Chapter 14
Unsupervised Learning

It would be a mistake to think that machine learning always requires examples with class labels. Far from it! Useful information can be gleaned even from examples whose classes are not known. This is sometimes called *unsupervised learning*, in contrast to the term *supervised learning* which is used when talking about induction from pre-classified examples.

While supervised learning focuses on induction of classifiers, unsupervised learning is interested in discovering useful properties of available data. Perhaps the most popular task looks for groups (called clusters) of similar examples. The centroids of these groups can then be used as gaussian centers for Bayesian or RBF classifiers, as predictors of unknown attribute values, and even as visualization tools for multidimensional data. Last but not least, techniques used in unsupervised learning can be used to create higher-level attributes from existing ones.

The chapter describes some practical techniques for unsupervised learning, explaining the basic algorithms, their behaviors in practical circumstances, and the benefits they offer.

14.1 Cluster Analysis

The fundamental task in unsupervised learning is *cluster analysis*. Here, the input is a set of examples, each described by a vector of attribute values—but no class labels. The output is a set of two or more clusters of examples.

Identifying Groups of Similar Examples Figure 14.1 shows a simple domain with a few examples described by two attributes: `weight` and `height`. An observer can easily see that the examples form three or four groups, depending on the subjective "level of resolution."

M. Kubat, *An Introduction to Machine Learning*,
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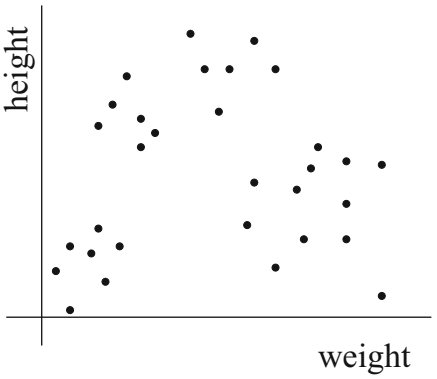


Fig. 14.1 A two-dimensional domain with clusters of examples

Visual identification of such groups in a two-dimensional space is easy, but in four or more dimensions, humans can neither visualize the data nor see the clusters. These can only be detected by cluster-analysis algorithms.

Representing Clusters by Centroids To begin with, we have to decide how the clusters are to be described. A few alternatives can be considered: it is possible to specify the clusters' locations, sizes, boundaries, and perhaps some other aspects. But the simplest approach relies on *centroids*.[1] If all attributes are numeric, the centroid is identified with the averages of the individual attributes. For instance, suppose a two-dimensional cluster consists of the following examples: $(2, 5), (1, 4), (3, 6)$. In this case, the centroid is described by vector $(2, 5)$ because the first attribute's average is $\frac{2+1+3}{3} = 2$ and the second attribute's average is $\frac{5+4+6}{3} = 5$.

The averages can be calculated even when the attributes are discrete if we know how to turn them into numeric ones. Here is a simple way of doing so. If the attribute can acquire three or more different values, we can replace each attribute-value pair with one boolean variable (say, `season=fall`, `season=winter`, etc.). The values of the boolean attributes are then represented by 0 or 1 instead of *false* and *true*, respectively.

What Should the Clusters Be Like? Clusters should not overlap each other: each example must belong to one and only one cluster. Within the same cluster, the examples should be relatively close to each other, certainly much closer than to the examples from the other clusters.

An important question will ask how many clusters the data contain. In Fig. 14.1, we noticed that the human observer discerns either three or four clusters. However, the scope of existing options is not limited to these two possibilities. At one extreme, the entire training set can be thought of as forming one big cluster; at the other,

[1] Machine learning professionals sometimes avoid the term "center" which might imply mathematical properties that are for the specific needs of cluster analysis largely irrelevant.

each example can be seen as representing its own single-example cluster. Practical implementations often side-step the problem by asking the user to supply the number of clusters by way of an input parameter. Sometimes, however, machine-learning software is expected to determine the number automatically.

Problems with Measuring Distances Algorithms for cluster analysis usually need a mechanism to evaluate the distance between an example and a cluster. If the cluster is described by its centroid, the Euclidean distance between the two vectors seems to offer a good way of doing so—assuming that we are aware of situations where this can be misleading. This last statement calls for an explanation.

Euclidean distance may be inconvenient in the case of discrete attributes, but we already know how to deal with them. More importantly, we must not forget that each attribute is likely to represent a different quantity, which renders the use geometric distance rather arbitrary: a 4-year difference in `age` is hard to compare with a 4-foot difference in `height`. Also the problem of scaling plays its role: if we replace feet with miles, the distances will change considerably.

We have encountered these problems earlier, in Chap. 3. In the context of cluster analysis, however, these issues tend to be less serious than in k-NN classifiers. Most of the time, engineers get around the difficulties by normalizing all attribute values into the unit interval, $x_i \in [0, 1]$. We will return to normalization in Sect. 14.2.

A More General Formula for Distances If the examples are described by a mixture of numeric and discrete attributes, we can rely on the sum of the squared distances along corresponding attributes. More specifically, the following expression is recommended (denoting by n the number of attributes):

$$d_M(\mathbf{x}, \mathbf{y}) = \sqrt{\Sigma_{i=1}^{n} d(x_i, y_i)} \tag{14.1}$$

In this formula, we will use $d(x_i, y_i) = (x_i - y_i)^2$ for continuous attributes. For discrete attributes (including boolean attributes), we put $d(x_i, y_i) = 0$ if $x_i = y_i$ and $d(x_i, y_i) = 1$ if $x_i \neq y_i$.

Which Cluster Should an Example Belong To? Let us suppose that each example is described by an attribute vector, $\mathbf{x}$, and that each cluster is defined by its centroid—which, too, is an attribute vector.

Suppose there are N clusters whose centroids are denoted by $\mathbf{c}_i$, where $i \in (1, N)$. The example $\mathbf{x}$ has a certain distance $d(\mathbf{x}, \mathbf{c}_i)$, from each centroid. If $d(\mathbf{x}, \mathbf{c}_P)$ is the smallest of these distances, it is natural to expect that $\mathbf{x}$ be placed in cluster $\mathbf{c}_P$.

