 13.2.3).

Mining Text Data

Text mining is an interdisciplinary field that draws on information retrieval, data mining, machine learning, statistics, and computational linguistics. A substantial portion of information is stored as text such as news articles, technical papers, books, digital libraries, email messages, blogs, and web pages. Hence, research in text mining has been very active. An important goal is to derive high-quality information from text. This is

typically done through the discovery of patterns and trends by means such as statistical pattern learning, topic modeling, and statistical language modeling. Text mining usually requires structuring the input text (e.g., parsing, along with the addition of some derived linguistic features and the removal of others, and subsequent insertion into a database). This is followed by deriving patterns within the structured data, and evaluation and interpretation of the output. "High quality" in text mining usually refers to a combination of relevance, novelty, and interestingness.

Typical text mining tasks include text categorization, text clustering, concept/entity extraction, production of granular taxonomies, sentiment analysis, document summarization, and entity-relation modeling (i.e., learning relations between named entities). Other examples include multilingual data mining, multidimensional text analysis, contextual text mining, and trust and evolution analysis in text data, as well as text mining applications in security, biomedical literature analysis, online media analysis, and analytical customer relationship management. Various kinds of text mining and analysis software and tools are available in academic institutions, open-source forums, and industry. Text mining often also uses WordNet, Sematic Web, Wikipedia, and other information sources to enhance the understanding and mining of text data.

Mining Web Data

The World Wide Web serves as a huge, widely distributed, global information center for news, advertisements, consumer information, financial management, education, government, and e-commerce. It contains a rich and dynamic collection of information about web page contents with hypertext structures and multimedia, hyperlink information, and access and usage information, providing fertile sources for data mining. **Web mining** is the application of data mining techniques to discover patterns, structures, and knowledge from the Web. According to analysis targets, web mining can be organized into three main areas: *web content mining*, *web structure mining*, and *web usage mining*.

Web content mining analyzes web content such as text, multimedia data, and structured data (within web pages or linked across web pages). This is done to understand the content of web pages, provide scalable and informative keyword-based page indexing, entity/concept resolution, web page relevance and ranking, web page content summaries, and other valuable information related to web search and analysis. Web pages can reside either on the *surface web* or on the *deep Web*. The *surface web* is that portion of the Web that is indexed by typical search engines. The *deep Web* (or *hidden Web*) refers to web content that is not part of the surface web. Its contents are provided by underlying database engines.

Web content mining has been studied extensively by researchers, search engines, and other web service companies. Web content mining can build links across multiple web pages for individuals; therefore, it has the potential to inappropriately disclose personal information. Studies on privacy-preserving data mining address this concern through the development of techniques to protect personal privacy on the Web.

Web structure mining is the process of using graph and network mining theory and methods to analyze the nodes and connection structures on the Web. It extracts patterns from hyperlinks, where a hyperlink is a structural component that connects a

web page to another location. It can also mine the document structure within a page (e.g., analyze the treelike structure of page structures to describe HTML or XML tag usage). Both kinds of web structure mining help us understand web contents and may also help transform web contents into relatively structured data sets.

Web usage mining is the process of extracting useful information (e.g., user click streams) from server logs. It finds patterns related to general or particular groups of users; understands users' search patterns, trends, and associations; and predicts what users are looking for on the Internet. It helps improve search efficiency and effectiveness, as well as promotes products or related information to different groups of users at the right time. Web search companies routinely conduct web usage mining to improve their quality of service.

Mining Data Streams

Stream data refer to data that flow into a system in vast volumes, change dynamically, are possibly infinite, and contain multidimensional features. Such data cannot be stored in traditional database systems. Moreover, most systems may only be able to read the stream once in sequential order. This poses great challenges for the effective mining of stream data. Substantial research has led to progress in the development of efficient methods for mining data streams, in the areas of mining frequent and sequential patterns, multidimensional analysis (e.g., the construction of stream cubes), classification, clustering, outlier analysis, and the online detection of rare events in data streams. The general philosophy is to develop single-scan or a-few-scan algorithms using limited computing and storage capabilities.

This includes collecting information about stream data in sliding windows or *tilted time windows* (where the most recent data are registered at the finest granularity and the more distant data are registered at a coarser granularity), and exploring techniques like microclustering, limited aggregation, and approximation. Many applications of stream data mining can be explored—for example, real-time detection of anomalies in computer network traffic, botnets, text streams, video streams, power-grid flows, web searches, sensor networks, and cyber-physical systems.

13.2 Other Methodologies of Data Mining

Due to the broad scope of data mining and the large variety of data mining methodologies, not all methodologies of data mining can be thoroughly covered in this book. In this section, we briefly discuss several interesting methodologies that were not fully addressed in the previous chapters. These methodologies are listed in Figure 13.3.

13.2.1 Statistical Data Mining

The data mining techniques described in this book are primarily drawn from computer science disciplines, including data mining, machine learning, data warehousing, and algorithms. They are designed for the efficient handling of huge amounts of data that are

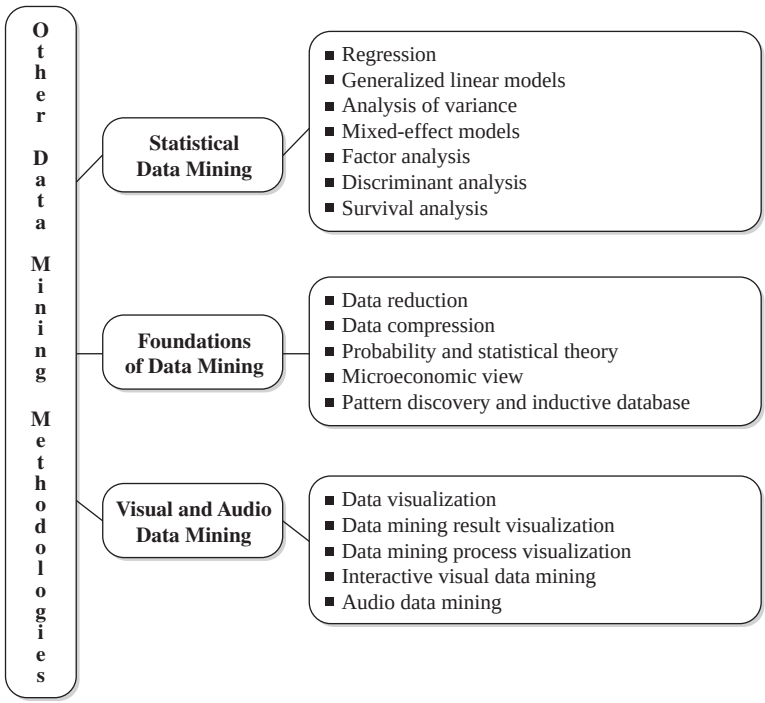

Figure 13.3 Other data mining methodologies.

typically multidimensional and possibly of various complex types. There are, however, many well-established statistical techniques for data analysis, particularly for numeric data. These techniques have been applied extensively to scientific data (e.g., data from experiments in physics, engineering, manufacturing, psychology, and medicine), as well as to data from economics and the social sciences. Some of these techniques, such as principal components analysis (Chapter 3) and clustering (Chapters 10 and 11), have already been addressed in this book. A thorough discussion of major statistical methods for data analysis is beyond the scope of this book; however, several methods are mentioned here for the sake of completeness. Pointers to these techniques are provided in the bibliographic notes (Section 13.8).

- **Regression**: In general, these methods are used to predict the value of a *response* (dependent) variable from one or more *predictor* (independent) variables, where the variables are numeric. There are various forms of regression, such as linear, multiple, weighted, polynomial, nonparametric, and robust (robust methods are useful when errors fail to satisfy normalcy conditions or when the data contain significant outliers).
- **Generalized linear models**: These models, and their generalization (*generalized additive models*), allow a *categorical* (nominal) response variable (or some transformation

of it) to be related to a set of predictor variables in a manner similar to the modeling of a numeric response variable using linear regression. Generalized linear models include logistic regression and Poisson regression.

- **Analysis of variance**: These techniques analyze experimental data for two or more populations described by a numeric response variable and one or more categorical variables (*factors*). In general, an ANOVA (single-factor analysis of variance) problem involves a comparison of k population or treatment means to determine if at least two of the means are different. More complex ANOVA problems also exist.
- **Mixed-effect models**: These models are for analyzing grouped data—data that can be classified according to one or more grouping variables. They typically describe relationships between a response variable and some covariates in data grouped according to one or more factors. Common areas of application include multilevel data, repeated measures data, block designs, and longitudinal data.
- **Factor analysis**: This method is used to determine which variables are combined to generate a given factor. For example, for many psychiatric data, it is not possible to measure a certain factor of interest directly (e.g., intelligence); however, it is often possible to measure other quantities (e.g., student test scores) that reflect the factor of interest. Here, none of the variables is designated as dependent.
- **Discriminant analysis**: This technique is used to predict a categorical response variable. Unlike generalized linear models, it assumes that the independent variables follow a multivariate normal distribution. The procedure attempts to determine several discriminant functions (linear combinations of the independent variables) that discriminate among the groups defined by the response variable. Discriminant analysis is commonly used in social sciences.
- **Survival analysis**: Several well-established statistical techniques exist for survival analysis. These techniques originally were designed to predict the probability that a patient undergoing a medical treatment would survive at least to time t. Methods for survival analysis, however, are also commonly applied to manufacturing settings to estimate the life span of industrial equipment. Popular methods include Kaplan-Meier estimates of survival, Cox proportional hazards regression models, and their extensions.
- **Quality control**: Various statistics can be used to prepare charts for quality control, such as Shewhart charts and CUSUM charts (both of which display group summary statistics). These statistics include the mean, standard deviation, range, count, moving average, moving standard deviation, and moving range.

13.2.2 Views on Data Mining Foundations

Research on the theoretical foundations of data mining has yet to mature. A solid and systematic theoretical foundation is important because it can help provide a coherent

framework for the development, evaluation, and practice of data mining technology. Several theories for the basis of data mining include the following:

- **Data reduction**: In this theory, the basis of data mining is to reduce the data representation. Data reduction trades accuracy for speed in response to the need to obtain quick approximate answers to queries on very large databases. Data reduction techniques include singular value decomposition (the driving element behind principal components analysis), wavelets, regression, log-linear models, histograms, clustering, sampling, and the construction of index trees.
- **Data compression**: According to this theory, the basis of data mining is to compress the given data by encoding in terms of bits, association rules, decision trees, clusters, and so on. Encoding based on the *minimum description length principle* states that the "best" theory to infer from a data set is the one that minimizes the length of the theory and of the data when encoded, using the theory as a predictor for the data. This encoding is typically in bits.
- **Probability and statistical theory**: According to this theory, the basis of data mining is to discover joint probability distributions of random variables, for example, Bayesian belief networks or hierarchical Bayesian models.
- **Microeconomic view**: The microeconomic view considers data mining as the task of finding patterns that are interesting only to the extent that they can be used in the decision-making process of some enterprise (e.g., regarding marketing strategies and production plans). This view is one of utility, in which patterns are considered interesting if they can be acted on. Enterprises are regarded as facing optimization problems, where the object is to maximize the utility or value of a decision. In this theory, data mining becomes a nonlinear optimization problem.
- **Pattern discovery and inductive databases**: In this theory, the basis of data mining is to discover patterns occurring in the data such as associations, classification models, sequential patterns, and so on. Areas such as machine learning, neural network, association mining, sequential pattern mining, clustering, and several other subfields contribute to this theory. A knowledge base can be viewed as a database consisting of data and patterns. A user interacts with the system by querying the data and the theory (i.e., patterns) in the knowledge base. Here, the knowledge base is actually an inductive database.

