

Appendix A

Keynotes

A.1 Cluster Analysis Reader's Digest

Clustering methods have been and are still the object of applied and theoretical research in many different fields such as statistical pattern recognition, data mining, image processing, biomedical sciences, etc. It is not the aim of this section to present a complete overview of clustering techniques, but rather to provide enough information to justify why a particular technique may be preferred (there is no universal best clustering algorithm, and choices and compromises have to be made). A good review of clustering techniques by Jain *et al.*, from a statistical pattern recognition viewpoint, can be found in [93]. The main concepts can also be found in Duda and Hart [60], Hastie *et al.* [82] and Kaufman and Rousseeuw [96] textbooks.

Most of the clustering algorithms are either partitional, or hierarchical methods. While partitional methods produce a single partition, hierarchical methods produce a nested series of partitions. In this sense, they provide a totally different data description and should not be considered as two competing techniques. However, as shall be seen, because of their different nature, the corresponding strategies for cluster validity assessment may be quite different.

A.1.1 Partitional Clustering Methods

Let us denote by $\mathcal{T} = \{T_k, k \in \{1, \dots, M\}\}$ the data set where each pattern T_k is a D -dimensional feature vector, and by $d_T : \mathcal{T} \times \mathcal{T} \rightarrow \mathbb{R}^+$ the dissimilarity measure. Assuming for the moment that the partition size c is given, the goal of a partitional clustering algorithm is to identify the partition $\mathcal{P}(\mathcal{T}) = \{\mathcal{T}_1, \dots, \mathcal{T}_c\}$ on \mathcal{T} that optimizes a criterion function. Parametric methods as mixture decomposition will not be addressed here since there is no *a priori* knowledge on the underlying probability distribution. (In these methods, the data set is assumed to be drawn from a mixture of c underlying parametric distributions, and the goal is to determine

the involved parameters. The standard algorithm is the Expectation-Maximization algorithm [46].) Hence, since there are approximately $c^M/c!$ ways of partitioning a set of M elements into c subsets (a Stirling number of the second kind), optimizing the criterion function by exhaustive search is intractable and iterative optimization procedures are needed.

The simplest and most widely used family of criteria function is the one of related minimum variance criteria [60, 96]. The energy to be minimized here is

$$E = \frac{1}{2} \sum_{m=1}^c n_m \langle d_m \rangle,$$

where n_m is the number of points in the m -th cluster, and

$$\langle d_m \rangle = \frac{1}{n_m^2} \sum_{T_i \in \mathcal{T}_m} \sum_{T_j \in \mathcal{T}_m} d_T(T_i, T_j)$$

is the average dissimilarity measure between points in the m -th cluster. If \mathcal{T} was a subset of a vector space, and d_T was the squared Euclidean distance, the resulting criteria would be the sum of variances of each cluster,

$$\sum_{m=1}^c \sum_{T \in \mathcal{T}_m} \|T - \langle T_m \rangle\|_2^2, \text{ where } \langle T_m \rangle = \frac{1}{n_m} \sum_{T \in \mathcal{T}_m} T.$$

Strictly speaking, this criterion only makes sense when clusters are isotropic, multivariate normally distributed. Moreover, the solution is not invariant to linear transformations of the data. Many variations on this method exists, taking any Minkowski metric or the squared Mahalanobis distance instead of the squared Euclidean distance [93]. Notice however that all of these methods are based on the notions of medoid or centroid (barycenter) of a set of points and this does not make sense unless patterns live in a vector space.

Related minimum variance criteria suffer from the problem that partitions that split large clusters may be favored over ones that maintain the integrity of natural clusters [60]. When natural clusters have very different number of points, the partition minimizing this criteria may not reveal the intrinsic structure of the data. Another weakness of these methods is the lack of ability to extract a very dense cluster embedded in the center of a diffuse cluster. Besides, the partition solution has to be found by iterative optimization procedures. These iterative procedures are to be initialized by a reasonable initial partition and solution can be trapped in local minima [93].

Other popular criterion functions, also defined only when patterns live in Euclidean (or Hermitian) spaces, and closely related to the previous ones, can be derived based on the within cluster scatter matrix $W(\mathcal{P}(\mathcal{T}))$, and the between cluster scatter matrix $B(\mathcal{P}(\mathcal{T}))$ [60],

$$\begin{aligned}
W(\mathcal{P}(\mathcal{T})) &= \sum_{m=1}^c \sum_{T \in \mathcal{T}_m} (T - \langle T_m \rangle) \cdot (T - \langle T_m \rangle)^T, \\
B(\mathcal{P}(\mathcal{T})) &= \sum_{m=1}^c n_m (\langle T_m \rangle - \langle T \rangle) \cdot (\langle T_m \rangle - \langle T \rangle)^T, \\
S &= \sum_{m=1}^c (T - \langle T \rangle) \cdot (T - \langle T \rangle)^T = W(\mathcal{P}(\mathcal{T})) + B(\mathcal{P}(\mathcal{T})),
\end{aligned}$$

where $\langle T \rangle$ is the barycenter of all patterns in the data set, and S is the total scatter matrix, which is a constant given the data, independent on the partition. One can define optimal partitions as minimizers of $\text{tr}[W(\mathcal{P}(\mathcal{T}))]$ (or equivalently maximizers of $\text{tr}[B(\mathcal{P}(\mathcal{T}))]$). This turns out to be a minimum variance criterion. Another possibility is to minimize $\det[W(\mathcal{P}(\mathcal{T}))]$ whose solution is invariant to linear transformations of the data. In any case, combinatorial optimization is intractable and one has to consider iterative procedures.

