

Chapter 2

Methodologies

In this section, we will develop three methodologies: the PROMETHEE II ranking method, the Hierarchical Cluster Analysis and the K-means analysis.

2.1 Ranking Methods

Multicriteria analysis, often called multiple criteria decision making (MCDM) by the American School and multicriteria decision aid (MCDA) by the European School, is a set of methods which allow the aggregation of several evaluation criteria in order to choose, rank, sort or describe a set of alternatives (Zopounidis 1999). The one basic conviction underlying every MCDA approach is that the explicit introduction of several criteria, each representing a particular dimension of the problem to be taken into account, is a better path for robust decision-making when facing multidimensional and ill-defined problems, than optimizing a single-dimensional objective function (such as cost-benefit analysis) (Costa et al. 1997). In contrast to the more classical operations research approaches, the multicriteria decision aid framework facilitates learning about the problem and the alternative courses of action, by enabling people to think about their values and preferences from several points of view (Costa et al. 1997).

Interest in MCDA increased as the sphere of application of quantitative management science moved from operational decision making situations, for which a more-or-less well-defined single objective function could be identified with little controversy (e.g. maximize profit), to more complex levels of managerial planning and decision making, which are naturally multidimensional problems (Costa et al. 1997). Multicriteria analysis now supports the structuring of a decision problem, the exploration of the concerns of decision actors, the evaluation of alternatives under different perspectives and the analysis of their robustness against uncertainty (Beinat and Nijkamp 1998).

MCDA can deal with mixed sets of data, quantitative and qualitative, including expert opinions (Mendoza and Martins 2006). The capability to accommodate these gaps in information and knowledge through qualitative data, expert opinions, or experiential knowledge is a distinct advantage (Mendoza and Martins 2006). This participatory environment accommodates the involvement and participation of multiple experts and stakeholders (Mendoza and Prabhu 2003).

As various alternatives are available, selecting the best among them which satisfies the manufacturer's requirement becomes more complex and time consuming. To choose an appropriate material with several criterion is a multi-objective task and it is a multi criteria decision making (MCDM) problem (Anojkumar et al. 2016). Many multivariate techniques are extensions of univariate analysis (analysis of single-variable distributions) and bivariate analysis (cross-classification, correlation, analysis of variance and simple regression used to analyze two variables) (Hair 2010). For example, simple regression (with one predictor variable) is extended in the multivariate case to include several predictor variables (Hair 2010). Likewise, the single dependent variable found in analysis of variance is extended to include multiple dependent variables in multivariate analysis of variance (Hair 2010). Some multivariate techniques (e.g. multiple regression and multivariate analysis of variance) provide a means of performing in a single analysis what once took multiple univariate analyses to accomplish (Hair 2010). Other multivariate techniques, however, are uniquely designed to deal with multivariate issues, such as factor analysis, which identifies the structure underlying a set of variables, or discriminant analysis, which differentiates among groups based on a set of variables (Hair 2010).

The PROMETHEE (Preference Ranking Organization Method for Enrichment Evaluation) belongs to the class of MCDA instruments. Several MCDA techniques have been developed over the years that deal with the ranking of numerous alternatives based on a variety of criteria. MCDA can be efficiently utilized in order to handle both qualitative and quantitative criteria (Stiakakis and Sifaleras 2013). In other words, the MCDA allows for the selection of the best from the analyzed alternatives. Their development was actually the result of the practitioner's motivation to provide academics and researchers with improved decision making processes suitable for real-life multiple criteria decision situations by taking advantage of the recent evolutions in computer technology and the mathematical techniques involved (Wiecek et al. 2008). An important objective of outranking methods is that the decision maker should be able to incorporate any argument into the process to achieve better awareness of the decision problem (Lerche and Geldermann 2015). In this book, following Kosmidou and Zopounidis (2008a, b), we will present one of the most recent MCDA techniques, the PROMETHEE II method.

2.1.1 PROMETHEE II Method

PROMETHEE II method is an outranking multi-criteria decision aid approach developed and presented for the first time by Brans (1982) at the University Laval, Quebec, Canada, during an organized conference on multi-criteria decision aid instruments by Nadeau and Landry. This method has attracted the increased attention of the researchers for practically complex problems and the growing records of conference presentations and academic papers can easily illustrate this. As the time passed, a number of extensions have been suggested with the aim of assisting researchers in dealing with more complex problems. Indeed, PROMETHEE methodology has effectively been applied in a variety of areas such as Banking, Business and Financial Management, Chemistry, Energy resources, Health, Investments, Industrial Location, and other fields. As Brans and Mareschal (2005) have pointed out, the above technique owes its success mainly to its particular friendliness of use and to its' mathematical properties.