These theories are not mutually exclusive. For example, pattern discovery can also be seen as a form of data reduction or data compression. Ideally, a theoretical framework should be able to model typical data mining tasks (e.g., association, classification, and clustering), have a probabilistic nature, be able to handle different forms of data, and consider the iterative and interactive essence of data mining. Further efforts are required to establish a well-defined framework for data mining that satisfies these requirements.

13.2.3 Visual and Audio Data Mining

Visual data mining discovers implicit and useful knowledge from large data sets using data and/or knowledge visualization techniques. The human visual system is controlled by the eyes and brain, the latter of which can be thought of as a powerful, highly parallel processing and reasoning engine containing a large knowledge base. Visual data mining essentially combines the power of these components, making it a highly attractive and effective tool for the comprehension of data distributions, patterns, clusters, and outliers in data.

Visual data mining can be viewed as an integration of two disciplines: data visualization and data mining. It is also closely related to computer graphics, multimedia systems, human–computer interaction, pattern recognition, and high-performance computing. In general, data visualization and data mining can be integrated in the following ways:

- **Data visualization**: Data in a database or data warehouse can be viewed at different granularity or abstraction levels, or as different combinations of attributes or dimensions. Data can be presented in various visual forms, such as boxplots, 3-D cubes, data distribution charts, curves, surfaces, and link graphs, as shown in the data visualization section of Chapter 2. Figures 13.4 and 13.5 from StatSoft show

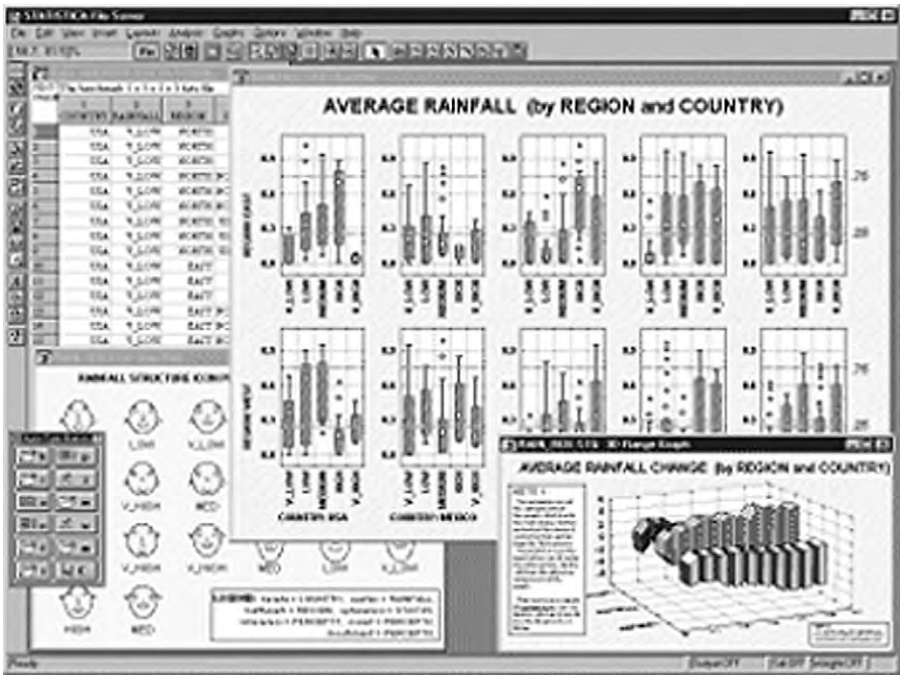

Figure 13.4 Boxplots showing multiple variable combinations in StatSoft. *Source:* *www.statsoft.com*.

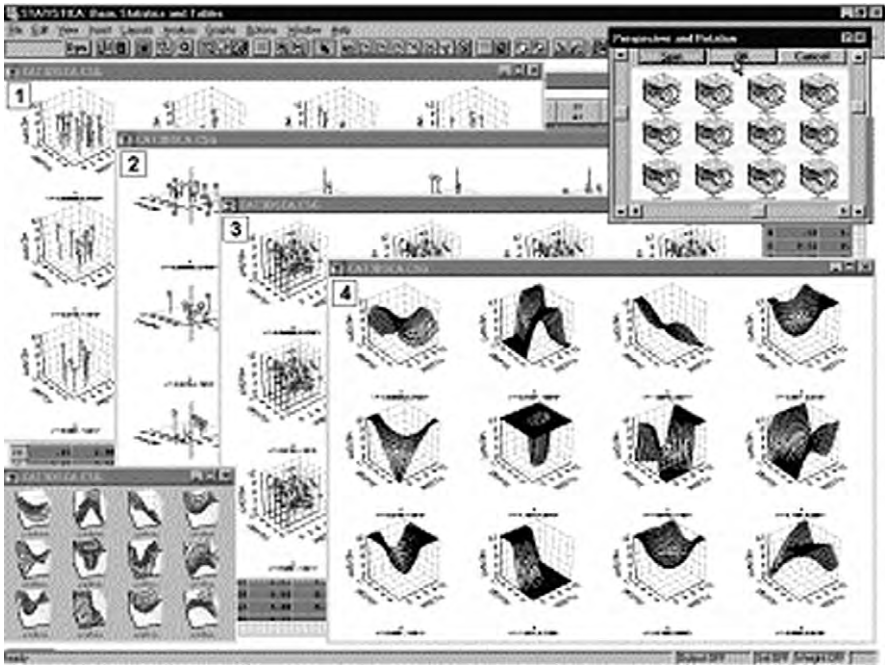

Figure 13.5 Multidimensional data distribution analysis in StatSoft. *Source: www.statsoft.com.*

data distributions in multidimensional space. Visual display can help give users a clear impression and overview of the data characteristics in a large data set.

- **Data mining result visualization**: Visualization of data mining results is the presentation of the results or knowledge obtained from data mining in visual forms. Such forms may include scatter plots and boxplots (Chapter 2), as well as decision trees, association rules, clusters, outliers, and generalized rules. For example, scatter plots are shown in Figure 13.6 from SAS Enterprise Miner. Figure 13.7, from MineSet, uses a plane associated with a set of pillars to describe a set of association rules mined from a database. Figure 13.8, also from MineSet, presents a decision tree. Figure 13.9, from IBM Intelligent Miner, presents a set of clusters and the properties associated with them.
- **Data mining process visualization**: This type of visualization presents the various processes of data mining in visual forms so that users can see how the data are extracted and from which database or data warehouse they are extracted, as well as how the selected data are cleaned, integrated, preprocessed, and mined. Moreover, it may also show which method is selected for data mining, where the results are stored, and how they may be viewed. Figure 13.10 shows a visual presentation of data mining processes by the Clementine data mining system.

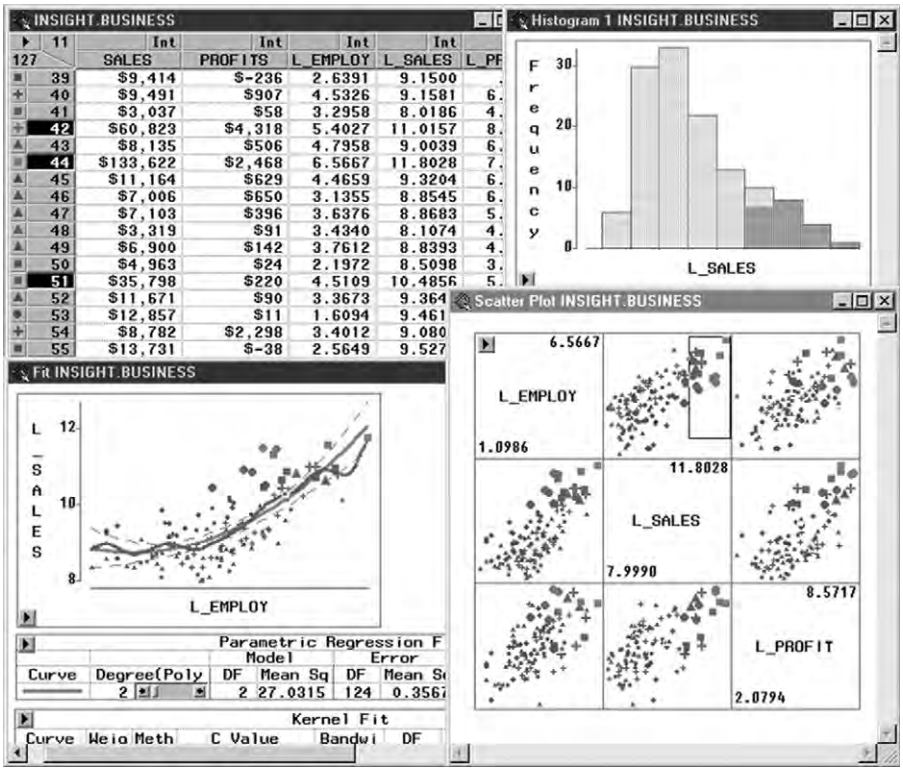

Figure 13.6 Visualization of data mining results in SAS Enterprise Miner.

- **Interactive visual data mining**: In (interactive) visual data mining, visualization tools can be used in the data mining process to help users make smart data mining decisions. For example, the data distribution in a set of attributes can be displayed using colored sectors (where the whole space is represented by a circle). This display helps users determine which sector should first be selected for classification and where a good split point for this sector may be. An example of this is shown in Figure 13.11, which is the output of a perception-based classification (PBC) system developed at the University of Munich.