A.1.2 Iterative Methods for Partitional Clustering

Most partitional methods are based on the definition of c elements from a pattern space called centroids, each defined to be a representative object of one of the clusters. The criterion function to be minimized is usually the sum of the average dissimilarities between each centroid and all of the other patterns of the same cluster. Typically, iterative methods begin by initialising a set of c centroids. Each pattern is then assigned to the cluster corresponding to its closest centroid (for the considered dissimilarity measure), and centroids are re-computed in order to minimize the criterion function. The iteration ends when centroids do not change. The computational efficiency of this approach depends on how easily centroids can be computed. The c -means algorithm [115] (also referred in the literature as k -means) runs typically in $O(M)$ [25]. Indeed in this algorithm the dissimilarity measure is the squared Euclidean distance and centroids are the clusters' barycenters, which can be easily computed using an update equation. A similar algorithm can be obtained by using the ℓ_1 -norm as dissimilarity measure. The centroids for this measure (which is more robust to outliers than the squared Euclidean distance) are the cluster medians.

When the dissimilarity measure does not lead to a closed form representation for the centroids, a method known as k -medoid which allows clustering with respect to any specified dissimilarity measure can be used [96]. In this method, centroids (the so-called medoids) are restricted to be patterns from the data set, and as before patterns are assigned to the cluster corresponding to its closest centroid. The goal is then to select, among all M patterns the c centroids which minimize the sum of the average dissimilarities between each centroid and all of the other patterns of the same cluster. A widely used implementation for the k -medoid method is the

Partitioning Around Medoids algorithm (PAM), by Kaufman and Rousseeuw [96]. PAM consists of two phases. In the first one, a method for selecting the initial set of c centrotypes or medoids is applied. The second phase is an iterative procedure where in each iteration the set of centrotypes is updated by analyzing all possible pairs of patterns such that one pattern is a centrotype and the other is not, and by swapping the pair which most reduces the value of the criterion function. The cost of a single iteration is $O(c(M - c)^2)$.

A.1.3 Hierarchical Clustering Methods

While partitional clustering algorithms construct a single partition with c clusters (a flat description), hierarchical methods deliver a recursive structure. Since they represent data in different ways, partitional and hierarchical methods do not really compete with one another. Indeed, when data is to be described in terms of classes, subclasses, sub-subclasses (e.g. a biological taxonomy), flat representations do not make sense and hierarchical methods are needed. There are, of course, many applications in which data is not inherently hierarchical, and one has to make a choice among clustering methods from both types. Hierarchical methods are more versatile than partitional methods and can deal with many differently shaped clusters, but generally they are more time consuming.

Depending on the direction they build the hierarchy, these clustering methods can be agglomerative (bottom-up) or divisive (top-down). The former, which are usually computationally simpler, start with each single point as a cluster, and iteratively merge the closest pair of clusters in the sense of a chosen dissimilarity measure. The generic algorithm is as follows [93].

1. Initialization: compute the proximity matrix (the matrix containing the dissimilarity between each pair of patterns).
2. Find the most similar pair of clusters using the proximity matrix. Merge these two clusters.
3. Update the proximity matrix according to this merging.
4. Repeat steps 2 and 3 until all patterns are in one cluster.

At each iteration step, two clusters are merged. The procedure builds up a tree or dendrogram, where leaves are the M elements of \mathcal{T} (step 1). At level l , this tree has $M - l$ nodes, each node being a cluster. At level $l + 1$, the closest clusters from level l are merged (step 2). By closest, we mean the pair \mathcal{T}_i and \mathcal{T}_j minimizing a given distance or proximity measure $\delta(\mathcal{T}_i, \mathcal{T}_j)$ between clusters. Different strategies for updating the proximity matrix lead to different hierarchical clustering methods. (Moreover, since all of these algorithms are merging methods, they admit a variational formulation and can be solved as an energy minimization problem; see [137], Chap. 3.) Lance and Williams [103] define a class of methods by specifying a generalized recurrence formula for updating the proximity matrix:

$$\delta(\mathcal{T}_i \cup \mathcal{T}_j, \mathcal{T}_k) = \alpha_i \delta(\mathcal{T}_i, \mathcal{T}_k) + \alpha_j \delta(\mathcal{T}_j, \mathcal{T}_k) + \beta \delta(\mathcal{T}_i, \mathcal{T}_j) + \gamma |\delta(\mathcal{T}_i, \mathcal{T}_k) - \delta(\mathcal{T}_j, \mathcal{T}_k)|,$$

where parameter values α_i , α_j , β and γ characterize the particular clustering method. Below we describe the most popular ones.

- Choosing $\alpha_i = \alpha_j = 1/2$, $\beta = 0$ and $\gamma = -1/2$, leads to the following distance between clusters:

$$\delta_{min}(\mathcal{T}_p, \mathcal{T}_q) = \min_{T_i \in \mathcal{T}_p, T_j \in \mathcal{T}_q} d_T(T_i, T_j).$$

The corresponding algorithm is known as *single-linkage algorithm* [93, 60]. Here the nearest-neighbor points determine the nearest subsets. If elements in \mathcal{T} are viewed as nodes of a graph, merging \mathcal{T}_p and \mathcal{T}_q corresponds to adding an edge between the nearest points in \mathcal{T}_p and \mathcal{T}_q . This procedure generates a tree, and if one lets the procedure evolve up to having a single cluster containing all points, the result is a *minimal spanning tree*.

- Taking $\alpha_i = \alpha_j = \gamma = 1/2$, $\beta = 0$, yields

$$\delta_{max}(\mathcal{T}_p, \mathcal{T}_q) = \max_{T_i \in \mathcal{T}_p, T_j \in \mathcal{T}_q} d_T(T_i, T_j).$$

The resulting algorithm is called *complete-linkage algorithm* [93, 60]. Here distance between two clusters is given by the farthest pair of points in the two clusters. This procedure produces a graph in which edges connect all of the nodes in a cluster. When the nearest clusters are merged, edges between every pair of nodes in the two clusters are added. If the diameter of a partition is defined as the largest diameter for clusters in the partition, then each iteration of the complete-linkage algorithm increases the diameter of the partition as little as possible.

