1 Introduction

Clustering is an important combinatorical optimization problem that must often be solved as a part of more complicated tasks in pattern recognition, image analysis and other fields of science and engineering [JD88, KR90, E92, GG92]. Clustering is also needed for designing a codebook in vector quantization. The clustering problem contains two subproblems: *determining the number* of clusters and *finding the location* of clusters.

The process of solving a pattern recognition problem (see Figure 1.1) typically involves the following steps [JD88, JMF99]:

(1) Pattern representation (including feature extraction and/or selection).

(2) Definition of a pattern proximity measure appropriate to the data [A73, DS76, MS83, JD88].

(3) Clustering or grouping.

(4) Data abstraction (if needed) [DS76].

(5) Assessment of output (if needed) [D87, D93, C95b, K01].

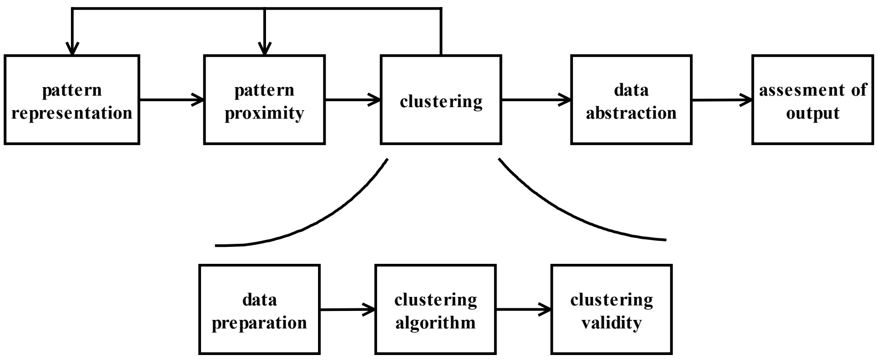


Figure 1.1. The steps of cluster analysis for pattern recognition.

The preprocessing of data objects improves the efficiency and the outcome of the clustering algorithm. With appropriate preprocessing, larger data sets can be clustered and, in addition, better clustering results can be achieved during the actual clustering. Although most of the preprocessing methods are designed to aid in the manipulation of the clusters, unsupervised learning may also focus on *description* tasks [T99]. The preprocessing of data (data preparation) can be considered as a separate task that takes place before actual clustering. It is common that a data set includes unnecessary features (noise and outliers) and asymmetrically scaled features [MS03]. If a data set is not properly preprocessed, it can be assumed that the outcome of clustering is suboptimal. Some preprocessing methods are:

(1) Indexing of the data [B75, FBF77, B80, B90, S91, Y93, NN97, B02, BM02] for nearest neighbor search.

(2) Projecting the data [FBS75, GK92, RK93, LC94, LC95a, BJS97, **P1**] for a nearest neighbor search.

(3) Using an *approximating and eliminating search algorithm* (*AESA*) [V86, MOV94, V94, V95, RP00].

(4) Scaling and weighting of the data [MS03].

(5) Selecting the features [GM86, F87, ZRL97, T99, T00, DCSL02].

(6) Using heuristic clustering to get an initial partition [S80, JD88].

(7) Filtering noise and outliers [BCQY97, RRS00, WC04].

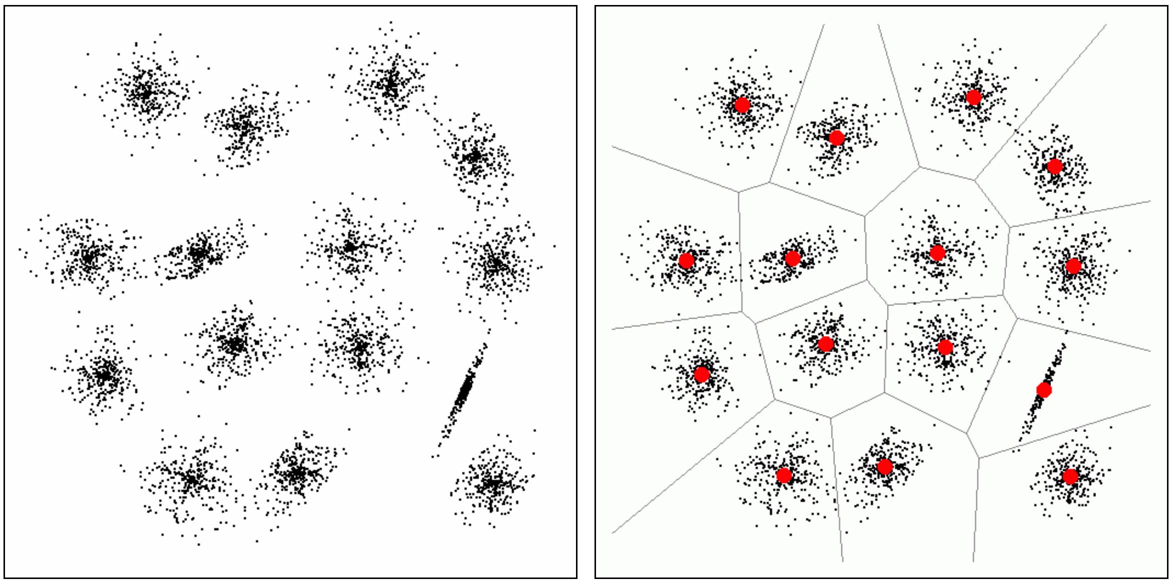


Figure 1.2. An example of clustering. On the left, a sample data set is shown. On the right, a clustering of the data set with 15 clusters and their centroids is shown.

Clustering entails partitioning a data set so that similar objects are grouped together and dissimilar objects are placed in separate groups; see Figure 1.2 for an example. The dots represent two-dimensional data points in Euclidean space. The 5000 data objects have been divided into 15 clusters separated by straight lines in the figure. The data objects separated by straight lines form a *partition* of the data. Centroids of the partition are represented by large dots.

Formally, the clustering problem is defined as follows: Given a set of N data vectors $X=\{x_1, x_2, \ldots, x_N\}$ in a K-dimensional space, clustering aims at solving the partition $P=\{p_1, p_2, \ldots, p_N\}$, which defines for each data vector the index of the cluster where it is assigned to. Cluster s_a is defined as the set of data vectors that belong to the same partition a:

$$s_a = \{x_i | p_i = a\}. \tag{1}$$

Clustering is then represented as the set of clusters $S = \{s_1, s_2, ..., s_M\}$. In vector quantization, the output of clustering is a codebook $C = \{c_1, c_2, \ldots, c_M\}$, which is usually the set of cluster centroids (code vectors).

The most important choice in clustering is the cost function f for evaluating the goodness of the clustering. For a given application, the criterion can be based on the principle of *minimum description length* (*MDL*) [R78, S78]. Otherwise, the criterion is based on certain assumptions of data normalization and spherical clusters. Basically, the function should correlate with high inter cluster distance and low intra cluster diversity. In the case of binary data, *stochastic complexity* has been applied [GKV97].

When data vectors belong to Euclidean space, a commonly used function is the *mean square error* (*MSE*) between the data vector and their cluster centroids. Given a partition P and the codebook C, the MSE is calculated as:

$$f(C,P) = \frac{1}{N}\sum_{i=1}^{N}\left\| x_i - c_{p_i} \right\|^2, \tag{2}$$

where p_i is the cluster (partition) index of the data vector x_i. From here on, the vectors are assumed to belong to Euclidean space and the mean square error (MSE) is used as the objective function. The number of clusters is also assumed to be known beforehand, unless otherwise stated.

2 Clustering algorithms

Clustering is an *NP-complete* [GJW82] combinatorical optimization problem, for which optimal solutions can be found by the *branch-and-bound* technique, but in exponential time [FN75, KNF75, FG88, W91, WL93, C95a, P97, GYZ98, GRS99, IA99, FV02, FVK02, MP02, **P5**]. The total number of different clusterings equals *Stirling's number of the second kind* [GKP94]. Suboptimal algorithms must therefore be used in practice.

Existing methods can be roughly divided into *heuristic*, *optimization, graph-theoretical* and *hierarchical* methods. The heuristic methods are usually fast but rough, and hence, they are not adequate alone. Instead, they can be used for creating an initial solution for more sophisticated algorithms. Optimization methods produce a partition that aims at minimizing an *a priori* chosen objective function, which is a goodness (of fit?) criterion for a partition [B99]. Hierarchical clustering methods start with an initial partition. After that, clusters are split or merged repeatedly. In hierarchical methods, an attempt is made to perform locally optimal steps, but this does not necessarily lead to the global optimal solution relative to any criterion function.

2.1 Algorithms

There are many heuristic clustering algorithms proposed in the literature [H75, S80, JD88]. They belong to the group of *partitional methods* that produce only one partition. An explicit objective function is not necessarily used since the object is to allocate the data vectors to the cluster they seem to fit best at the moment. Usually, each data vector is considered only once in a greedy manner, and it is allocated to a cluster or it is not allocated at all. These algorithms tend to produce rather weak solutions. Three simple heuristic methods are *leader* [H75, S80], *nearest neighbor clustering* [JD88] and *joiner* [H75, S80].

Optimization methods [K04a] are usually based on *k-means* [F65], which is also referred to by several other names, such as *c-means* [M67], *generalized Lloyd algorithm* (*GLA*) [L57], *Linde-Buzo-Gray* algorithm (*LBG*) [LBG80] or *iterative self-organizing data analysis technique* (*ISODATA*) [BH65]. These are slightly different variations on each other but the main concept is nevertheless the same. *K-means* applies two optimization steps iteratively: (i) it calculates an optimal partition for the given codebook, and (ii) calculates a new codebook as the cluster centroids. These steps are based on two optimality conditions:

(1) *Nearest neighbor condition*: for a given codebook, the optimal clustering of the data set is obtained by mapping each data vector to its nearest code vector in the codebook (or cluster representative) with respect to the evaluation function.

(2) *Centroid condition*: for a given partition, the optimal code vector (cluster representative) is the centroid (average vector) of the data vectors within the partition.

Each iteration of the *k-means* algorithm decreases the distortion; however, the process leads only to a *local optimum* that depends on the initial codebook, with *M* random data vectors, that was used. Several other techniques have also been proposed for generating an initial codebook [LBG80, YG88, GG92, NT92, BM93, KKZ94, AR96, PLL99]. Thus, *k-means* can fine-tune a codebook. It can also be integrated in many other of the more complicated algorithms discussed later in this thesis.

