Data Exploration

The word "data" is derived from the Latin word *dare*, which means "something given"—an observation or a fact about a subject. (Interestingly, the Sanskrit word *dAta* also means "given"). Data science helps decipher the hidden useful relationships within data. Before venturing into any advanced analysis of data using statistical, machine learning, and algorithmic techniques, it is essential to perform basic data exploration to study the basic characteristics of a dataset. Data exploration helps with understanding data better, to prepare the data in a way that makes advanced analysis possible, and sometimes to get the necessary insights from the data faster than using advanced analytical techniques.

Simple pivot table functions, computing statistics like mean and deviation, and plotting data as a line, bar, and scatter charts are part of data exploration techniques that are used in everyday business settings. Data exploration, also known as exploratory data analysis, provides a set of tools to obtain fundamental understanding of a dataset. The results of data exploration can be extremely powerful in grasping the structure of the data, the distribution of the values, and the presence of extreme values and the interrelationships between the attributes in the dataset. Data exploration also provides guidance on applying the right kind of further statistical and data science treatment.

Data exploration can be broadly classified into two types—descriptive statistics and data visualization. Descriptive statistics is the process of condensing key characteristics of the dataset into simple numeric metrics. Some of the common quantitative metrics used are mean, standard deviation, and correlation. Visualization is the process of projecting the data, or parts of it, into multi-dimensional space or abstract images. All the useful (and adorable) charts fall under this category. Data exploration in the context of data science uses both descriptive statistics and visualization techniques.

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3.1 OBJECTIVES OF DATA EXPLORATION

In the data science process, data exploration is leveraged in many different steps including preprocessing or data preparation, modeling, and interpretation of the modeling results.

1. *Data understanding*: Data exploration provides a high-level overview of each attribute (also called variable) in the dataset and the interaction between the attributes. Data exploration helps answers the questions like what is the typical value of an attribute or how much do the data points differ from the typical value, or presence of extreme values.
2. *Data preparation*: Before applying the data science algorithm, the dataset has to be prepared for handling any of the anomalies that may be present in the data. These anomalies include outliers, missing values, or highly correlated attributes. Some data science algorithms do not work well when input attributes are correlated with each other. Thus, correlated attributes need to be identified and removed.
3. *Data science tasks*: Basic data exploration can sometimes substitute the entire data science process. For example, scatterplots can identify clusters in low-dimensional data or can help develop regression or classification models with simple visual rules.
4. *Interpreting the results*: Finally, data exploration is used in understanding the prediction, classification, and clustering of the results of the data science process. Histograms help to comprehend the distribution of the attribute and can also be useful for visualizing numeric prediction, error rate estimation, etc.

3.2 DATASETS

Throughout the rest of this chapter (and the book) a few classic datasets, which are simple to understand, easy to explain, and can be used commonly across many different data science techniques, will be introduced. The most popular datasets used to learn data science is probably the *Iris dataset*, introduced by Ronald Fisher, in his seminal work on discriminant analysis, "The use of multiple measurements in taxonomic problems" (Fisher, 1936). Iris is a flowering plant that is found widely, across the world. The genus of Iris contains more than 300 different species. Each species exhibits different physical characteristics like shape and size of the flowers and leaves. The *Iris dataset* contains 150 observations of three different species, *Iris setosa*, *Iris virginica*, and *I. versicolor*, with 50 observations each. Each observation consists of four attributes: sepal length, sepal width, petal length, and petal width. The fifth attribute, the label, is the name of the species observed, which takes the values *I. setosa*, *I. virginica*, and *I. versicolor*. The petals are the brightly

colored inner part of the flowers and the sepals form the outer part of the flower and are usually green in color. However, in an Iris flower, both sepals and petals are bright purple in color, but can be distinguished from each other by differences in the shape (Fig. 3.1).

All four attributes in the Iris dataset are numeric continuous values measured in centimeters. One of the species, *I. setosa*, can be easily distinguished from the other two using simple rules like the petal length is less than 2.5 cm. Separating the *virginica* and *versicolor* classes requires more complex rules that involve more attributes. The dataset is available in all standard data science tools, such as RapidMiner, or can be downloaded from public websites such as the University of California Irvine—Machine Learning repository[2] (Bache & Lichman, 2013). This dataset and other datasets used in this book can be accessed from the book companion website: www.IntroDataScience.com.
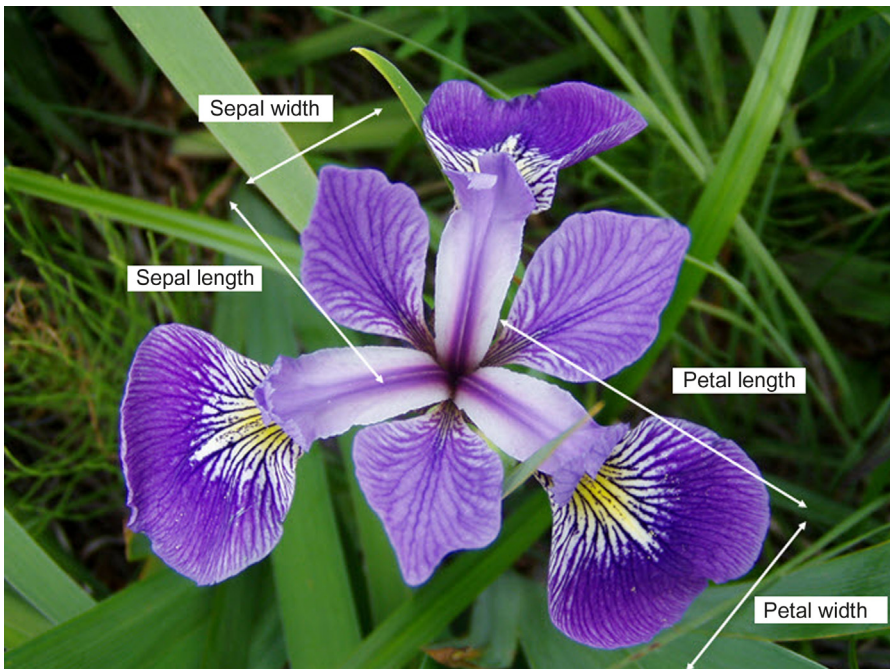

FIGURE 3.1

Iris versicolor. Source: Photo by Danielle Langlois. July 2005 (Image modified from original by marking parts. "Iris versicolor 3." Licensed under Creative Commons Attribution-Share Alike 3.0 via Wikimedia Commons.[1])

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[1] http://commons.wikimedia.org/wiki/File:Iris_versicolor_3.jpg#mediaviewer/File:Iris_versicolor_3.jpg.
[2] https://archive.ics.uci.edu/ml/datasets.html.

The Iris dataset is used for learning data science mainly because it is simple to understand, explore, and can be used to illustrate how different data science algorithms approach the problem on the same standard dataset. The dataset extends beyond two dimensions, with three class labels, of which one class is easily separable (*I. setosa*) just by visual exploration, while classifying the other two classes is slightly more challenging. It helps to reaffirm the classification results that can be derived based on visual rules, and at the same time sets the stage for data science to build new rules beyond the limits of visual exploration.

3.2.1 Types of Data

Data come in different formats and types. Understanding the properties of each attribute or feature provides information about what kind of operations can be performed on that attribute. For example, the temperature in weather data can be expressed as any of the following formats:

- Numeric centigrade (31°C, 33.3°C) or Fahrenheit (100°F, 101.45°F) or on the Kelvin scale
- Ordered labels as in hot, mild, or cold
- Number of days within a year below 0°C (10 days in a year below freezing)

All of these attributes indicate temperature in a region, but each have different data types. A few of these data types can be converted from one to another.

Numeric or Continuous
Temperature expressed in Centigrade or Fahrenheit is numeric and continuous because it can be denoted by numbers and take an infinite number of values between digits. Values are ordered and calculating the difference between the values makes sense. Hence, additive and subtractive mathematical operations and logical comparison operators like greater than, less than, and equal to, operations can be applied.

An integer is a special form of the numeric data type which does not have decimals in the value or more precisely does not have infinite values between consecutive numbers. Usually, they denote a count of something, number of days with temperature less than 0°C, number of orders, number of children in a family, etc.

If a zero point is defined, numeric data become a *ratio* or *real* data type. Examples include temperature in Kelvin scale, bank account balance, and income. Along with additive and logical operations, ratio operations can be performed with this data type. Both integer and ratio data types are categorized as a *numeric* data type in most data science tools.