Audio data mining uses audio signals to indicate the patterns of data or the features of data mining results. Although visual data mining may disclose interesting patterns using graphical displays, it requires users to concentrate on watching patterns and identifying interesting or novel features within them. This can sometimes be quite tiresome. If patterns can be transformed into sound and music, then instead of watching pictures, we can listen to pitchs, rhythm, tune, and melody to identify anything interesting or unusual. This may relieve some of the burden of visual concentration and be more

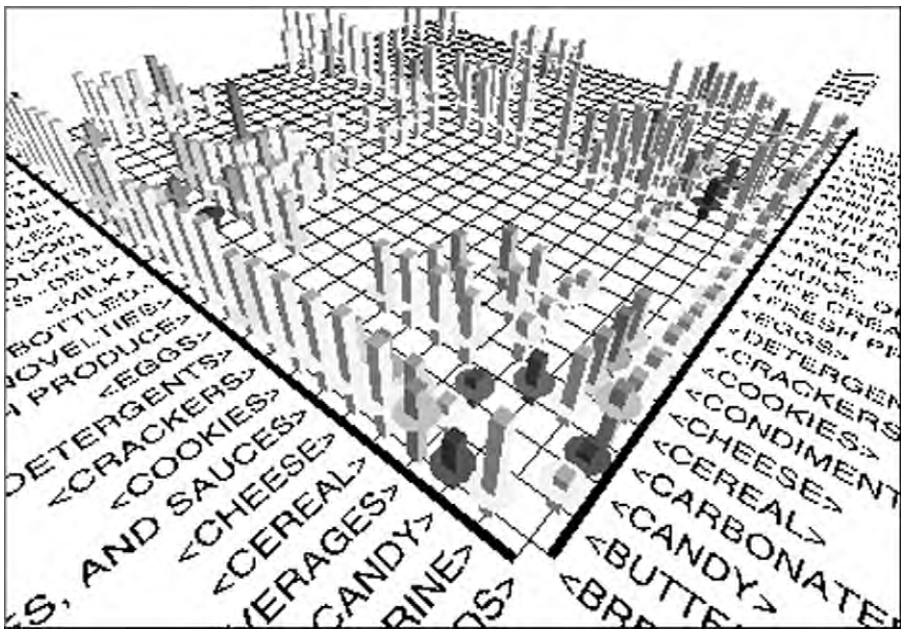

Figure 13.7 Visualization of association rules in MineSet.

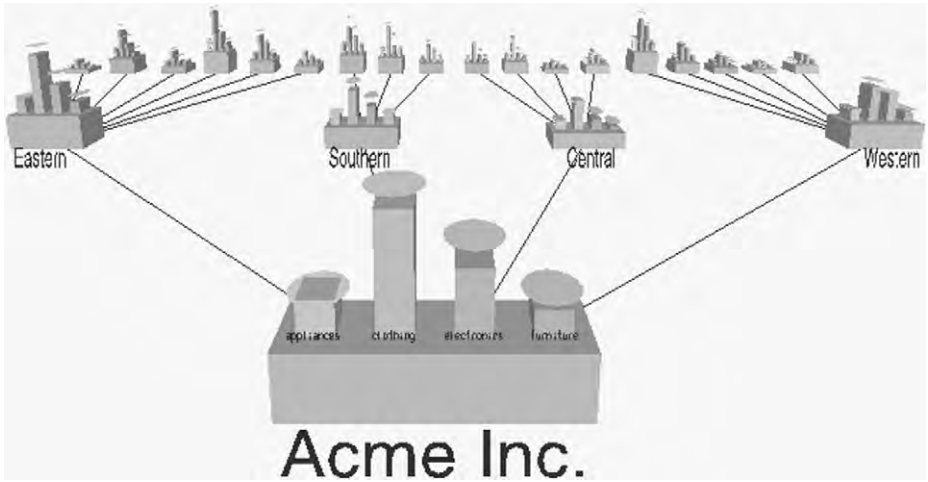

Figure 13.8 Visualization of a decision tree in MineSet.

Figure 13.9 Visualization of cluster groupings in IBM Intelligent Miner.

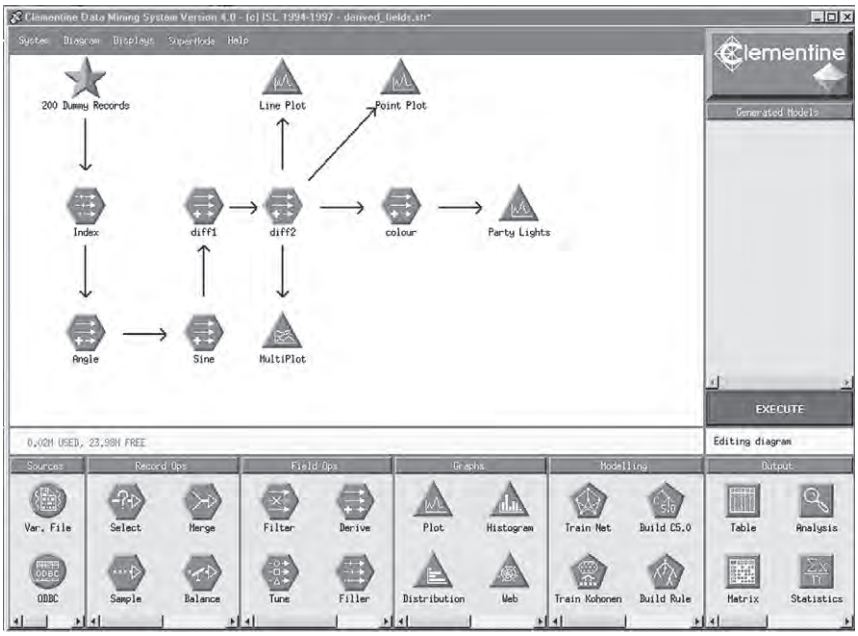

Figure 13.10 Visualization of data mining processes by Clementine.

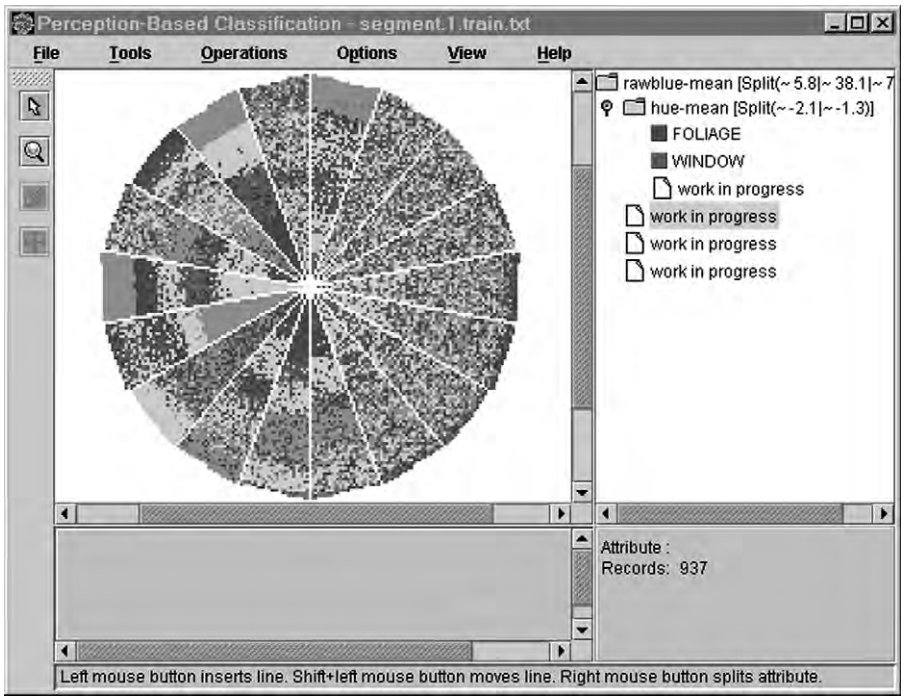

Figure 13.11 Perception-based classification, an interactive visual mining approach.

relaxing than visual mining. Therefore, audio data mining is an interesting complement to visual mining.

13.3 Data Mining Applications

In this book, we have studied principles and methods for mining relational data, data warehouses, and complex data types. Because data mining is a relatively young discipline with wide and diverse applications, there is still a nontrivial gap between general principles of data mining and application-specific, effective data mining tools. In this section, we examine several application domains, as listed in Figure 13.12. We discuss how customized data mining methods and tools should be developed for such applications.

13.3.1 Data Mining for Financial Data Analysis

Most banks and financial institutions offer a wide variety of banking, investment, and credit services (the latter include business, mortgage, and automobile loans and credit cards). Some also offer insurance and stock investment services.

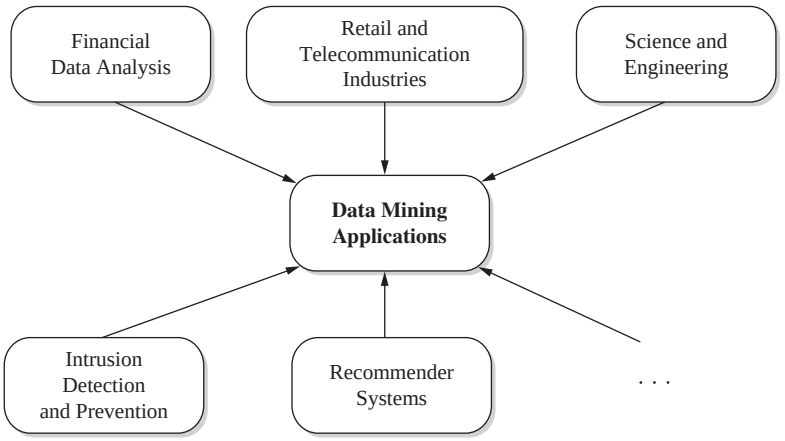

Figure 13.12 Common data mining application domains.

Financial data collected in the banking and financial industry are often relatively complete, reliable, and of high quality, which facilitates systematic data analysis and data mining. Here we present a few typical cases.

- **Design and construction of data warehouses for multidimensional data analysis and data mining:** Like many other applications, data warehouses need to be constructed for banking and financial data. Multidimensional data analysis methods should be used to analyze the general properties of such data. For example, a company's financial officer may want to view the debt and revenue changes by month, region, and sector, and other factors, along with maximum, minimum, total, average, trend, deviation, and other statistical information. Data warehouses, data cubes (including advanced data cube concepts such as multifeature, discovery-driven, regression, and prediction data cubes), characterization and class comparisons, clustering, and outlier analysis will all play important roles in financial data analysis and mining.
- **Loan payment prediction and customer credit policy analysis:** Loan payment prediction and customer credit analysis are critical to the business of a bank. Many factors can strongly or weakly influence loan payment performance and customer credit rating. Data mining methods, such as attribute selection and attribute relevance ranking, may help identify important factors and eliminate irrelevant ones. For example, factors related to the risk of loan payments include loan-to-value ratio, term of the loan, debt ratio (total amount of monthly debt versus total monthly income), payment-to-income ratio, customer income level, education level, residence region, and credit history. Analysis of the customer payment history may find that, say, payment-to-income ratio is a dominant factor, while education level and debt ratio are not. The bank may then decide to adjust its loan-granting policy so

as to grant loans to those customers whose applications were previously denied but whose profiles show relatively low risks according to the critical factor analysis.

- **Classification and clustering of customers for targeted marketing:** Classification and clustering methods can be used for customer group identification and targeted marketing. For example, we can use classification to identify the most crucial factors that may influence a customer's decision regarding banking. Customers with similar behaviors regarding loan payments may be identified by multidimensional clustering techniques. These can help identify customer groups, associate a new customer with an appropriate customer group, and facilitate targeted marketing.
- **Detection of money laundering and other financial crimes:** To detect money laundering and other financial crimes, it is important to integrate information from multiple, heterogeneous databases (e.g., bank transaction databases and federal or state crime history databases), as long as they are potentially related to the study. Multiple data analysis tools can then be used to detect unusual patterns, such as large amounts of cash flow at certain periods, by certain groups of customers. Useful tools include data visualization tools (to display transaction activities using graphs by time and by groups of customers), linkage and information network analysis tools (to identify links among different customers and activities), classification tools (to filter unrelated attributes and rank the highly related ones), clustering tools (to group different cases), outlier analysis tools (to detect unusual amounts of fund transfers or other activities), and sequential pattern analysis tools (to characterize unusual access sequences). These tools may identify important relationships and patterns of activities and help investigators focus on suspicious cases for further detailed examination.