Addressing a classification problem requires the development of a classification model that aggregates the characteristics of the alternatives to provide recommendations on the assignment of the alternatives to the predefined classes. The significance of classification problems has motivated the development of a plethora of techniques for constructing classification models. Statistical techniques have been dominating the field for many years, but during the last two decades other approaches have become popular mainly from the field of machine learning (Andreopoulou et al. 2014a).

Also, the contributions of MCDA are mainly focused on the study of multicriteria classification problems (MCPs). MCPs can be distinguished from traditional classification problems studied within the statistical and machine learning framework in two aspects (Zopounidis and Doumpos 2002). The first aspect involves the nature of the characteristics describing the alternatives, which are assumed to have the form of decision criteria providing not only a description of the alternatives but also some additional preferential information. The second aspect involves the nature of the predefined classification which is defined in ordinal rather than nominal terms. Classification models developed through statistical and machine learning techniques often fail to address this issues focusing solely on the accuracy of the results obtained from the model.

Within the MCDA several criteria aggregation forms have been proposed for developing decision models. These include relational forms, value functions, and rule-based models.

The PROMETHEE II method is part of the outranking relations theory (Brans and Vinke 1985; Brans et al. 1986; Siskos and Zopounidis 1987; Brans et al. 1987; Brans et al. 1998; Zopounidis 2001). Relational models are based on the construction of an outranking relation that is used to compare the alternatives with some reference profiles characterizing each class. The reference profiles are either typical examples (alternatives) of each class or examples that define the upper/lower bounds of the classes. Some typical examples of this approach include methods

such as ELECTRE TRI (Roy and Bouyssou 1993), PROAFTN (Belacel 2000), PAIRCLAS (Doumpos and Zopounidis 2004), and PROMETHEE TRI (Figueira et al. 2004). The main advantage of this approach is that it enables the decision maker (DM) to take into account the non-compensatory character of the decision process and to identify alternatives with special characteristics through the incorporation of the incomparability relation in the analysis. On other hand, the construction of the outranking relation requires the specification of a considerable amount of information which is not always easy to obtain (Andreopoulou et al. 2014a; Zopounidis et al. 2014). Brans (2015) presents a brief overview of OR from 1937 till now, the role of the outranking procedures in the field of MCDA and the PROMETHEE methodology including its extensions being of course stressed.

Value functions have also been quite popular as a criteria aggregation model in classification problems. This approach provides a straightforward methodology to perform the classification of the alternatives. Each alternative is evaluated according to the constructed value function and its global evaluation is compared to some value cut-off points in order to perform the assignment to one of the predefined classes. Due to their simplicity linear or additive value functions are usually considered (Jacquet-Lagrange 1995; Zopounidis and Doumpos 1999, 2000; Lemonakis and Strikos 2012). These provide a simple evaluation mechanism which is generally easy to understand and implement. However, there has been criticism on the assumptions underlying the use of such simple models and their ability to capture the interactions between the criteria.

The PROMETHEE methodology gives the researcher the ability to solve a decision problem where a finite set of comparable alternatives is to be evaluated according to several and often opposing criteria. The implementation of the PROMETHEE method involves the construction of an evaluation table (Table 2.1), in which the alternatives are estimated on the preferred criteria and ranked from the best to the worst. The PROMETHEE methods are considered to provide solutions for multicriteria problems of the form (2.1) and their associated evaluation table.

$$\max \{ g_1(a), g_2(a), g_3(a), \dots, g_j(a), \dots, g_k(a) | a \in A \} \quad (2.1)$$

where:

A is a finite set of possible alternatives $\{\alpha_1, \alpha_2, \dots, \alpha_i, \dots, \alpha_n\}$ ($\alpha_1, \alpha_2, \dots, \alpha_i, \dots, \alpha_n$) & $\{g_1(*), g_2(*), \dots, g_j(*), \dots, g_k(*)\}$ is a set of evaluation criteria.

Additional requirements for the application of PROMETHEE are the consideration of the relative significance of the selected criteria (i.e., the weights) and the information on the individually defined preference function of the decision-maker, regarding the comparison of the alternatives in terms of each single criterion.