There are many variants of the *k-means* algorithm that include fast implementations [HLC91, WG94, CKS95, M95, CL96, KFN96, F97, BJLS98, KFN00, Z01, KMNPSW02, LVV03]. The fuzzy variant is known as *fuzzy c-means* [D73, DL94, CCLH97, OZ00, WCS01]. Among many other variants, there are *simulated annealing* [KGV83, ZG89, HPLSH01] and *deterministic annealing* [RGF90, HB97] variants. These methods are based on interesting theories but it does not mean that they would work well in practice.(this sentence, still, seems like it is an abrupt change of tone to the rest of the paper. The author takes a subjective position about the interest of these theories) Among those, simulated annealing is probably the one that works best in practice.

The best clustering results, in term of minimizing the distortion function, have been obtained by the *genetic algorithm* (*GA*) [H75, G89, MC96], which uses agglomerative methods in the crossover. The method was first reported by [FKKN97] using an effective but rather slow algorithm. The algorithm was then simplified and made faster [F00]. It is noted that the use of random crossover is not sufficient to be superior to the other clustering methods.

An alternative approach has been offered by the *randomized local search* algorithm (*RLS*) [FK00, FXK03]. In terms of minimizing the distortion function, it is almost as good as genetic algorithms but the *RLS* method is much simpler to implement. It uses a simple trial-and-error approach in which new candidate solutions are generated by random swapping of the code vectors and then uses *k*-means for fine-tuning the candidate solutions. The *RLS* algorithm has been successfully applied to the classification of bacteria [FGGKKLN00].

The graph-theoretical methods can be divided into three categories:

(1) Methods where the initial partition is the singleton partition and a hierarchical sequence of partitions obtained by agglomeration [KHK99,

HK01, **P2**].

(2) Methods that produce a connected graph from which a clustering is obtained by cutting inconsistent edges [Z71, J78, T80a, T80b, U82, U83, KN86, KNT87, SC91a, SC91b].

(3) Methods that produce an unconnected graph where the connected components correspond to the clusters [U82].

Hierarchical methods [K99] are either *divisive* or *agglomerative*. Divisive methods start by putting all data vectors in a single cluster. New clusters are created by dividing existing ones. This approach involves two main design problems: which cluster to divide, and how the division is performed. The division can be made along a selected dimension of the vector space as in the *median cut* algorithm [H82], or along the principal axis [WZ91]. The latter approach has been studied and a method has been proposed for locally fine-tuning the cluster boundaries after the divisions have been made [FKN97]. The divisive methods can be fast, e.g., $O(N \cdot \log N)$, but more complicated than the agglomerative methods.

Agglomerative clustering is simple to implement and it provides better clustering results than the divisive approach. It can also be combined with *k-means* as proposed [GPF95], or used as the merge phase in the split-and-merge algorithm [KFN98], which results in a good time-distortion performance.

Another clustering method is the *self-organizing map* (*SOM*) [K88, K95], which is commonly applied to data mining and to the visualization of complex data sets. SOM can also be used for clustering [NF88, CTC94]. Unfortunately, for large clustering problems *SOM* is inferior to the majority of other, noteworthy methods (noteworthy is redundant, you could leave it out for clarity's sake) [K04a]. Furthermore, the clustering results depend strongly on the parameter setup [F99].

2.2 Unknown number of clusters

Determination of the number of clusters in data requires that one has both an algorithm that searches for the correct clustering of data and has a criterion that is capable of recognizing the number of clusters [DB79, I80, FK97, SYK97, BP98, KF02b, KLL04, SWJ04, WC04, X04]. The simplest approach is to loop the number of clusters, use an existing algorithm for a fixed number of clusters in the loop, and then select the best solution using some criterion. This *brute force* search is guaranteed to work (assuming that the criterion is valid) but it is also slow.

The *stepwise clustering* algorithm, which reduces the workload required by the brute force approach, has been proposed [KF02b]. The idea is to utilize the previous solution as a starting point when solving the next clustering problem that has a different number of clusters. A stopping criterion is applied to estimate the potential improvement of the algorithm and to stop the iteration when the estimated improvement stays below a predefined threshold value.

There are also methods that solve the number and location of the clusters jointly. The c*ompetitive agglomeration* algorithm (*CA*) [FK97] decreases the number of clusters until there are no clusters smaller than a predefined threshold value. The drawback is that the threshold value must experimentally be determined. Another approach is the *dynamic local search* [KF02a] that solves the number and location of the clusters jointly. The algorithm uses a set of basic operations, such as cluster addition, removal and swapping.

2.3 Fast search methods

In the clustering problem, one typically needs to search for the *nearest neighbor* (*NN*) during the process. The nearest neighbor search problem involves searching for a set of K-dimensional vectors $C = \{c_i\}$ that are nearest to a given target vector x with respect to a distance function d. A large part of the running time of the search is due to the computation of the O(K) distance function. A *full search* solution involves calculating the distance between the data vector, x, and every code vector, c_i, in order to find the nearest to x; however, the full search solution comes at the cost of O(NK). (a ';' should separate two complete clauses, not a clause and a phrase.

In the search of nearest code vector in Euclidean space, several speed-up methods have been introduced that reduce the computation required by distance calculations [FN75, S75, BS76, FBF77, WL83, BG85, V89, S90a, S90b, CH91, MNS91, O91, OB91, GK92, HBSH92, RP92, RK93, EE94, LC94, CK95, LC95a, LC95b, LC95c, LS95, DE96, BJS97, RP97, AMNSW98, GG98, KS98, SC98, BBS99, KFN00, RP00, S00, TSL00, WL00, Y00, BBK01, CNBM01, HC01, AP02, BM02, KMNPSW02, M02, BN03, HS03a, HS03b, M03, SR03, K04b].

The *triangular inequality elimination* (*TIE*) technique presented by Chen and Hsieh [CH91] maintains the distances between all code vectors and then reduces the number of distance calculations by a condition derived from the triangle inequality.

The *partial distortion search* (*PDS*) proposed by Bei and Gray [BG85] terminates a single distance calculation immediately when the partial distance exceeds the shortest distance previously found. Let s_a be the cluster for which one seeks the nearest neighbor. One uses full search to calculate the distance values $d_{a,j}$ between s_a and all other clusters s_j. Let $d_{\min}$ be the distance of the best candidate found so far. The distance is calculated cumulatively by summing up the squared differences in each dimension. In *PDS*, one utilizes the fact that the cumulative summation is nondecreasing, since the individual terms are nonnegative. The calculation is therefore terminated and the candidate is rejected if the partial distance value exceeds the current minimum $d_{\min}$.

The *mean-distance-ordered partial search* (*MPS*) technique introduced by Ra and Kim [RK93] applies two different techniques to speed-up the search of the nearest code vector. First, it uses a fast precondition for checking whether the distance calculation to a given candidate cluster can be omitted. Second, it sorts the codebook according to the component means of the code vectors and derives limits for the search.

An interesting approach for clustering is to use *graph theoretical methods* [GR69, U82, JD88, OM95, EPY97, BCQY97, KHK99, HS00, HK01, B04]. For example, by first creating a complete undirected graph where the nodes correspond to the data vectors and the edges correspond to vector distances according to a given *similarity* or *dissimilarity* measure. The resulting graph can be trimmed to a *minimum spanning tree*, which can be interpreted as one large cluster. The clustering can then be generated by iteratively dividing the cluster by removing the longest edges from the graph. In the final graph, clusters can be determined by finding the separate components of the graph [GR69]. This algorithm can be seen as a variation of split-based methods with a similar criterion to the criterion in *single-linkage* agglomerative clustering.

Many agglomerative clustering algorithms construct a sparse graph and then perform the clustering on this graph [JD88, KHK99, HK01]. Two main characteristics of these approaches are that

(1) the methods construct undirected graphs, and

(2) the methods neglect the original data after building the weighted graph (meaning that weights of the new edges are determined by the weights of current edges).

Generating and utilizing the graph efficiently is problematic for this approach. For example, standard solutions for solving minimum spanning tree takes O(N^2) time, which would prevent any speed-up.

A *k-nearest neighbor graph* (*kNN graph*) is defined as a weighted, directed graph in which every node represents a single cluster and the edges correspond to pointers to neighbor clusters. A pointer maintains the index of the neighbor cluster and the corresponding distance. Every node has exactly k edges to the k nearest clusters according to a given distance function. The distance of clusters is defined by the merge cost function of the agglomerative clustering, see Eq. (3) below. Note that this is not the only possible definition of the graph: Other definitions have been given in [AM93, CBC00].

2.4 Multilevel thresholding

Multilevel thresholding, which is needed in the compression of the medical images [KOKKNN98], can be seen as a 1-dimensional special case of the clustering problem. The time complexity in the 1-dimensional case of clustering is expected to be lower than in the general case. For example, the time complexity of the *GLA* (for vector quantization in the multidimensional space) is O(NM) while the time complexity of its 1-dimensional counter-part, the *Lloyd-Max quantizer* (*LMQ*) [LS55, L57], is only O(N).

Over the years, many thresholding techniques have been proposed [KR79, O79, P80, WH84, KSW85, T85, B86, KI86, SSWC88, A89, PP89, LSP90, B92, CW92, TC92, PP93, AST94, CWY94, BM95, YCC95, YC97, CSS98, GLC98, Y99, ST00, LCC01, SS01, Y02]. The thresholding methods can be categorized in six groups according to the information they explore. These categories are [SS04]

(1) histogram shape-based methods where the peaks, valleys and curvatures of the smoothed histogram are analyzed;

(2) clustering-based methods where the gray level samples are clustered in two parts as background and foreground or, alternately, are modeled as two Gaussian distributions;

(3) entropy-based methods that use the cross-entropy between the original and binarized image;

(4) object attribute-based methods that search for a measure of similarity between the gray-level and binarized images, such as fuzzy similarity, shape, edges, or the number of objects;

(5) spatial methods that use the probability mass function models, which take into account the correlation between pixels on a global scale; and

(6) local methods that do not determine a single value of threshold, but adapt the threshold value depending upon the local image characteristics instead. (see note on last page).