13.3.2 Data Mining for Retail and Telecommunication Industries

The retail industry is a well-fit application area for data mining, since it collects huge amounts of data on sales, customer shopping history, goods transportation, consumption, and service. The quantity of data collected continues to expand rapidly, especially due to the increasing availability, ease, and popularity of business conducted on the Web, or **e-commerce**. Today, most major chain stores also have web sites where customers can make purchases online. Some businesses, such as Amazon.com (*www.amazon.com*), exist solely online, without any brick-and-mortar (i.e., physical) store locations. Retail data provide a rich source for data mining.

Retail data mining can help identify customer buying behaviors, discover customer shopping patterns and trends, improve the quality of customer service, achieve better customer retention and satisfaction, enhance goods consumption ratios, design more effective goods transportation and distribution policies, and reduce the cost of business.

A few examples of data mining in the retail industry are outlined as follows:

- **Design and construction of data warehouses:** Because retail data cover a wide spectrum (including sales, customers, employees, goods transportation, consumption,

and services), there can be many ways to design a data warehouse for this industry. The levels of detail to include can vary substantially. The outcome of preliminary data mining exercises can be used to help guide the design and development of data warehouse structures. This involves deciding which dimensions and levels to include and what preprocessing to perform to facilitate effective data mining.

- **Multidimensional analysis of sales, customers, products, time, and region:** The retail industry requires timely information regarding customer needs, product sales, trends, and fashions, as well as the quality, cost, profit, and service of commodities. It is therefore important to provide powerful multidimensional analysis and visualization tools, including the construction of sophisticated data cubes according to the needs of data analysis. The *advanced data cube structures* introduced in Chapter 5 are useful in retail data analysis because they facilitate analysis on multidimensional aggregates with complex conditions.
- **Analysis of the effectiveness of sales campaigns:** The retail industry conducts sales campaigns using advertisements, coupons, and various kinds of discounts and bonuses to promote products and attract customers. Careful analysis of the effectiveness of sales campaigns can help improve company profits. Multidimensional analysis can be used for this purpose by comparing the amount of sales and the number of transactions containing the sales items during the sales period versus those containing the same items before or after the sales campaign. Moreover, association analysis may disclose which items are likely to be purchased together with the items on sale, especially in comparison with the sales before or after the campaign.
- **Customer retention—analysis of customer loyalty:** We can use customer loyalty card information to register sequences of purchases of particular customers. Customer loyalty and purchase trends can be analyzed systematically. Goods purchased at different periods by the same customers can be grouped into sequences. Sequential pattern mining can then be used to investigate changes in customer consumption or loyalty and suggest adjustments on the pricing and variety of goods to help retain customers and attract new ones.
- **Product recommendation and cross-referencing of items:** By mining associations from sales records, we may discover that a customer who buys a digital camera is likely to buy another set of items. Such information can be used to form product recommendations. *Collaborative recommender systems* (Section 13.3.5) use data mining techniques to make personalized product recommendations during live customer transactions, based on the opinions of other customers. Product recommendations can also be advertised on sales receipts, in weekly flyers, or on the Web to help improve customer service, aid customers in selecting items, and increase sales. Similarly, information, such as "hot items this week" or attractive deals, can be displayed together with the associative information to promote sales.
- **Fraudulent analysis and the identification of unusual patterns:** Fraudulent activity costs the retail industry millions of dollars per year. It is important to (1) identify potentially fraudulent users and their atypical usage patterns; (2) detect attempts to gain fraudulent entry or unauthorized access to individual and organizational

accounts; and (3) discover unusual patterns that may need special attention. Many of these patterns can be discovered by multidimensional analysis, cluster analysis, and outlier analysis.

As another industry that handles huge amounts of data, the **telecommunication industry** has quickly evolved from offering local and long-distance telephone services to providing many other comprehensive communication services. These include cellular phone, smart phone, Internet access, email, text messages, images, computer and web data transmissions, and other data traffic. The integration of telecommunication, computer network, Internet, and numerous other means of communication and computing has been under way, changing the face of telecommunications and computing. This has created a great demand for data mining to help understand business dynamics, identify telecommunication patterns, catch fraudulent activities, make better use of resources, and improve service quality.

Data mining tasks in telecommunications share many similarities with those in the retail industry. Common tasks include constructing large-scale data warehouses, performing multidimensional visualization, OLAP, and in-depth analysis of trends, customer patterns, and sequential patterns. Such tasks contribute to business improvements, cost reduction, customer retention, fraud analysis, and sharpening the edges of competition. There are many data mining tasks for which customized data mining tools for telecommunication have been flourishing and are expected to play increasingly important roles in business.

Data mining has been popularly used in many other industries, such as *insurance, manufacturing, and health care*, as well as for the *analysis of governmental and institutional administration data*. Although each industry has its own characteristic data sets and application demands, they share many common principles and methodologies. Therefore, through effective mining in one industry, we may gain experience and methodologies that can be transferred to other industrial applications.

13.3.3 Data Mining in Science and Engineering

In the past, many scientific data analysis tasks tended to handle relatively small and homogeneous data sets. Such data were typically analyzed using a "*formulate hypothesis, build model, and evaluate results*" paradigm. In these cases, statistical techniques were typically employed for their analysis (see Section 13.2.1). Massive data collection and storage technologies have recently changed the landscape of scientific data analysis. Today, scientific data can be amassed at much higher speeds and lower costs. This has resulted in the accumulation of huge volumes of high-dimensional data, stream data, and heterogenous data, containing rich spatial and temporal information. Consequently, scientific applications are shifting from the "*hypothesize-and-test*" paradigm toward a "*collect and store data, mine for new hypotheses, confirm with data or experimentation*" process. This shift brings about new challenges for data mining.

Vast amounts of data have been collected from scientific domains (including geosciences, astronomy, meteorology, geology, and biological sciences) using sophisticated

telescopes, multispectral high-resolution remote satellite sensors, global positioning systems, and new generations of biological data collection and analysis technologies. Large data sets are also being generated due to fast numeric simulations in various fields such as climate and ecosystem modeling, chemical engineering, fluid dynamics, and structural mechanics. Here we look at some of the challenges brought about by emerging scientific applications of data mining.

- **Data warehouses and data preprocessing**: Data preprocessing and data warehouses are critical for information exchange and data mining. Creating a warehouse often requires finding means for resolving inconsistent or incompatible data collected in multiple environments and at different time periods. This requires reconciling semantics, referencing systems, geometry, measurements, accuracy, and precision. Methods are needed for integrating data from heterogeneous sources and for identifying events.

  For instance, consider climate and ecosystem data, which are spatial and temporal and require cross-referencing geospatial data. A major problem in analyzing such data is that there are too many events in the spatial domain but too few in the temporal domain. For example, El Nino events occur only every four to seven years, and previous data on them might not have been collected as systematically as they are today. Methods are also needed for the efficient computation of sophisticated spatial aggregates and the handling of spatial-related data streams.

- **Mining complex data types**: Scientific data sets are heterogeneous in nature. They typically involve semi-structured and unstructured data, such as multimedia data and georeferenced stream data, as well as data with sophisticated, deeply hidden semantics (e.g., genomic and proteomic data). Robust and dedicated analysis methods are needed for handling spatiotemporal data, biological data, related concept hierarchies, and complex semantic relationships. For example, in bioinformatics, a research problem is to identify regulatory influences on genes. *Gene regulation* refers to how genes in a cell are switched on (or off) to determine the cell's functions. Different biological processes involve different sets of genes acting together in precisely regulated patterns. Thus, to understand a biological process we need to identify the participating genes and their regulators. This requires the development of sophisticated data mining methods to analyze large biological data sets for clues about regulatory influences on specific genes, by finding DNA segments ("regulatory sequences") mediating such influence.

- **Graph-based and network-based mining**: It is often difficult or impossible to model several physical phenomena and processes due to limitations of existing modeling approaches. Alternatively, labeled graphs and networks may be used to capture many of the spatial, topological, geometric, biological, and other relational characteristics present in scientific data sets. In graph or network modeling, each object to be mined is represented by a vertex in a graph, and edges between vertices represent relationships between objects. For example, graphs can be used to model chemical structures, biological pathways, and data generated by numeric

simulations such as fluid-flow simulations. The success of graph or network modeling, however, depends on improvements in the scalability and efficiency of many graph-based data mining tasks such as classification, frequent pattern mining, and clustering.

- **Visualization tools and domain-specific knowledge**: High-level graphical user interfaces and visualization tools are required for scientific data mining systems. These should be integrated with existing domain-specific data and information systems to guide researchers and general users in searching for patterns, interpreting and visualizing discovered patterns, and using discovered knowledge in their decision making.

Data mining in engineering shares many similarities with data mining in science. Both practices often collect massive amounts of data, and require data preprocessing, data warehousing, and scalable mining of complex types of data. Both typically use visualization and make good use of graphs and networks. Moreover, many engineering processes need real-time responses, and so mining data streams in real time often becomes a critical component.

Massive amounts of human communication data pour into our daily life. Such communication exists in many forms, including news, blogs, articles, web pages, online discussions, product reviews, twitters, messages, advertisements, and communications, both on the Web and in various kinds of social networks. Hence, **data mining in social science and social studies** has become increasingly popular. Moreover, user or reader feedback regarding products, speeches, and articles can be analyzed to deduce general opinions and sentiments on the views of those in society. The analysis results can be used to predict trends, improve work, and help in decision making.

Computer science generates unique kinds of data. For example, computer programs can be long, and their execution often generates huge-size traces. Computer networks can have complex structures and the network flows can be dynamic and massive. Sensor networks may generate large amounts of data with varied reliability. Computer systems and databases can suffer from various kinds of attacks, and their system/data accessing may raise security and privacy concerns. These unique kinds of data provide fertile land for data mining.

Data mining in computer science can be used to help monitor system status, improve system performance, isolate software bugs, detect software plagiarism, analyze computer system faults, uncover network intrusions, and recognize system malfunctions. Data mining for software and system engineering can operate on static or dynamic (i.e., stream-based) data, depending on whether the system dumps traces beforehand for postanalysis or if it must react in real time to handle online data.

Various methods have been developed in this domain, which integrate and extend methods from machine learning, data mining, software/system engineering, pattern recognition, and statistics. Data mining in computer science is an active and rich domain for data miners because of its unique challenges. It requires the further development of sophisticated, scalable, and real-time data mining and software/system engineering methods.