The weights are typically arbitrary positive numbers, determined independently from the measurement units of the criteria. These numbers actually represent the relative significance of each criterion. The higher becomes the value of the weight, the higher the significance of the relevant criterion and conversely. According to Macharis et al. (2004), the selection of the weights is of high importance in the case

Table 2.1 Evaluation Table

a	g1(*)	g2(*)	...	gj(*)	...	gk(*)
$\alpha 1$	g1($\alpha 1$)	g2($\alpha 1$)	...	gj($\alpha 1$)	...	gk($\alpha 1$)
$\alpha 2$	g1($\alpha 2$)	g2($\alpha 2$)	...	gj($\alpha 2$)	...	gk($\alpha 2$)
.
.
.
αi	g1(αi)	g2(αi)	...	gj(αi)	...	gk(αi)
.
.
.
αn	g1(αn)	g2(αn)	...	gj(αn)	...	gk(αn)

Source Brans and Mareschal (2005)

of multicriteria decision analysis, since it reflects the decision-makers' insights and priorities.

The preference structure of PROMETHEE is based on pair wise comparisons. This means that a separate preference function for each criterion must be defined for all pairs of alternatives, reflecting the degree of preference for an alternative a over b. Vincke and Brans (1985) suggested six specific types of preference functions, provided in the appendix section, from which the researcher can easily define its preference structure. No matter, which is the preference function, the decision maker has to define the values of q, p and σ parameters. In contrast to q which is an indifference threshold that corresponds to the largest deviation, p is a strict preference threshold with the smallest deviation, capable of generating a full preference sufficiently for the decision maker. As far as the σ parameter is concerned it represents an intermediate value between q and p.

According to Brans et al. (1986), this preference degree for all couples of actions, can be represented by the preferred index of the following form:

$$\Pi(\alpha, \beta) = \frac{\sum_{j=1}^n w_j P_j(a, b)}{\sum_{j=1}^n w_j}$$

where:

w_j is the weight for each criterion

$P_j(a, b)$ expresses the degree at which bank a is preferred to bank b, when all the criteria are considered at once. Its value varies between 0 and 1.

A value equal to unity for the index will imply a strong preference of a bank a over b, while a zero value will imply a weak preference respectively. From the preference functions described above, this study utilized the Gaussian form for all the selected criteria. This function requires only for the parameter σ to be specified

and at the same time, due to the lack of discontinuities, it gives robust and stable results.

As for the ranking of alternative actions, two flows should be defined, the leaving and the entering flow, briefly described below:

$$\Phi^+(\alpha) = \sum_{b \in X} \pi(a, b)$$

$$\Phi^-(\alpha) = \sum_{b \in X} \pi(b, a)$$

where:

X is the total of alternative solutions

The leaving flow $\phi + (a)$ expresses how an alternative a dominates all the other alternatives of X (the outranking character of a). On the other hand, the entering flow $\phi - (a)$ measures how an alternative a is surpassed by all the other alternatives of X (the outranked character of a). According to PROMETHEE I partial ranking an action a is favoured over an action b , (aPb) if the leaving and entering flows of action a are greater and smaller respectively than those of action b :

$$\begin{aligned} aPb \text{ if : } & \phi + (a) > \phi + (b) \quad \text{and} \quad \phi - (a) < \phi - (b) \quad \text{or} \\ & \phi + (a) > \phi + (b) \quad \text{and} \quad \phi - (a) = \phi - (b) \quad \text{or} \\ & \phi + (a) = \phi + (b) \quad \text{and} \quad \phi - (a) < \phi - (b). \end{aligned}$$

In the case that the leaving and entering flows of two actions a and b are the same, the indifference situation can be written with the following expression (aIb):

$$aIb \text{ if : } \phi + (a) = \phi + (b) \quad \text{and} \quad \phi - (a) = \phi - (b)$$

There is also the possibility for two alternative actions to be incomparable, (aRb), if the entering flow of action a is worse than the corresponding flow of action b , while the opposite is implied by the leaving flow:

$$\begin{aligned} aRb \text{ if : } & \phi + (a) > \phi + (b) \quad \text{and} \quad \phi - (a) > \phi - (b) \quad \text{or} \quad \phi + (a) < \phi + (b) \quad \text{and} \\ & \phi - (a) < \phi - (b) \end{aligned}$$

In this paper we utilized only the PROMETHEE II method which provides a complete ranking of the comparable alternatives from the best to the worst. The net flow implied by $\Phi(a)$, which is the difference between the two flows, corresponds to a value function for which the higher the value the higher the attractiveness of alternative a . For each action $a \in X$ the net flow can be described as follows:

$$\Phi(a) = \Phi^+(a) - \Phi^-(a)$$

The outranking relations in PROMETHEE II method are such that:

$$\begin{aligned} \alpha \text{PIIb} & \text{ if } \Phi(a) > \Phi(b), \\ \alpha \text{IIIb} & \text{ if } \Phi(a) = \Phi(b) \end{aligned}$$

When, αPIIb , alternative α is preferred over b .