Categorical or Nominal

Categorical data types are attributes treated as distinct symbols or just names. The color of the iris of the human eye is a categorical data type because it takes a value like black, green, blue, gray, etc. There is no direct relationship among the data values, and hence, mathematical operators except the logical or "is equal" operator cannot be applied. They are also called a nominal or polynominal data type, derived from the Latin word for *name*.

An ordered nominal data type is a special case of a categorical data type where there is some kind of order among the values. An example of an ordered data type is temperature expressed as hot, mild, cold.

Not all data science tasks can be performed on all data types. For example, the neural network algorithm does not work with categorical data. However, one data type can be converted to another using a type conversion process, but this may be accompanied with possible loss of information. For example, credit scores expressed in poor, average, good, and excellent categories can be converted to either 1, 2, 3, and 4 or average underlying numerical scores like 400, 500, 600, and 700 (scores here are just an example). In this type conversion, there is no loss of information. However, conversion from numeric credit score to categories (poor, average, good, and excellent) does incur loss of information.

3.3   DESCRIPTIVE STATISTICS

Descriptive statistics refers to the study of the aggregate quantities of a dataset. These measures are some of the commonly used notations in everyday life. Some examples of descriptive statistics include average annual income, median home price in a neighborhood, range of credit scores of a population, etc. In general, descriptive analysis covers the following characteristics of the sample or population dataset (Kubiak & Benbow, 2006):

Characteristics of the Dataset	Measurement Technique
Center of the dataset	Mean, median, and mode
Spread of the dataset	Range, variance, and standard deviation
Shape of the distribution of the dataset	Symmetry, skewness, and kurtosis

The definition of these metrics will be explored shortly. Descriptive statistics can be broadly classified into univariate and multivariate exploration depending on the number of attributes under analysis.

3.3.1 Univariate Exploration

Univariate data exploration denotes analysis of one attribute at a time. The example Iris dataset for one species, *I. setosa*, has 50 observations and 4 attributes, as shown in Table 3.1. Here some of the descriptive statistics for sepal length attribute are explored.

Measure of Central Tendency
The objective of finding the central location of an attribute is to quantify the dataset with one central or most common number.

- *Mean*: The mean is the arithmetic average of all observations in the dataset. It is calculated by summing all the data points and dividing by the number of data points. The mean for sepal length in centimeters is 5.0060.
- *Median*: The median is the value of the central point in the distribution. The median is calculated by sorting all the observations from small to large and selecting the mid-point observation in the sorted list. If the number of data points is even, then the average of the middle two data points is used as the median. The median for sepal length is in centimeters is 5.0000.
- *Mode*: The mode is the most frequently occurring observation. In the dataset, data points may be repetitive, and the most repetitive data point is the mode of the dataset. In this example, the mode in centimeters is 5.1000.

Table 3.1 Iris Dataset and Descriptive Statistics (Fisher, 1936)				
Observation	**Sepal Length**	**Sepal Width**	**Petal Length**	**Petal Width**
1	5.1	3.5	1.4	0.2
2	4.9	3.1	1.5	0.1
. . .	. . .	. . .	. . .	. . .
49	5	3.4	1.5	0.2
50	4.4	2.9	1.4	0.2
Statistics	**Sepal Length**	**Sepal Width**	**Petal Length**	**Petal Width**
Mean	5.006	3.418	1.464	0.244
Median	5.000	3.400	1.500	0.200
Mode	5.100	3.400	1.500	0.200
Range	1.500	2.100	0.900	0.500
Standard deviation	0.352	0.381	0.174	0.107
Variance	0.124	0.145	0.030	0.011

In an attribute, the mean, median, and mode may be different numbers, and this indicates the shape of the distribution. If the dataset has outliers, the mean will get affected while in most cases the median will not. The mode of the distribution can be different from the mean or median, if the underlying dataset has more than one natural normal distribution.

Measure of Spread

In desert regions, it is common for the temperature to cross above 110°F during the day and drop below 30°F during the night while the average temperature for a 24-hour period is around 70°F. Obviously, the experience of living in the desert is not the same as living in a tropical region with the same average daily temperature around 70°F, where the temperature within the day is between 60°F and 80°F. What matters here is not just the central location of the temperature, but the *spread* of the temperature. There are two common metrics to quantify spread.

- *Range:* The range is the difference between the maximum value and the minimum value of the attribute. The range is simple to calculate and articulate but has shortcomings as it is severely impacted by the presence of outliers and fails to consider the distribution of all other data points in the attributes. In the example, the range for the temperature in the desert is 80°F and the range for the tropics is 20°F. The desert region experiences larger temperature swings as indicated by the range.
- *Deviation:* The variance and standard deviation measures the spread, by considering all the values of the attribute. Deviation is simply measured as the difference between any given value (x_i) and the mean of the sample (μ). The variance is the sum of the squared deviations of all data points divided by the number of data points. For a dataset with N observations, the variance is given by the following equation:

$$\text{Variance} = s^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2 \tag{3.1}$$

Standard deviation is the square root of the variance. Since the standard deviation is measured in the same units as the attribute, it is easy to understand the magnitude of the metric. High standard deviation means the data points are spread widely around the central point. Low standard deviation means data points are closer to the central point. If the distribution of the data aligns with the *normal distribution*, then 68% of the data points lie within one standard deviation from the mean. Fig. 3.2 provides the univariate summary of the Iris dataset with all 150 observations, for each of the four numeric attributes.

				Min	Max	Average	Deviation
Sepal Length	Real	0		4.300	7.900	5.843	0.828
Sepal Width	Real	0		2	4.400	3.054	0.434
Petal Length	Real	0		1	6.900	3.759	1.764
Petal Width	Real	0		0.100	2.500	1.199	0.763

FIGURE 3.2
Descriptive statistics for the Iris dataset.

3.3.2   Multivariate Exploration

Multivariate exploration is the study of more than one attribute in the dataset simultaneously. This technique is critical to understanding the relationship between the attributes, which is central to data science methods. Similar to univariate explorations, the measure of central tendency and variance in the data will be discussed.

Central Data Point

In the Iris dataset, each data point as a set of all the four attributes can be expressed:

observation i: {sepal length, sepal width, petal length, petal width}

For example, observation one: {5.1, 3.5, 1.4, 0.2}. This observation point can also be expressed in four-dimensional Cartesian coordinates and can be plotted in a graph (although plotting more than three dimensions in a visual graph can be challenging). In this way, all 150 observations can be expressed in Cartesian coordinates. If the objective is to find the most "typical" observation point, it would be a data point made up of the mean of each attribute in the dataset independently. For the Iris dataset shown in Table 3.1, the central mean point is {5.006, 3.418, 1.464, 0.244}. This data point may not be an actual observation. It will be a hypothetical data point with the most typical attribute values.

Correlation

Correlation measures the statistical relationship between two attributes, particularly dependence of one attribute on another attribute. When two attributes are highly correlated with each other, they both vary at the same rate with each other either in the same or in opposite directions. For example, consider average temperature of the day and ice cream sales. Statistically, the two attributes that are correlated are dependent on each other and one may be used to predict the other. If there are sufficient data, future sales of ice cream can be predicted if the temperature forecast is known. However, correlation between two attributes does not imply causation, that is, one doesn't necessarily cause the other. The ice cream sales and the shark attacks are correlated, however there is no causation. Both ice cream sales and shark attacks are influenced by the third attribute—the summer season. Generally, ice cream sales spikes as temperatures rise. As more people go to beaches during summer, encounters with sharks become more probable.