13.3.4 Data Mining for Intrusion Detection and Prevention

The security of our computer systems and data is at continual risk. The extensive growth of the Internet and the increasing availability of tools and tricks for intruding and attacking networks have prompted **intrusion detection and prevention** to become a critical component of networked systems. An intrusion can be defined as any set of actions that threaten the integrity, confidentiality, or availability of a network resource (e.g., user accounts, file systems, system kernels, and so on). Intrusion detection systems and intrusion prevention systems both monitor network traffic and/or system executions for malicious activities. However, the former produces reports whereas the latter is placed in-line and is able to actively prevent/block intrusions that are detected. The main functions of an intrusion prevention system are to identify malicious activity, log information about said activity, attempt to block/stop activity, and report activity.

The majority of intrusion detection and prevention systems use either *signature-based detection* or *anomaly-based detection.*

- **Signature-based detection**: This method of detection utilizes *signatures*, which are attack patterns that are preconfigured and predetermined by domain experts. A signature-based intrusion prevention system monitors the network traffic for matches to these signatures. Once a match is found, the intrusion detection system will report the anomaly and an intrusion prevention system will take additional appropriate actions. Note that since the systems are usually quite dynamic, the signatures need to be updated laboriously whenever new software versions arrive or changes in network configuration or other situations occur. Another drawback is that such a detection mechanism can only identify cases that match the signatures. That is, it is unable to detect new or previously unknown intrusion tricks.
- **Anomaly-based detection**: This method builds models of normal network behavior (called *profiles*) that are then used to detect new patterns that significantly deviate from the profiles. Such deviations may represent actual intrusions or simply be new behaviors that need to be added to the profiles. The main advantage of anomaly detection is that it may detect novel intrusions that have not yet been observed. Typically, a human analyst must sort through the deviations to ascertain which represent real intrusions. A limiting factor of anomaly detection is the high percentage of false positives. New patterns of intrusion can be added to the set of signatures to enhance signature-based detection.

Data mining methods can help an intrusion detection and prevention system to enhance its performance in various ways as follows.

- **New data mining algorithms for intrusion detection**: Data mining algorithms can be used for both signature-based and anomaly-based detection. In signature-based detection, training data are labeled as either "normal" or "intrusion." A classifier can then be derived to detect known intrusions. Research in this area has

included the application of classification algorithms, association rule mining, and cost-sensitive modeling. Anomaly-based detection builds models of normal behavior and automatically detects significant deviations from it. Methods include the application of clustering, outlier analysis, and classification algorithms and statistical approaches. The techniques used must be efficient and scalable, and capable of handling network data of high volume, dimensionality, and heterogeneity.

- **Association, correlation, and discriminative pattern analyses help select and build discriminative classifiers**: Association, correlation, and discriminative pattern mining can be applied to find relationships between system attributes describing the network data. Such information can provide insight regarding the selection of useful attributes for intrusion detection. New attributes derived from aggregated data may also be helpful such as summary counts of traffic matching a particular pattern.
- **Analysis of stream data**: Due to the transient and dynamic nature of intrusions and malicious attacks, it is crucial to perform intrusion detection in the data stream environment. Moreover, an event may be normal on its own, but considered malicious if viewed as part of a sequence of events. Thus, it is necessary to study what sequences of events are frequently encountered together, find sequential patterns, and identify outliers. Other data mining methods for finding evolving clusters and building dynamic classification models in data streams are also necessary for real-time intrusion detection.
- **Distributed data mining**: Intrusions can be launched from several different locations and targeted to many different destinations. Distributed data mining methods may be used to analyze network data from several network locations to detect these distributed attacks.
- **Visualization and querying tools**: Visualization tools should be available for viewing any anomalous patterns detected. Such tools may include features for viewing associations, discriminative patterns, clusters, and outliers. Intrusion detection systems should also have a graphical user interface that allows security analysts to pose queries regarding the network data or intrusion detection results.

In summary, computer systems are at continual risk of breaks in security. Data mining technology can be used to develop strong intrusion detection and prevention systems, which may employ signature-based or anomaly-based detection.

13.3.5 Data Mining and Recommender Systems

Today's consumers are faced with millions of goods and services when shopping online. **Recommender systems** help consumers by making product recommendations that are likely to be of interest to the user such as books, CDs, movies, restaurants, online news articles, and other services. Recommender systems may use either a *content-based* approach, a *collaborative* approach, or a *hybrid* approach that combines both content-based and collaborative methods.

The **content-based approach** recommends items that are similar to items the user preferred or queried in the past. It relies on product features and textual item descriptions. The **collaborative approach** (or *collaborative filtering approach*) may consider a user's social environment. It recommends items based on the opinions of other customers who have similar tastes or preferences as the user. Recommender systems use a broad range of techniques from information retrieval, statistics, machine learning, and data mining to search for similarities among items and customer preferences. Consider Example 13.1.

Example 13.1 **Scenarios of using a recommender system.** Suppose that you visit the web site of an online bookstore (e.g., Amazon) with the intention of purchasing a book that you have been wanting to read. You type in the name of the book. This is not the first time you have visited the web site. You have browsed through it before and even made purchases from it last Christmas. The web store remembers your previous visits, having stored click stream information and information regarding your past purchases. The system displays the description and price of the book you have just specified. It compares your interests with other customers having similar interests and recommends additional book titles, saying *"Customers who bought the book you have specified also bought these other titles as well."* From surveying the list, you see another title that sparks your interest and decide to purchase that one as well.

Now suppose you go to another online store with the intention of purchasing a digital camera. The system suggests additional items to consider based on previously mined sequential patterns, such as *"Customers who buy this kind of digital camera are likely to buy a particular brand of printer, memory card, or photo editing software within three months."* You decide to buy just the camera, without any additional items. A week later, you receive coupons from the store regarding the additional items. ■

An advantage of recommender systems is that they provide *personalization* for customers of e-commerce, promoting one-to-one marketing. Amazon, a pioneer in the use of collaborative recommender systems, offers "a personalized store for every customer" as part of their marketing strategy. Personalization can benefit both consumers and the company involved. By having more accurate models of their customers, companies gain a better understanding of customer needs. Serving these needs can result in greater success regarding cross-selling of related products, upselling, product affinities, one-to-one promotions, larger baskets, and customer retention.

The recommendation problem considers a set, C, of users and a set, S, of items. Let u be a utility function that measures the usefulness of an item, s, to a user, c. The utility is commonly represented by a rating and is initially defined only for items previously rated by users. For example, when joining a movie recommendation system, users are typically asked to rate several movies. The space $C \times S$ of all possible users and items is huge. The recommendation system should be able to extrapolate from known to unknown ratings so as to predict item–user combinations. Items with the highest predicted rating/utility for a user are recommended to that user.

"*How is the utility of an item estimated for a user*?" In content-based methods, it is estimated based on the utilities assigned by the same user to other items that are similar. Many such systems focus on recommending items containing textual information, such as web sites, articles, and news messages. They look for commonalities among items. For movies, they may look for similar genres, directors, or actors. For articles, they may look for similar terms. Content-based methods are rooted in information theory. They make use of keywords (describing the items) and user profiles that contain information about users' tastes and needs. Such profiles may be obtained explicitly (e.g., through questionnaires) or learned from users' transactional behavior over time.

A collaborative recommender system tries to predict the utility of items for a user, u, based on items previously rated by other users who are similar to u. For example, when recommending books, a collaborative recommender system tries to find other users who have a history of agreeing with u (e.g., they tend to buy similar books, or give similar ratings for books). Collaborative recommender systems can be either memory (or heuristic) based or model based.

Memory-based methods essentially use heuristics to make rating predictions based on the entire collection of items previously rated by users. That is, the unknown rating of an item–user combination can be estimated as an aggregate of ratings of the most similar users for the same item. Typically, a k-nearest-neighbor approach is used, that is, we find the k other users (or neighbors) that are most similar to our target user, u. Various approaches can be used to compute the similarity between users. The most popular approaches use either Pearson's correlation coefficient (Section 3.3.2) or cosine similarity (Section 2.4.7). A weighted aggregate can be used, which adjusts for the fact that different users may use the rating scale differently. Model-based collaborative recommender systems use a collection of ratings to learn a model, which is then used to make rating predictions. For example, probabilistic models, clustering (which finds clusters of like-minded customers), Bayesian networks, and other machine learning techniques have been used.

Recommender systems face major challenges such as scalability and ensuring quality recommendations to the consumer. For example, regarding scalability, collaborative recommender systems must be able to search through millions of potential neighbors in real time. If the site is using browsing patterns as indications of product preference, it may have thousands of data points for some of its customers. Ensuring quality recommendations is essential to gain consumers' trust. If consumers follow a system recommendation but then do not end up liking the product, they are less likely to use the recommender system again.

As with classification systems, recommender systems can make two types of errors: false negatives and false positives. Here, *false negatives* are products that the system fails to recommend, although the consumer would like them. *False positives* are products that are recommended, but which the consumer does not like. False positives are less desirable because they can annoy or anger consumers. Content-based recommender systems are limited by the features used to describe the items they recommend.

Another challenge for both content-based and collaborative recommender systems is how to deal with new users for which a buying history is not yet available.

Hybrid approaches integrate both content-based and collaborative methods to achieve further improved recommendations. The Netflix Prize was an open competition held by an online DVD-rental service, with a payout of $1,000,000 for the best recommender algorithm to predict user ratings for films, based on previous ratings. The competition and other studies have shown that the predictive accuracy of a recommender system can be substantially improved when blending multiple predictors, especially by using an ensemble of many substantially different methods, rather than refining a single technique.

Collaborative recommender systems are a form of **intelligent query answering**, which consists of analyzing the intent of a query and providing generalized, neighborhood, or associated information relevant to the query. For example, rather than simply returning the book description and price in response to a customer's query, returning additional information that is related to the query but that was not explicitly asked for (e.g., book evaluation comments, recommendations of other books, or sales statistics) provides an intelligent answer to the same query.

13.4 Data Mining and Society

For most of us, data mining is part of our daily lives, although we may often be unaware of its presence. Section 13.4.1 looks at several examples of "ubiquitous and invisible" data mining, affecting everyday things from the products stocked at our local supermarket, to the ads we see while surfing the Internet, to crime prevention. Data mining can offer the individual many benefits by improving customer service and satisfaction as well as lifestyle, in general. However, it also has serious implications regarding one's right to privacy and data security. These issues are the topic of Section 13.4.2.

13.4.1 Ubiquitous and Invisible Data Mining

Data mining is present in many aspects of our daily lives, whether we realize it or not. It affects how we shop, work, and search for information, and can even influence our leisure time, health, and well-being. In this section, we look at examples of such **ubiquitous** (or ever-present) **data mining**. Several of these examples also represent **invisible data mining**, in which "smart" software, such as search engines, customer-adaptive web services (e.g., using recommender algorithms), "intelligent" database systems, email managers, ticket masters, and so on, incorporates data mining into its functional components, often unbeknownst to the user.

From grocery stores that print personalized coupons on customer receipts to online stores that recommend additional items based on customer interests, data mining has innovatively influenced what we buy, the way we shop, and our experience while shopping. One example is Wal-Mart, which has hundreds of millions of customers visiting its tens of thousands of stores every week. Wal-Mart allows suppliers to access data on

their products and perform analyses using data mining software. This allows suppliers to identify customer buying patterns at different stores, control inventory and product placement, and identify new merchandizing opportunities. All of these affect which items (and how many) end up on the stores' shelves—something to think about the next time you wander through the aisles at Wal-Mart.