When extended to multilevel thresholding, many of these methods have high computational complexity since they carry out an exhaustive search, which takes O(N^{M-1}) time. A faster algorithm based on Otsu's method was proposed by Liao et al. [LCC01]. However, it still requires O(N^{M-1}) time. Faster O($N \cdot \mathrm{sqrt}(M \cdot \log N) + N \cdot \log N$) and O($N^2 M$) time algorithms have been developed for multilevel thresholding by Aggarwal et al. [AST94] and by Kundu [K98] respectively.

The best, known method uses *dynamic programming* [B57] and has the time complexity O(NM) for globally optimal scalar quantizers [W91, WZ93]. This method is based on monotonicity properties of optimal scalar quantizers. The same technique can also be adopted to multilevel thresholding because the problem statement is equal. Thus, optimal multilevel thresholding can be calculated ultimately in O(NM) time.

3 Agglomerative clustering

Agglomerative clustering [LW67, CO72, BS93] generates clusters by a sequence of merge operations. Clustering starts by initializing each data vector as its own cluster. Two clusters are merged at each step and the process is repeated until the desired number of clusters has been obtained. The *single linkage* (*SL*) [SS73] method determines the cluster pair to be merged based on the two closest vectors. The *complete linkage* (*CL*) [SS73] method determines the cluster pair to be merged based on the two furthest vectors. *Ward's* method [W63] selects the cluster pair to be merged so that the merge increases the given objective function value least. In the vector quantization context, this is also known as the *pairwise nearest neighbor* (*PNN*) method, attributed to Equitz [E89].

The algorithm is straightforward to implement in its basic form and, in comparison to *k*-means, it gives better results (i.e., it has a codebook with a lower MSE value). The *PNN* method also has the advantage that the hierarchical approach produces multiple codebooks of different sizes as a side-product. Thus, the *PNN* method can be applied to joint minimization of distortion and entropy of code vector indices [FGP90, GPF91, GPF95, KS98]. The algorithm can also be used as a part of hybrid method such as a *genetic algorithm* [FKKN97, F00, KFN03, FV03], or an iterative *split-and-merge* method [KFN98].

3.1 PNN method

The basic structure of the *exact PNN* method is shown in Figure 3.1. The method starts by initializing each data vector x_i as its own code vector c_i. In each step of the algorithm, the size of the codebook is reduced by merging two nearby clusters. The cost of merging two clusters s_a and s_b (*merge cost*), which is also the *distance* between these clusters, is defined as the increase in the distortion of the codebook if the clusters are merged [W63, E89]:

$$d_{a,b} = \frac{n_a n_b}{n_a + n_b} \cdot \left\| c_a - c_b \right\|^2, \tag{3}$$

where n_a and n_b denote the sizes of the corresponding clusters s_a and s_b. This minimizes the increase of MSE caused by the merge operation. The cost function is symmetric ($d_{a,b} = d_{b,a}$) and can be calculated in $O(K)$ time, assuming that n_a, n_b, c_a, and c_b are known.

The costs for merging three clusters are illustrated in Figure 3.2. The cost values are: $d_{a,b} = 32{,}40$; $d_{b,c} = 56{,}25$ and $d_{a,c} = 90{,}75$. It can be observed that, in this case, it is better to merge the central cluster (b) with the smaller cluster (a) than with the larger cluster (c) even though the latter is closer in respect of the Euclidean distance.

```
PNN(X, M) → C, P
    $s_i \leftarrow \{x_i\} \ \forall\, i \in [1,N]$;
    $m \leftarrow N$;
    REPEAT
        $(s_a, s_b) \leftarrow$ NearestClusters();
        MergeClusters($s_a, s_b$);
        $m \leftarrow m-1$;
        UpdateDataStructures();
    UNTIL $m=M$;
```

Figure 3.1. Structure of the exact *PNN* method.

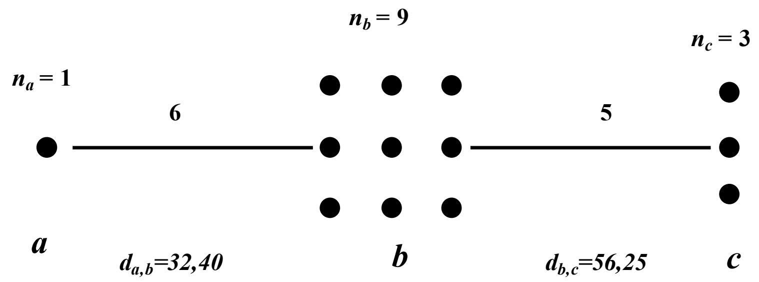


Figure 3.2. Illustration of the distances between the clusters s_a, s_b and s_c, where the Euclidean distance between the clusters s_a and s_b is $\|a-b\|^2 = 6$ and similarly between the clusters s_b and s_c the distance is $\|b-c\|^2 = 5$.

The exact variant of the *PNN* method applies a local optimization strategy: all possible cluster pairs are considered and the one (s_a, s_b) increasing the distortion least is chosen:

$$a,b = \arg \min_{\substack{i,j\in[1,N] \\ i\neq j}} d_{i,j} . \tag{4}$$

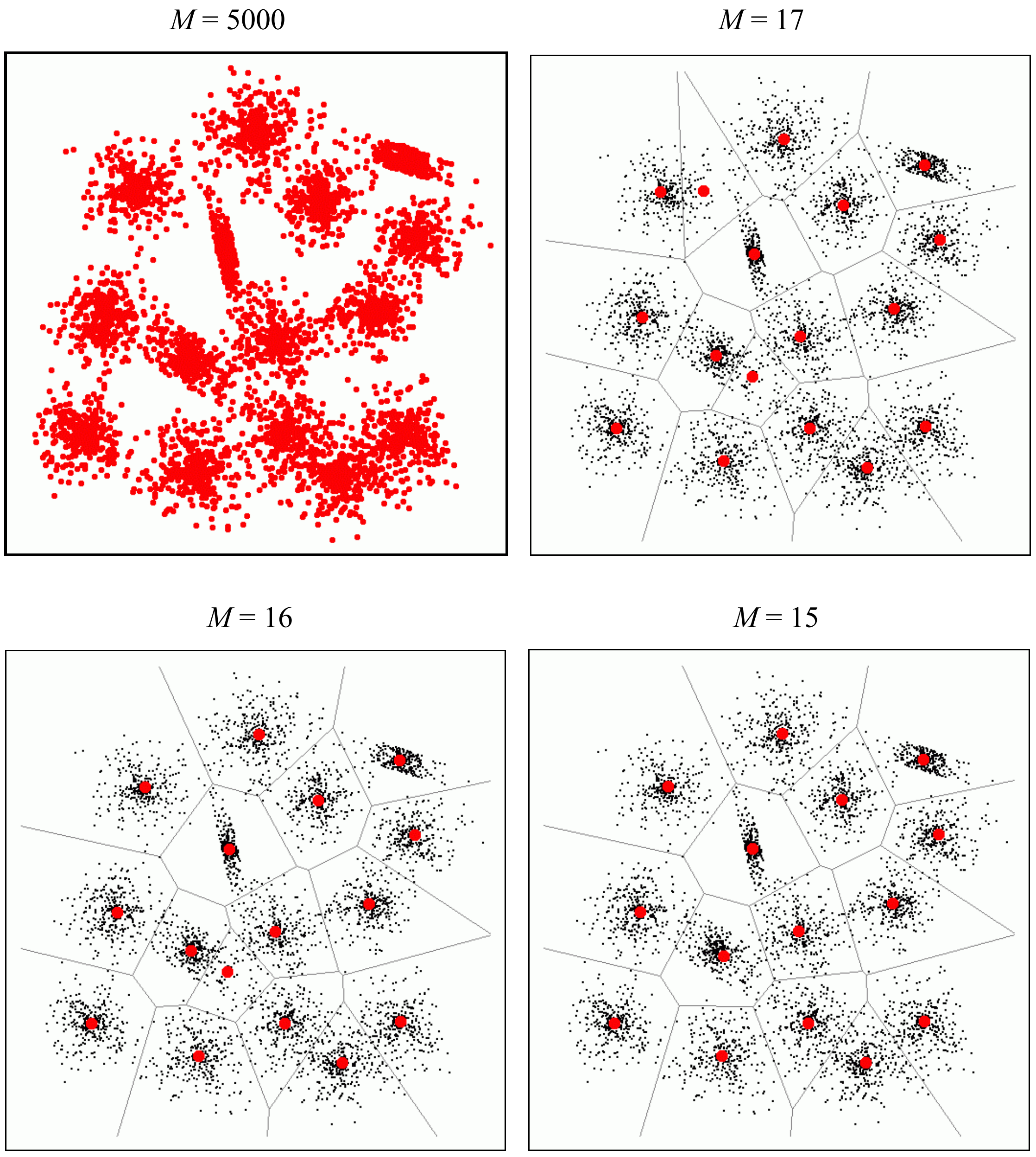
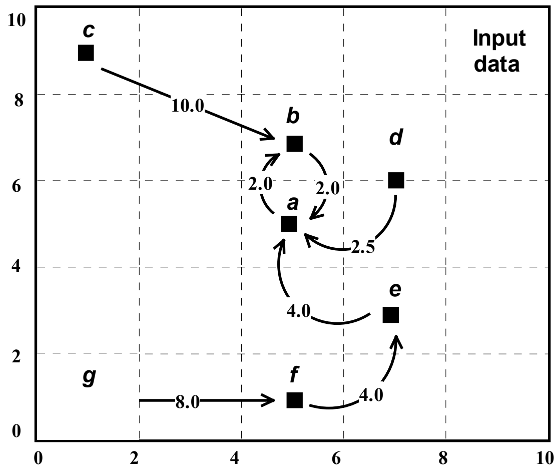


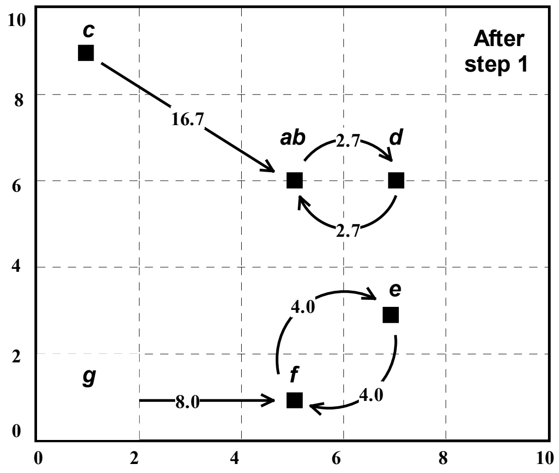
Figure 3.3. Illustration of the agglomeration of the *PNN* method for the data set S_2. The final clustering has 15 separate clusters.