Correlation between two attributes is commonly measured by the Pearson correlation coefficient (r), which measures the strength of *linear* dependence (Fig. 3.3). Correlation coefficients take a value from $-1 \leq r \leq 1$. A value closer to 1 or -1 indicates the two attributes are highly correlated, with perfect correlation at 1 or -1. Perfect correlation also exists when the attributes are governed by formulas and laws. For example, observations of the values of gravitational force and the mass of the object (Newton's second law) or the quantity of the products sold and total revenue (price* volume = revenue). A correlation value of 0 means there is no linear relationship between two attributes.
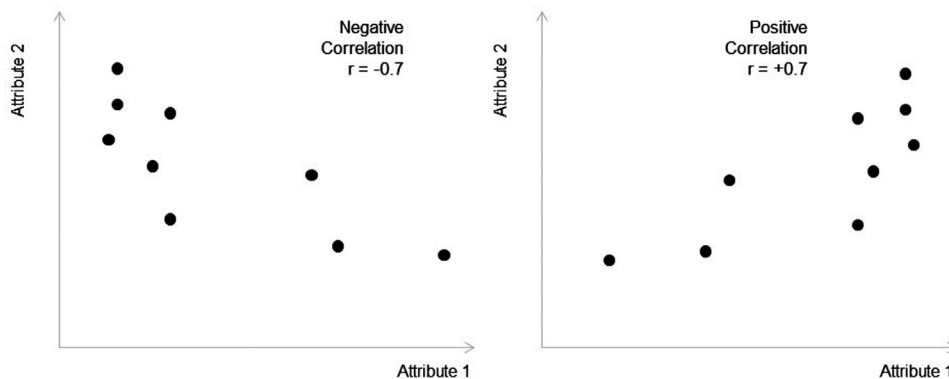

FIGURE 3.3
Correlation of attributes.

The Pearson correlation coefficient between two attributes x and y is calculated with the formula:

$$
\begin{aligned}
r_{xy} &= \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2 \sum_{i=1}^{n}(y_i - \overline{y})^2}} \\
&= \frac{\sum_{i=1}^{N}(x_i - \overline{x})(y_i - \overline{y})}{N \times s_x \times s_y}
\end{aligned}
\tag{3.2}
$$

where s_x and s_y are the standard deviations of random variables x and y, respectively. The Pearson correlation coefficient has some limitations in quantifying the strength of correlation. When datasets have more complex nonlinear relationships like quadratic functions, only the effects on linear relationships are considered and quantified using correlation coefficient. The presence of outliers can also skew the measure of correlation. Visually, correlation can be observed using scatterplots with the attributes in each Cartesian coordinate (Fig. 3.3). In fact, visualization should be the first step in understanding correlation because it can identify nonlinear relationships and show any outliers in the dataset. Anscombe's quartet (Anscombe, 1973) clearly illustrates the limitations of relying only on the correlation coefficient to understand the data (Fig. 3.4). The quartet consists of four different datasets, with two attributes (x, y). All four datasets have the same mean, the same variance for x and y, and the same correlation coefficient between x and y, but look drastically different when plotted on a chart. This evidence illustrates the necessity of visualizing the attributes instead of just calculating statistical metrics.

3.4 DATA VISUALIZATION

Visualizing data is one of the most important techniques of data discovery and exploration. Though visualization is not considered a data science technique, terms like visual mining or pattern discovery based on visuals are increasingly used in the context of data science, particularly in the business world. The discipline of data visualization encompasses the methods of expressing data in an abstract visual form. The visual representation of data provides easy comprehension of complex data with multiple attributes and their underlying relationships. The motivation for using data visualization includes:

- *Comprehension of dense information*: A simple visual chart can easily include thousands of data points. By using visuals, the user can see the big picture, as well as longer term trends that are extremely difficult to interpret purely by expressing data in numbers.
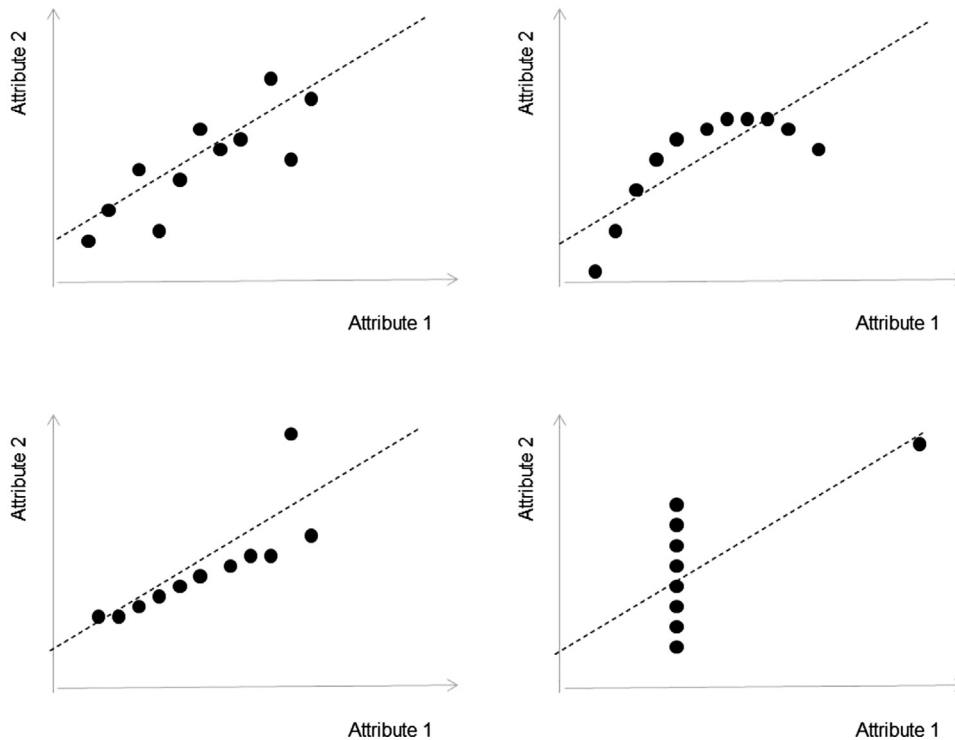
FIGURE 3.4

Anscombe's Quartet: descriptive statistics versus visualization. Source*: Adapted from: Anscombe, F. J., 1973. Graphs in statistical analysis*, American Statistician, 27*(1), pp. 19—20.*

- *Relationships*: Visualizing data in Cartesian coordinates enables exploration of the relationships between the attributes. Although representing more than three attributes on the *x*, *y*, and *z*-axes is not feasible in Cartesian coordinates, there are a few creative solutions available by changing properties like the size, color, and shape of data markers or using flow maps (Tufte, 2001), where more than two attributes are used in a two-dimensional medium.

Vision is one of the most powerful senses in the human body. As such, it is intimately connected with cognitive thinking (Few, 2006). Human vision is trained to discover patterns and anomalies even in the presence of a large volume of data. However, the effectiveness of the pattern detection depends on how effectively the information is visually presented. Hence, selecting suitable visuals to explore data is critically important in discovering and comprehending hidden patterns in the data (Ware, 2004). As with descriptive statistics, visualization techniques are also categorized into: univariate visualization, multivariate visualization and visualization of a large number of attributes using parallel dimensions.

Some of the common data visualization techniques used to analyze data will be reviewed. Most of these visualization techniques are available in commercial spreadsheet software like MS Excel. RapidMiner, like any other data science tool, offers a wide range of visualization tools. To maintain consistency with rest of the book, all further visualizations are output from RapidMiner using the Iris dataset. Please review Chapter 15, Getting Started With RapidMiner, to become familiar with RapidMiner.

3.4.1 Univariate Visualization

Visual exploration starts with investigating one attribute at a time using uni-variate charts. The techniques discussed in this section give an idea of how the attribute values are distributed and the shape of the distribution.

Histogram

A histogram is one of the most basic visualization techniques to understand the frequency of the occurrence of values. It shows the distribution of the data by plotting the frequency of occurrence in a range. In a histogram, the attribute under inquiry is shown on the horizontal axis and the frequency of occurrence is on the vertical axis. For a continuous numeric data type, the range or *binning* value to group a range of values need to be specified. For example, in the case of human height in centimeters, all the occurrences between 152.00 and 152.99 are grouped under 152. There is no optimal number of bins or bin width that works for all the distributions. If the bin width is too small, the distribution becomes more precise but reveals the noise due to sampling. A general rule of thumb is to have a number of bins equal to the square root or cube root of the number of data points.

Histograms are used to find the central location, range, and shape of distribution. In the case of the petal length attribute in the Iris dataset, the data is multimodal (Fig. 3.5), where the distribution does not follow the bell curve pattern. Instead, there are two peaks in the distribution. This is due to the fact that there are 150 observations of three *different* species (hence, distributions) in the dataset. A histogram can be *stratified* to include different classes in order to gain more insight. The enhanced histogram with class labels shows the dataset is made of three different distributions (Fig. 3.6). *I. setosa's* distribution stands out with a mean around 1.25 cm and ranges from 1−2 cm. *I. versicolor* and *I. virginica's* distributions overlap *I. setosa's* have separate means.