For instance, suppose that we use the Euclidean distance, and that there are three clusters. If the centroids are $\mathbf{c}_1 = (3, 4)$, $\mathbf{c}_2 = (4, 6)$ and $\mathbf{c}_3 = (5, 7)$, and if the example is $\mathbf{x} = (4, 4)$, then the Euclidean distances are $d(\mathbf{x}, \mathbf{c}_1) = 1$, $d(\mathbf{x}, \mathbf{c}_2) = 2$, and $d(\mathbf{x}, \mathbf{c}_3) = \sqrt{10}$. Since $d(\mathbf{x}, \mathbf{c}_1)$ is the smallest of the three values, we conclude that $\mathbf{x}$ should belong to $\mathbf{c}_1$.

Benefit 1: Estimating Missing Values The knowledge of the clusters can help us estimate missing attribute values. Returning to Fig. 14.1, the reader will notice that if `weight` is low, the example is bound to belong to the bottom-left cluster. In this case, also `height` is likely to be low because it is low in all examples found in this cluster. This aspect tends to be even more strongly pronounced in realistic data described by multiple attributes.

In example descriptions, some attribute values are sometimes unknown. As a simple way of dealing with this issue, Sect. 10.4 suggested that the missing value be estimated as the average or the most frequent value encountered in the training set. However, an estimate of the missing value as the average or the most frequent value of the given cluster is sounder because it uses more information about the nature of the domain.

Benefit 2: Reducing the Size of RBF Networks and Bayesian Classifiers Cluster analysis can assist such techniques as Bayesian learners and radial-basis-function networks. The reader will recall that these paradigms operate with centers.[2] In the simplest implementation, the centers are identified with the attribute vectors of the individual examples. In domains with millions of examples, however, this would lead to impractically big classifiers. The engineer then prefers to divide the training set into N clusters, and to identify the gaussian centers with the centroids of the clusters.

Benefit 3: A Simple Classifier Finally, the knowledge of data clusters may be useful in supervised learning. It is quite common that all (or almost all) examples in a cluster belong to the same class. In that case, the developer of a supervised-learning software may decide first to identify the clusters, and then label each cluster with its dominant class.

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

- What is the main difference between unsupervised learning and supervised learning?
- What is a cluster of examples? Define some mechanisms to describe the clusters. How can we measure the distance between an example and a cluster?
- Summarize the main benefits of cluster analysis.

[2] For instance, the section on RBF networks denoted these centers by μ_i's.

14.2 A Simple Algorithm: *k*-Means

Perhaps the simplest algorithm to detect clusters of data is known under the name *k-means*. The "*k*" in the name denotes the requested number of clusters—a parameter whose value is supplied by the user.

The Outline of the Algorithm The pseudocode of the algorithm is provided in Table 14.1. The first step creates *k* initial clusters such that each example finds itself in one and only one cluster. After this, the coordinates of all centroids are calculated. Let us note that the problem of initialization is somewhat more complicated than that. We will return to this issue presently.

In the next step, *k-means* investigates one example at a time, calculating its distances from all centroids. The nearest centroid then defines the cluster to which the example should belong. If the example already *is* that cluster, nothing needs to be done; otherwise, the example is transferred from the current (wrong) cluster to the right one. After the relocation, the centroids of the two affected clusters (the one that lost the example, and the one that gained it) have to be recalculated. The procedure is graphically illustrated by the single-attribute domain from Fig. 14.2. Here, two examples find themselves in the wrong cluster and are therefore relocated. Note how, after the example relocation, the vertical bars (separating the clusters), and also the centroids, change their locations.

Termination The good thing about the algorithm described in Table 14.1 is that the process is guaranteed to reach a situation where each example finds itself in the nearest cluster so that, from this moment on, no further transfers are needed. The clusters do not overlap. Since this is usually achieved in a manageable number of steps, no sophisticated termination criterion is needed here.

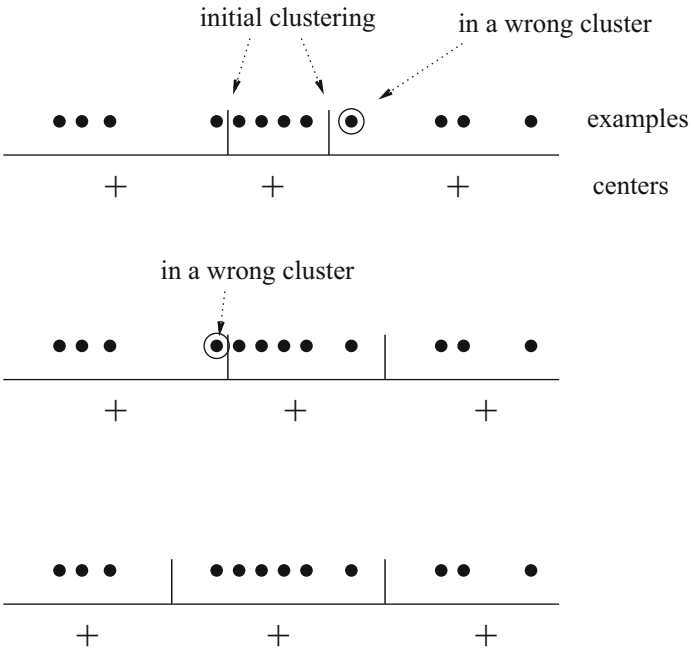
Table 14.1 The clustering algorithm *k-means*

Input: a set of examples without class labels
user-set constant *k*

1. Create *k* initial clusters. For each, calculate the coordinates of its centroid, C_i, as the numeric averages of the attribute values in the examples it contains.
2. Choose an example, **x**, and find its distances from all centroids. Let *j* be the index of the *nearest centroid*.
3. If **x** already finds itself in the *j*-th cluster, do nothing. Otherwise, move **x** from its current cluster to the *j*-th cluster and recalculate the centroids.
4. Unless a stopping criterion has been satisfied, repeat the last two steps for another example.

Stopping criterion: each training example already finds itself in the nearest cluster.

