

3.8. DATA CLUSTERING AND VISUALIZATION

Table 3.8.1

Six commonly used clustering methods

 For each method, the coefficients α_i , β and γ in equation (3.8.11) are given.

Method	α_i	β	γ
Single link	$\frac{1}{2}$	0	$-\frac{1}{2}$
Complete link	$\frac{1}{2}$	0	$\frac{1}{2}$
Average link	$n_i/(n_i + n_j)$	0	0
Weighted-average link	$\frac{1}{2}$	0	0
Centroid	$n_i/(n_i + n_j)$	$-n_i n_j/(n_i + n_j)^2$	0
Sum of squares	$(n_i + n_k)/(n_i + n_j + n_k)$	$-n_k/(n_i + n_j + n_k)$	0

In some cases it can be advantageous to use $I^{1/2}$ in the distance-matrix generation; this can enhance the sensitivity of the clustering to weak peaks (Butler *et al.*, 2019).

3.8.3. Cluster analysis

Cluster analysis uses \mathbf{d} (or \mathbf{s} , or δ) to partition the patterns into groups based on the similarity of their diffraction profiles. Associated with cluster are a number of important ancillary techniques all of which will be discussed here. A flowchart of these methods is shown in Fig. 3.8.4.

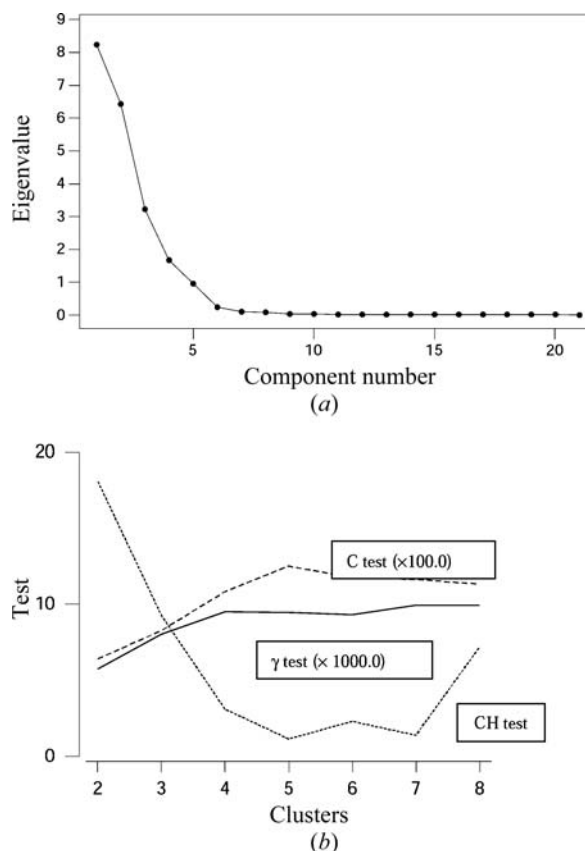
3.8.3.1. Dendrograms

Using \mathbf{d} and \mathbf{s} , agglomerative, hierarchical cluster analysis is now carried out, in which the patterns are put into clusters as defined by their distances from each other. [Gordon (1981, 1999) and Everitt *et al.* (2001) provide excellent and detailed introductions to the subject. Note that the two editions of Gordon's monograph are quite distinct and complementary.] The method begins with a situation in which each pattern is considered to be in a separate cluster. It then searches for the two patterns with the shortest distance between them, and joins them into a single cluster. This continues in a stepwise fashion until all the patterns form a single cluster. When two clusters (C_i and C_j) are merged, there is the problem of defining the distance between the newly formed cluster $C_i \cup C_j$ and any other cluster C_k . There are a number of different ways of doing this, and each one gives rise to a different clustering of the patterns, although often the difference can be quite small. A general algorithm has been proposed by Lance & Williams (1967), and is summarized in a simplified form by Gordon (1981). The distance from the new cluster formed by merging C_i and C_j to any other cluster C_k is given by

$$d(C_i \cup C_j, C_k) = \alpha_i d(C_i, C_k) + \alpha_j d(C_j, C_k) + \beta d(C_i, C_j) + \gamma |d(C_i, C_k) - d(C_j, C_k)|. \quad (3.8.11)$$

There are many possible clustering methods. Table 3.8.1 defines six commonly used clustering methods, defined in terms of the parameters α , β and γ . All these methods can be used with powder data; in general, the group-average-link or single-link formalism is the most effective, although differences between the methods are often slight.

The results of cluster analysis are usually displayed as a dendrogram, a typical example of which is shown in Fig. 3.8.6(a), where a set of 13 powder patterns is analysed using the centroid method. Each pattern begins at the bottom of the plot as a separate cluster, and these amalgamate in stepwise fashion linked by horizontal tie bars. The height of the tie bar represents a similarity measure as measured by the relevant distance. As an


Figure 3.8.2

Four different methods of estimating the number of clusters present in a set of 23 powder patterns for the drug doxazosin. A total of five polymorphs are present, as well as two mixtures of these polymorphs. (a) A scree plot from the eigenvalue analysis of the correlation matrix; (b) the use of the C test (the coefficients have been multiplied by 100.0), which gives an estimate of five clusters using its local maximum. The γ test estimates that there are seven clusters and the CH test has a local maximum at seven clusters. Numerical details are given in Table 3.8.2.

indication of the differences that can be expected in the various algorithms used for dendrogram generation, Fig. 3.8.6(e) shows the same data analysed using the single-link method: the resulting clustering is slightly different: the similarity measures are larger, and, in consequence, the tie bars are higher on the graph. [For further examples see Barr *et al.* (2004b,c) and Barr, Dong, Gilmore & Faber (2004).]

3.8.3.2. Estimating the number of clusters

An estimate of the number of clusters present in the data set is needed. In terms of the dendrogram, this is equivalent to 'cutting the dendrogram' *i.e.* the placement of a horizontal line across it such that all the clusters as defined by tie lines above this line remain independent and unlinked. The estimation of the number of clusters is an unsolved problem in classification methods. It is easy to see why: the problem depends on how similar the patterns need to be in order to be classed as the same, and how much variability is allowed within a cluster. We use two approaches: (a) eigenvalue analysis of matrices ρ and \mathbf{A} , and (b) those based on cluster analysis.

Eigenvalue analysis is a well used technique: the eigenvalues of the relevant matrix are sorted in descending order and when a fixed percentage (typically 95%) of the data variability has been accounted for, the number of eigenvalues is selected. This is shown graphically *via* a scree plot, an example of which is shown in Fig. 3.8.2.