- Taking $\alpha_i = n_i/(n_i + n_j)$, $\alpha_j = n_j/(n_i + n_j)$, and $\beta = \gamma = 0$, leads to a group averaging method, where

$$\delta_{avg}(\mathcal{T}_p, \mathcal{T}_q) = \frac{1}{n_p n_q} \sum_{T_i \in \mathcal{T}_p} \sum_{T_j \in \mathcal{T}_q} d_T(T_i, T_j).$$

- Some clustering methods based on barycenters, such as Ward's minimum variance method [176], can also be represented in terms of Lance and Williams formula. For Ward's method, $\alpha_i = (n_i + n_k)/(n_i + n_j + n_k)$, $\alpha_j = (n_j + n_k)/(n_i + n_j + n_k)$, $\beta = -n_k/(n_i + n_j + n_k)$, $\gamma = 0$, and the corresponding cluster proximity measure is

$$\delta_{ward}(\mathcal{T}_p, \mathcal{T}_q) = \frac{n_p n_q}{n_p + n_q} \|\langle T_p \rangle - \langle T_q \rangle\|_2^2,$$

where $\langle T_p \rangle$ and $\langle T_q \rangle$ denote the barycenters of \mathcal{T}_p and \mathcal{T}_q respectively.

Time and memory complexity of the algorithms given by the Lance and Williams formula are studied in [44]. Overall, the time required for hierarchical clustering is $O(M^2 \log M)$, and the memory complexity is $O(M^2)$.

In practice, if clusters are compact and well separated, all methods yield the same results. However, when this is not the case, the resulting partitions may be quite different. Depending on the cluster proximity measure, different methods of clustering can be more or less successful with different types of clusters. Single-linkage algorithms suffer from the chaining effect: A single corrupted point somewhere in between two compact clusters can lead to an unwanted merging between them [93, 60]. However, this property is very useful if one wants to detect elongated clusters.

The complete-linkage algorithm tends to produce compact clusters with small diameters. However, patterns assigned to a cluster can be much closer to patterns in other clusters [82, 60].

The single-linkage and the complete-linkage algorithms are both sensitive to outliers since they rely on extremal measures. One way to reduce the influence of outliers is using δ_{avg} as cluster proximity measure though the improvement is often not good enough. Besides, average methods have another drawback compared to single or complete linkage methods: they are not invariant under monotone transformations on the dissimilarity measure d_T (invariance of the former ones is a consequence of being based on extremal values) [82].

To end this section, let us make a few general remarks. In Sect. A.1.1, one of the main assumptions is that the number of clusters c was given, for partitional clustering algorithms. Then, the goal was to find the c -partition on the data optimizing a global criterion (in practice iterative methods are used and the convergence to a global minimum is not ensured). Agglomerative hierarchical clustering methods perform well in making local decisions about cluster merging since they make use of the proximity matrix. As the hierarchy is built by means of local optimization, the level corresponding to a c -partition will not correspond in general to a global optimum (unless clusters are compact and well separated). For instance, Ward's method will not lead to the same c -partition as a c -means method, despite the fact that both attempt to minimize variance. In this sense, one would rather say that partitional methods are better than hierarchical methods. But how to be sure that there are exactly c groups of patterns in the data? Is the criterion function well adapted to the shape of clusters that are present in the data? From this viewpoint, hierarchical clustering may be more appealing than partitional ones. Another argument in favor of hierarchical clustering methods is their versatility and their ability to cope with differently shaped clusters. For instance, the single linkage algorithm can deal with non-isotropic, elongated or concentric clusters while partitional methods like c -means can only deal with isotropic clusters. Since their outputs are nested series of partitions, ranging from M clusters to one single cluster, one can imagine methods to determine the number of clusters as stopping rules in the merging process. If stopping rules are correctly designed, hierarchical methods would also be able to detect clusters having different densities or different number of points.

A.1.4 Cluster Validity Analysis and Stopping Rules

The great variety of clustering methods that have been proposed in the recent past has been followed by an increasing interest in clustering validation methods. In [73], a comprehensive study of these techniques is presented.

Cluster validity analysis deals with assessing the validity of classifications obtained from the application of clustering procedures. There are different validation approaches [58, 73] depending on the amount of prior information on the data. This section deals with *internal validation tests*, which consist in determining if the structure is intrinsically adapted to the data. In other words, internal tests are derived from some *internal criteria* measuring the suitability of the clustering structure for the original data set with no other information than the data themselves.

Classical issues in cluster validity analysis are the assessment of individual cluster validity and the assessment of a whole partition. (In some applications validity of a dendrogram also needs to be assessed. This problem is not addressed here.) These two issues are briefly summarized next.

A.1.4.1 Partition Validity Assessment

A relevant question to address in order to assess the validity of a partition, is deriving the number of clusters [58], denoted by c . Notice that by solving this problem, it cannot be ensured that the c clusters are valid clusters. The most common approach to decide how many clusters are best consists in finding partitions for $c = 1, \dots, c_{max}$ and optimizing a measure $G(c)$ of partition adequacy, which is usually based on the within-cluster and between-cluster variability. When applied to hierarchical clustering methods these cluster validity assessment techniques are known as *global stopping rules* because the choice of c can be seen as stopping the merging process (in the agglomerative case) at a certain level of the dendrogram.

When dealing with hierarchical classifications, another approach to determine the most appropriate number of clusters are *local stopping rules*. In the agglomerative case, these rules are *merging criteria* to decide whether two clusters should be merged. Usually, the merging process is continued until it is decided, for the first time, that two clusters should not be aggregated.

Milligan and Cooper [125], and Dubes [58], present comparative studies of some stopping rules. Milligan and Cooper's paper provides a particularly comprehensive Monte-Carlo evaluation of these rules, by comparing thirty local and global stopping rules. In their simulation experiment, only strongly clustered data sets (internally cohesive and well separated clusters) were considered. Hence, since clustering this kind of data should not be a challenging problem, techniques that do not perform well on it are also expected to be inefficient when dealing with any data set. The main conclusion of this experiment is that only five or maybe six of the compared rules perform quite well on strongly clustered data. One can also observe that the majority of the stopping rules described in the study are based on heuristics and lack of theoretical foundation. Those derived from rigorous statistical techniques, assume

in general hypotheses on the data which are unrealistic in most real applications (e.g. multivariate normal distribution for the patterns). In order to briefly illustrate the considered stopping rules, it is worth describing Calinski and Harabasz's index [26] and Duda and Hart's rule [60], since these methods provided the best results.