Quartile

A *box whisker* plot is a simple visual way of showing the distribution of a continuous variable with information such as quartiles, median, and outliers,
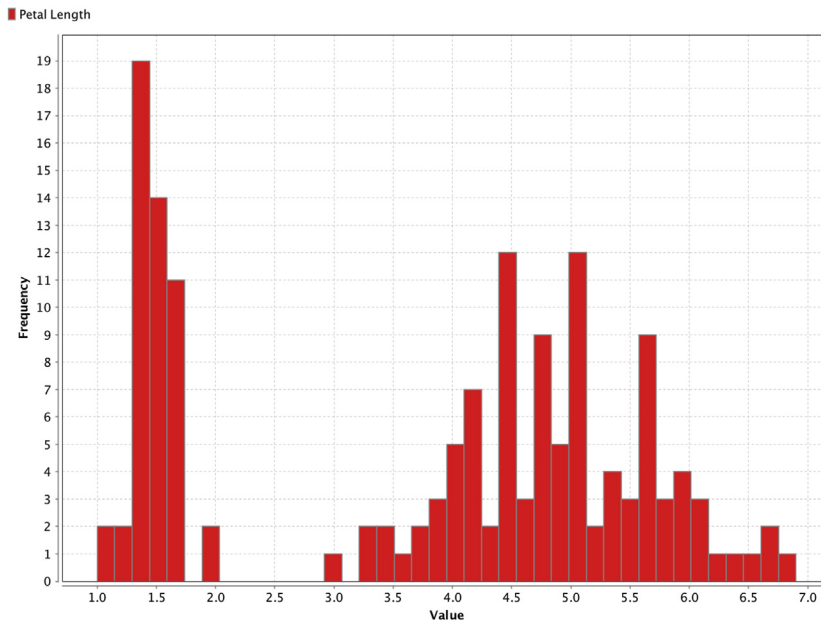
FIGURE 3.5
Histogram of petal length in Iris dataset.

overlaid by mean and standard deviation. The main attraction of box whisker or quartile charts is that distributions of multiple attributes can be compared side by side and the overlap between them can be deduced. The quartiles are denoted by Q1, Q2, and Q3 points, which indicate the data points with a 25% bin size. In a distribution, 25% of the data points will be below Q1, 50% will be below Q2, and 75% will be below Q3.

The Q1 and Q3 points in a box whisker plot are denoted by the edges of the box. The Q2 point, the median of the distribution, is indicated by a cross line within the box. The outliers are denoted by circles at the end of the whisker line. In some cases, the mean point is denoted by a solid dot overlay followed by standard deviation as a line overlay.

Fig. 3.7 shows that the quartile charts for all four attributes of the Iris dataset are plotted side by side. Petal length can be observed as having the broadest range and the sepal width has a narrow range, out of all of the four attributes.

One attribute can also be selected—petal length—and explored further using quartile charts by introducing a class label. In the plot in Fig. 3.8, we can see the distribution of three species for the petal length measurement. Similar to the previous comparison, the distribution of multiple species can be compared.
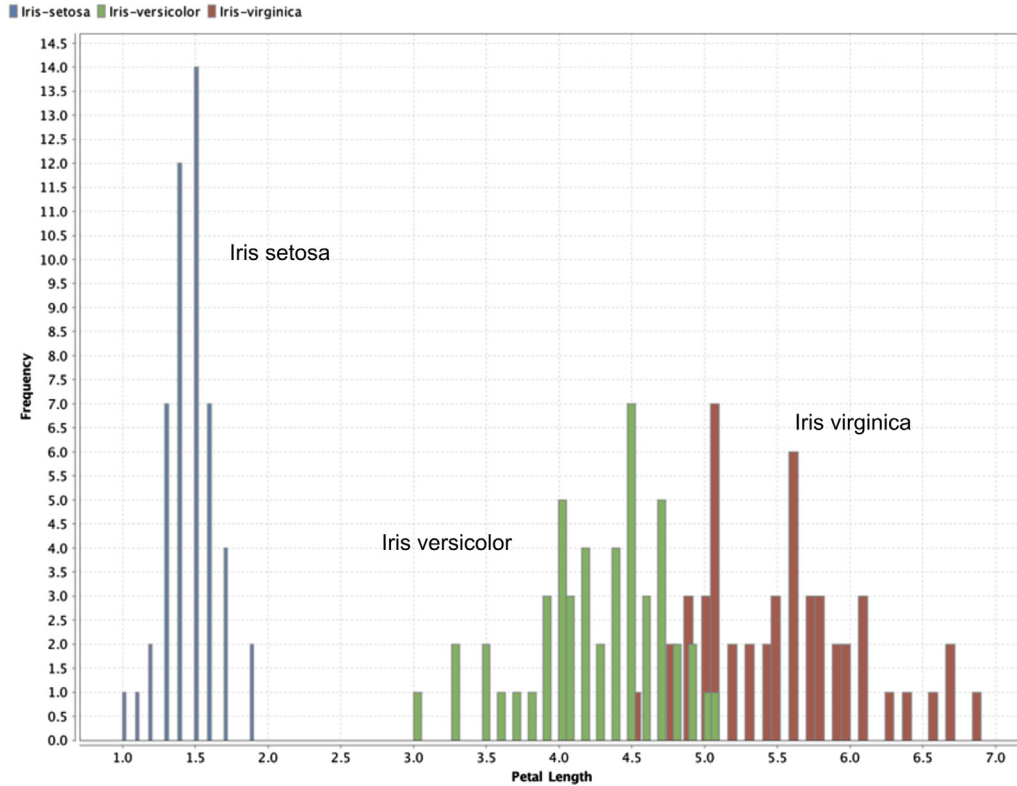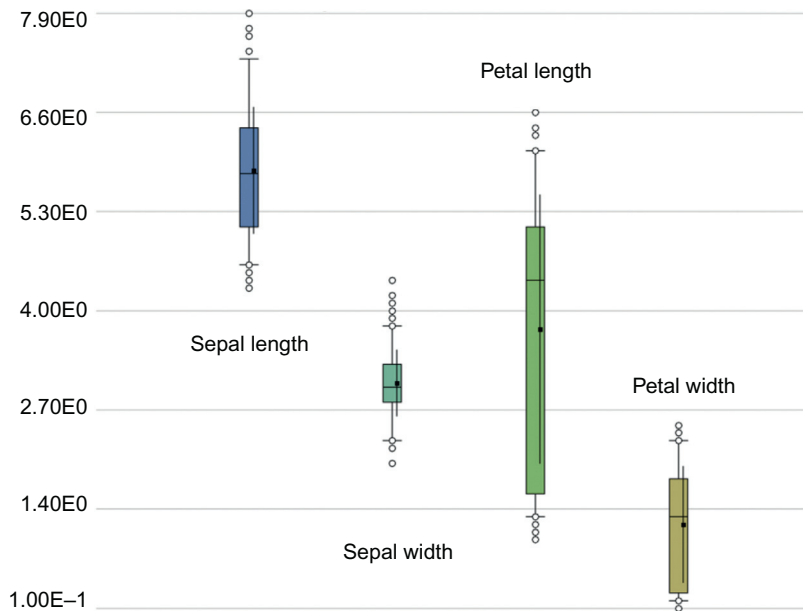
FIGURE 3.6
Class-stratified histogram of petal length in Iris dataset.

Distribution Chart

For continuous numeric attributes like petal length, instead of visualizing the actual data in the sample, its normal distribution function can be visualized instead. The normal distribution function of a continuous random variable is given by the formula:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{(x-\mu)^2/2\sigma^2} \tag{3.3}$$

where μ is the mean of the distribution and σ is the standard deviation of the distribution. Here an inherent assumption is being made that the measurements of petal length (or any continuous variable) follow the normal distribution, and hence, its distribution can be visualized instead of the actual values. The normal distribution is also called the *Gaussian distribution* or "bell curve" due to its bell shape. The normal distribution function

FIGURE 3.7

Quartile plot of Iris dataset.

shows the probability of occurrence of a data point within a range of values. If a dataset exhibits normal distribution, then 68.2% of data points will fall within one standard deviation from the mean; 95.4% of the points will fall within 2σ and 99.7% within 3σ of the mean. When the normal distribution curves are stratified by class type, more insight into the data can be gained. Fig. 3.9 shows the normal distribution curves for petal length measurement for each Iris species type. From the distribution chart, it can be inferred that the petal length for the *I. setosa* sample is more distinct and cohesive than *I. versicolor* and *I. virginica.* If there is an unlabeled measurement with a petal length of 1.5 cm, it can be predicted that the species is *I. setosa*. However, if the petal length measurement is 5.0 cm, there is no clear prediction, as the species could be either *Iris versicolor* and *I. virginica*.