Data mining has shaped the online shopping experience. Many shoppers routinely turn to online stores to purchase books, music, movies, and toys. Recommender systems, discussed in Section 13.3.5, offer personalized product recommendations based on the opinions of other customers. Amazon.com was at the forefront of using such a personalized, data mining–based approach as a marketing strategy. It has observed that in traditional brick-and-mortar stores, the hardest part is getting the customer into the store. Once the customer is there, he or she is likely to buy something, since the cost of going to another store is high. Therefore, the marketing for brick-and-mortar stores tends to emphasize drawing customers in, rather than the actual in-store customer experience. This is in contrast to online stores, where customers can "walk out" and enter another online store with just a click of the mouse. Amazon.com capitalized on this difference, offering a "personalized store for every customer." They use several data mining techniques to identify customer's likes and make reliable recommendations.

While we are on the topic of shopping, suppose you have been doing a lot of buying with your credit cards. Nowadays, it is not unusual to receive a phone call from one's credit card company regarding suspicious or unusual patterns of spending. Credit card companies use data mining to detect fraudulent usage, saving billions of dollars a year.

Many companies increasingly use data mining for **customer relationship management (CRM)**, which helps provide more customized, personal service addressing individual customer's needs, in lieu of mass marketing. By studying browsing and purchasing patterns on web stores, companies can tailor advertisements and promotions to customer profiles, so that customers are less likely to be annoyed with unwanted mass mailings or junk mail. These actions can result in substantial cost savings for companies. The customers further benefit in that they are more likely to be notified of offers that are actually of interest, resulting in less waste of personal time and greater satisfaction.

Data mining has greatly influenced the ways in which people use computers, search for information, and work. Once you get on the Internet, for example, you decide to check your email. Unbeknownst to you, several annoying emails have already been deleted, thanks to a spam filter that uses classification algorithms to recognize spam. After processing your email, you go to Google (*www.google.com*), which provides access to information from billions of web pages indexed on its server. Google is one of the most popular and widely used Internet search engines. Using Google to search for information has become a way of life for many people.

Google is so popular that it has even become a new verb in the English language, meaning "to search for (something) on the Internet using the Google search engine or, by extension, any comprehensive search engine."[1] You decide to type in some keywords

[1] *http://open-dictionary.com*.

for a topic of interest. Google returns a list of web sites on your topic, mined, indexed, and organized by a set of data mining algorithms including PageRank. Moreover, if you type "Boston New York," Google will show you bus and train schedules from Boston to New York; however, a minor change to "Boston Paris" will lead to flight schedules from Boston to Paris. Such smart offerings of information or services are likely based on the frequent patterns mined from the click streams of many previous queries.

While you are viewing the results of your Google query, various ads pop up relating to your query. Google's strategy of tailoring advertising to match the user's interests is one of the typical services being explored by every Internet search provider. This also makes you happier, because you are less likely to be pestered with irrelevant ads.

Data mining is omnipresent, as can be seen from these daily-encountered examples. We could go on and on with such scenarios. In many cases, data mining is invisible, as users may be unaware that they are examining results returned by data mining or that their clicks are actually fed as new data into some data mining functions. For data mining to become further improved and accepted as a technology, continuing research and development are needed in the many areas mentioned as challenges throughout this book. These include efficiency and scalability, increased user interaction, incorporation of background knowledge and visualization techniques, effective methods for finding interesting patterns, improved handling of complex data types and stream data, real-time data mining, web mining, and so on. In addition, the *integration* of data mining into existing business and scientific technologies, to provide domain-specific data mining tools, will further contribute to the advancement of the technology. The success of data mining solutions tailored for e-commerce applications, as opposed to generic data mining systems, is an example.

13.4.2 Privacy, Security, and Social Impacts of Data Mining

With more and more information accessible in electronic forms and available on the Web, and with increasingly powerful data mining tools being developed and put into use, there are increasing concerns that data mining may pose a threat to our privacy and data security. However, it is important to note that many data mining applications do not even touch personal data. Prominent examples include applications involving natural resources, the prediction of floods and droughts, meteorology, astronomy, geography, geology, biology, and other scientific and engineering data. Furthermore, most studies in data mining research focus on the development of scalable algorithms and do not involve personal data.

The focus of data mining technology is on the *discovery of general or statistically significant patterns*, not on specific information regarding individuals. In this sense, we believe that the real privacy concerns are with unconstrained access to individual records, especially access to privacy-sensitive information such as credit card transaction records, health-care records, personal financial records, biological traits, criminal/justice investigations, and ethnicity. For the data mining applications that do involve personal data, in many cases, simple methods such as removing sensitive IDs from data may protect the privacy of most individuals. Nevertheless, privacy concerns exist wherever

personally identifiable information is collected and stored in digital form, and data mining programs are able to access such data, even during data preparation.

Improper or nonexistent disclosure control can be the root cause of privacy issues. To handle such concerns, numerous data security-enhancing techniques have been developed. In addition, there has been a great deal of recent effort on developing *privacy-preserving* data mining methods. In this section, we look at some of the advances in protecting privacy and data security in data mining.

"*What can we do to secure the privacy of individuals while collecting and mining data?*" Many **data security–enhancing techniques** have been developed to help protect data. Databases can employ a *multilevel security model* to classify and restrict data according to various security levels, with users permitted access to only their authorized level. It has been shown, however, that users executing specific queries at their authorized security level can still infer more sensitive information, and that a similar possibility can occur through data mining. *Encryption* is another technique in which individual data items may be encoded. This may involve *blind signatures* (which build on public key encryption), *biometric encryption* (e.g., where the image of a person's iris or fingerprint is used to encode his or her personal information), and *anonymous databases* (which permit the consolidation of various databases but limit access to personal information only to those who need to know; personal information is encrypted and stored at different locations). Intrusion detection is another active area of research that helps protect the privacy of personal data.

Privacy-preserving data mining is an area of data mining research in response to privacy protection in data mining. It is also known as *privacy-enhanced* or *privacy-sensitive* data mining. It deals with obtaining valid data mining results without disclosing the underlying sensitive data values. Most privacy-preserving data mining methods use some form of transformation on the data to perform privacy preservation. Typically, such methods reduce the granularity of representation to preserve privacy. For example, they may generalize the data from individual customers to customer groups. This reduction in granularity causes loss of information and possibly of the usefulness of the data mining results. This is the natural trade-off between information loss and privacy. Privacy-preserving data mining methods can be classified into the following categories.

- **Randomization methods**: These methods add noise to the data to mask some attribute values of records. The noise added should be sufficiently large so that individual record values, especially sensitive ones, cannot be recovered. However, it should be added skillfully so that the final results of data mining are basically preserved. Techniques are designed to derive aggregate distributions from the perturbed data. Subsequently, data mining techniques can be developed to work with these aggregate distributions.
- **The *k*-anonymity and *l*-diversity methods**: Both of these methods alter individual records so that they cannot be uniquely identified. In the *k-anonymity method*, the granularity of data representation is reduced sufficiently so that any given record maps onto at least *k* other records in the data. It uses techniques like generalization and suppression. The *k*-anonymity method is weak in that, if there is a homogeneity

of sensitive values within a group, then those values may be inferred for the altered records. The *l-diversity model* was designed to handle this weakness by enforcing intragroup diversity of sensitive values to ensure anonymization. The goal is to make it sufficiently difficult for adversaries to use combinations of record attributes to exactly identify individual records.

- **Distributed privacy preservation**: Large data sets could be partitioned and distributed either *horizontally* (i.e., the data sets are partitioned into different subsets of records and distributed across multiple sites) or *vertically* (i.e., the data sets are partitioned and distributed by their attributes), or even in a combination of both. While the individual sites may not want to share their entire data sets, they may consent to limited information sharing with the use of a variety of protocols. The overall effect of such methods is to maintain privacy for each individual object, while deriving aggregate results over all of the data.
- **Downgrading the effectiveness of data mining results**: In many cases, even though the data may not be available, the output of data mining (e.g, association rules and classification models) may result in violations of privacy. The solution could be to downgrade the effectiveness of data mining by either modifying data or mining results, such as hiding some association rules or slightly distorting some classification models.

Recently, researchers proposed new ideas in privacy-preserving data mining such as the notion of **differential privacy**. The general idea is that, for any two data sets that are close to one another (i.e., that differ only on a tiny data set such as a single element), a given *differentially private algorithm* will behave approximately the same on both data sets. This definition gives a strong guarantee that the presence or absence of a tiny data set (e.g., representing an individual) will not affect the final output of the query significantly. Based on this notion, a set of differential privacy-preserving data mining algorithms have been developed. Research in this direction is ongoing. We expect more powerful privacy-preserving data publishing and data mining algorithms in the near future.

Like any other technology, data mining can be misused. However, we must not lose sight of all the benefits that data mining research can bring, ranging from insights gained from medical and scientific applications to increased customer satisfaction by helping companies better suit their clients' needs. We expect that computer scientists, policy experts, and counterterrorism experts will continue to work with social scientists, lawyers, companies, and consumers to take responsibility in building solutions to ensure data privacy protection and security. In this way, we may continue to reap the benefits of data mining in terms of time and money savings and the discovery of new knowledge.

13.5 Data Mining Trends

The diversity of data, data mining tasks, and data mining approaches poses many challenging research issues in data mining. The development of efficient and effective data

mining methods, systems and services, and interactive and integrated data mining environments is a key area of study. The use of data mining techniques to solve large or sophisticated application problems is an important task for data mining researchers and data mining system and application developers. This section describes some of the trends in data mining that reflect the pursuit of these challenges.

- **Application exploration:** Early data mining applications put a lot of effort into helping businesses gain a competitive edge. The exploration of data mining for businesses continues to expand as e-commerce and e-marketing have become mainstream in the retail industry. Data mining is increasingly used for the exploration of applications in other areas such as web and text analysis, financial analysis, industry, government, biomedicine, and science. Emerging application areas include data mining for counterterrorism and mobile (wireless) data mining. Because generic data mining systems may have limitations in dealing with application-specific problems, we may see a trend toward the development of more application-specific data mining systems and tools, as well as invisible data mining functions embedded in various kinds of services.
- **Scalable and interactive data mining methods:** In contrast with traditional data analysis methods, data mining must be able to handle huge amounts of data efficiently and, if possible, interactively. Because the amount of data being collected continues to increase rapidly, scalable algorithms for individual and integrated data mining functions become essential. One important direction toward improving the overall efficiency of the mining process while increasing user interaction is **constraint-based mining**. This provides users with added control by allowing the specification and use of constraints to guide data mining systems in their search for interesting patterns and knowledge.
- **Integration of data mining with search engines, database systems, data warehouse systems, and cloud computing systems:** Search engines, database systems, data warehouse systems, and cloud computing systems are mainstream information processing and computing systems. It is important to ensure that data mining serves as an essential data analysis component that can be smoothly integrated into such an information processing environment. A data mining subsystem/service should be tightly coupled with such systems as a seamless, unified framework or as an invisible function. This will ensure data availability, data mining portability, scalability, high performance, and an integrated information processing environment for multidimensional data analysis and exploration.
- **Mining social and information networks:** Mining social and information networks and link analysis are critical tasks because such networks are ubiquitous and complex. The development of scalable and effective knowledge discovery methods and applications for large numbers of network data is essential, as outlined in Section 13.1.2.
- **Mining spatiotemporal, moving-objects, and cyber-physical systems:** Cyber-physical systems as well as spatiotemporal data are mounting rapidly due to the

popular use of cellular phones, GPS, sensors, and other wireless equipment. As outlined in Section 13.1.3, there are many challenging research issues realizing real-time and effective knowledge discovery with such data.