Also, when αIIIb , the decision maker is indifferent between alternatives α and b .

The net flow is the number that is used for the comparison between the cases in order to obtain the ranking. Each case with a higher net flow is considered superior in ranking.

In fact, there exist two types of the PROMETHEE methodology, the PROMETHEE I that ranks partially and also, the PROMETHEE II, which performs a full and complete ranking, based on all of the input data. In contrast to PROMETHEE I, incomparabilities are now absent between the alternatives. As a result, the alternative with the higher net flow is identified as the one optimizing all the criteria.

In general, the PROMETHEE methods include the three following steps (Brans and Mareschal 1994):

1. Enrichment of the preference structure. The notion of generalized criteria is introduced in order to take into account the amplitudes of the deviations between the evaluations. This step is crucial. Yet it can easily be understood by the decision maker because all the additional parameters to be defined have an economical significance. Moreover, the scaling effects are entirely handled in this first step.
2. Enrichment of the dominance relation. A valued outranking relation is built taking into account all the criteria. For each pair of alternatives, the overall degree of preference of one alternative over the other is obtained.
3. Exploitation for decision aid. PROMETHEE I provides a partial ranking of A , including possible incomparabilities. PROMETHEE II provides a complete ranking of A . It can look more efficient but in fact the information used is more disputable.

Multiattribute utility theory is not the only framework about multicriteria decision problems. In this approach, the cardinal approach, we aggregate numbers (the monodimensional utilities) representing an absolute evaluation of a given alternative with respect to a given criterion (Grabish 1995). As for the relational approach, the alternatives are compared two by two and the degree of preference of one alternative over the other, with respect to a criterion (relative evaluation) is expressed with a number. All these preference relations are then aggregated to take into account all the criteria (Grabish 1995). This approach has been developed essentially by Roy (1968, 1972) (ELECTRE methods) with ordinary crisp relations and then by Fodor and Roubens (1992) with fuzzy preference relations.

In Chap. 3, three examples will be presented using PROMETHEE II method. The first case study deals with skiing centers, the second case study is about 20 agrotourism enterprises and the third one regards 20 aquaculture units. These entities are ranked according to certain qualitative characteristics.

2.2 Cluster Generation Methods

Cluster analysis describes a set of multivariate methods and techniques that seek to classify data, often into groups, types, profiles, and so on (Leonard and Droege, 2008). For example, cluster analysis can be used to develop taxonomies or typological frameworks, to explore data to unravel complex underlying patterns, and may also be understood as a type of data reduction procedure (Leonard and Droege). Because of its utility, and due to advances in software technology, studies using cluster analysis have been surging in number since its introduction in the early 1960s (Leonard and Droege). Aldenderfer and Blashfield (1984) suggest that the popularity of cluster analysis can be attributed to its applicability to all scientific disciplines that rely on classification systems to guide research and understanding (Leonard and Droege). Cluster analysis is relevant to research in biology, medicine, education, archaeology, psychology, and other sciences because all such scientific disciplines rely in some way on classification (Leonard and Droege).

Classification refers to the assignment of a finite set of alternatives into groups. The alternatives belonging into different groups have different characteristics, without being possible to establish any kind of preference relation between them (i.e. the groups provide a description of the alternatives without any further information) (Doumpos and Zopounidis 2002).

Cluster analysis strategy is to detect structures, non visible and will always form clusters with the objects not considering the true existence of any structure in the data (Arabatzis and Kokkinakis 2005). The cluster solution is completely dependent among the variables used as the basis for the similarity measure and the method. When a cluster solution is identified the researcher should furthermore examine the fundamental structure represented in the defined clusters. Moreover, in the case that a single member cluster appears, the researcher must decide if it represents a valid structural component in the sample or if it should be deleted as unrepresentative (Hair et al. 1998). The formation of clusters/groups is based on ad hoc simple calculative procedures (Kinnear and Taylor 1996), although with substantial mathematical identities, they are no more than clever algorithms, and their result has to be translated with practical rules, mainly objective.