3.4.2 Multivariate Visualization

The multivariate visual exploration considers more than one attribute in the same visual. The techniques discussed in this section focus on the relationship of one attribute with another attribute. These visualizations examine two to four attributes simultaneously.
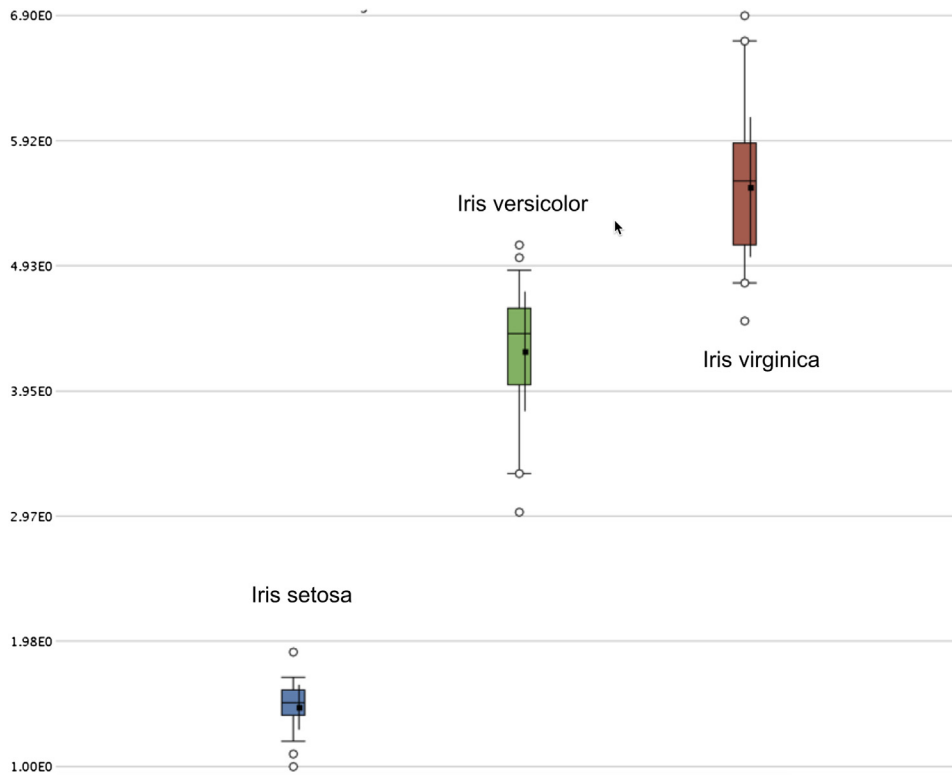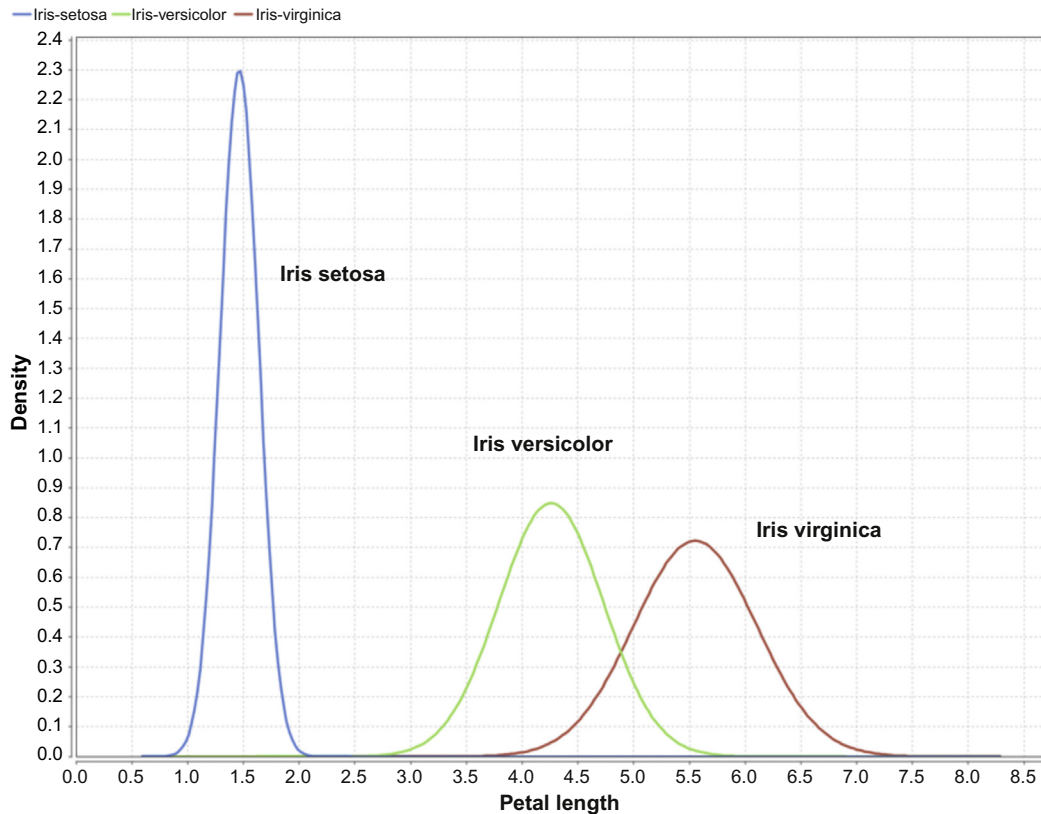
FIGURE 3.8
Class-stratified quartile plot of petal length in Iris dataset.

Scatterplot

A scatterplot is one of the most powerful yet simple visual plots available. In a scatterplot, the data points are marked in Cartesian space with attributes of the dataset aligned with the coordinates. The attributes are usually of continuous data type. One of the key observations that can be concluded from a scatterplot is the existence of a relationship between two attributes under inquiry. If the attributes are linearly correlated, then the data points align closer to an imaginary straight line; if they are not correlated, the data points are scattered. Apart from basic correlation, scatterplots can also indicate the existence of patterns or groups of clusters in the data and identify outliers in the data. This is particularly useful for low-dimensional datasets. Chapter 13: Anomaly detection, provides techniques for finding outliers in high-dimensional space.

Fig. 3.10 shows the scatterplot between petal length (*x*-axis) and petal width (*y*-axis). These two attributes are slightly correlated, because this is a measurement of the same part of the flower. When the data markers are colored to

FIGURE 3.9

Distribution of petal length in Iris dataset.

indicate different species using class labels, more patterns can be observed. There is a cluster of data points, all belonging to species *I. setosa*, on the lower left side of the plot. *I. setosa* has much smaller petals. This feature can be used as a rule to predict the species of unlabeled observations. One of the limitations of scatterplots is that only two attributes can be used at a time, with an additional attribute possibly shown in the color of the data marker. However, the colors are usually reserved for class labels.