- **Mining multimedia, text, and web data:** As outlined in Section 13.1.3, mining such kinds of data is a recent focus in data mining research. Great progress has been made, yet there are still many open issues to be solved.
- **Mining biological and biomedical data:** The unique combination of complexity, richness, size, and importance of biological and biomedical data warrants special attention in data mining. Mining DNA and protein sequences, mining high-dimensional microarray data, and biological pathway and network analysis are just a few topics in this field. Other areas of biological data mining research include mining biomedical literature, link analysis across heterogeneous biological data, and information integration of biological data by data mining.
- **Data mining with software engineering and system engineering:** Software programs and large computer systems have become increasingly bulky in size sophisticated in complexity, and tend to originate from the integration of multiple components developed by different implementation teams. This trend has made it an increasingly challenging task to ensure software robustness and reliability. The analysis of the executions of a buggy software program is essentially a data mining process—tracing the data generated during program executions may disclose important patterns and outliers that could lead to the eventual automated discovery of software bugs. We expect that the further development of data mining methodologies for software/system debugging will enhance software robustness and bring new vigor to software/system engineering.
- **Visual and audio data mining:** Visual and audio data mining is an effective way to integrate with humans' visual and audio systems and discover knowledge from huge amounts of data. A systematic development of such techniques will facilitate the promotion of human participation for effective and efficient data analysis.
- **Distributed data mining and real-time data stream mining:** Traditional data mining methods, designed to work at a centralized location, do not work well in many of the distributed computing environments present today (e.g., the Internet, intranets, local area networks, high-speed wireless networks, sensor networks, and cloud computing). Advances in distributed data mining methods are expected. Moreover, many applications involving stream data (e.g., e-commerce, Web mining, stock analysis, intrusion detection, mobile data mining, and data mining for counterterrorism) require dynamic data mining models to be built in real time. Additional research is needed in this direction.
- **Privacy protection and information security in data mining:** An abundance of personal or confidential information available in electronic forms, coupled with increasingly powerful data mining tools, poses a threat to data privacy and security. Growing interest in data mining for counterterrorism also adds to the concern.

Further development of privacy-preserving data mining methods is foreseen. The collaboration of technologists, social scientists, law experts, governments, and companies is needed to produce a rigorous privacy and security protection mechanism for data publishing and data mining.

With confidence, we look forward to the next generation of data mining technology and the further benefits that it will bring.

13.6 Summary

- Mining complex data types poses challenging issues, for which there are many dedicated lines of research and development. This chapter presents a high-level overview of **mining complex data types**, which includes *mining sequence data* such as time series, symbolic sequences, and biological sequences; *mining graphs and networks*; and mining other kinds of data, including *spatiotemporal and cyber-physical system data*, *multimedia, text and Web data*, and *data streams*.
- Several well-established **statistical methods** have been proposed for data analysis such as regression, generalized linear models, analysis of variance, mixed-effect models, factor analysis, discriminant analysis, survival analysis, and quality control. Full coverage of statistical data analysis methods is beyond the scope of this book. Interested readers are referred to the statistical literature cited in the bibliographic notes (Section 13.8).
- Researchers have been striving to build **theoretical foundations** for data mining. Several interesting proposals have appeared, based on data reduction, data compression, probability and statistics theory, microeconomic theory, and pattern discovery–based inductive databases.
- **Visual data mining** integrates data mining and data visualization to discover implicit and useful knowledge from large data sets. Visual data mining includes *data visualization*, *data mining result visualization*, *data mining process visualization,* and *interactive visual data mining*. **Audio data mining** uses audio signals to indicate data patterns or features of data mining results.
- Many customized data mining tools have been developed for **domain-specific applications**, including finance, the retail and telecommunication industries, science and engineering, intrusion detection and prevention, and recommender systems. Such application domain-based studies integrate domain-specific knowledge with data analysis techniques and provide mission-specific data mining solutions.
- **Ubiquitous data mining** is the constant presence of data mining in many aspects of our daily lives. It can influence how we shop, work, search for information, and use a computer, as well as our leisure time, health, and well-being. In **invisible data mining**, "smart" software, such as search engines, customer-adaptive web services

(e.g., using recommender algorithms), email managers, and so on, incorporates data mining into its functional components, often unbeknownst to the user.

- A major social concern of data mining is the issue of *privacy and data security*. **Privacy-preserving data mining** deals with obtaining valid data mining results without disclosing underlying sensitive values. Its goal is to ensure privacy protection and security while preserving the overall quality of data mining results.
- **Data mining trends** include further efforts toward the exploration of new application areas; improved scalable, interactive, and constraint-based mining methods; the integration of data mining with web service, database, warehousing, and cloud computing systems; and mining social and information networks. Other trends include the mining of spatiotemporal and cyber-physical system data, biological data, software/system engineering data, and multimedia and text data, in addition to web mining, distributed and real-time data stream mining, visual and audio mining, and privacy and security in data mining.

13.7 Exercises

13.1 Sequence data are ubiquitous and have diverse applications. This chapter presented a general overview of sequential pattern mining, sequence classification, sequence similarity search, trend analysis, biological sequence alignment, and modeling. However, we have not covered sequence clustering. Present an overview of methods for *sequence clustering*.

13.2 This chapter presented an overview of sequence pattern mining and graph pattern mining methods. Mining tree patterns and partial order patterns is also studied in research. *Summarize the methods for mining structured patterns*, including sequences, trees, graphs, and partial order relationships. Examine what kinds of structural pattern mining have not been covered in research. Propose applications that can be created for such new mining problems.

13.3 Many studies analyze homogeneous information networks (e.g., social networks consisting of friends linked with friends). However, many other applications involve *heterogeneous information networks* (i.e., networks linking multiple types of object such as research papers, conference, authors, and topics). What are the major differences between methodologies for mining heterogeneous information networks and methods for their homogeneous counterparts?

13.4 Research and describe a *data mining application* that was not presented in this chapter. Discuss how different forms of data mining can be used in the application.

13.5 Why is the establishment of *theoretical foundations* important for data mining? Name and describe the main theoretical foundations that have been proposed for data mining. Comment on how they each satisfy (or fail to satisfy) the requirements of an ideal theoretical framework for data mining.

13.6 (**Research project**) Building a theory of data mining requires setting up a *theoretical framework* so that the major data mining functions can be explained under this framework. Take one theory as an example (e.g., data compression theory) and examine how the major data mining functions fit into this framework. If some functions do not fit well into the current theoretical framework, can you propose a way to extend the framework to explain these functions?

13.7 There is a strong linkage between *statistical data analysis* and data mining. Some people think of data mining as automated and scalable methods for statistical data analysis. Do you agree or disagree with this perception? Present one statistical analysis method that can be automated and/or scaled up nicely by integration with current data mining methodology.

13.8 What are the differences between *visual data mining* and *data visualization*? Data visualization may suffer from the data abundance problem. For example, it is not easy to visually discover interesting properties of network connections if a social network is huge, with complex and dense connections. Propose a visualization method that may help people see through the network topology to the interesting features of a social network.

13.9 Propose a few implementation methods for *audio data mining*. Can we integrate audio and *visual data mining* to bring fun and power to data mining? Is it possible to develop some video data mining methods? State some scenarios and your solutions to make such integrated audiovisual mining effective.

13.10 General-purpose computers and domain-independent relational database systems have become a large market in the last several decades. However, many people feel that generic data mining systems will not prevail in the data mining market. What do you think? For data mining, should we focus our efforts on developing *domain-independent* data mining tools or on developing *domain-specific* data mining solutions? Present your reasoning.

13.11 What is a *recommender system*? In what ways does it differ from a customer or product-based clustering system? How does it differ from a typical classification or predictive modeling system? Outline one method of collaborative filtering. Discuss why it works and what its limitations are in practice.

13.12 Suppose that your local bank has a data mining system. The bank has been studying your debit card usage patterns. Noticing that you make many transactions at home renovation stores, the bank decides to contact you, offering information regarding their special loans for home improvements.

(a) Discuss how this may conflict with your right to *privacy*.

(b) Describe another situation in which you feel that data mining can infringe on your privacy.

(c) Describe a *privacy-preserving data mining* method that may allow the bank to perform customer pattern analysis without infringing on its customers' right to privacy.

(d) What are some examples where data mining could be used to help society? Can you think of ways it could be used that may be detrimental to society?

13.13 What are the major challenges faced in bringing data mining research to *market*? Illustrate one data mining research issue that, in your view, may have a strong impact on the market and on society. Discuss how to approach such a research issue.

13.14 Based on your view, what is the most *challenging research problem* in data mining? If you were given a number of years and a good number of researchers and implementors, what would your plan be to make good progress toward an effective solution to such a problem?

13.15 Based on your experience and knowledge, suggest a *new frontier* in data mining that was not mentioned in this chapter.

13.8 Bibliographic Notes

For mining complex data types, there are many research papers and books covering various themes. We list here some recent books and well-cited survey or research articles for references.

Time-series analysis has been studied in statistics and computer science communities for decades, with many textbooks such as Box, Jenkins, and Reinsel [BJR08]; Brockwell and Davis [BD02]; Chatfield [Cha03b]; Hamilton [Ham94]; and Shumway and Stoffer [SS05]. A fast subsequence matching method in time-series databases was presented by Faloutsos, Ranganathan, and Manolopoulos [FRM94]. Agrawal, Lin, Sawhney, and Shim [ALSS95] developed a method for fast **similarity search** in the presence of noise, scaling, and translation in time-series databases. Shasha and Zhu present an overview of the methods for high-performance discovery in time series [SZ04].

Sequential pattern mining methods have been studied by many researchers, including Agrawal and Srikant [AS95]; Zaki [Zak01]; Pei, Han, Mortazavi-Asl, et al. [PHM-A$^+$04]; and Yan, Han, and Afshar [YHA03]. The study on **sequence classification** includes Ji, Bailey, and Dong [JBD05] and Ye and Keogh [YK09], with a survey by Xing, Pei, and Keogh [XPK10]. Dong and Pei [DP07] provide an overview on **sequence data mining** methods.