Although cluster analysis is conceptually simple to understand, some features of cluster analysis methods can be confusing (Leonard and Droege). This is largely due to the diversity of applications of cluster analysis across disciplines (Kogan 2007); many of the evolutionary stages of cluster analysis have occurred in silos and are somewhat discipline specific, without much cohesion or translation of developments and findings across disciplines (Leonard and Droege). There is no

detailed, uniform protocol (i.e., step-by-step progression) in conducting cluster analysis, which makes it different from multivariate procedures such as multivariate analysis of variance (MANOVA) and factor analysis (Leonard and Droege). The researcher using cluster analysis for the first time will likely be confronted with a set of choices and options that will need to be customized to her or his own unique research problem (Leonard and Droege). This is not to suggest that cluster analysis is a haphazard collection of procedures (Leonard and Droege). In fact, several authors have proposed guidelines for conducting CA in a step-by-step manner (Leonard and Droege).

According to Milligan (1996, 2007), there are seven steps in conducting cluster analysis:

1. Composition of the dataset
2. Selection of variables
3. Decisions about standardizing variables
4. Selecting a measure of association (or similarity measure)
5. Selecting a clustering method
6. Determining the number of clusters
7. Interpretation, testing and replication

Within each step, there are multiple options for implementation (Leonard and Droege). Unless one is an expert in cluster analysis or has a thorough statistical background, choosing from among the possible options can be challenging (Leonard and Droege). At this point in the evolution of cluster analysis, it is rare for a researcher to find a straightforward, direct path through the series of steps involved in completing cluster analysis (Leonard and Droege). This is not intended to discourage researchers from trying cluster analysis, but it may be advisable to anticipate these challenges and not be alarmed if and when they emerge (Leonard and Droege). It is also important to clearly state that it is unlikely that this article will provide a pharmacy researcher with all the information he or she would need to successfully complete cluster analysis; chances are that one would need to consult additional sources directly, although the reference list contains many useful sources (Leonard and Droege).

Cluster analysis can be performed either with the technique of hierarchical cluster analysis or with the technique of k-means cluster analysis (Everitt 1993). Furthermore, both hierarchical clustering and k-means generate “hard” solutions that define partitions of the data (Ahlquist and Breunig 2012). There is no foundation in statistical theory on which to prefer a particular clustering solution over another and no possibility of evaluating the uncertainty around a particular observation’s assignment to a given cluster (Ahlquist and Breunig 2012). The choice of both the number of clusters to focus on and the substantive interpretations assigned to them is solely the responsibility of the analyst (Ahlquist and Breunig 2012).

Initially, cluster randomized designs were widely regarded as lacking statistical precision (Raudenbush 1997). Cluster analysis is a descriptive method, used mostly as an exploratory implement that without any statistical basis at which to draw

statistical assumptions from a sample to a population (Hair et al. 1998). In most real life clustering situations, an applied researcher is faced with the dilemma of selecting the number of clusters or partitions in the final solution (Everitt 1979; Sneath and Sokal 1973). Virtually all clustering procedures provide little if any information as to the number of clusters present in the data (Milligan and Cooper 1985). A theoretical consideration which underlies many of the hierarchical methods is that some of these algorithms invoke the ultrametric inequality in the solution process (Milligan 1980). Pvcust is an add-on package for a statistical software R to assess the uncertainty in hierarchical cluster analysis (Suzuki and Shimodaira 2006). Pvcust can be used easily for general statistical problems, such as DNA microarray analysis, to perform the bootstrap analysis of clustering, which has been popular in phylogenetic analysis (Suzuki and Shimodaira 2006). Most (although by no means all) investigators are now warier of the whole area, having become aware of the varied and difficult problems facing the cluster analysis user in practice (Everitt 1979). Various qualitative guidelines have been proposed for deciding at what point in the clustering process clusters become non-significant (e.g., Thorndike 1953; Marriot 1971; Mojena 1977; Struass 1982). Everitt (1980), noting that the determination of the number of significant groups in a cluster analysis is a “formidable problem,” has identified three principal difficulties encountered in deriving adequate significance tests: (1) specification of a suitable null hypothesis; (2) determination of the sampling distribution of the distance or similarity measure used; and (3) development of a flexible test procedure.