Let us consider an almost trivial domain where 13 examples are described by a single numeric attribute. Suppose the examples have been initially divided into the three groups indicated here by the *vertical bars*. The following sequence shows how two examples (marked by *circles*) are moved from one cluster to another.



After the second transfer, the clusters are perfect and the calculations can stop.

Fig. 14.2 Illustration of the *k-means* procedure in a domain with one numeric attribute

Numeric Example In Table 14.2, a set of nine two-dimensional examples has been randomly divided into three groups (because the user specified $k = 3$), each containing the same number of examples. The table also provides the centroids for each group. *k-means* goes through these examples systematically, one by one—in this concrete case, starting with group-2. For each example, its distance from each centroid is calculated. It turns out that the first example from group-2 already finds itself in the right cluster. However, the second example is closer to group-1 than to group-2 and, for this reason, has to be transferred from its original cluster to group-1. After this, the affected centroids are recalculated.

Table 14.2 Illustration of the *k-means* procedure in a domain with two attributes

The table below contains three initial groups of vectors. The task is to find "ideal" clusters using the *k-means* ($k = 3$).

	Group-1	Group-2	Group-3
	(2, 5)	(4, 3)	(1, 5)
	(1, 4)	(3, 7)	(3, 1)
	(3, 6)	(2, 2)	(2, 3)
Centroids:	(2, 5)	(3, 4)	(2, 3)

Let us pick the first example in group-2. The Euclidean distances between this example, (4, 3), and the centroids of the three groups are $\sqrt{8}$, $\sqrt{2}$, and $\sqrt{4}$, respectively. This means that the centroid of group-2 is the one nearest to the example. Since this is where the example already is, *k-means* does not do anything.

Let us now proceed to the second example in group-2, (3, 7). In this case, the distances are $\sqrt{5}$, $\sqrt{9}$, and $\sqrt{17}$, respectively. Since the centroid of group-1 has the smallest distance, the example is moved from group-2 to group-1. After this, the averages of the two affected groups are recalculated.

Here are the new clusters:

	Group-1	Group-2	Group-3
	(2, 5)	(4, 3)	(1, 5)
	(1, 4)	(2, 2)	(3, 1)
	(3, 6)		(2, 3)
	(3, 7)		
Averages:	(2.25, 5.25)	(3, 2.5)	(2, 3)

The process continues as long as any example transfers are needed.

The Need for Normalization The reader will recall that, when discussing *k*-NN classifiers, Chap. 3 argued that inappropriate attribute scaling will distort the distances between attribute vectors. The same concern can be raised in cluster analysis. It is therefore always a good idea to normalize the vectors so that all numeric attributes have values from the same range, say, from 0 to 1.

The simplest way of doing so is to determine for the given attribute its maximum (*MAX*) and minimum (*MIN*) value in the training set. Then, each value of this attribute is re-calculated using the following formula:

$$x = \frac{x - MIN}{MAX - MIN} \tag{14.2}$$

As for boolean attributes, their values can simply be replaced with 1 and 0 for *true* and *false*, respectively. Finally, an attribute that acquires n discrete values (such as `season`, which has four different values) can be replaced with n boolean attributes, one for each value—and, again, for the values of these boolean attributes, 1 or 0 are used.

Computational Aspects of Initialization To reach its goal, the *k-means* needs to go through a certain number of transfers of examples from wrong clusters to the right clusters. How many such transfers are needed depends on the contents of the initial clusters. At least in theory, it *can* happen that the randomly created initial clusters are already perfect, and not a single example needs to be moved. This, of course, is an extreme, but the reader surely understands that if the initialization is "lucky," fewer relocations have to be carried out than otherwise. Initialization matters in the sense that a better starting point ensures that the solution is found sooner.

How to Initialize In some domains, we can take advantage of some background knowledge about the problem at hand. For instance, seeking to create initial clusters in a database of a company's employees, the data analyst may speculate that it makes sense to group them by their age, salary, or some other intuitive criterion, and that the groups thus obtained will be good initial clusters.

In other applications, however, no such guidelines exist. The simplest procedure then picks k random training examples and regards them as *code vectors* to define initial centroids. The initial clusters are then created by associating each of the examples with its nearest code vector.

A More Serious Problem with Initialization There is another issue, and a more serious one than the computational costs. The thing is, also the *composition* of the resulting clusters (once the *k-means* has completed its work) may depend on initialization. Choose a different set of initial code vectors, and the technique may generate a different set of clusters.

The point is illustrated in Fig. 14.3. Suppose that the user wants two clusters ($k = 2$). If he chooses as code vectors the examples denoted by **x** and **y** then the initial clusters created with the help of these two examples are already perfect.

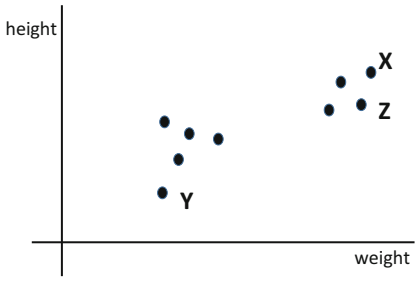


Fig. 14.3 Suppose $k = 2$. If the code vectors are [**x**,**y**], the initial clusters for k-means will be different than when the code vectors are [**x**,**z**]

The situation changes when we choose for the code vectors examples **x** and **z**. In this event, the two initial clusters will have a very different composition, and *k-means* is likely to converge on a different set of clusters. The phenomenon will be more pronounced if there are "outliers," examples that do not apparently belong to any of the two clusters.

Summary of the Main Problems The good thing about *k-means* is that it is easy to explain and easy to implement. Yet this simplicity comes at a price. The technique is sensitive to initialization; the user is expected to provide the number of clusters (though he may not know how many clusters there are); and, as we will see, some clusters can never be identified, in this manner. The next sections will take a look at some techniques to overcome these shortcomings.

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

- Describe the principle of the *k-means* algorithm. What is the termination criterion?
- What would be the consequence if we did not normalize the training set? Write down the simple normalization formula.
- Describe some methods for the initialization of *k-means*. What are the main consequences of good or bad initialization?