Methods for **analysis of biological sequences** including **Markov chains** and **hidden Markov models** are introduced in many books or tutorials such as Waterman [Wat95]; Setubal and Meidanis [SM97]; Durbin, Eddy, Krogh, and Mitchison [DEKM98]; Baldi and Brunak [BB01]; Krane and Raymer [KR03]; Rabiner [Rab89]; Jones and Pevzner [JP04]; and Baxevanis and Ouellette [BO04]. Information about BLAST (see also Korf, Yandell, and Bedell [KYB03]) can be found at the NCBI web site *www.ncbi.nlm.nih.gov/BLAST/*.

Graph pattern mining has been studied extensively, including Holder, Cook, and Djoko [HCD94]; Inokuchi, Washio, and Motoda [IWM98]; Kuramochi and Karypis [KK01]; Yan and Han [YH02, YH03a]; Borgelt and Berthold [BB02]; Huan, Wang, Bandyopadhyay, et al. [HWB$^+$04]; and the Gaston tool by Nijssen and Kok [NK04].

There has been a great deal of research on **social and information network analysis**, including Newman [New10]; Easley and Kleinberg [EK10]; Yu, Han, and Faloutsos [YHF10]; Wasserman and Faust [WF94]; Watts [Wat03]; and Newman, Barabasi, and Watts [NBW06]. **Statistical modeling of networks** is studied popularly such as Albert and Barbasi [AB99]; Watts [Wat03]; Faloutsos, Faloutsos, and Faloutsos [FFF99]; Kumar, Raghavan, Rajagopalan, et al. [KRR+00]; and Leskovec, Kleinberg, and Faloutsos [LKF05]. **Data cleaning, integration, and validation by information network analysis** was studied by many, including Bhattacharya and Getoor [BG04] and Yin, Han, and Yu [YHY07, YHY08].

Clustering, ranking, and classification in networks has been studied extensively, including in Brin and Page [BP98]; Chakrabarti, Dom, and Indyk [CDI98]; Kleinberg [Kle99]; Getoor, Friedman, Koller, and Taskar [GFKT01]; Newman and M. Girvan [NG04]; Yin, Han, Yang, and Yu [YHYY04]; Yin, Han, and Yu [YHY05]; Xu, Yuruk, Feng, and Schweiger [XYFS07]; Kulis, Basu, Dhillon, and Mooney [KBDM09]; Sun, Han, Zhao, et al. [SHZ+09]; Neville, Gallaher, and Eliassi-Rad [NGE-R09]; and Ji, Sun, Danilevsky et al. [JSD+10]. **Role discovery and link prediction in information networks** have been studied extensively as well, such as by Krebs [Kre02]; Kubica, Moore, and Schneider [KMS03]; Liben-Nowell and Kleinberg [L-NK03]; and Wang, Han, Jia, et al. [WHJ+10].

Similarity search and OLAP in information networks has been studied by many, including Tian, Hankins, and Patel [THP08] and Chen, Yan, Zhu, et al. [CYZ+08]. **Evolution of social and information networks** has been studied by many researchers, such as Chakrabarti, Kumar, and Tomkins [CKT06]; Chi, Song, Zhou, et al. [CSZ+07]; Tang, Liu, Zhang, and Nazeri [TLZN08]; Xu, Zhang, Yu, and Long [XZYL08]; Kim and Han [KH09]; and Sun, Tang, and Han [STH+10].

Spatial and spatiotemporal data mining has been studied extensively, with a collection of papers by Miller and Han [MH09], and was introduced in some textbooks, such as Shekhar and Chawla [SC03] and Hsu, Lee, and Wang [HLW07]. Spatial clustering algorithms have been studied extensively in Chapters 10 and 11 of this book. Research has been conducted on spatial warehouses and OLAP, such as by Stefanovic, Han, and Koperski [SHK00], and spatial and spatiotemporal data mining, such as by Koperski and Han [KH95]; Mamoulis, Cao, Kollios, Hadjieleftheriou, et al. [MCK+04]; Tsoukatos and Gunopulos [TG01]; and Hadjieleftheriou, Kollios, Gunopulos, and Tsotras [HKGT03]. **Mining moving-object data** has been studied by many, such as Vlachos, Gunopulos, and Kollios [VGK02]; Tao, Faloutsos, Papadias, and Liu [TFPL04]; Li, Han, Kim, and Gonzalez [LHKG07]; Lee, Han, and Whang [LHW07]; and Li, Ding, Han, et al. [LDH+10]. For the bibliography of temporal, spatial, and spatiotemporal data mining research, see a collection by Roddick, Hornsby, and Spiliopoulou [RHS01].

Multimedia data mining has deep roots in image processing and pattern recognition, which have been studied extensively in many textbooks, including Gonzalez and Woods [GW07]; Russ [Rus06]; Duda, Hart, and Stork [DHS01]; and Z. Zhang and R. Zhang [ZZ09]. Searching and mining of multimedia data has been studied by many (see, e.g., Fayyad and Smyth [FS93]; Faloutsos and Lin [FL95]; Natsev, Rastogi, and

Shim [NRS99]; and Zaïane, Han, and Zhu [ZHZ00]). An overview of image mining methods is given by Hsu, Lee, and Zhang [HLZ02].

Text data analysis has been studied extensively in information retrieval, with many textbooks and survey articles such as Croft, Metzler, and Strohman [CMS09]; S. Buttcher, C. Clarke, G. Cormack [BCC10]; Manning, Raghavan, and Schutze [MRS08]; Grossman and Frieder [GR04]; Baeza-Yates and Riberio-Neto [BYRN11]; Zhai [Zha08]; Feldman and Sanger [FS06]; Berry [Ber03]; and Weiss, Indurkhya, Zhang, and Damerau [WIZD04]. Text mining is a fast-developing field with numerous papers published in recent years, covering many topics such as topic models (e.g., Blei and Lafferty [BL09]); sentiment analysis (e.g., Pang and Lee [PL07]); and contextual text mining (e.g., Mei and Zhai [MZ06]).

Web mining is another focused theme, with books like Chakrabarti [Cha03a], Liu [Liu06], and Berry [Ber03]. Web mining has substantially improved search engines with a few influential milestone works, such as Brin and Page [BP98]; Kleinberg [Kle99]; Chakrabarti, Dom, Kumar, et al. [CDK+99]; and Kleinberg and Tomkins [KT99]. Numerous results have been generated since then, such as search log mining (e.g., Silvestri [Sil10]); blog mining (e.g., Mei, Liu, Su, and Zhai [MLSZ06]); and mining online forums (e.g., Cong, Wang, Lin, et al. [CWL+08]).

Books and surveys on stream data systems and stream data processing include Babu and Widom [BW01]; Babcock, Babu, Datar, et al. [BBD+02]; Muthukrishnan [Mut05]; and Aggarwal [Agg06].

Stream data mining research covers stream cube models (e.g., Chen, Dong, Han, et al. [CDH+02]), stream frequent pattern mining (e.g., Manku and Motwani [MM02] and Karp, Papadimitriou and Shenker [KPS03]), stream classification (e.g., Domingos and Hulten [DH00]; Wang, Fan, Yu, and Han [WFYH03]; Aggarwal, Han, Wang, and Yu [AHWY04b]), and stream clustering (e.g., Guha, Mishra, Motwani, and O'Callaghan [GMMO00] and Aggarwal, Han, Wang, and Yu [AHWY03]).

There are many books that discuss **data mining applications**. For financial data analysis and financial modeling, see, for example, Benninga [Ben08] and Higgins [Hig08]. For retail data mining and customer relationship management, see, for example, books by Berry and Linoff [BL04] and Berson, Smith, and Thearling [BST99]. For telecommunication-related data mining, see, for example, Horak [Hor08]. There are also books on scientific data analysis, such as Grossman, Kamath, Kegelmeyer, et al. [GKK+01] and Kamath [Kam09].

Issues in the **theoretical foundations of data mining** have been addressed by many researchers. For example, Mannila presents a summary of studies on the foundations of data mining in [Man00]. The data reduction view of data mining is summarized in *The New Jersey Data Reduction Report* by Barbará, DuMouchel, Faloutos, et al. [BDF+97]. The data compression view can be found in studies on the minimum description length principle, such as Grunwald and Rissanen [GR07].

The pattern discovery point of view of data mining is addressed in numerous machine learning and data mining studies, ranging from association mining, to decision tree induction, sequential pattern mining, clustering, and so on. The probability theory point of view is popular in the statistics and machine learning literature, such

as Bayesian networks and hierarchical Bayesian models in Chapter 9, and probabilistic graph models (e.g., Koller and Friedman [KF09]). Kleinberg, Papadimitriou, and Raghavan [KPR98] present a microeconomic view, treating data mining as an optimization problem. Studies on the inductive database view include Imielinski and Mannila [IM96] and de Raedt, Guns, and Nijssen [RGN10].

Statistical methods for data analysis are described in many books, such as Hastie, Tibshirani, Friedman [HTF09]; Freedman, Pisani, and Purves [FPP07]; Devore [Dev03]; Kutner, Nachtsheim, Neter, and Li [KNNL04]; Dobson [Dob01]; Breiman, Friedman, Olshen, and Stone [BFOS84]; Pinheiro and Bates [PB00]; Johnson and Wichern [JW02b]; Huberty [Hub94]; Shumway and Stoffer [SS05]; and Miller [Mil98].

For **visual data mining**, popular books on the visual display of data and information include those by Tufte [Tuf90, Tuf97, Tuf01]. A summary of techniques for visualizing data is presented in Cleveland [Cle93]. A dedicated visual data mining book, *Visual Data Mining: Techniques and Tools for Data Visualization and Mining*, is by Soukup and Davidson [SD02]. The book *Information Visualization in Data Mining and Knowledge Discovery*, edited by Fayyad, Grinstein, and Wierse [FGW01], contains a collection of articles on visual data mining methods.

Ubiquitous and invisible data mining has been discussed in many texts including John [Joh99], and some articles in a book edited by Kargupta, Joshi, Sivakumar, and Yesha [KJSY04]. The book *Business @ the Speed of Thought: Succeeding in the Digital Economy* by Gates [Gat00] discusses e-commerce and customer relationship management, and provides an interesting perspective on data mining in the future. Mena [Men03] has an informative book on the use of data mining to detect and prevent crime. It covers many forms of criminal activities, ranging from fraud detection, money laundering, insurance crimes, identity crimes, and intrusion detection.

Data mining issues regarding **privacy and data security** are addressed popularly in literature. Books on privacy and security in data mining include Thuraisingham [Thu04]; Aggarwal and Yu [AY08]; Vaidya, Clifton, and Zhu [VCZ10]; and Fung, Wang, Fu, and Yu [FWFY10]. Research articles include Agrawal and Srikant [AS00]; Evfimievski, Srikant, Agrawal, and Gehrke [ESAG02]; and Vaidya and Clifton [VC03]. Differential privacy was introduced by Dwork [Dwo06] and studied by many such as Hay, Rastogi, Miklau, and Suciu [HRMS10].

There have been many discussions on **trends and research directions of data mining** in various forums. Several books are collections of articles on these issues such as Kargupta, Han, Yu, et al. [KHY+08].