Scatter Multiple

A *scatter multiple* is an enhanced form of a simple scatterplot where more than two dimensions can be included in the chart and studied simultaneously. The primary attribute is used for the *x*-axis coordinate. The secondary axis is shared with more attributes or dimensions. In this example (Fig. 3.11), the values on the *y*-axis are shared between sepal length, sepal
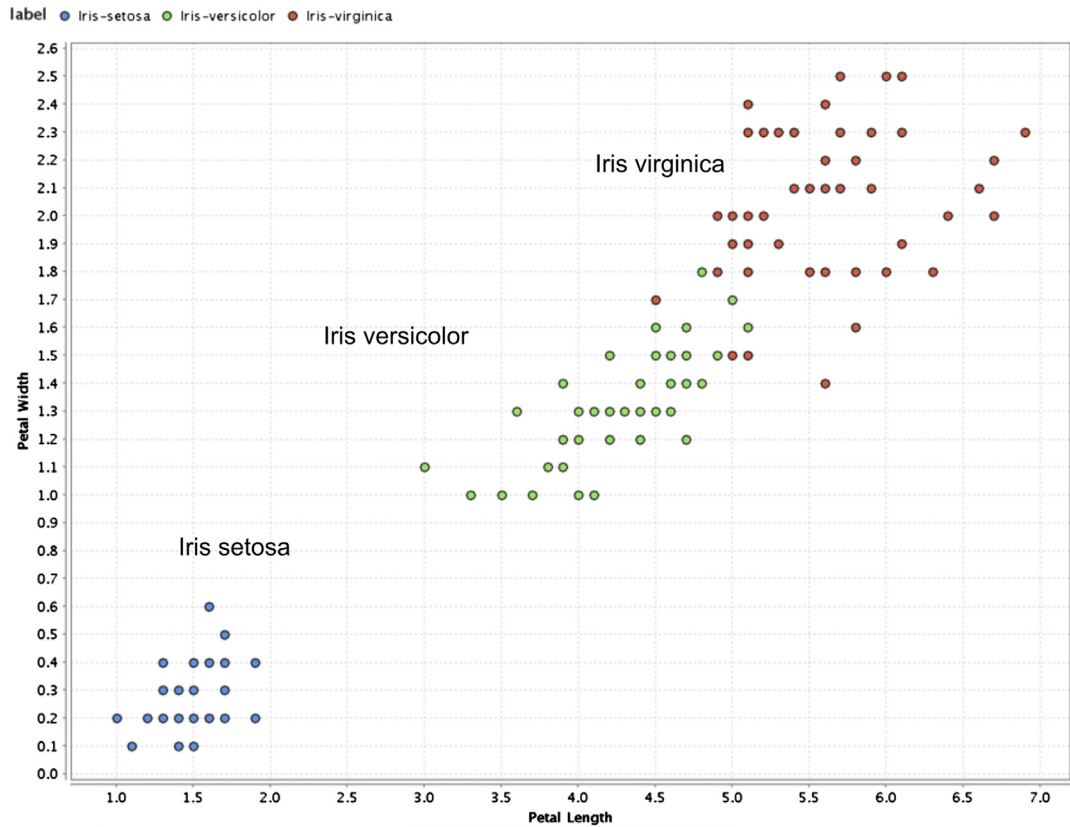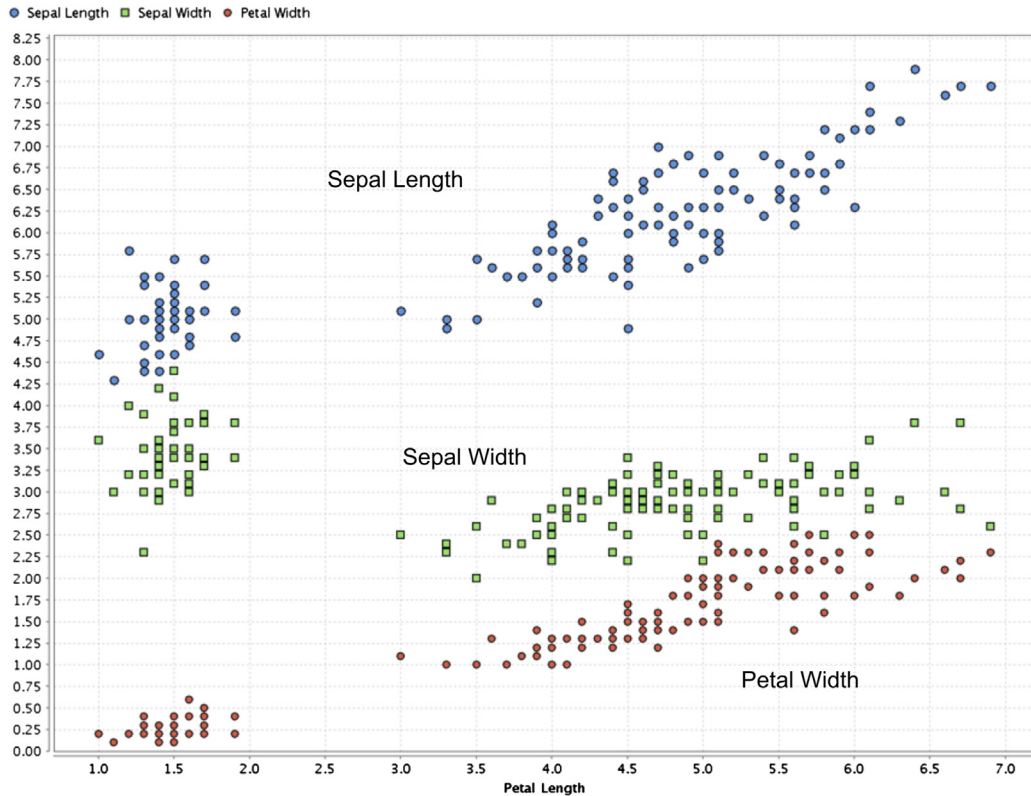
FIGURE 3.10
Scatterplot of Iris dataset.

width, and petal width. The name of the attribute is conveyed by colors used in data markers. Here, sepal length is represented by data points occupying the topmost part of the chart, sepal width occupies the middle portion, and petal width is in the bottom portion. Note that the data points are *duplicated for each attribute in the y-axis*. Data points are color-coded for each dimension in *y*-axis while the *x*-axis is anchored with one attribute—petal length. All the attributes sharing the y-axis should be of the same unit or normalized.

Scatter Matrix
If the dataset has more than two attributes, it is important to look at combinations of all the attributes through a scatterplot. A *scatter matrix* solves this need by comparing all combinations of attributes with individual scatterplots and arranging these plots in a matrix.

FIGURE 3.11

Scatter multiple plot of Iris dataset.

A scatter matrix for all four attributes in the Iris dataset is shown in Fig. 3.12. The color of the data point is used to indicate the species of the flower. Since there are four attributes, there are four rows and four columns, for a total of 16 scatter charts. Charts in the diagonal are a comparison of the attribute with itself; hence, they are eliminated. Also, the charts below the diagonal are mirror images of the charts above the diagonal. In effect, there are six distinct comparisons in scatter multiples of four attributes. Scatter matrices provide an effective visualization of comparative, multivariate, and high-density data displayed in small multiples of the similar scatterplots (Tufte, 2001).

Bubble Chart

A *bubble chart* is a variation of a simple scatterplot with the addition of one more attribute, which is used to determine the size of the data point. In the Iris dataset, petal length and petal width are used for *x* and *y*-axis, respectively
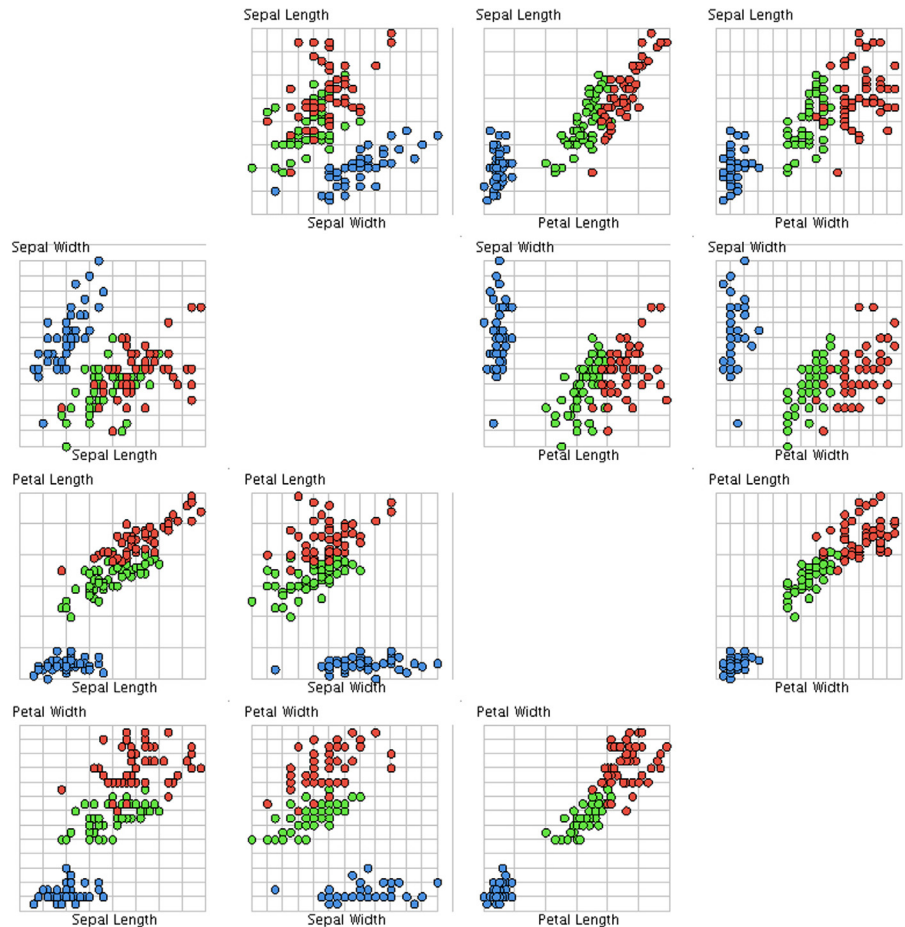
FIGURE 3.12
Scatter matrix plot of Iris dataset.

and sepal width is used for the size of the data point. The color of the data point represents a species class label (Fig. 3.13).