14.3 More Advanced Versions of *k*-Means

The previous section described the baseline version of *k-means* and explained its main weaknesses: sensitivity to initialization, and lack of flexibility in deciding about the number of clusters. Let us now take a look at some improvements meant to address these shortcomings.

Quality of the Clusters An engineer always needs to be able to evaluate and compare alternative solutions. And thus also for the topic addressed by this section, we need a criterion to help us choose between different sets of clusters. Primarily, the criterion should reflect the fact that we want clusters that minimize the average distance between examples and the centroids of "their" clusters.

Let us denote by $d(\mathbf{x}, \mathbf{c})$ the distance between example **x** and the centroid, **c**, of the cluster to which **x** belongs. If all attributes are numeric, and if they all have been normalized, then $d(\mathbf{x}, \mathbf{c})$ can be evaluated either by the Euclidean distance or by the more general Eq. (14.1).

The following formula (in which *SD* stands for *summed distances*) sums up the distances of all examples from their clusters' centroids. Here, $\mathbf{x}_i^{(j)}$ denotes the *i*-th example in the *j*-th cluster, *K* is the number of clusters, n_j is the number of examples in the *j*-th cluster, and $\mathbf{c}_j$ is the *j*-th cluster's centroid.

$$SD = \sum_{j=1}^{K} \sum_{i=1}^{n_j} d(\mathbf{x}_i^{(j)}, \mathbf{c}_j) \tag{14.3}$$

In cluster analysis, we seek to minimize *SD*. When calculating this quantity, we must not forget that the value obtained by Eq. (14.3) will go down if we increase the number of clusters (and thus decrease their average size), reaching $SD = 0$ in the extreme case when each cluster is identified with one and only one training example. The formula is therefore useful only if we compare solutions that have similar numbers of clusters.

Using Alternative Initializations Knowing that the composition of the resulting clusters depends on the algorithm's initialization, we can suggest a simple improvement. We will define two or more sets of initial code vectors, and apply *k-means* separately to each of them. After this, we will evaluate the quality of all the alternative data partitionings thus obtained, using the criterion defined by Eq. (14.3). The best solution is the one for which we get the lowest value. This solution is then retained, and the others discarded.

Experimenting with Different Values of *k* One obvious weakness of *k-means* is the requirement that the user should provide the value of *k*. This is easier said than done because, more often than not, the engineer has no idea into how many clusters the available data naturally divide. Unless more sophisticated techniques are used (about these, see later), the only way out is to try a few different values, and then pick the best according to an appropriate criterion (such as the one defined in Eq. (14.3)). As we already know, the shortcoming of this criterion is that it tends to give preference to small clusters. For this reason, data analysts often normalize the value of *SD* by *k*, the number of clusters.

Post-processing: Merging and Splitting Clusters The quality of the set of clusters created by *k-means* can often be improved by post-processing techniques that either increase the number of clusters by splitting, or decrease the number by merging.

As for merging, two neighboring clusters will be merged if their mutual distance is small. To find out whether the distance merits the merging, we simply calculate the distance of two centroids, and then compare it with the average cluster-to-cluster distance calculated by the following sum, where $\mathbf{c}_i$ and $\mathbf{c}_j$ are centroids:

$$S = \sum_{i \neq j} d(\mathbf{c}_i, \mathbf{c}_j) \tag{14.4}$$

Conversely, splitting makes sense when the average example-to-example distance within some cluster is high. The concrete solution is not easy to formalize because once we have specified that cluster C is to be split into C_1 and C_2, we need to decide which of C's examples will go to the first cluster and which to the second. Very often, however, it is perfectly acceptable to identify in C two examples with the greatest mutual distance, and then treat them as the code vectors of newly created C_1 and C_2, respectively.

Hierarchical Application of *k*-Means Another modification relies on recursive calls. The technique begins with running *k-means* for $k = 2$, obtaining two clusters. After this, *k-means* is applied to each of these two clusters separately, again with $k = 2$. The process is continued until an appropriate termination criterion has been satisfied— for instance, the maximum number of clusters the user wants to obtain, or the minimum distance between neighboring clusters.

This hierarchical version side-steps one serious shortcoming of *k-means*: the necessity to provide the number of clusters because, in this case, this is found automatically. This is particularly useful when the goal is to identify the gaussian centers in Bayesian classifiers or in RBF networks.

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

- Discuss some shortcomings of the *k-means* algorithm, and describe the simple techniques for overcoming them.
- Specify how you would implement the cluster-splitting and cluster-merging techniques described in this section.
- Explain the principle of hierarchical application of *k-means*.

14.4 Hierarchical Aggregation

Just as any other machine-learning technique, *k-means* has not only advantages, but also shortcomings. To avoid at least some of the latter, we need an alternative, an approach which is likely to prove useful in situations where *k-means* fails.

Another Serious Limitation of *k*-Means By minimizing the distance between the examples and the centroids of the clusters to which these examples belong, *k-means* essentially guarantees that it will discover "convex" clusters. Most of the time, this is indeed what we want. Such clusters can be useful in the context of Bayesian classifiers and the RBF networks where they reduce, sometimes very significantly, the number of employed gaussian centers.

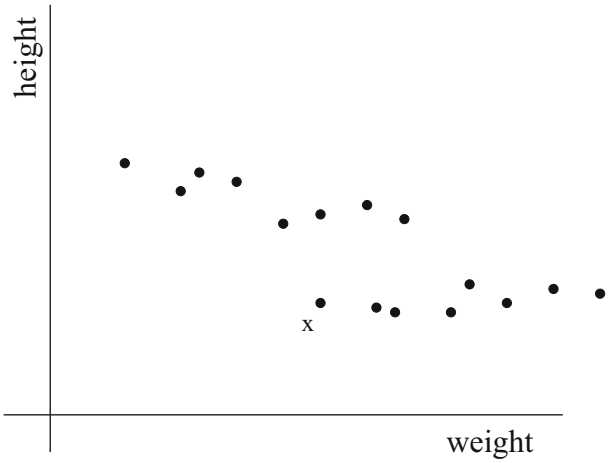


Fig. 14.4 Note that the leftmost examples in the "bottom" cluster are closer to the "upper" cluster's centroid than to its own. In a domain of this kind *k-means* will not find the best solution

This approach, however, will do a poor job if the clusters are of a different ("non-convex") nature. To see the point, consider the clusters in Fig. 14.4. Here, the leftmost example, **x**, in the bottom cluster is closer to the centroid of the upper cluster, and *k-means* would therefore relocate it accordingly—and yet we feel that this would not do justice to the nature of the two groups.