The code vector (c_a) of the combined cluster (s_a) is calculated as the weighted average of the code vectors (c_a and c_b) of the merged clusters s_a and s_b:

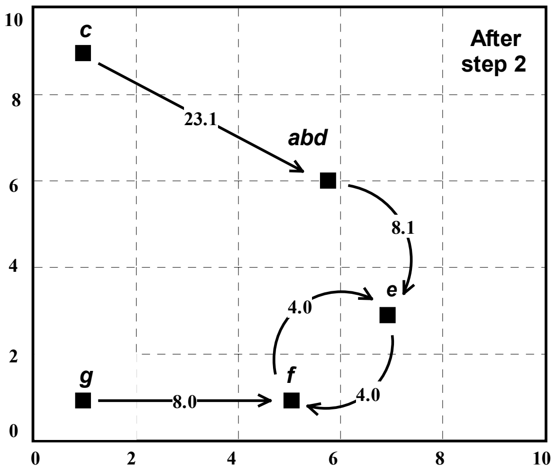
$$c_a \leftarrow \frac{n_a c_a + n_b c_b}{n_a + n_b}. \tag{5}$$



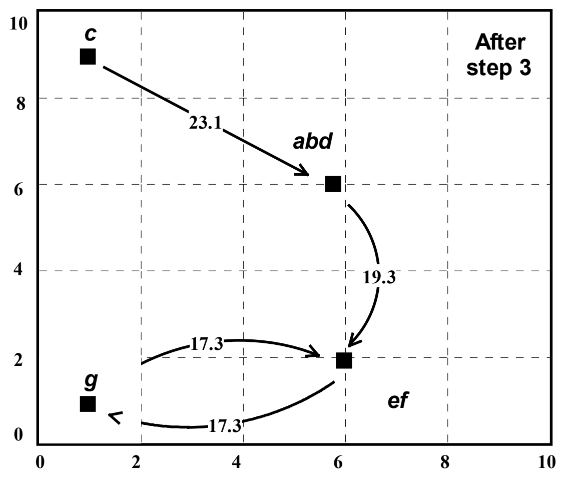
cluster	*a*	*b*	*c*	*d*	*e*	*f*	*g*	min	*NN*
a	--	2.0	16.0	2.5	4.0	8.0	16.0	2.0	*b*
b	2.0	--	10.0	2.5	10.0	18.0	26.0	2.0	*a*
c	16.0	10.0	--	22.5	36.0	40.0	32.0	10.0	*b*
d	2.5	2.5	22.5	--	4.5	14.5	30.5	2.5	*a*
e	4.0	10.0	36.0	4.5	--	4.0	20.0	4.0	*a*
f	8.0	18.0	40.0	14.5	4.0	--	8.0	4.0	*e*
g	16.0	26.0	32.0	30.5	20.0	8.0	--	8.0	*f*



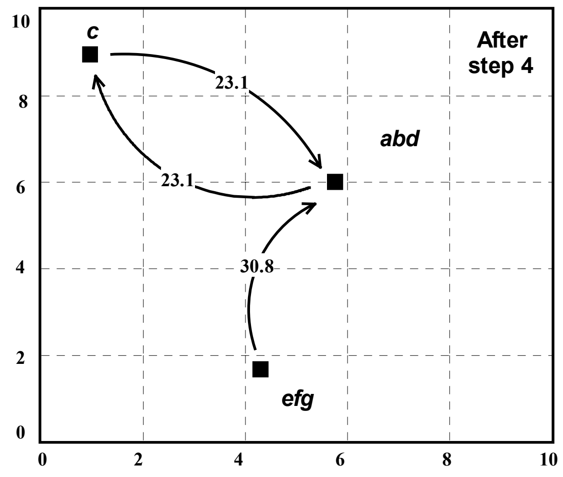
cluster	*ab*	*c*	*d*	*e*	*f*	*G*	min	*NN*
ab	--	16.7	2.7	8.7	16.7	27.3	2.7	*d*
c	16.7	--	22.5	36.0	40.0	32.0	16.7	*ab*
d	2.7	22.5	--	4.5	14.5	30.5	2.7	*ab*
e	8.7	36.0	4.5	--	4.0	20.0	4.0	*f*
f	16.7	40.0	14.5	4.0	--	8.0	4.0	*e*
g	27.3	32.0	30.5	20.0	8.0	--	8.0	*f*



cluster	*abd*	*c*	*e*	*f*	*g*	min	*NN*
abd	--	23.1	8.1	19.1	35.1	8.1	*e*
c	23.1	--	36.0	40.0	32.0	23.1	*abd*
e	8.1	36.0	--	4.0	20.0	4.0	*f*
f	19.1	40.0	4.0	--	8.0	4.0	*e*
g	35.1	32.0	20.0	8.0	--	8.0	*f*



cluster	*abd*	*c*	*ef*	*g*	min	*NN*
abd	--	23.1	19.3	35.1	19.3	*ef*
c	23.1	--	49.3	32.0	23.1	*abd*
ef	19.3	49.3	--	17.3	17.3	*g*
g	35.1	32.0	17.3	--	17.3	*ef*



cluster	*abd*	*c*	*efg*	min	*NN*
abd	--	23.1	30.8	23.1	*c*
c	23.1	--	48.7	23.1	*abd*
efg	30.8	48.7	--	30.8	*abd*

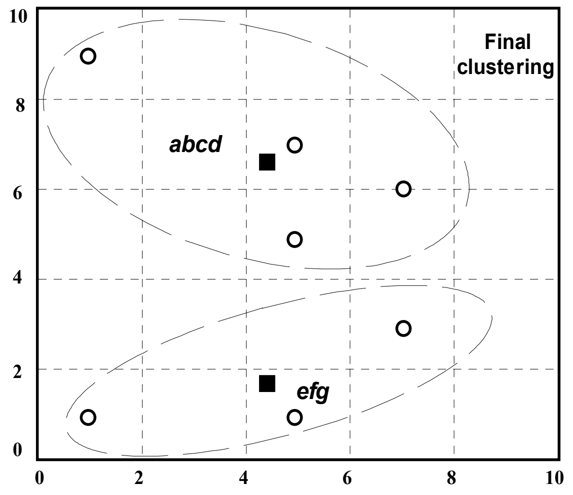


Figure 3.4. *PNN* example. At the end of the agglomeration there are two clusters left.

The clusters are then merged and the process is repeated until the codebook reaches the desired size, M. It should also be noted that, although a single merge operation is always performed optimally, the whole process does not guarantee an optimal codebook. An illustration of the agglomeration of the *PNN* method for a sample data set is shown in Figure 3.3. On the top left, the initial phase after each data vector has been assigned to its own cluster (M=5000) is shown. On the top right, the clustering before the last two merge steps (M=17) is shown. On the bottom left, the clustering before the last merge step (M=16) is shown. Finally, on the bottom right, the final clustering (M=15) is shown. The code vectors are presented by large dots.

A detailed example of the *exact PNN* method is illustrated in Figure 3.4. In the matrix, all pairwise distances of the clusters are shown. On the right hand side of the matrix, the nearest neighbor cluster and the associated distance for each cluster are shown. Note that these data structures are not maintained by the basic *PNN* algorithm. At the beginning there are seven clusters: *a*, *b*, *c*, *d*, *e*, *f*, and *g*. During each step of the algorithm, two clusters are always merged. Thus after the first step, there are six clusters left: *ab*, *c*, *d*, *e*, *f*, and *g*. At the end of the agglomeration, there are only two clusters left: *abcd* and *efg*.

A drawback of the *PNN* method is its relatively high running time in its basic form [SO97]. There are almost N steps to be performed by the algorithm because, typically, $M<<N$. Straightforward implementation [E89] recalculates all pairwise distances of the clusters at each step of the algorithm for finding the pair of clusters to be merged in the algorithm. No additional data structures are required, but the algorithm takes $O(N^3K)$ time [SO97] because there are $O(N)$ steps and in each step there are $O(N^2)$ cost function values to be calculated. Therefore, the algorithm is very slow for large data sets.

3.2 Using a distance matrix

To reduce the number of the calculations of the merge cost function of Eq. (3), pairwise distances can be stored in an $N×N$ matrix; see Figure 3.5. A strictly upper triangular matrix, which is shown in gray, is only used because the distances between the clusters are symmetrical. The minimum value is searched for from the distance matrix and the corresponding cluster pair is merged. New merge cost values are then calculated between the new cluster and remaining clusters, only. Thus, the number of the calculations per iteration falls from $O(N^2)$ to $O(N)$, but the search for the minimum still takes $O(N^2)$. The time complexity of using the distance matrix is thus $O(N^2K+N^3)$, where the first term originates from the calculations of the merge cost values and the second term originates from the search for the minimum [SO97]. The disadvantage of this approach is its quadratic memory consumption.

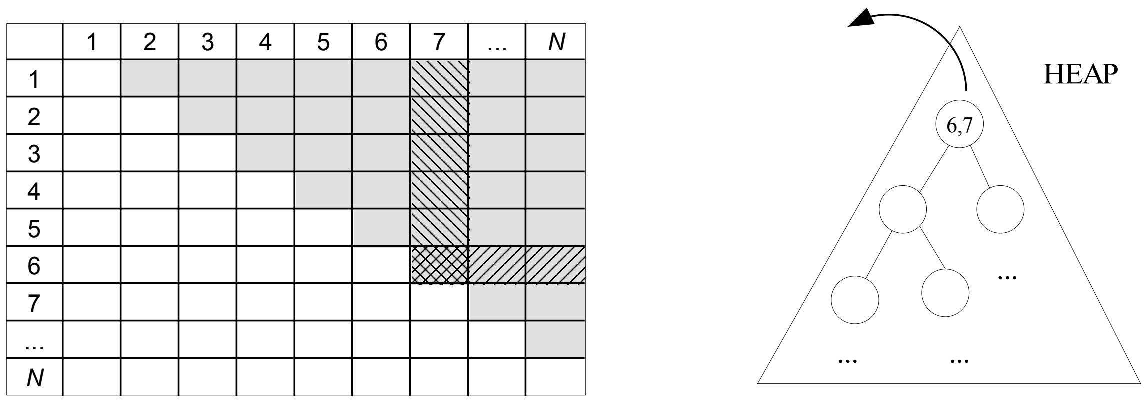


Figure 3.5. Distance matrix. A strictly upper triangular matrix shown in gray is only used because the distances between the clusters are symmetrical.