- Calinski and Harabasz propose a *global stopping rule* for assessing partitions, by choosing the partition size c that maximizes the index

$$G(c) = \frac{\frac{1}{c-1} \text{tr} [B(\mathcal{P}(T))]}{\frac{1}{M-c} \text{tr} [W(\mathcal{P}(T))]},$$

where $B(\mathcal{P}(T))$ and $W(\mathcal{P}(T))$ are respectively the between- and within-cluster scatter matrices of a c -partition \mathcal{P} , defined in section A.1.1. The index $G(c)$ is the ratio between the total within-cluster sum of squared distances about the centroids, and the total between-cluster sum of squared distances. This index is only defined for sets of patterns living in an Euclidean space. Moreover, since the index is based on the sum of squares criterion, it has a tendency to partition the data into hyperspherical shaped clusters, having roughly equal numbers of patterns [73] (this is probably the main reason for its first position in Milligan and Cooper's ranking, since their data was strongly clustered, and clusters contained almost the same numbers of points and were pretty isotropic).

- Duda and Hart proposed the $Je(2)/Je(1)$ *local stopping rule* for deciding whether or not a cluster should be split into two subclusters. The rule consists in computing the ratio between the total within sum of squared distances about the centroids of the two clusters for the two-cluster solution ($Je(2)$), and the within sum of squared distances about the centroid when only one cluster is present ($Je(1)$). The method considers a null hypothesis, assuming that all patterns come from a normal distribution, whose mean and variances are empirically estimated over the whole data set. The null hypothesis of one single cluster is rejected if $Je(2)/Je(1)$ is smaller than a specified critical value, fixed by a significance level for the hypothesis testing. While considering a normal distribution as a null hypothesis and using the sum of squared distances may not be well adapted to real clustering problems (particularly when the number of patterns in the data set is not as large to be well represented by an asymptotic distribution), the proposed *a contrario* formulation is appealing from our point of view.

To finish the discussion on partition validity assessment we quote one of Bock's conclusions from his work on significance tests in cluster analysis [24], where a comparison between global and local methods is made.

Some care is needed when applying any test for clustering, bearing in mind that different types of clusters may be present simultaneously in the data, and that the number of clusters is, in some sense, dependent on the intended level of information compression. Thus, a global application of a cluster test to a large or high-dimensional data set will not be advisable in most cases. However, a local application (...) to a specific part of the data will often be useful for providing evidence for or against a prospective clustering tendency.

A.1.4.2 Validity Assessment of Individual Clusters

The problem is now to decide, among the candidate clusters furnished by the clustering procedure, which ones correspond to natural clusters. But what does a natural cluster look like? As pointed out by Gordon [73], it may be difficult to specify a relevant definition of an ideal cluster for a particular data set. However, clusters must reveal structure in the data and can be detected as opposed to a complete absence of structure. Thus, in order to decide whether the candidate clusters are significant, they can be compared to some appropriate random distribution. This leads to a general methodology for cluster validity analysis based on the statistical approach of hypothesis testing [24, 72, 73]. Following Bock [24], this framework consists of these stages:

1. Design a null hypothesis \mathcal{H} for the absence of class structure in the data (a *background model*, or *null model*), meaning that patterns are sampled from a homogeneous population. Then, heterogeneity or clustering structure are involved in the alternative hypothesis \mathcal{A} .
2. Define a test statistic, which will be used as a validity index to discriminate between \mathcal{H} and \mathcal{A} .
3. If, for a given significance level (error probability) α , the test statistic of the observed data exceeds the corresponding critical value c_α , the null hypothesis \mathcal{H} is rejected, in favor of \mathcal{A} .

This general framework can be adapted for assessing the validity of individual clusters. A general approach within this framework is the Monte-Carlo validation, which is described in [73]. Assume one wants to assess the validity of an observed cluster \mathcal{T}_i having n patterns in a data set having M patterns. In the Monte-Carlo validation method, data sets of M patterns are simulated under the background model, and classified using the same clustering procedure that was used to classify the original data. The test statistic is computed for those clusters having n patterns, and the distribution of the test statistic is estimated. Then, using the value of the test statistic of \mathcal{T}_i , one can compute the significance level of rejecting \mathcal{H} . Two popular test statistics are the maximum F test and the U statistic (see Bock [24] and Gordon [73]).

Appropriate null models for data are the subject of the study presented in [72]. These models, which specify the distribution of patterns in the absence of structure in the data, can be of two types.

- *Standard (data-independent) null models.* Two well known standard null models are the *Poisson model* and the *Unimodal model* [24]. The main problem with the Poisson model is the choice of the region R within which patterns are uniformly distributed (standard choices for normalized data are the unit hypercube and the unit hypersphere). The Unimodal model assumes that the joint distribution of the variables describing the patterns is unimodal, but the choice of the distribution may not be easy.
- *Data-influenced null models.* Here the data is used to influence the specification of the null model. Examples of these null models are the Poisson model where R is chosen to be the convex hull of the data set, or the *Ellipsoidal model*, which is

a multivariate normal distribution, whose mean and covariance matrix are given by the data set.

In [72], Gordon concludes that the results of the tests depend considerably on the choice of the null model and that in general the results based on data-influenced null models are more relevant than those obtained using a standard null model.

A.2 Three classical methods for object detection based on spatial coherence

This section addresses some issues of the generalized Hough transform [14], whose variations are probably the most widely used techniques in object detection. Two frequently used techniques for robust transformation estimation will also be described: geometric hashing[102, 184] and the RANSAC algorithm [64].

A.2.1 The Generalized Hough Transform

In [14] Ballard proposed a generalization of the Hough transform [85] allowing the detection of arbitrary planar shapes undergoing similarity transformations. Most object detection and recognition systems using transformations clustering are based on the generalized Hough transform. The basic idea is to quantize the transformation space into D -dimensional cells. Each transformation point T_i is quantized and then votes for one of these cells. In practice, noise and image quantization induce localization errors in the extracted features and one has to take into account uncertainty in computing T_i . Thus, each pairing of model and image features defines a volume of possible transformations, so it should cast a vote into each cell intersecting this volume (see [75] for an error analysis when using line segments as features).