To deal with data of this kind, we need another technique, one capable of identifying clusters such as those in Fig. 14.4.

An Alternative Way of Measuring Inter-Cluster Distance In the previous section, the distance between two clusters was evaluated as the Euclidean distance between their centroids. However, for the needs of the approach described below, we will suggest another mechanism: we will measure the distances between all pairs of examples, **[x,y]**, such that **x** comes from the first cluster and **y** from the second. The smallest value found among all these example-to-example distances then defines the distance between the two clusters.

Returning to Fig. 14.4, the reader will agree that, along this new distance metric, example **x** is closer to the bottom cluster than to the upper clusters. This means that the limitation mentioned in the previous paragraph has been in this particular case eliminated. The price for this improvement is increased computational costs: if N_A is the number of examples in the first cluster, and N_B the number of examples in the second, then $N_A \times N_B$ example-to-example distances have to be evaluated. Most of the time, however, the clusters are not going to so big as to make this an issue.

Numeric Example For the sake of illustration of how this new distance metric is calculated, consider the following two clusters, A and B.

A
$\mathbf{x}_1 = (1, 0)$
$\mathbf{x}_2 = (2, 2)$

B
$\mathbf{y}_1 = (3, 3)$
$\mathbf{y}_2 = (4, 4)$

Table 14.3 The basic algorithm of *hierarchical aggregation*

Input: a set of examples without labels

1. Let each example form one cluster. For N examples, this means creating N clusters, each containing a single example.
2. Find a pair of clusters with the smallest cluster-to-cluster distance. Merge the two clusters into one, thus reducing the total number of clusters to $N - 1$.
3. Unless a termination criterion is satisfied, repeat the previous step.

Using the Euclidean formula, we calculate the individual example-to-example distances as follows:

$$d(\mathbf{x}_1, \mathbf{y}_1) = \sqrt{13},$$
$$d(\mathbf{x}_1, \mathbf{y}_2) = \sqrt{25},$$
$$d(\mathbf{x}_2, \mathbf{y}_1) = \sqrt{2},$$
$$d(\mathbf{x}_2, \mathbf{y}_2) = \sqrt{8}.$$

Observing that the smallest of these values is $d(\mathbf{x}_2, \mathbf{y}_1) = \sqrt{2}$, we conclude that the distance between the two clusters is $d(A, B) = \sqrt{2}$.

Hierarchical Aggregation For domains such as the one in Fig. 14.4, the clustering technique known as *hierarchical aggregation* is recommended. The principle is summarized by the pseudocode in Table 14.3.

In the first step, each example defines its own cluster. This means that in a domain with N examples, we have N initial clusters. In a series of the subsequent steps, hierarchical aggregation always identifies a pair of clusters that have the smallest mutual distance along the distance metric from the previous paragraphs. These clusters are then merged. At an early stage, this typically amounts to merging pairs of neighboring examples. Later, this results either in adding an example to its nearest cluster, or in merging two neighboring clusters. The first few steps are illustrated in Fig. 14.5.

The process continues until an appropriate termination criterion is satisfied. One possibility is to stop when the number of clusters drops below a user-specified threshold. Alternatively, one can base the stopping criterion on the cluster-to-cluster distance (finish when the smallest of these distances exceeds a certain value).

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

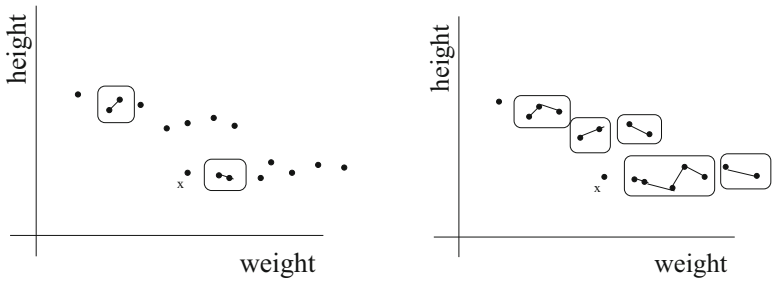


Fig. 14.5 Hierarchical aggregation after first two steps (*left*) and after first nine steps (*right*). Note how the clusters are gradually developed

- What kind of clusters cannot be detected by the *k-means* algorithm?
- What distance metric is used in hierarchical aggregation? What are the advantages and disadvantages of this metric?
- Describe the principle of the hierarchical-aggregation approach to clustering. For what kind of clusters is it particularly suited?

14.5 Self-Organizing Feature Maps: Introduction

Let us now introduce yet another approach to unsupervised learning, this time borrowing from the field of neural networks. The technique is known as a *self-organizing feature map, SOFM*.[3] Another name commonly used in this context is *Kohonen networks*, to honor its inventor.

The Idea Perhaps the best way to explain the nature of SOFM is to use, as a metaphor, the principle of physical attraction. A *code vector*, initially generated by a random-number generator, is subjected to the influence of a sequence of examples (attribute vectors), each "pulling" the vector in a different direction. In the long run, the code vector settles in a location that represents a compromise over all these conflicting forces.

The whole network consists of a set of *neurons* arranged in a two-dimensional matrix such as the one shown in Fig. 14.6. Each node (a neuron) in this matrix represents a code vector that has the same length (the same number of attributes) as the training examples. At the bottom is an input attribute vector that is connected to all neurons in parallel. The idea is to achieve by training a situation where neighboring neurons respond similarly to similar input vectors. For the sake of simplicity, the input vector in the picture only has two attributes, x_1 and x_2. In reality, it can have a great many.