Kurita's method [K91] stores all pairwise distances into a matrix but utilizes a heap structure for searching the minimum distance; see Figure 3.5. The merged clusters can be found by taking the smallest element from the top of the heap in O(log$N$) time. Although the number of the elements in the heap is even O(N^2) in the beginning, the search can be done nevertheless in O(log$N$) time because O(log(N^2)) = O(2log$N$). Only O(N) distance updates are needed after each merge step; each of these updates takes O(K+log$N$) time. There, the first term (K) originates from the time for the calculation of the merge cost and the second term is attributed to the heap operation. *Kurita's* method thus runs in O(N^2K+N^2·log N) time; however, it still requires O(N^2) memory, which is impractical for large data sets.

3.3 Fast exact PNN

A much faster variant of the *PNN* method can be implemented by maintaining, for each cluster, a pointer to its nearest neighbor [FKSC00]. The nearest neighbor nn_a for a cluster s_a is defined as the cluster minimizing the merge cost:

$$nn_a = \arg\min_{\substack{j\in[1,N]\\ j\neq a}} d_{a,j}\,. \qquad (6)$$

The nearest neighbor property is not symmetrical, (i.e., $nn_a=b$ does not imply $nn_b=a$). The nearest neighbor of the cluster a is the cluster b, according to Eq. (3), but the nearest neighbor of the cluster b is the cluster c (see Figure 3.6 where the nearest neighbor pointers are illustrated). In this way, only a few nearest neighbor searches are needed in each iteration. The method is denoted as the *fast exact PNN*. Its implementation details are given next.

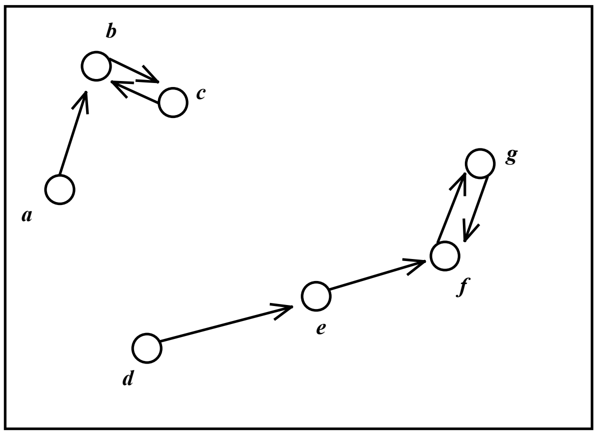


Figure 3.6. Nearest neighbor pointers, which reduce the amount of the nearest neighbor search in each iteration.

For each cluster s_j, one maintains the cluster size n_j, the corresponding cluster center c_j, and the pointer to its nearest neighbor nn_j. The nearest neighbor pointer is assigned with the cost value d_j. The cost values of pointers indicate the amount of increase in the distortion if the cluster s_j is merged to s_{nn_j}. For each data vector the algorithm maintains the index of the cluster p_i, which the data vector belongs to.

In the initialization, each data vector x_i is assigned to its own cluster of the size one and the cluster center c_i is initialized to the data vector itself:

$$p_i \leftarrow i; n_i \leftarrow 1; c_i \leftarrow x_i \; for \; all \; i \in [1, N]. \tag{7}$$

In order to generate the nearest neighbor table for the cluster centers, one must find the nearest neighbor nn_i for every cluster. This is done by considering all other clusters as tentative neighbors and by selecting the one that minimizes Eq. (3). There are $O(N^2)$ pairs to be considered and thus, the initialization phase takes $O(N^2K)$ time in total.

The optimal cluster pair (s_a and s_b) to be merged is the cluster that has the minimum d_j-distance according to Eq. (3) and its nearest neighbor nn_j:

$$a \leftarrow \arg\min_{j \in [1,N]} d_j \; ; \; b \leftarrow nn_a \, . \tag{8}$$

This pair can be found in $O(N)$ time using linear search in the nearest neighbor table. The merge of the clusters is then performed as follows. First, one updates the partition indices so that the combined cluster replaces s_a, and the cluster s_b becomes obsolete:

$$p_i \leftarrow a \text{ for all } i = 1, 2, ..., N \text{ such that } p_i = b. \tag{9}$$

In order to minimize rounding errors it is advantageous to calculate the new code vector as the centroid of the cluster. This can now be easily done by the aid of the partition indices p_i:

$$c_a \leftarrow \frac{1}{n_a} \cdot \sum_{p_i = a} x_i . \tag{10}$$

The above steps can be performed at most in O(NK) time.

The nearest neighbor nn_a for the merged cluster (now s_a) must be resolved by calculating the merge cost values of Eq. (3) between the new cluster and all other remaining clusters. This can be done in an O(NK) time.

As mentioned before, the nearest neighbor function is not symmetrical. Therefore, one must also resolve the nearest neighbor pointer for all clusters whose nearest neighbor was, before the merge, either *a,* or *b* ($nn_i=a$, or $nn_i=b$). This takes O(NK) time for a single cluster and (according to practical tests) there are approximately 3-5 clusters on average to be updated at each step of the algorithm, see [FKSC00]. The overall time complexity of the update operation is thus O(τNK), where τ denotes the number of clusters whose nearest neighbor pointer must be resolved. To sum up, the time complexity of the *fast exact PNN* method is O(τN^2K).

The range of τ is [0-N] and is closely related to the *kissing number problem* (also sometimes called the *Newton number*, *contact number*, *coordination number*, or *ligancy*), which asks the maximum number of spheres of radius one that can simultaneously touch the unit sphere in K-dimensional Euclidean space [MTTV97, CS98, W04]. The cluster merge cost values of Eq. (3), however, are not Euclidean and therefore the kissing number only applies in cases when all cluster sizes are equal. This is the case at least in the initial stage of the *PNN* method, if all clusters have same initial frequencies. Usually the initial frequency of the cluster is one, but this is not necessarily always the case (see the data sets in Section 5).

In the worst case, the same cluster can be the nearest neighbor for all the other clusters, and thus τ=O(N). This situation could appear when there is one small cluster and all the rest are large. This cannot happen in the exact *PNN* method; however, it has been reported to be possible in other situations [F00]. Thus, this is not common in practice and the connection to the kissing number (even as an open problem in the general case) indicates that τ is a function of the vector dimension K.

In a favorable case, two merged clusters are chosen randomly. Since each cluster has only one nearest neighbor pointer, a randomly chosen cluster is the nearest neighbor for one cluster for the average case. The average number of the updated pointers is therefore two because there are two clusters involved in the merge operation. However, the merged clusters are not chosen randomly, rather they tend to be located in areas of high concentrations of clusters. Thus, in practice, τ is greater than two. Ultimately, τ can be zero when two clusters far away from other clusters are merged because then it is possible that the merged new cluster is not the nearest neighbor of any other cluster.

cluster	*a*	*b*	*c*	*d*	*e*	*f*	*g*	min	*NN*
a	--	2.0	16.0	2.5	4.0	8.0	16.0	2.0	*b*
b	2.0	--	10.0	2.5	10.0	18.0	26.0	2.0	*a*
c	16.0	10.0	--	22.5	36.0	40.0	32.0	10.0	*b*
d	2.5	2.5	22.5	--	4.5	14.5	30.5	2.5	*a*
e	4.0	10.0	36.0	4.5	--	4.0	20.0	4.0	*a*
f	8.0	18.0	40.0	14.5	4.0	--	8.0	4.0	*e*
g	16.0	26.0	32.0	30.5	20.0	8.0	--	8.0	*f*

Figure 3.7. Initial distance matrix of the *PNN* example shown in Figure 3.4. The cells shown in gray contain the cluster distance to the nearest neighbor for each cluster.

The initial distance matrix of the *PNN* example shown in Figure 3.4 is illustrated in Figure 3.7. The cluster pair *a* and *b* will be merged in the first step because their merge cost is smallest. After the merge, the distance matrix is updated before the search for the next cluster pair to be merged. In the *original PNN* variant (full search), the whole matrix is recalculated during the next iteration since nothing is stored. In the *distance matrix* variant, only the values of the rows and the columns for the merged cluster *ab* must be calculated and stored in the distance matrix. In the *fast exact PNN* method, only the values of the rows and the columns for the clusters *ab*, *c*, *d* and *e* are recalculated because the nearest neighbor pointers must be updated for those clusters. In this method, only the nearest neighbor pointers to the nearest neighbors and the corresponding distance values are stored in the nearest neighbor table.

3.4 Lazy PNN

The number of distance calculations can be reduced further by delaying the update of the nearest neighbor pointers. The method is based on the *monotony property*; see [KFN99]. Suppose that the current minimal merge cost is $d(s_a, s_b)$ and the clusters s_a and s_b are merged. It is possible that the centroid of the merged cluster (c_{a+b}) becomes closer to the centroid of the third cluster s_c than c_c was in respect of the original cluster centroids (c_a and c_b); see Figure 3.8. However, the monotony property states that the merge cost $d(s_{a+b}, s_c)$ cannot be smaller than $\min\{d(s_a, s_c), d(s_b, s_c)\}$. So the minimum cluster distortion d never decreases due to the merge of the optimal cluster pair. This is formalized in the following lemma [KFN99]:

Lemma 3.1. Consider three clusters s_a, s_b, s_c with centroids c_a, c_b, c_c and the number of objects in these clusters n_a, n_b, n_c. Assume that $d(s_a, s_b) \le d(s_a, s_c) \le d(s_b, s_c)$ and n_a, n_b, $n_c \ge 1$. Then it holds that $d(s_a, s_c) \le d(s_{a+b}, s_c)$.