As with all techniques based on histograms in multidimensional spaces, the generalized Hough method is very sensitive to the choice of quantization precision (this remark also holds for Lamdan and Wolfson's Geometric Hashing [184, 102] described in Sect. A.2). Most of the time, the cell size is chosen by problem specific *ad hoc* arguments (see [113] for an example). However, in the general case, quantization effects may lead to several problems:

- Similar transformation points may vote for different cells. In order to reduce this problem, either votes are counted by adding the votes of neighboring cells (using a sliding window) in the case of no uncertainty in T_i , or, when uncertainty is considered, a vote is cast into each cell intersecting the uncertainty volume.
- In the plane similarity case, for instance, if one wants to do a fine discretization of the 4-D transformation space in order to perform accurate detection, the search space is too large for an exhaustive search. Coarse to fine techniques applied to transformation clustering, first introduced by Stockman [169], can deal with this complexity problem, but there is no reason why the most voted cells at the finer scale should correspond to the most voted ones at coarser scales.
- From the detection viewpoint, the size of the cells is also crucial. Indeed, if quantization is too fine, cells will not have enough votes and correct instances will be missed (false negatives). On the other hand, choosing a very coarse quantization increases the likelihood of large clusters occurring at random (false positives).

These remarks partially motivate our decision to use the clustering techniques described in Chap. 7, along with the validity assessment method proposed in the same

chapter. Indeed, the proposed methodology does not suffer from quantization problems.

The generalized Hough transform is with geometric hashing [102, 182, 184], and the alignment method [89] one of the most popular voting schemes. Given two shapes, the geometric hashing method aims at determining if there is a transformed subset of the features from one shape that matches a subset of the features of the other one. The alignment method is a similar voting method. The generalized Hough transform method, instead of voting over all possible configurations of shapes, consists in voting over all possible transformations mapping a shape to another one. As for all techniques based on histograms in multidimensional spaces, these voting methods are very sensitive to the choice of quantization precision (too large bins may lead to false matches, and too small bins may produce misses). Besides, most of the time, the size of the hash table and the amount of parameters (the size of the bins in the voting stage, the threshold for the amount of votes in each bin, *etc.*) are crippling. The complexity of these voting schemes increases with the invariance degree; affine invariant shape retrieval in large databases is intractable. All these properties make the local features not suitable for shape retrieval in large databases.

A.2.2 Geometric Hashing

In order to illustrate the geometric hashing algorithm, we present the case of similarity or affine transformations.

A query shape \mathcal{S} is searched in a set of shapes.

Preprocessing (off line). For each shape \mathcal{S}'_i in the set of shapes:

1. Extract local invariant features from \mathcal{S}'_i . Assume n such features are found.
2. For each local basis b_j (e.g. a pair of points for similarity transformations, three non-collinear points for affine transformations) of features:
 - a. Compute the quantized coordinates (u, v) of all the remaining features, in the local basis.
 - b. Use the couple (u, v) as an index in a hash table, and write the information (i, b_j) in the corresponding bin (i is the index that identifies \mathcal{S}'_i).

Recognition stage (on line). For the query shape \mathcal{S} :

1. Extract local invariant features from \mathcal{S} . Assume n such features are found.
2. Choose arbitrarily a local basis (two or three points, depending on the considered invariance).
3. Compute the quantized coordinates (u, v) of all the remaining features, in the local basis.
4. For each of these coordinates, go to the corresponding bin in the hash table, and cast a vote for each pair (i, b_j) inscribed in the bin.

5. Keep only the pairs (i, b_j) which received more than a certain number of votes. Each of these pairs stands for a potential match.
6. For each potential match, compute the best transformation (in the least squares sense) between all corresponding features, and check if the query features and the features from the corresponding shape are well aligned. If not, go to (2) and choose another basis.

For affine invariant shape recognition, time complexity for the preprocessing stage is $O(n^4)$ for each shape in the set of shapes. If the access time to the hash table is $O(1)$, time complexity for the recognition stage is between $O(m)$ (when the first query basis chosen at random corresponds to a model in the set of shapes) and $O(m^4)$ (when no basis from the query shape corresponds to a model in the set of shapes).

A.2.3 A RANSAC-based Approach

The RANDOM SAMPLE CONSENSUS (RANSAC) algorithm by Fischler and Bolles [64], is certainly one of the most popular robust estimators in computer vision. It has proved very successful in stereo vision tasks, such as estimating homographies and fundamental matrices [81]. The main reason for its success is its ability to deal with large proportions of outliers. Roughly speaking, in its general form, the RANSAC procedure to fit a model consists in randomly selecting a minimal subset of the data (*i.e.* a subset allowing to instantiate the model), then computing the number of inliers consistent with the instantiated model. These two steps are repeated for N minimal subsets of the data. The model having the largest number of inliers is chosen and refined by re-estimating it from the corresponding set of inliers.

Our framework deals with M meaningful matches, and usually M is small enough to test for all corresponding similarity or affine transformations. Hence, using the same ideas, an elementary algorithm would be as follows:

1. For each element in the set of M pairs of local frames corresponding to meaningful matches:
 - a. Compute the associated transformation T ;
 - b. Apply T to all query local frames, and compute their distances to their corresponding scene local frames;
 - c. Compute the number of inliers consistent with T , *i.e.* the pairs for which the distance is less than d pixels;
2. Choose the transformation T having the largest number of inliers;
3. Re-estimate T for all pairs of local frames determined as inliers (with a least squares method, for instance).

One can iterate this procedure on the set of outliers in order to find other (less dominant) transformations.