[3] In statistics, and in neural networks, scientists often use the term *feature* instead of *attribute*.

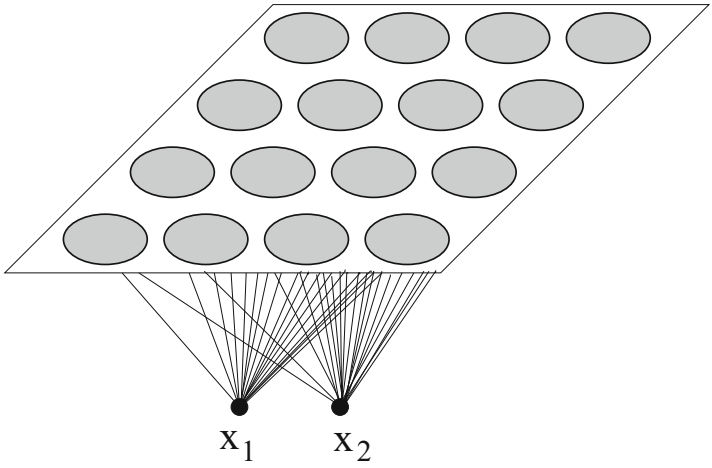


Fig. 14.6 General schema of a Kohonen network

How to Model Attraction Each neuron is described by a weight vector, $\mathbf{w} = (w_1, \ldots, w_n)$ where n is the number of attributes describing the examples. If $\mathbf{x} = (x_1 \ldots, x_n)$ is the example, and if $\eta \in (0, 1)$ is a user-specified learning rate, then the individual weights are modified according to the following formula:

$$w_i = w_i + \eta(x_i - w_i) \tag{14.5}$$

Note that the i-th weight is increased if $x_i > w_i$ because the term in the parentheses is then positive (and η is always positive). Conversely, the weight is decreased if $x_i < w_i$ because then the term is negative. It is in this sense that we say that the weight vector is attracted to $\mathbf{x}$. How strongly it is attracted is determined by the value of the learning rate.

Numeric Example Suppose that an example $\mathbf{x} = (0.2, 0.8)$ has been presented, and suppose that the winning neuron has the weights $\mathbf{w} = (0.3, 0.7)$. If the learning rate is $\eta = 0.1$, then the new weights are calculated as follows:

$$w_1 = w_1 + \eta(x_1 - w_1) = 0.3 + 0.1(0.2 - 0.3) = 0.3 - 0.01 = 0.29$$
$$w_2 = w_2 + \eta(x_2 - w_2) = 0.7 + 0.1(0.8 - 0.7) = 0.7 + 0.01 = 0.71$$

Note that the first weight originally had a greater value than the first attribute. By the force of the attribute's attraction, the weight has been reduced. Conversely, the second weight was originally smaller than the corresponding attribute, but the attribute's "pull" increases it.

Which Weight Vectors Are to Be Attracted by the Example Once an example, $\mathbf{x}$, has been presented to the neural matrix, a two-step process is launched. The task of the first step, a "competition," is to identify in the matrix the neuron whose weight

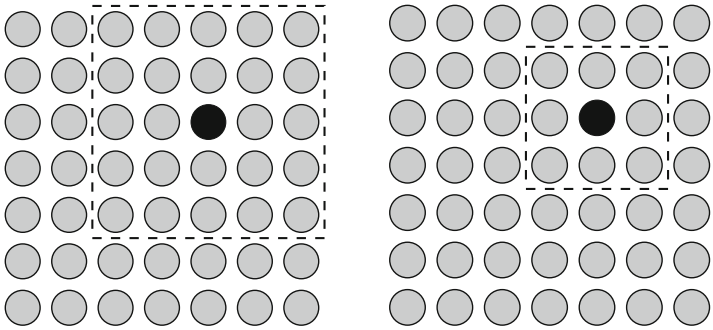


Fig. 14.7 The idea of "neighborhood" in the Kohonen network

vector is most similar to **x**. To this end, the Euclidean distance is used—smaller distance means greater similarity. Once the winner has been established, the second step updates the weights of this winning neuron as well as the weights of all neurons in the winner's physical neighborhood.

A Note on "Neighborhood" Figure 14.7 illustrates what is meant by the neighborhood of the winning code vector, $\mathbf{c}_{winner}$. Informally, the neighborhood consists of a set of neurons within a specific physical distance (in the matrix) from $\mathbf{c}_{winner}$. Note that this results in a situation where the weights of all neurons in the neighborhood are modified in a like manner.

Usually, the size of the neighborhood is not fixed. Rather, it is a common practice to reduce it over time as indicated in the right part of Fig. 14.7. Ultimately, the neighborhood will degenerate to the single neuron, the one that has won the competition. The idea is to start with a coarse approximation that is later fine-tuned.

Why Does It Work? The idea motivating the self-organizing feature map is to make sure that code vectors physically close to each other in the neural matrix respond to similar examples. This is why the same weight-updating formula is applied to all neurons in the winner's neighborhood.

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

- Describe the general architecture of self-organizing feature maps. Relate the notion of a *code vector* to that of a *neuron* in the matrix.
- Explain the two steps of the self-organizing algorithm: competition, and weight adjustment. Comment also on the role of the learning rate, η.
- What is meant by the *neighborhood* of the winning code vector? Is its size always constant?

14.6 Some Important Details

Having outlined the principle, let us now take a look at some details without which the technique would underperform.