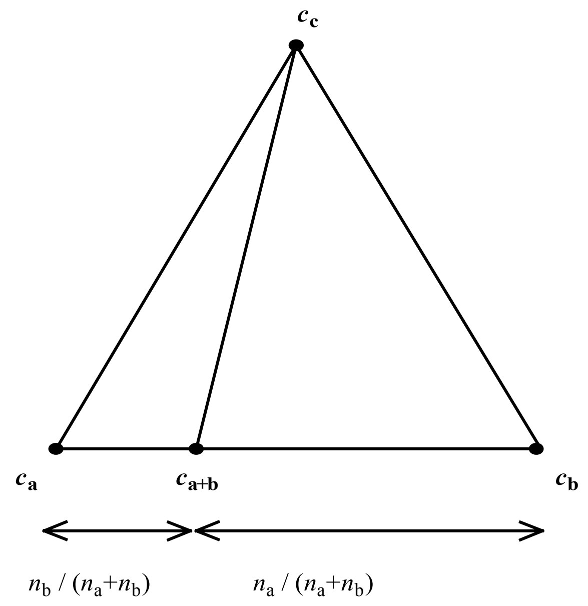


Figure 3.8. Illustration of the three clusters in 2-dimensional space. Here c_a and c_b are the centroids of the two clusters to be merged, c_{a+b} is the centroid of the merged cluster, and c_c is the centroid of any other cluster.

For example, assume that the nearest neighbor for a cluster s_i was s_a before the merge of the two clusters s_a and s_b, and s_x after the merge. From the monotony property one knows that $d_{i,a} \le d_{i,a+b}$. One therefore does not need the exact cluster distance because the previous cluster distance value serves as a lower bound. In practice, one can assume that the nearest neighbor after the merge is s_{a+b} so the previous cost function value $d_{i,a}$ (or $d_{i,b}$) can be used as a lower bound. The cluster dissimilarity value is labeled as outdated. It will be updated only if it becomes a candidate for being the smallest distance of all. In this way, one can reduce the computation by about 35% while preserving the exactness of the *PNN* method [KFN99].

3.5 Inexact variants

Several inexact variants of the *PNN* method have been considered in the literature. These variants decrease the running time at the cost of increased distortion. Equitz proposed an $O(NK \cdot \log N)$ time variant, which he referred as the *fast PNN* [E89]. It uses a KD-tree [B75, FBF77] for localizing the search for the code vectors. The algorithm merges several vector pairs at the same time. The KD-tree structure and the corresponding partition of the 2-dimensional space are illustrated in Figure 3.9. All data vectors are assigned to the buckets of the KD-tree so that the similar data vectors are in the same bucket. The method; however, has not gained as much popularity as the *exact PNN* method, probably because of its more complex implementation and suboptimal results.

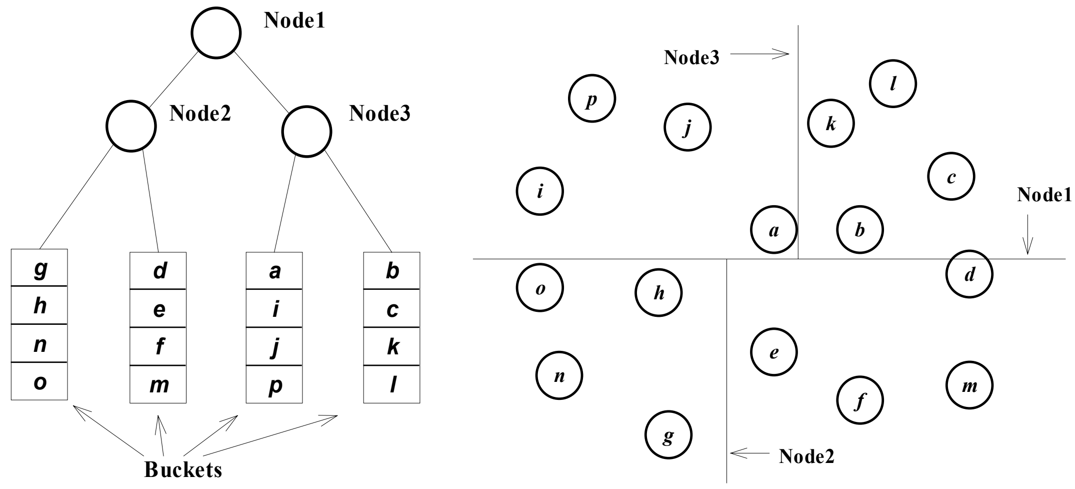


Figure 3.9. KD-tree and the corresponding partition.

Another possibility is to generate a preliminary codebook of size M_0 ($N > M_0 > M$) using the *GLA* with a random initialization of the data vectors. Any other fast algorithm could be used as well. The *exact PNN* method is then applied until the codebook reaches its final size M [GPF95]. The *exact PNN* method has now only (M_0 - M) steps, and the time complexity of this method is thus $O(NM_0) + O(M_0^3)$, where the first term is due to the *GLA* and the second term is due to the *PNN* method.

Thus, one has several different possibilities to combine the *GLA* and the *PNN* method:

(1) *Random initialization + GLA*
(2) *PNN*
(3) *PNN + GLA*
(4) *GLA + PNN*
(5) *GLA + PNN + GLA*.

In the first case, one uses the *GLA* by itself with a random initialization, which can be done very fast by choosing random data vectors as cluster centroids. In the second case, one uses the *PNN* method by itself. Since it has quadratic running time, this method is quite slow with a large data set. In the third case, *exact PNN* method is used first. After that, one fine-tunes the codebook with the *GLA*. In that way, one gets better codebooks than with the *PNN* method or the *GLA* alone.

Table 3.1. Time complexities of the different scenarios of combining the *PNN* and G*LA*.

Combination:	**Time complexity**	
	In general	Assuming $M_0 = O(M)$
Random + GLA	$O(gNMK)$	$O(gNMK)$
PNN	$O(\tau N^2 K)$	$O(\tau N^2 K)$
PNN + GLA	$O(\tau N^2 K) + O(gNMK)$	$O(\tau N^2 K)$
GLA + PNN	$O(gNM_0K) + O(\tau M_0^2 K)$	$O(gNMK)$
GLA + PNN + GLA	$O(gNM_0K) + O(\tau M_0^2 K) + O(gNMK)$	$O(gNMK)$

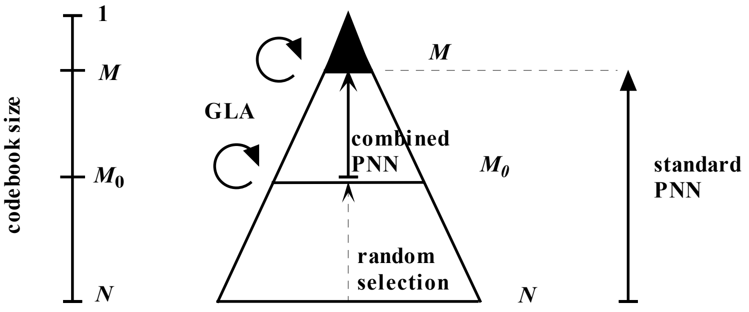


Figure 3.10. Different scenarios of combining the *PNN* and *GLA*.

In the fourth case, one first uses the *GLA* to generate a preliminary codebook of size M_0, and then applies the *exact PNN* method until the codebook reaches the final size, *M*. In this way, one can speed-up the *PNN* method remarkably yielding to $O(NM_0K) + O(\tau M_0^2 K)$ time complexity. Unfortunately, then the exactness of the *PNN* method cannot be preserved. In the fifth case, one first uses the *GLA* to generate a preliminary codebook of size M_0 and then applies the *exact PNN* method until the codebook reaches the final size, *M*. The codebook is finally fine-tuned with the *GLA*. Thus, one can speed-up the *PNN* method like in the third case. Even though the exactness of the *PNN* method is then lost, one can still get with this method a better codebook compared to the fourth case. The time complexities of the different combination scenarios are summarized in Table 3.1, where *g* denotes the number of iterations of the *GLA*. For illustration of these variants, see Figure 3.10.

3.6 Genetic algorithm

Genetic algorithms (*GA*) are based on the model of natural selection that occurs in nature. The main idea is to maintain a set of solutions (called a *population of individuals*) that are iteratively manipulated using *genetic operations* (*crossover* and *mutations*) and *selection*. Each initial solution is created by selecting M random data vectors as the code vectors and by calculating the optimal partition. Crossing the best solutions of the current population then creates the solutions for the next population. The number of iterations and the population size are the main parameters of the algorithm.

Several *genetic algorithms* have been previously considered for the clustering problem [DK95, PMJ95, MC96, S96, FKKN97, KM99, F00, TY00, KFN03]. The best, known (or best, known) *genetic algorithms* use a crossover method, which is based on the *PNN* method [FKKN97, F00, KFN03]. The crossover proposed in [F00] will be described below.

The *PNN crossover* starts by merging two parent codebooks by taking their union. The new partition of a data vectors is then constructed based on the existing partitions P^1 and P^2 [F00]. The partition of the data vector x_i is either p_i^1 or p_i^2. The one with the smaller distance to x_i is chosen. In this way, the new partition can be generated using $2{\cdot}N$ distance calculations only. The new codebook is then updated in respect to the new partition. This procedure gives a solution in which the size of the codebook is twice the size of the final codebook. A final task is to reduce the codebook size from $2{\cdot}M$ to M using the exact *PNN* method with the following two differences. First, one does not perform the *PNN* method for a full data set. Rather, one starts from an initial solution of $2{\cdot}M$ clusters at most. The crossover can therefore be performed in $O(\tau M^2)$ time instead of the original $O(\tau N^2)$ time. Second, the partition data is also updated during the crossover and, therefore, the partition is not needed to be recalculated after the *PNN* method. Figure 3.11 illustrates the *PNN* crossover.

The revised version of [F00] has three vital improvements over [FKKN97]: (i) The representation of solution is revised so that one does not merge only the codebooks, but maintain both partition and codebook for each solution. In this way, the partition of a new solution can efficiently be computed from those of the parent solutions. Access to the partition also gives a more precise initialization for the *PNN* method, which results in higher quality candidate solutions. (ii) Empty partitions are removed before the application of the *PNN* method, which is vital for avoiding the worst-case behavior of the *PNN* method. (iii) Since the new candidate solutions are already close to a local minimum, the *GLA* iterations are extremely fast using the activity detection technique [KFN99].