2.2.1 *Hierarchical Cluster Analysis*

Hierarchical cluster analysis produces a unique set of nested categories or clusters by sequentially pairing variables, clusters, or variables and clusters (Bridges 1966). At each step, beginning with the correlation matrix, all clusters and unclustered variables are tried in all possible pairs, and that pair producing the highest average intercorrelation within the trial cluster is chosen as the new cluster (Bridges 1966). In contrast to other types of cluster analysis in which a single set of mutually exclusive and exhaustive clusters is formed, this technique proceeds sequentially from tighter, less inclusive clusters through larger more inclusive clusters and is continued until all variables are clustered in a single group (Bridges 1966). A graph, constructed like the taxonomic dendrogram of the biological systematist, shows the class-inclusive relations between clusters and the value of the clustering criterion associated with each (Bridges 1966).

An important characteristic of hierarchical procedures is that the results at an earlier stage are always nested within the results at a later stage, creating a similarity to a tree (Arabatzis and Kokkinakis 2005). However, divisions or fusions of clusters once made are irrevocable, so that when an agglomerative algorithm has joined two objects they cannot subsequently be separated. The disadvantage of this technique

lies in the fact that an exchange of elements between the groups is impossible when the “tree structure” is building up (Gerstengarbe et al. 1999).

Hierarchical cluster analysis is primarily an exploratory rather than confirmatory or inferential activity. In fact, Kaufman and Rousseeuw (2005) suggest that “it is permissible to try several algorithms on the same data because cluster analysis is mostly used as a descriptive or exploratory tool....we just want to see what the data are trying to tell us.” There are many attributes on which to measure similarity and difference across objects and, given some set of attributes, numerous algorithms for identifying clusters (Ahlquist and Breunig 2012).

Hierarchical analysis uses intuitively plausible procedures based on various distance metrics to either merge or partition observations into clusters (Ahlquist and Breunig 2012).

Hierarchical procedure involves the construction of a hierarchy of a tree like structure that helps to indicate the number of clusters within the cases (Andreopoulou et al. 2014b). In order to determine the final number of the clusters (stopping rule) large increases in the average within-cluster distance are identified. The prior cluster solution is then selected on the logic that its combination caused a substantial decrease in similarity (Hair et al. 1998).

Hierarchical cluster analysis is a method for finding the underlying structure of objects through an iterative process that associates (agglomerative methods) or dissociates (divisive methods) object by object, and that is halted when all objects have been processed (Steinbach et al. 2003; Almeida et al. 2007). The agglomerative procedure starts with each object in a separate cluster and then combines the clusters sequentially, reducing the number of clusters at each step until all objects belong to only one cluster (Almeida et al. 2007).

It begins with each object on its own and proceeding to combine them into clusters that maximize within-cluster similarity and between-cluster difference, as determined by a distance metric. Several different metrics can be employed and the literature provides little theoretical guidance about their appropriateness, though Milligan (1980, 1981) surveys Monte Carlo experiments, concluding that Ward’s linkage is a useful distance metric.

Among the five most popular agglomerative algorithms used to develop clusters is the Ward’s method. In Ward’s method is a clustering procedure seeking to form the partitions in a manner that minimizes the loss associated with each grouping and to quantify that loss in terms of an error sum-of-squares criterion (ESS) (Everitt 1993). Ward’s method is designed to form clusters that have minimum within-cluster sum-of-squares (Waller et al. 1998). The complete linkage method forms clusters in which each entity is more similar to other members of its cluster than to all members of other clusters (Waller et al. 1998). The average linkage method forms clusters that each entity has a greater mean similarity with all members of its cluster than to all members of other clusters (Waller et al. 1998).

The divisive methods start with all of the objects in one cluster, and then proceed to their partition into smaller clusters until there is one object per cluster (Downs and Barnard 2002; Bratchell 1989; Almeida et al. 2007). This means that for N objects, the process involves $N - 1$ clustering steps.

In hierarchical cluster analysis there are two important choices when defining a method: the type of similarity measure between objects and/or groups, and the linkage technique (Bratchell 1989). The first task is to determine a numerical value for the similarity between objects, constructing a similarity matrix (Almeida et al. 2007). The most popular ways to determine the similarity between objects use the Euclidean distance and the correlation coefficient, but there are many alternatives for similarity indicators (Kellner et al. 2004; Brereton 2004).