Normalization The technique does not work well unless all vectors have been normalized to unit length (i.e., length equal to 1). This applies both to the vectors describing the examples, and to the weight vectors of the neurons. Fortunately, normalization to unit length is easy to carry out. Suppose an example is described as follows:

$$\mathbf{x} = (x_1, \ldots, x_n)$$

To obtain unit length, we divide each attribute's value by the length of the original attribute vector, $\mathbf{x}$:

$$x_i := \frac{x_i}{\sqrt{\Sigma_j x_j^2}} \tag{14.6}$$

Numeric Example Suppose we want to normalize the two-dimensional vector $\mathbf{x} = (5, 5)$. The length of this vector is $l(\mathbf{x}) = \sqrt{x_1^2 + x_2^2} = \sqrt{25 + 25} = \sqrt{50}$. Dividing the value of each attribute by this length results in the following normalized version of the vector:

$$\mathbf{x}' = (\frac{5}{\sqrt{50}}, \frac{5}{\sqrt{50}}) = (\sqrt{\frac{25}{50}}, \sqrt{\frac{25}{50}}) = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$$

That the length of $\mathbf{x}'$ is equal to 1 is easy to verify: using the Pythagorean Theorem, we calculate it as $\sqrt{x_1^2 + x_2^2} = \sqrt{\frac{1}{2} + \frac{1}{2}} = 1$. We can see that the new attribute vector indeed has unit length.

Initialization The first step in SOFM is the initialization of the neurons' weights. Usually, this initialization is carried out by a random-number generator that chooses the values from an interval that spans equally the positive and negative domains, say, $[-1, 1]$. After this, the weight vector is normalized to unit length as explained above.

Another thing to be decided is the learning rate, η. Usually, a small number is used, say, $\eta = 0.1$. Sometimes, however, it is practical to start with a relatively high value such as $\eta = 0.9$, and then gradually decrease it. The point is to modify the weights more strongly at the beginning, during the period of early approximation. After this, smaller values are used so as to fine-tune the results.

The Algorithm The general principle of self-organizing feature maps is summarized by the pseudocode in Table 14.4. To begin with, all examples are normalized

Table 14.4 The basic algorithm of self-organizing feature maps

Input: set of examples without labels
a learning rate, η.
a set of randomly initialized neurons arranged in a matrix

1. Normalize all training examples to unit length.
2. Present a training example, and find its nearest code vector, $\mathbf{c}_{winner}$
3. Modify the weights of $\mathbf{c}_{winner}$, as well as the weights of the code vectors in the neighborhood of $\mathbf{c}_{winner}$, using the formula $w_i = w_i + \eta(x_i - w_i)$. After this, re-normalize the weight vectors.
4. Unless a stopping criterion is met, present another training example, identify $\mathbf{c}_{winner}$, and repeat the previous step.

Comments:
1. η usually begins with a relatively high value from $(0, 1)$, then gradually decreases.
2. Every now and then, the size of the neighborhood is reduced.

to unit length. Initial code vectors are created by a random-number generator and then normalized, too.

In the algorithm's main body, training examples are presented one by one. After the presentation of example $\mathbf{x}$, the algorithm identifies a neuron whose weight vector, $\mathbf{c}_{winner}$, is the closest to $\mathbf{x}$ according to the Euclidean distance. Then, the weights of $\mathbf{c}_{winner}$ as well as those of all neurons in its neighborhood in the matrix are modified using Eq. (14.5), and then re-normalized. The algorithm is usually run for a predefined number of epochs.[4]

In the course of this procedure, the value of the learning rate is gradually decreased. Occasionally, the size of the neighborhood is reduced, too.

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

- Which vectors have to be normalized? What is the goal of this normalization? Write down the formula that is used to this end.
- What is the subject of initialization? What values are used?
- Summarize the algorithm of self-organizing feature maps.

[4]Recall that one epoch means that all training examples have been presented once.

14.7 Why Feature Maps?

Let us now turn our attention to some practical benefits of self-organizing feature maps.

Reducing Dimensionality The technique introduced in the previous section essentially maps the original N-dimensional space of the original attribute vectors to the two-dimensional space of the neural matrix: each example has its winning neuron, and the winner can be described by its two coordinates in the matrix. These coordinates can be seen as new description of the original examples.

Creating Higher-Level Features Reducing the number of attributes is of vital importance in applications where the number of attributes is prohibitively high, especially if most of these attributes are either irrelevant or redundant. For instance, this may the case in the field of computer vision where each image (i.e., an example) can be described by hundreds of thousands of pixels.

Having studied Chap. 7, the reader understands that a direct application of, say, perceptron learning to attribute vectors of extreme length is unlikely to succeed: in a domain of this kind, a classifier that does well on a training set tends to fail miserably on testing data. The mathematical explanation of this failure is that the countless attributes render the problem's VC-dimension so high as to prevent learnability unless the training set is unrealistically large. Advanced machine learning applications therefore seek to reduce the dimensionality either by attribute selection or, which is more relevant to this chapter, by way of mapping the multi-dimensional problem to a smaller space. This is accomplished by creating new features as functions of the original features.

What New Features Can Thus Be Created One might take this idea a step further. Here is a simple suggestion, just to offer inspiration. Suppose the training examples are described by 100 attributes, and suppose we have a reason to suspect that some attributes are mutually dependent whereas quite a few others are irrelevant.

In such a domain, the dimensionality is likely to be unnecessarily high, and any attempt to reduce it is welcome. One way to do so is to extract, say, five different subsets of the attributes, and then redescribe the training examples five times, each time using a different attribute set. After this, each of these newly obtained training sets is subjected to SOFM which then maps each multi-dimensional space to two dimensions. Since this is done five times, we obtain $5 \times 2 = 10$ new attributes.

Visualization Human brain has no problem visualizing two- or three-dimensional data, and then develop an opinion about the similarity (or mutual distance) of concrete examples, about the examples' distribution, or about the groups they tend to form. However, this becomes impossible when there are more than three attributes.

This is when self-organizing feature maps can be practical. By mapping each example onto a two-dimensional matrix, we may be able to visualize at least some of the relations inherent in the data. For instance, similar attribute vectors are likely

to be mapped to the same neuron, or at least to neurons that are physically close to each other. Similar observations can be made about general data distribution. In this sense, feature maps can be regarded as a useful visualization tool.

Initializing k-Means Each of the weight vectors in the neural matrix can be treated as a code vector. The mechanism of SOFM makes it possible to find reasonably good values of these vectors—which can then be used to initialize such cluster-analysis methods as *k-means*. Whether this is a practical approach is another question because SOFM is a computationally expensive technique.