Even for this simple version of the algorithm, two problems arise: the choice of the distance threshold d , and the minimum number of inliers a model should have in order to be valid. The distance threshold d is usually chosen empirically. Otherwise, it can be chosen by considering a significance level α , corresponding to the probability that a point is an inlier [81], which requires hypothesizing a model for the distribution of distances. Concerning the minimum number of inliers to assess model validity, generally it is also fixed by means of arbitrary rules. It seems reasonable to us that this minimum number of inliers depends on the distance threshold, but as far as we know no effort has been done to establish this relation.

A.3 On the Negative Association of Multinomial Distributions

This section presents the notion of *negative association* (a strong notion of negative dependence) and summarizes some relevant consequences first reported by Joag-Dev and Proschan in [94]. Some proofs are also completed when they were just outlined in the original paper. The result is then applied to multinomial distributions.

Definition 20 (Negative association). A set $\mathcal{X} = \{X_1, \dots, X_n\}$ of real random variables is said to be negatively associated (NA) if for every two disjoint index sets $I, J \subset \{1, \dots, n\}$,

$$\mathbb{E}[f(X_i, i \in I)g(X_j, j \in J)] \leq \mathbb{E}[f(X_i, i \in I)] \cdot \mathbb{E}[g(X_j, j \in J)],$$

for all non-decreasing functions $f : \mathbb{R}^{\#I} \rightarrow \mathbb{R}$, $g : \mathbb{R}^{\#J} \rightarrow \mathbb{R}$ (a function $h : \mathbb{R}^k \rightarrow \mathbb{R}$ is said to be non-decreasing if $h(x_1, \dots, x_k) \geq h(y_1, \dots, y_k)$ whenever $x_1 \leq y_1, \dots, x_k \leq y_k$).

Remark 7. Negative association is a natural generalization of negative correlation.

The negatively associated set $\mathcal{X} = \{X_1, \dots, X_n\}$ verifies the following properties:

Property 1. For any non-decreasing functions $f_i, i \in \{1, \dots, n\}$,

$$\mathbb{E}\left[\prod_{i=1}^n f_i(X_i)\right] \leq \prod_{i=1}^n \mathbb{E}[f_i(X_i)].$$

Proof. Define $f(x_1, \dots, x_{n-1}) = \prod_{i=1}^{n-1} f_i(x_i)$ and $g(x_n) = f_n(x_n)$ for all $(x_1, \dots, x_n) \in \mathbb{R}^n$. Since f and g are both non-decreasing, it follows from Definition 20 that

$$\mathbb{E}\left[\prod_{i=1}^n f_i(X_i)\right] \leq \mathbb{E}\left[\prod_{i=1}^{n-1} f_i(X_i)\right] \mathbb{E}[f_n(X_n)].$$

Using induction yields the desired result. \square

Property 2. For all $(x_1, \dots, x_n) \in \mathbb{R}^n$,

$$\Pr(X_i \geq x_i \forall i \in \{1, \dots, n\}) \leq \prod_{i=1}^n \Pr(X_i \geq x_i).$$

This follows immediately from Property 1 for $f_i(x) = \chi_{[x \geq x_i]}$, the indicator function of event $[x \geq x_i]$. The following property is obvious from Definition 20:

Property 3. Non-decreasing functions defined on disjoint subsets of a set of NA random variables are NA.

Property 4. The union of independent sets of NA random variables is NA.

Proof. Let \mathbf{X} and \mathbf{Y} be independent vectors such that for each one its components are sets of NA random variables. Let $(\mathbf{X}_1, \mathbf{X}_2)$ and $(\mathbf{Y}_1, \mathbf{Y}_2)$ denote arbitrary partitions of \mathbf{X} and \mathbf{Y} respectively. Hence, the vector (\mathbf{X}, \mathbf{Y}) is NA if and only if $\mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)] \leq \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)] \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)]$. Now,

$$\begin{aligned} \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)] &= \mathbb{E}\{\mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1, \mathbf{Y}_2]\} \\ &= \sum_{(y_1, y_2)} \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2] \\ &\quad \cdot \Pr(\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2). \end{aligned}$$

Since $(\mathbf{X}_1, \mathbf{X}_2)$ and $(\mathbf{Y}_1, \mathbf{Y}_2)$ are independent, $\{f(\mathbf{X}_1, \mathbf{Y}_1)|\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2\}$ and $\{g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2\}$ are parametric functions of random vectors \mathbf{X}_1 and \mathbf{X}_2 respectively. Thus, because of the negative association of \mathbf{X} ,

$$\begin{aligned} \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2] &\leq \\ \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)|\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2] \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1 = y_1, \mathbf{Y}_2 = y_2]. \end{aligned}$$

Hence,

$$\mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)] \leq \mathbb{E}\{\mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)|\mathbf{Y}_1, \mathbf{Y}_2] \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1, \mathbf{Y}_2]\}$$

Now, since the conditional expectations

$$\mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)|\mathbf{Y}_1, \mathbf{Y}_2] \text{ and } \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1, \mathbf{Y}_2]$$

are respectively \mathbf{Y}_1 and \mathbf{Y}_2 measurable functions, it follows that

$$\begin{aligned} h_1(\mathbf{Y}_1) &\equiv \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)|\mathbf{Y}_1, \mathbf{Y}_2] = \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)|\mathbf{Y}_1], \\ h_2(\mathbf{Y}_2) &\equiv \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_1, \mathbf{Y}_2] = \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)|\mathbf{Y}_2]. \end{aligned}$$

Finally, using that \mathbf{Y} is NA,

$$\begin{aligned} \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)g(\mathbf{X}_2, \mathbf{Y}_2)] &\leq \mathbb{E}[h_1(\mathbf{Y}_1)h_2(\mathbf{Y}_2)] \\ &\leq \mathbb{E}[h_1(\mathbf{Y}_1)] \mathbb{E}[h_2(\mathbf{Y}_2)] \\ &= \mathbb{E}[f(\mathbf{X}_1, \mathbf{Y}_1)] \mathbb{E}[g(\mathbf{X}_2, \mathbf{Y}_2)]. \quad \square \end{aligned}$$

These results yield the following proposition.