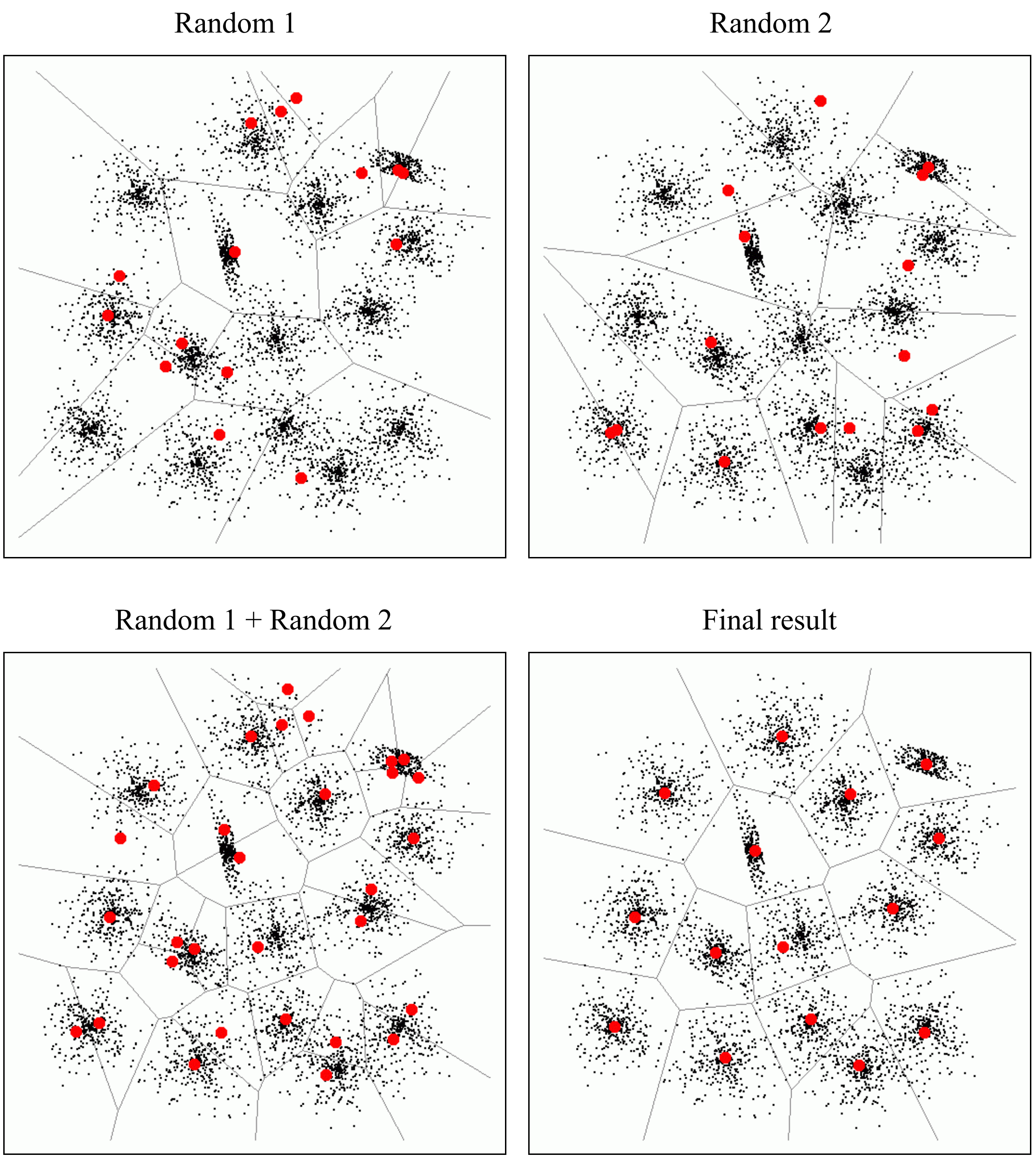


Figure 3.11. Illustration of the use of the *PNN* method as a deterministic crossover method in the *genetic algorithm* for the data set S_2. Panels on top left and right show two initial codebooks, which have been generated randomly among the data vectors (M=15). The panel on bottom left shows the codebook after combining two initial codebooks (M=30). On the bottom right the final codebook after the 15 merge steps of the *PNN* method (M=15) is shown.

According to the experiments in [F00], the *genetic algorithm* with the *PNN crossover* method outperforms all the comparative methods, including the previous variants of the genetic algorithm. The only other method that has been reported to give better results is the *self-adaptive genetic algorithm* (*SAGA)* [KFN03], which still uses the *PNN crossover* as the key component. The use of the *PNN* method as a deterministic crossover method also achieves a fast convergence with a rather small population size. The algorithm is therefore remarkably faster than any of the previously reported genetic algorithms.

3.7 Summary

The results of the *PNN* method are quite good; in general, they are better than the results of the opposite hierarchical methods performing divisions of greater clusters. The *PNN* method does not suffer from bad data sets as *k-means* does. It can be expected that the results of the *PNN* method are quite good, in general. The hierarchical property of the *PNN* method also makes it possible to get the clustering results of many different levels with the same effort. It is the best, known clustering method when used with the *genetic algorithm* as a crossover method. The *PNN* method is simple and it can be easily applied to many other problems.

On the other hand, the *PNN* method is slow. The running time of the best *PNN* algorithm is lower bounded by $\Omega(N^2)$ and there are not any clear, simple and practical ways to speed-up the algorithm. Since the merge phase is based on the local optimization strategy and is a greedy heuristic, there is no guarantee of the global optimum. If the number of the clusters is small, the result can remain quite far away from the best possible result. Thus, there is a need for improvement, but it is not obvious how this could be done.

4 Summary of the publications

In the first paper [**P1**], we study methods for speeding-up the *pairwise nearest neighbor* method. We consider two different speed-up methods. The first is the *partial distortion search* (*PDS*) originally proposed by Bei and Gray [BG85] for *k*-means. It terminates a single distance calculation immediately when the partial distance exceeds the shortest distance that has been found so far. Since the idea is independent of the chosen metrics, it can, therefore, also be directly applied to the *PNN* method.

The second method is the *mean-distance-ordered partial search* (*MPS*) technique introduced by Ra and Kim [RK93]. This technique uses the component means of the vectors to derive a precondition for the distance calculations and, in this way, a large number of the distance calculations can be omitted completely. Although this idea utilizes properties of the Euclidean space, we will show that the precondition can also be generalized for the distance calculations in the *PNN* method.

When combining all the speed-up methods discussed in this paper, one can reduce the run time to 8-15% of the basic version of the *PNN* method in the case of four favorable training sets. We can reduce the run time to about 50% of the basic version in the case of the less favorable sets (residual vectors). When the dimensions of the vectors are very large (256 or greater), the run time can be reduced to 2% of the basic version. We also demonstrate that the improvements are applicable within hybrid methods such as the *GLA-PNN-GLA*, and the *GA with PNN crossover*.

In the second paper [**P2**], we propose an algorithm for fast agglomerative clustering using a *k* nearest neighbor graph. In our approach, every node in the graph represents a cluster. The edges of the graph represent inter cluster connections between nearby clusters. The graph has a linear space complexity and it is used as a search structure for reducing the number of distance calculations. The proposed approach has two specific problems: how to generate the graph efficiently, and how to utilize it. We propose solutions for the first problem by considering a *KD-tree* [B75], [FBF77], *divide-and-conquer* [PS85], and *projection-based search* [RK93]. It appears that the *projection-based heuristic* works reasonably well in most cases. The *divide-and-conquer* approach is faster in the case of some high dimensional image data sets, and the *KD-tree* is faster in the case of 3-dimensional color clustering.

We also study the second problem and found that a relatively small neighborhood size (k=3...6) is sufficient to produce clustering with similar quality to that of a full search. At the same time, significantly fewer distance calculations and operations are needed and, therefore, remarkable speed-up is achieved. The running time is comparable to that of the *k-means* with a lower distortion than that with the *k-means*. The improvement due to the neighborhood graph is significant.

In the third paper [**P3**], we introduce a new *multilevel thresholding* algorithm for image processing. The algorithm is derived from the *pairwise nearest neighbor* (*PNN*) method. The time complexity of the *PNN* method is lower bounded by $\Omega(N^2)$ in vector quantization. It is therefore not self-evident that the *PNN* method could be useful in real-time applications. For example, if the implementation is made poorly, the time complexity is $O(N^2)$ as in [CC03]. Our contribution is to show that *PNN thresholding* can be implemented in $O(N \cdot \log N)$ time.

Unlike in vector quantization, the one-dimensionality of the histogram of the image can be utilized so that the neighbor classes can be determined by using a simple linked list structure. This allows constant time updates of the data structures. At the same time, we use a heap structure for the search of the minimum cost class pair. The proposed method works in real time for any number of thresholds. Experiments also show that the proposed method, when combined with the *Lloyd-Max quantizer*, provides MSE values that are much closer to that of *optimal thresholding* than using *LMQ* alone. The difference is small when a low number of thresholds are needed (M = 2 or 3), but the difference is significant when the number of thresholds is higher (from M = 10 to M = 20).

In the fourth paper [**P4**], we propose a more general approach for agglomerative clustering called *iterative shrinking* (*IS*) that generates the clustering by a sequence of cluster removal operations. In the *IS* method, clusters are removed one at a time by reassigning the vectors in the removed cluster to the remaining nearby clusters. The *PNN* method can be considered a special case of the *IS* method since it removes one cluster and forces the vectors to move to the same neighbor-cluster. In the *IS* method, the vectors can be reassigned more freely. Apart from the difference in the removal operation, we follow the local optimization strategy of the *PNN* method and always remove the cluster that increases the cost function value least.

Experimental results show that the proposed method achieves better results than the comparative methods at the cost of slower speed. The time complexity of the method varies from $O(N^2)$ to $O(N^2 \cdot \log^2 N)$ depending on the variant. The proposed method was also applied as a crossover method in the *genetic algorithm* (*GAIS*). Experiments indicate that the proposed combination outperforms other clustering algorithms in terms of minimizing distortion. The *iterative shrinking* method also extends to the case where the number of the clusters must be determined simply by changing the optimization function. This does not add to the complexity since the solutions for variable number of clusters can be found during a single run of the proposed algorithm.