A Brief Mention of "Deep Learning" Let us also remark that methods for automated creation of higher-level features from very long attribute vectors are used in so-called *deep learning*. In essence, deep learning is a neural-networks technique that organizes the neurons in many layers, many more that we have seen in the context of multi-layer perceptrons in Chap. 5. It is in this sense the networks are "deep," and this is what gave the paradigm its name.

The top layers of these networks are trained by a supervised learning technique such as the backpropagation of error that the reader already knows. By contrast, the task for the lower layers is to create a reasonable set of features. It is conceivable that self-organizing feature maps be used to this end; in reality, more advanced techniques are usually preferred, but their detailed treatment is outside the scope of an introductory textbook.

One has to be cautions, though. The circumstance that a concrete paradigm is popular does not mean that it is a panacea that will solve all machine-learning problems. Far from it. If the number of features is manageable, and if the size of the training set is limited, then classical approaches will do just as well as deep learning, or even better.[5]

What Have You Learned?

To make sure you understand the topic, try to answer the following questions. If needed, return to the appropriate place in the text.

- In what way can the SOFM technique help us visualize the data?
- Explain how the SOFM technique can be used to reduce the number of attributes and to create new, higher-level features. Where can this be used?
- What is the principle of *deep learning*?

[5] A bulldozer is more powerful than a spade, and yet the gardener prefers the spade most of the time.

14.8 Summary and Historical Remarks

- In some machine-learning tasks, we have to deal with example vectors that do not have class labels. Still, useful knowledge can be induced for them by the techniques of *unsupervised learning*.
- The simplest task in unsupervised learning is *cluster analysis*. The goal is to find a way that naturally divides the training set into groups of similar examples. Each example should be more similar to examples in its group than to examples from any other group.
- One of the simplest *cluster analysis* techniques is known under the name of *k-means*. Once an initial clustering has been created, the algorithm accepts one example at a time, and evaluates its distance from the centroid of its own cluster as well as the distances from the centroids of the other clusters. If the example appears to find itself in a wrong cluster, it is transferred to a better one. The technique converges in a finite number of steps.
- The quality of the clusters discovered by *k-means* is sensitive to initialization and to the user-specified value of *k*. Methods to improve this quality by subsequent merging and splitting, and by alternative initializations sometimes have to be considered. Also hierarchical implementations of *k-means* are useful.
- In some domains, the shapes of the data clusters make it impossible for *k-means* to find them. For instance, this was the case of the training set shown in Fig. 14.4. In this event, the engineer will may give preference to some other clustering technique such as *hierarchical aggregation* that creates the clusters in a bottom-up manner, always merging the clusters with the smallest mutual distance.
- In the case of *hierarchical aggregation*, it is impractical to identify the distance between two clusters with the distance between their centroids. Instead, we use the minimum distance between **[x,y]** where **x** belongs to one cluster and **y** to the other.
- One of the problems facing the *k-means* algorithm is the question of how to define the initial *code vectors*. One way to address this issue is by the technique of *self-organizing feature maps*.
- As an added bonus, self-organizing feature maps are capable of converting a high-dimensional feature space onto only two attributes. They can also be used for the needs of data visualization.

Historical Remarks The problems of cluster analysis have been studied since the 1960s. The *k-means* algorithm was described by McQueen [58] and hierarchical aggregation by Murty and Krishna [71]. The idea of merging and splitting clusters (not necessarily those obtained by *k-means* was studied by Ball and Hall [2]. The technique of SOFM, self-organizing feature maps, was developed by Kohonen [45]. In this book, however, only a very simple version of the technique was presented.

14.9 Solidify Your Knowledge

The exercises are to solidify the acquired knowledge. The suggested thought experiments will help the reader see this chapter's ideas in a different light and provoke independent thinking. Computer assignments will force the readers to pay attention to seemingly insignificant details they might otherwise overlook.

Exercises

1. Look at the three initial clusters of two-dimensional vectors in Table 14.5. Calculate the coordinates of their centroids.
2. Using the Euclidean distance, decide whether all of the examples from group 1 are where they belong. You will realize that one of them is not. Move it to a more appropriate group and recalculate the centroids.
3. Normalize the examples in Table 14.5 using Eq. (14.2).
4. Suppose the only information you have is the set of the nine training examples from Table 14.5, and suppose that you want to run the *k-means* algorithm for $k = 3$ clusters. What will be the composition of the three initial clusters if your code vectors are $(1, 4)$, $(3, 6)$, and $(3, 5)$?
5. Consider the three clusters from Table 14.5. Which pair of clusters will be merged by the hierarchical-aggregation technique?

Give It Some Thought

1. At the beginning of this chapter, we specified the benefits of cluster analysis. Among these was the possibility of identifying neurons in RBF networks with clusters instead of examples. In the case of *k-means*, this is straightforward: each gaussian center is identified with one cluster's centroid. However, how would you benefit (in RBF networks) from the clusters obtained by hierarchical aggregation?
2. Try to invent a machine-learning algorithm that first pre-processes the training examples using some cluster-analysis technique, and then uses them for classification purposes.

Table 14.5 An initial set of three clusters

Group 1	Group 2	Group 3
$(1, 4)$	$(4, 3)$	$(4, 5)$
$(3, 6)$	$(6, 7)$	$(3, 1)$
$(3, 5)$	$(2, 2)$	$(2, 3)$

3. Explain how self-organizing feature maps can be used to define the code vectors with which *k-means* sometimes starts. Will it be more meaningful to use the opposite approach (initialize SOFM) by *kmeans*)?

Computer Assignments

1. Write a program that accepts as input a training set of unlabeled examples, chooses among them k random code vectors, and creates the clusters using the *k-means* technique.
2. Write a program that decides whether a pair of clusters (obtained by *k-means*) should be merged. The easiest way of doing so is to compare the distance between the two clusters with the average cluster-to-cluster distance in the given clustering.
3. Write a program that creates the clusters using the *hierarchical aggregation* technique described in Sect. 14.4. Do not forget that the distance between clusters is evaluated differently than in the case of *k-means*.
4. Write a program that accepts a set of unlabeled training examples and subjects them to the technique of self-organizing feature maps.