Proposition 14. A random vector $\mathbf{X} = (X_1, \dots, X_n)$ having a multinomial distribution of index M and parameter $\mathbf{p} = (p_1, \dots, p_n)$ (denoted by $\mathbf{X} \sim \text{Mult}(M, \mathbf{p})$), is NA.

Proof. The variable \mathbf{X} can be decomposed as

$$\mathbf{X} = \sum_{k=1}^M \mathbf{Y}_k,$$

where each $\mathbf{Y}_k \sim Mult(1, \mathbf{p})$, and the \mathbf{Y}_k 's are mutually independent. Since, for all $k \in \{1, \dots, M\}$, all elements in \mathbf{Y}_k are zero except for one whose value is 1, vector \mathbf{Y}_k is NA. Indeed, for all I, J disjoint subsets of $\{1, \dots, n\}$, for all non-decreasing functions $f : \mathbb{R}^{\#I} \rightarrow \mathbb{R}, g : \mathbb{R}^{\#J} \rightarrow \mathbb{R}$,

$$\begin{aligned} \mathbb{E}[f(\mathbf{Y}_{k,i}, i \in I)g(\mathbf{Y}_{k,j}, j \in J)] &\leq \mathbb{E}[f(\mathbf{Y}_{k,i}, i \in I)] \cdot \mathbb{E}[g(\mathbf{Y}_{k,j}, j \in J)] \\ &\Leftrightarrow \mathbb{E}[(f(\mathbf{Y}_{k,i}, i \in I) - f(0, \dots, 0))(g(\mathbf{Y}_{k,j}, j \in J) - g(0, \dots, 0))] \\ &\leq \mathbb{E}[f(\mathbf{Y}_{k,i}, i \in I) - f(0, \dots, 0)] \cdot \mathbb{E}[g(\mathbf{Y}_{k,j}, j \in J) - g(0, \dots, 0)]. \end{aligned}$$

The last inequality is true: the right member is non-negative because $f(\mathbf{Y}_{k,i}, i \in I) - f(0, \dots, 0)$ and $g(\mathbf{Y}_{k,j}, j \in J) - g(0, \dots, 0)$ are non-negative, and the left member is zero since $(f(\mathbf{Y}_{k,i}, i \in I) - f(0, \dots, 0))$ and $(g(\mathbf{Y}_{k,j}, j \in J) - g(0, \dots, 0))$ cannot be non-zero at the same time.

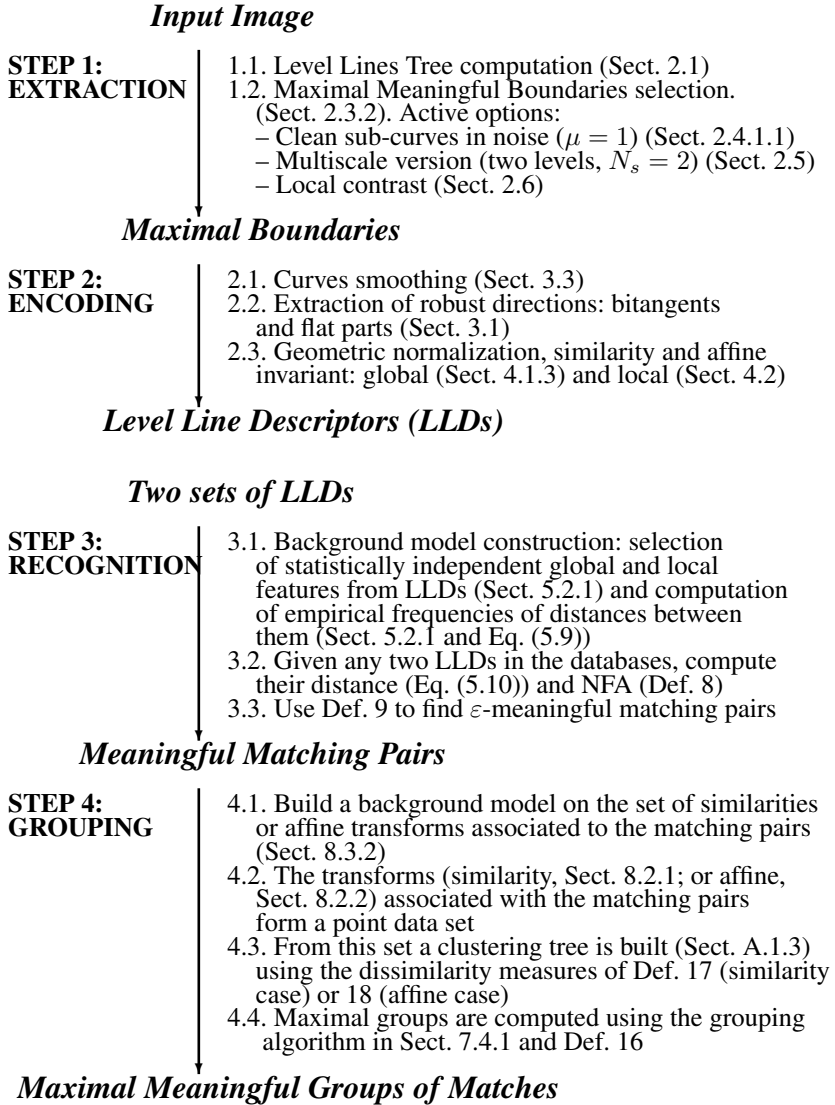
Then, using Property 4, it follows that $\{\mathbf{Y}_1, \dots, \mathbf{Y}_M\}$ is NA. Finally, for all $l \in \{1, \dots, n\}$, $X_l = \sum_{k=1}^M \mathbf{Y}_{k,l}$ are non-decreasing functions defined on disjoint subsets of $\{\mathbf{Y}_1, \dots, \mathbf{Y}_M\}$. This proves that \mathbf{X} is NA (Property 3). \square

Remark 8. Applying Property A.3 to the random vector \mathbf{X} proves Lem. 7, stated in Sect. 7.3.