In the fifth paper [P5], we present an optimal clustering algorithm that was motivated by the *PNN* method. Optimal clustering can be found by considering all possible merge sequences and finding the one that minimizes the optimization function. The idea can be implemented as a *branch-and-bound* (*BB*) *technique* that uses a search tree for finding the optimal clustering. We present also two suboptimal, but polynomial, time variants from the branch-and-bound technique.

The time complexity of the optimal algorithm is still exponential despite the non-redundant search tree and the designed bounding criterion. The practical usability of the algorithm is therefore limited to small, special cases only. The two polynomial time algorithms from the branch-and-bound technique offer a good compromise between the optimal algorithm and the *PNN* method. They can operate with larger data sets than the optimal branch-and-bound technique.

The contributions of the papers can be briefly summarized as follows. All the ideas have been developed through the teamwork of all authors. The author of this thesis is responsible for all the new implementations in this work, has run most of the experiments in this thesis and has made significant contributions to the writing of the papers. The order of the authors is determined by the estimated overall contribution to the writing of the papers.

5 Summary of results

Next, the results of the proposed methods used in this thesis are summarized. For the comparisons, the following methods are selected:

(1) The *fast exact PNN* method [FKSC00].

(2) The *PNN with the speed-up* methods [**P1**].

(3) The *graph-based PNN* method [**P2**].

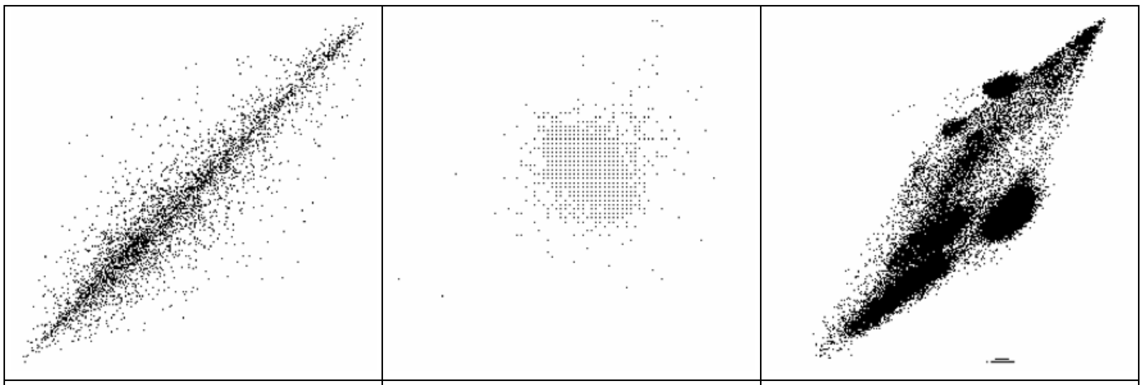
(4) The *iterative shrinking* method [**P4**].

(5) The *k-means* algorithm [KFN00].

(6) The *genetic algorithm* with *iterative shrinking* as crossover (*GAIS*) [**P4**].

Spatial vectors:	Spatial residual vectors:	Color vectors:
Bridge (256×256) K=16, N=4096	*Miss America* (360×288) K=16, N=6480	*House* (256×256) K=3, N=34112*

Figure 5.1. Image data sets used in this thesis. *Duplicate training vectors are combined and frequency information is stored. Note that when duplicate vectors are merged, all distance and merge cost calculations must always be multiplied by the frequency of the data vectors representing multiple instances of the original data set.

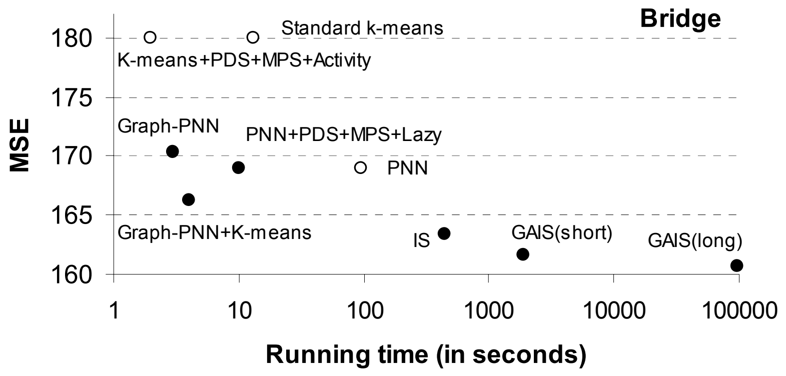


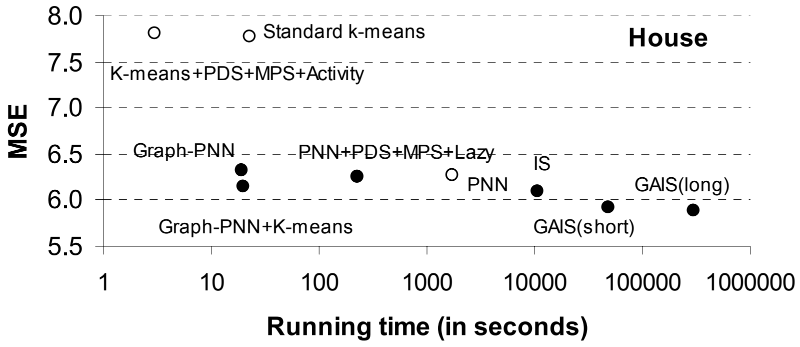
Data set *Bridge*	Data set *Miss America*	Data set *House*

Figure 5.2. Two-dimensional plots of the image data sets used in the experiments.

The experiments were performed for three data sets generated from different images; see Figures 5.1 and 5.2. The gray-scale image *Bridge* was divided into non-overlapping 4×4 pixel blocks. The data set *House* consists of color values of the *RGB* image. The third data set, *Miss America*, has been obtained by subtracting two subsequent image frames of the original video image sequence, and then constructing 4×4 spatial pixel blocks from the residuals. Only the first two frames have been used. In the two-dimensional plots, only the data of the first two dimensions of the image data sets are shown and the scale of each axis is from 0 to the maximum value of that dimension. The algorithms are coded in *DJGPP C* Version 2.01 and are run on a 450 MHz Pentium III personal computer that uses Microsoft Windows 98 Operating system.

Memory consumption of the methods is linear, except for the *GA* that stores *S* codebooks and mappings, and thus the *GA* consumes $O(NK + S(MK+N))$ space. Figure 5.3 illustrates the MSE values for the different methods as a function of running time. The summary of the MSE values and the running times as a function of codebook size is summarized in Table 5.1. Comparisons that are more detailed (or comparisons that are more detailed or more comparisons that are detailed?) are included in the individual papers.





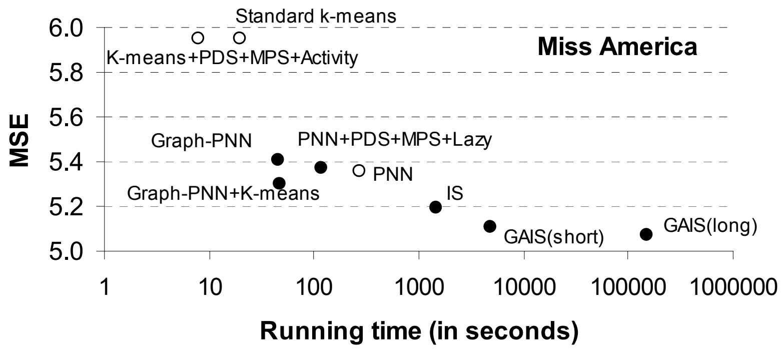


Figure 5.3. MSE values for the different methods as a function of running time.

Table 5.1. MSE values and running times for the different methods as a function of codebook size.

Bridge	MSE						Running time (in seconds)					
M	32	64	128	256	512	1024	32	64	128	256	512	1024
PNN	326.24	264.91	214.88	168.92	121.68	72.61	96	96	96	96	95	92
P1	326.24	264.91	214.88	168.92	121.68	72.61	11	10	10	10	10	9
P2	325.04	267.48	217.22	171.11	123.90	74.92	3	3	4	3	3	3
P4	318.07	258.36	209.42	163.38	117.41	70.52	469	465	459	444	413	362

House	MSE						Running time (in seconds)					
M	32	64	128	256	512	1024	32	64	128	256	512	1024
PNN	24.13	15.18	9.83	6.27	3.91	2.38	1734	1737	1736	1742	1736	1743
P1	24.04	15.27	9.85	6.26	3.92	2.39	230	231	230	226	227	229
P2	27.85	16.20	10.09	6.37	4.00	2.43	20	20	20	20	20	20
P4	23.65	14.83	9.56	6.09	3.79	2.29	10508	10449	10555	10569	10409	10113

Miss America	MSE						Running time (in seconds)					
M	32	64	128	256	512	1024	32	64	128	256	512	1024
PNN	9.04	7.81	6.60	5.36	4.11	2.85	268	266	268	270	269	264
P1	9.04	7.81	6.60	5.37	4.11	2.84	117	117	117	117	117	116
P2	9.04	7.83	6.64	5.44	4.19	2.90	48	47	47	47	47	47
P4	8.92	7.69	6.43	5.19	3.95	2.72	1580	1577	1553	1466	1390	1220

6 Conclusions

The main contributions of this thesis can be summarized as follows:

We have developed several speed-up improvements for the *PNN* method based on projection-based search, partial distortion search, and the use of a k nearest neighbor graph. The last idea could also be applied to other clustering algorithms that require a large number of distance calculations.

An efficient $O(N \cdot \log N)$ time implementation of the *PNN* method has been given for the 1-dimensional special case.

A generalization of the merge phase was proposed by introducing similar decremental clustering algorithms based on a slightly improved cluster removal operation. The results are systematically better than that of the *PNN* method although the differences are often small. However, in certain cases, the difference between the proposed *iterative shrinking* approach and the *PNN* method was decisive: the proposed method found the correct number of clusters (15), whereas the *PNN* method found only 14 clusters.

The merge approach of the *PNN* method was also used for generating optimal clustering, although the result is mainly theoretical. The idea, however, can have practical implications as was shown by introducing two polynomial time variants, motivated by the proposed optimal branch-and-bound algorithm.

7 References

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