Density Chart

Density charts are similar to the scatterplots, with one more dimension included as a background color. The data point can also be colored to visualize one dimension, and hence, a total of four dimensions can be visualized in a density chart. In the example in Fig. 3.14, petal length is used for the *x*-axis, sepal length for the *y*-axis, sepal width for the background color, and class label for the data point color.
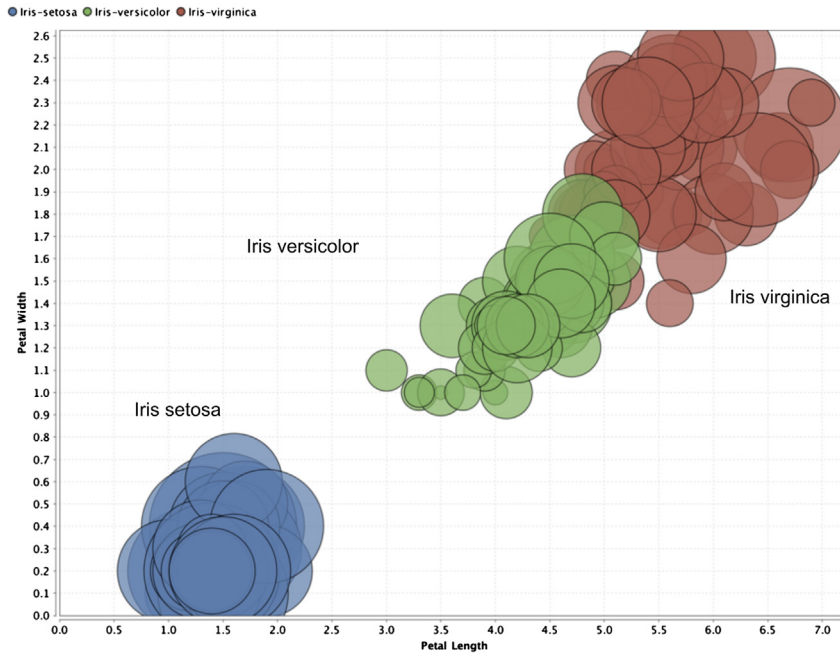
FIGURE 3.13
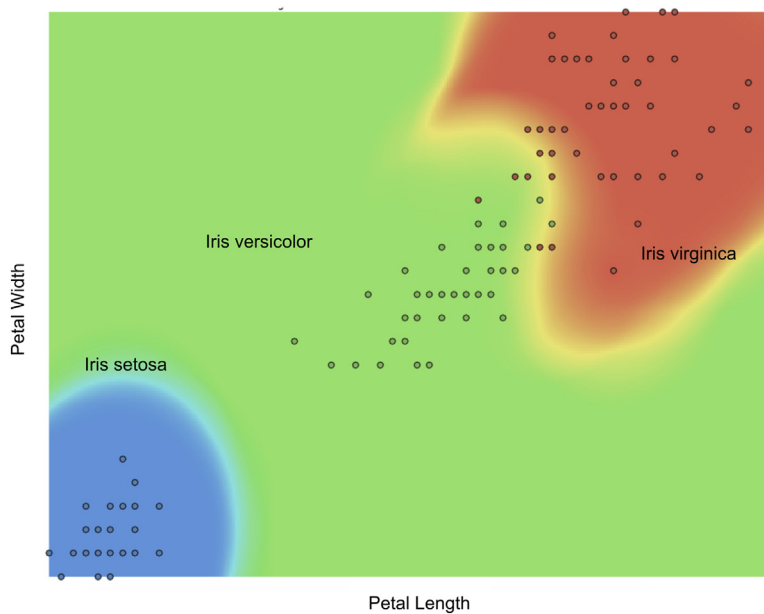Bubble chart of Iris dataset.

FIGURE 3.14
Density chart of a few attributes in the Iris dataset.

3.4.3 Visualizing High-Dimensional Data

Visualizing more than three attributes on a two-dimensional medium (like a paper or screen) is challenging. This limitation can be overcome by using transformation techniques to project the high-dimensional data points into parallel axis space. In this approach, a Cartesian axis is shared by more than one attribute.

Parallel Chart

A *parallel chart* visualizes a data point quite innovatively by transforming or projecting multi-dimensional data into a two-dimensional chart medium. In this chart, every attribute or dimension is linearly arranged in one coordinate (*x*-axis) and all the measures are arranged in the other coordinate (*y*-axis). Since the *x*-axis is multivariate, each data point is represented as a *line* in a parallel space.

In the case of the Iris dataset, all four attributes are arranged along the *x*-axis. The *y*-axis represents a generic distance and it is "shared" by all these attributes on the *x*-axis. Hence, parallel charts work only when attributes share a common unit of numerical measure or when the attributes are normalized. This visualization is called a *parallel axis* because all four attributes are represented in four parallel axes parallel to the *y*-axis.

In a parallel chart, a class label is used to color each data *line* so that one more dimension is introduced into the picture. By observing this parallel chart in Fig. 3.15, it can be noted that there is overlap between the three species on the sepal width attribute. So, sepal width cannot be the metric used to differentiate these three species. However, there is clear separation of species in petal length. No observation of *I. setosa* species has a petal length above 2.5 cm and there is little overlap between the *I. virginica* and *I. versicolor* species. Visually, just by knowing the petal length of an unlabeled observation, the species of Iris flower can be predicted. The relevance of this rule as a predictor will be discussed in the later chapter on Classification.

Deviation Chart

A *deviation chart* is very similar to a *parallel chart*, as it has parallel axes for all the attributes on the *x*-axis. Data points are extended across the dimensions as lines and there is one common *y*-axis. Instead of plotting all data lines, deviation charts only show the mean and standard deviation statistics. For each class, deviation charts show the mean line connecting the mean of each attribute; the standard deviation is shown as the band above and below the mean line. The mean line does not have to correspond to a data point (line). With this method, information is elegantly displayed, and the essence of a parallel chart is maintained.
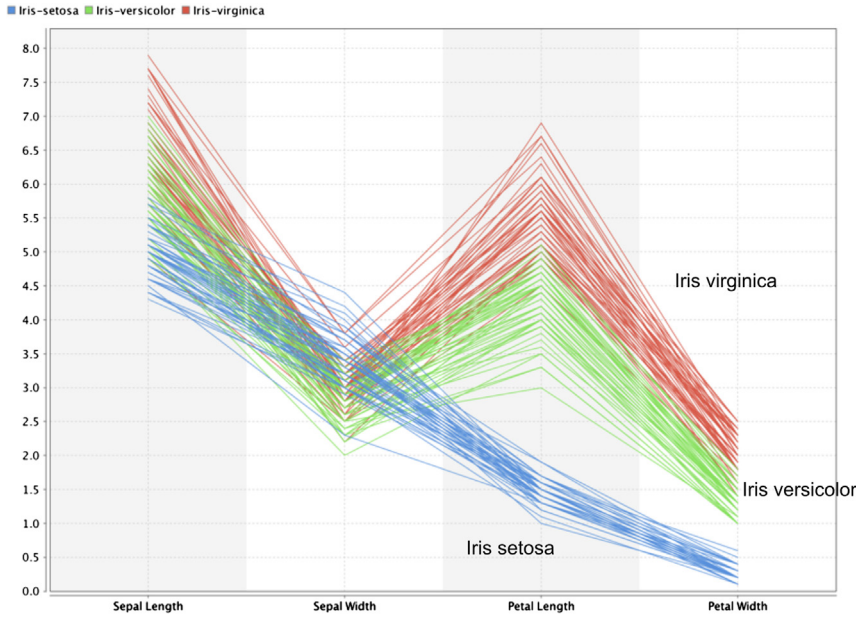
FIGURE 3.15
Parallel chart of Iris dataset.