The next step is to group or ungroup the objects. The most common approach is an agglomerative technique, whereby single objects are gradually connected to each other in groups. The first connection corresponds necessarily to the most similar pair of objects. Once the first group is formed, it is necessary to define the similarity between the new group and the remaining objects (Brereton 2004). This step requires a new choice among a variety of available techniques. Some of the most used linkage algorithms are complete-linkage (or furthest-neighbor), single linkage (or nearest-neighbor), average-linkage (between groups and within groups), centroid method and Ward's-linkage (Downs and Barnard 2002; Kellner et al. 2004; Smolinski et al. 2002). In single linkage, when a new group is formed, the corresponding distance to any other group is the minimal Euclidean distance of all possible distances between each object of the former group and each object of the latter (Almeida et al. 2007).

Once the similarity measure and the linkage method are defined, the agglomeration of objects and groups in each step of the process follows the order of larger similarity (Brereton 2004). The structure obtained by hierarchical clustering is often presented in the form of a dendrogram where each linkage step in the clustering process is represented by a connection line (Downs and Barnard 2002; Smolinski et al. 2002).

It is widely accepted that the average-linkage, centroid and Ward's methods are sensitive to the shape and size of clusters. Thus, they can easily fail when clusters have complicated forms departing from the hyperspherical shape (Downs and Barnard 2002). Complete-linkage is not strongly affected by outliers, but can break large clusters, and has trouble with convex shapes (Steinbach et al. 2003). The single linkage methodology, on the other hand, displays total insensibility to shape and size of clusters (Downs and Barnard 2002). However, there are also shortcomings associated with single linkage, which is the sensitivity to the presence of outliers and the difficulty in dealing with severe differences in the density of clusters (Almeida et al. 2007).

Hierarchical cluster analysis can further be subdivided into 2 methods: agglomerative and divisive (Leonard and Droege). Agglomerative methods use algorithms to join cases based on their similarity, and divisive methods use algorithms that separate cases based on their differences (Leonard and Droege). With either method, hierarchical cluster analysis is sequential (Leonard and Droege). Essentially, the hierarchical algorithm sorts through the dataset in a serial manner, seeking to divide (divisive methods) or fuse (agglomerative methods) 2 cases at a time (Leonard and Droege). This also means that when cases are joined or separated, hierarchical cluster analysis methods do not return to those 2 cases again

(Leonard and Droege). This is where the term “hierarchical” applies: Once a match or separation is achieved, it remains in place for the remainder of the analysis (Leonard and Droege). This process continues until all cases are assigned to a cluster. hierarchical cluster analysis involves many more computations than non-hierarchical methods, and this may be an issue with very large datasets (Leonard and Droege). Advances in computer technology may eventually obviate this consideration, but for now, extremely large datasets may be inappropriate for hierarchical cluster analysis methods (Aldenderfer and Blashfield 1984).

The application of different methods, which may involve different similarity measures, different linkage techniques, etc., leads to dendrograms with different structures (Almeida et al. 2007). Apparently, a good approach would be to use different methods of cluster analysis and compare the results, but due to an excessive wealth of options it is frequently more convenient to use well founded a priori choices (Almeida et al. 2007).

In Chap. 3, two examples will be presented using hierarchical cluster analysis. The first case study deals with 20 wood enterprises and the second one is about 20 enterprises which promote the Renewable Energy Sources. These entities are classified according to certain qualitative and quantitative characteristics.

2.2.2 *K-Means Analysis*

K-means cluster analysis is an example of a nonhierarchical cluster analysis method, where k is equal to the number of clusters the researcher wishes to impose upon the data (Leonard and Droege). Because k is determined a priori, k-means cluster analysis does not “suffer” from the issue of imposing a single partition only once and never visiting the partition again (Leonard and Droege).

Within traditional cluster analysis, relocation methods such as k-means require that the analyst posit the number of clusters in the data in advance and then proceed to iteratively move observations among clusters until an optimal allocation can be identified (Ahlquist and Breunig 2012). For example, k-means iteratively moves observations from one cluster to another to minimize the total squared distance from k “centroids” or “prototypes” (Ahlquist and Breunig 2012).

A generic outline that describes all k-means algorithms is presented below (Blashfield and Aldenderfer 1988; Darken and Moody 1990; Waller et al. 1998):

1. Initialize the seed values for a prespecified number (k) of clusters. These seed values represent the cluster centroids. If computationally feasible, cluster centroids from a prior hierarchical cluster analysis (e.g. Ward’s method or group average) can be used as seeds. This method of initializing the k-means seed values has been recommended by Milligan, who—when summarizing the findings of a previous Monte Carlo study—concluded that “the k-means algorithms do no seem to be very desirable if random starting seeds must be used”

2. Allocate each data point in the sample to the cluster with the nearest centroid. Proximity is defined using Euclidean distances.
3. If a cluster increased in size during the last data pass, that is, if new data points were allocated to the cluster, then recomputed the cluster centroid.
4. Alternate steps 2 and 3 until no data points change clusters.