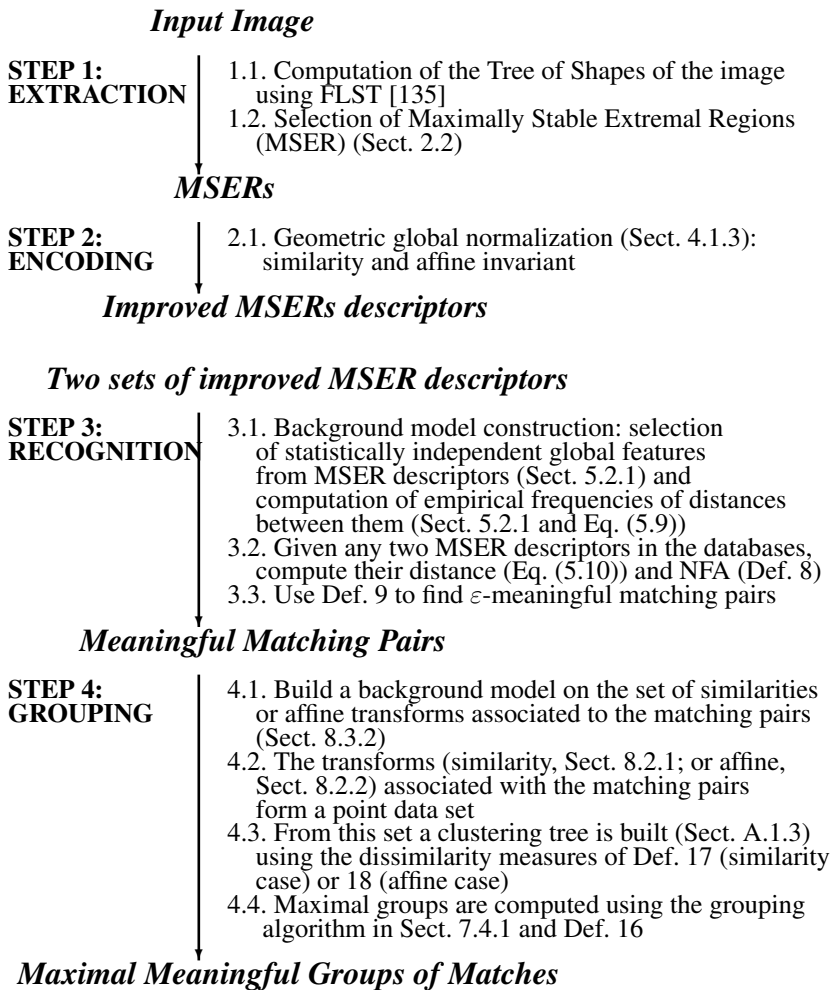
Appendix B

Algorithms

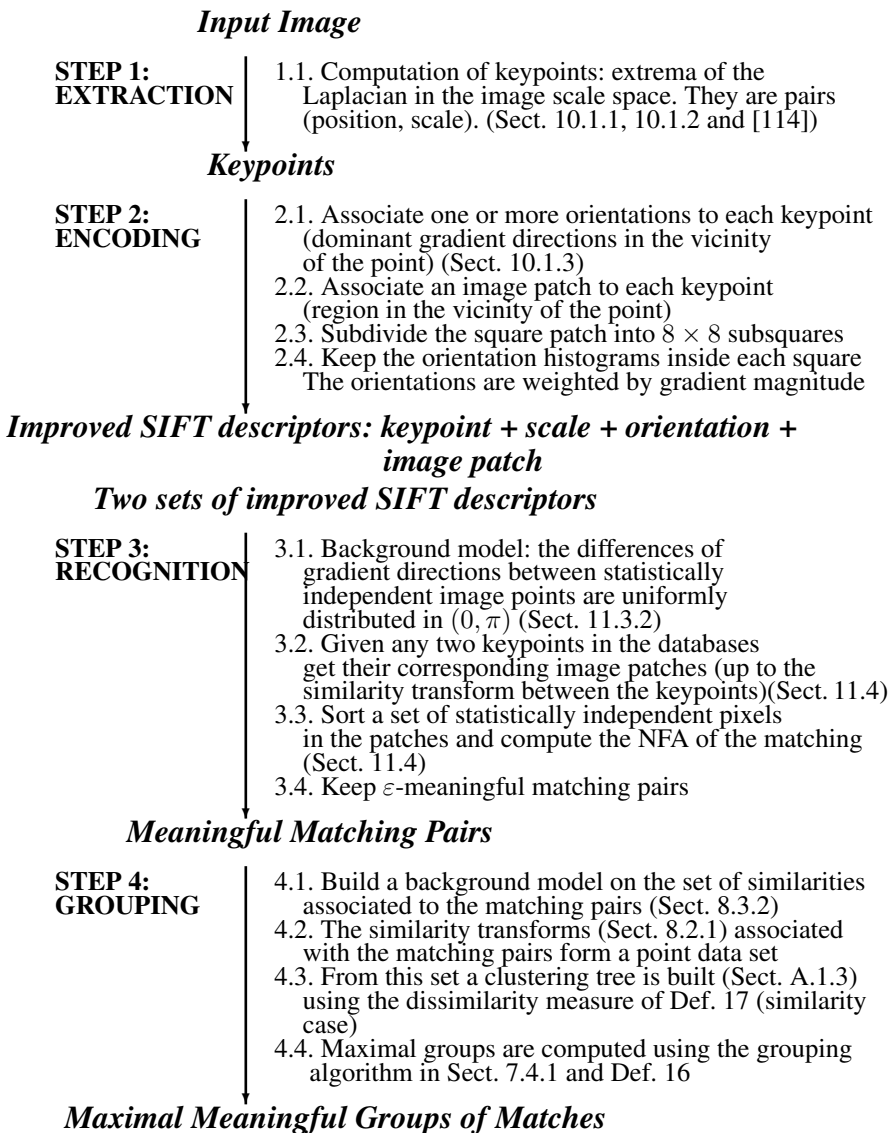
B.1 LLD Method Summary



B.2 Improved MSER Method Summary



B.3 Improved SIFT Method Summary



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