In Fig. 3.16, a deviation chart for the Iris dataset stratified by species is shown. It can be observed that the petal length is a good predictor to classify the species because the mean line and the standard deviation bands for the species are well separated.

Andrews Curves

An *Andrews plot* belongs to a family of visualization techniques where the high-dimensional data are projected into a vector space so that each data point takes the form of a line or curve. In an Andrews plot, each data point X with d dimensions, $X = (x_1, x_2, x_3, \ldots, x_d)$, takes the form of a Fourier series:

$$f_x(t) = \frac{x_1}{\sqrt{2}} + x_2\sin(t) + x_3\cos(t) + x_4\sin(2t) + x_5\cos(2t) + \cdots \tag{3.4}$$

This function is plotted for $-\pi < t < \pi$ for each data point. Andrews plots are useful to determine if there are any outliers in the data and to identify potential patterns within the data points (Fig. 3.17). If two data points are similar, then the curves for the data points are closer to each other. If curves are far apart and belong to different classes, then this information can be used classify the data (Garcia-Osorio & Fyfe, 2005).
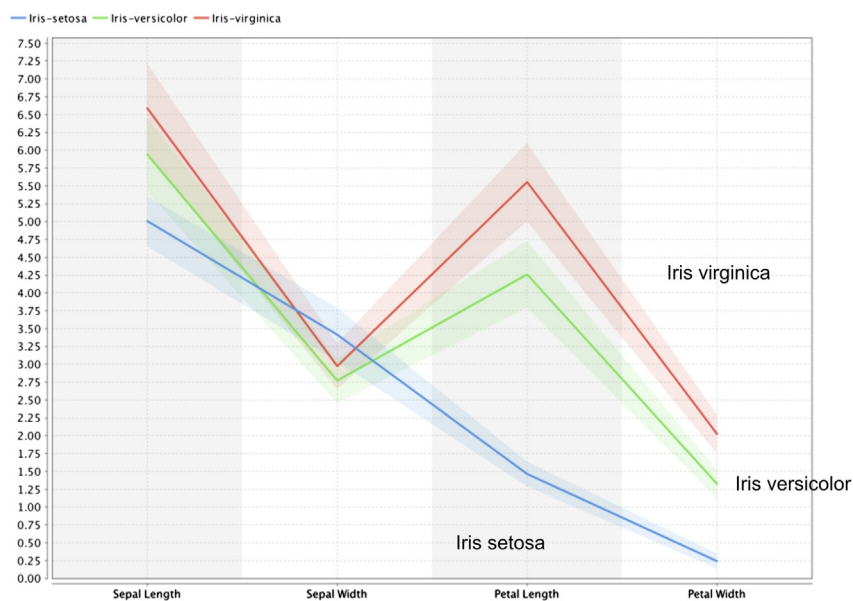
FIGURE 3.16
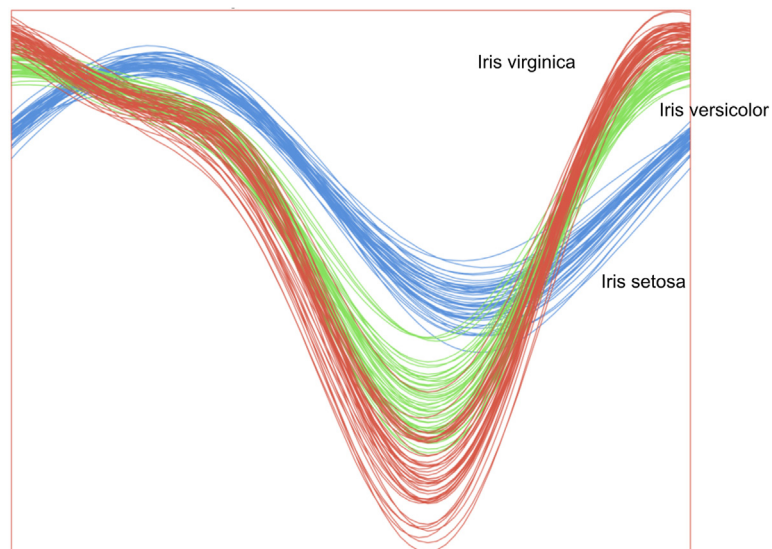Deviation chart of Iris dataset.

FIGURE 3.17
Andrews curves of Iris dataset.

Many of the charts and visuals discussed in this chapter explore the multivariate relationships within the dataset. They form the set of classic data visualizations used for data exploration, postprocessing, and understanding data science models. Some new developments in the area of visualization deals with networks and connections within the data objects (Lima, 2011). To better analyze data extracted from graph data, social networks, and integrated applications, connectivity charts are often used. Interactive exploration of data using visualization software provides an essential tool to observe multiple attributes at the same time but has limitations on the number of attributes used in visualizations. Hence, dimensional reduction using techniques discussed in Chapter 14, Feature Selection, can help in visualizing higher-dimensional data by reducing the dimensions to a critical few.

3.5 ROADMAP FOR DATA EXPLORATION

If there is a new dataset that has not been investigated before, having a structured way to explore and analyze the data will be helpful. Here is a roadmap to inquire a new dataset. Not all steps may be relevant for every dataset and the order may need to be adjusted for some sets, so this roadmap is intended as a guideline.

1. *Organize the dataset*: Structure the dataset with standard rows and columns. Organizing the dataset to have objects or instances in rows and dimensions or attributes in columns will be helpful for many data analysis tools. Identify the target or "class label" attribute, if applicable.
2. *Find the central point for each attribute*: Calculate *mean*, *median*, and *mode* for each attribute and the class label. If all three values are very different, it may indicate the presence of an outlier, or a multimodal or nonnormal distribution for an attribute.
3. *Understand the spread of each attribute*: Calculate the *standard deviation* and *range* for an attribute. Compare the standard deviation with the mean to understand the spread of the data, along with the max and min data points.
4. *Visualize the distribution of each attribute*: Develop the *histogram* and *distribution* plots for each attribute. Repeat the same for class-stratified histograms and distribution plots, where the plots are either repeated or color-coded for each class.
5. *Pivot the data*: Sometimes called dimensional slicing, a pivot is helpful to comprehend different values of the attributes. This technique can stratify by class and drill down to the details of any of the attributes. Microsoft Excel and Business Intelligence tools popularized this technique of data analysis for a wider audience.

6. *Watch out for outliers*: Use a scatterplot or quartiles to find outliers. The presence of outliers skews some measures like mean, variance, and range. Exclude outliers and rerun the analysis. Notice if the results change.
7. *Understand the relationship between attributes*: Measure the *correlation* between attributes and develop a correlation matrix. Notice what attributes are dependent on each other and investigate why they are dependent.
8. *Visualize the relationship between attributes*: Plot a quick scatter matrix to discover the relationship between multiple attributes at once. Zoom in on the attribute pairs with simple two-dimensional scatterplots stratified by class.
9. *Visualize high-dimensional datasets*: Create *parallel charts* and *Andrews curves* to observe the class differences exhibited by each attribute. *Deviation charts* provide a quick assessment of the spread of each class for each attribute.

References

Anscombe, F. J. (1973). Graphs in statistical analysis. *American Statistician, 27*(1), 17−21.

Bache, K., & Lichman, M. (2013) *University of California, School of Information and Computer Science*. Retrieved from UCI Machine Learning Repository <http://archive.ics.uci.edu/ml>.

Few, S. (2006). *Information dashboard design: The effective visual communication of data*. Sebastopol, CA: O'Reilly Media.

Fisher, R. A. (1936). The use of multiple measurements in taxonomic problems. *Annals of Human Genetics, 7*, 179−188, 10.1111/j.1469-1809.1936.tb02137.x.

Garcia-Osorio, C., & Fyfe, C. (2005). Visualization of high-dimensional data via orthogonal curves. *Journal of Universal Computer Science, 11*(11), 1806−1819.

Kubiak, T., & Benbow, D. W. (2006). *The certified six sigma black belt handbook*. Milwaukee, WI: ASQ Quality Press.

Lima, M. (2011). *Visual complexity: Mapping patterns of information*. New York: Princeton Architectural Press.

Tufte, E. R. (2001). *The visual display of quantitative information*. Cheshire, CT: Graphics Press.

Ware, C. (2004). *Information visualization: Perception for design*. Waltham, MA: Morgan Kaufmann.