The aim of the k-means algorithm is to generate clusters with minimum within-cluster sum of squares (Hartigan 1975). Unfortunately, there is no guarantee that this aim will be realized when the number of input vectors is moderate or large or when the number of clusters is larger than two (Waller et al. 1998). With more than two clusters there is an exponentially increasing number of initial data partitions from which to start the algorithm (Waller et al. 1998). The Hartigan and Wong (1979) algorithm that was used in the present study finds local optima such that, given the initial cluster seed values, the obtained clusters have minimum sums of squares. Alternative seeds may produce tighter clusters and thus the quality of the solution is sensitive to the initial cluster centroids (Waller et al. 1998).

The K-means algorithm requires three user-specified parameters: number of clusters K , cluster initialization, and distance metric (Jain 2010). The most critical choice is K (Jain 2010). While no perfect mathematical criterion exists, a number of heuristics are available for choosing K (Jain 2010). Typically, K-means is run independently for different values of K and the partition that appears the most meaningful to the domain expert is selected (Jain 2010). Different initializations can lead to different final clustering because K-means only converges to local minima (Jain 2010). One way to overcome the local minima is to run the K-means algorithm, for a given K , with multiple different initial partitions and choose the partition with the smallest squared error (Jain 2010).

K-means is typically used with the Euclidean metric for computing the distance between points and cluster centers (Jain 2010). As a result, K-means finds spherical or ball-shaped clusters in data (Jain 2010). K-means with Mahalanobis distance metric has been used to detect hyper-ellipsoidal clusters (Mao and Jain 1996), but this comes at the expense of higher computational cost (Jain 2010). A variant of K-means using the Itakura–Saito distance has been used for vector quantization in speech processing (Linde et al. 1980) and K-means with L1 distance was proposed in (Kashima et al. 2008). Banerjee et al. (2004) exploits the family of Bregman distances for K-means.

K-Means is a standard technique for clustering, used in a wide array of applications and even as way to initialize the more expensive EM clustering algorithm (Bishop 1995; Cheeseman and Stutz 1996; Meila and Heckerman 1998). Furthermore, regardless of which clustering algorithm is being used, K-Means is employed internally by our initialization refinement method (Bradley and Fayyad 1998).

The k-means algorithm is defined over continuous data (Niknam and Amiri 2010). The k-means algorithm gave better results only when the initial partitions were close to the final solution (Niknam and Amiri 2010). In other words, the results of k-means highly depend on the initial state and reach to local optimal solution. In order to overcome this problem, a lot of studies have done in clustering

(Kao et al. 2008; Cao and Krzysztof 2008; Zalik 2008; Krishna 1999; Mualik and Bandyopadhyay 2000; Fathian and Amiri 2007; Laszlo and Mukherjee 2007; Shelokar et al. 2004; Ng and Wong 2002; Sung and Jin 2000; Niknam et al. 2008; Niknam et al. 2008; Niknam et al. 2008).

The k-means algorithm has the following important properties (Huang 1998):

5. It is efficient in processing large data sets.
6. It often terminates at a local optimum (MacQueen 1967; Selim and Ismail 1984).
7. It works only on numeric values.
8. The clusters have convex shapes (Anderberg 1973).

There exist a few variants of the k-means algorithm which differ in selection of the initial k means, dissimilarity calculations and strategies to calculate cluster means (Anderberg 1973; Bobrowski and Bezdek 1991). The sophisticated variants of the k-means algorithm include the well-known ISODATA algorithm (Ball and Hall 1967) and the fuzzy k-means algorithms (Ruspini 1969, 1973; Bezdek 1981). One difficulty in using the k-means algorithm is that the number of clusters has to be specified (Anderberg 1973; Milligan and Cooper 1985). Some variants like ISODATA include a procedure to search for the best k at the cost of some performance (Huang 1998).

In Chap. 3, three examples will be presented using k-means analysis. The first case study deals with 20 government agencies in National Parks, the second one is about the agricultural exploitations of 50 prefectures and the third one deals with 20 agrifood entities. These entities are classified according to certain quantitative and qualitative characteristics.

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Multicriteria and Clustering

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