Modern hierarchical, agglomerative clustering algorithms

Daniel Müllner

This paper presents algorithms for hierarchical, agglomerative clustering which perform most efficiently in the general-purpose setup that is given in modern standard software. Requirements are: (1) the input data is given by pairwise dissimilarities between data points, but extensions to vector data are also discussed (2) the output is a "stepwise dendrogram", a data structure which is shared by all implementations in current standard software. We present algorithms (old and new) which perform clustering in this setting efficiently, both in an asymptotic worst-case analysis and from a practical point of view. The main contributions of this paper are: (1) We present a new algorithm which is suitable for any distance update scheme and performs significantly better than the existing algorithms. (2) We prove the correctness of two algorithms by Rohlf and Murtagh, which is necessary in each case for different reasons. (3) We give well-founded recommendations for the best current algorithms for the various agglomerative clustering schemes.

Keywords: clustering, hierarchical, agglomerative, partition, linkage

1 Introduction

Hierarchical, agglomerative clustering is an important and well-established technique in unsupervised machine learning. Agglomerative clustering schemes start from the partition of the data set into singleton nodes and merge step by step the current pair of mutually closest nodes into a new node until there is one final node left, which comprises the entire data set. Various clustering schemes share this procedure as a common definition, but differ in the way in which the measure of inter-cluster dissimilarity is updated after each step. The seven most common methods are termed single, complete, average (UPGMA), weighted (WPGMA, McQuitty), Ward, centroid (UPGMC) and median (WPGMC) linkage (see Everitt et al., 2011, Table 4.1). They are implemented in standard numerical and statistical software such as R (R Development Core Team, 2011), MATLAB (The MathWorks, Inc., 2011), Mathematica (Wolfram Research, Inc., 2010), SciPy (Jones et al., 2001).

The stepwise, procedural definition of these clustering methods directly gives a valid but inefficient clustering algorithm. Starting with Gower's and Ross's observation (Gower and Ross, 1969) that single linkage clustering is related to the minimum spanning tree of a graph in 1969, several authors have contributed algorithms to reduce the computational complexity of agglomerative clustering, in particular Sibson (1973), Rohlf (1973), Anderberg (1973, page 135), Murtagh (1984), Day and Edelsbrunner (1984, Table 5).

Even when software packages do not use the inefficient primitive algorithm (as SciPy (Eads, 2007) and the R (R Development Core Team, 2011) methods hclust and agnes do), the author found that implementations largely use suboptimal algorithms rather than improved methods suggested in theoretical work. This paper is to advance the theory further up to a point where the algorithms can be readily used in the standard setting, and in this way bridge the gap between the theoretical advances that have been made and the existing software implementations, which are widely used in science and industry.

The main contributions of this paper are:

- We present a new algorithm which is suitable for any distance update scheme and performs significantly better than the existing algorithms for the "centroid" and "median" clustering schemes.
- We prove the correctness of two algorithms, a single linkage algorithm by Rohlf (1973) and Murtagh's nearest-neighbor-chain algorithm (Murtagh, 1985, page 86). These proofs were still missing, and we detail why the two proofs are necessary, each for different reasons.
- These three algorithms (together with an alternative by Sibson, 1973) are the best currently available ones, each for its own subset of agglomerative clustering schemes. We justify this carefully, discussing potential alternatives.

The specific class of clustering algorithms which is dealt with in this paper has been characterized by the acronym SAHN (sequential, agglomerative, hierarchic, nonoverlapping methods) by Sneath and Sokal (1973, § 5.4, 5.5). The procedural definition (which is given in Figure 1 below) is not the only possibility for a SAHN method, but this method together with the seven common distance update schemes listed above is most widely used. The scope of this paper is contained further by practical considerations: We consider methods here which comply to the input and output requirements of the general-purpose clustering functions in modern standard software:

- The input to the algorithm is the list of $\binom{N}{2}$ pairwise dissimilarities between N points. (We mention extensions to vector data in Section 6.)
- The output is a so called *stepwise dendrogram* (see Section 2.2), in contrast to laxly specified output structure or weaker notions of (non-stepwise) dendrograms in earlier literature.

The first item has always been a distinctive characteristic to previous authors since the input format broadly divides into the *stored matrix approach* (Anderberg, 1973, § 6.2) and the *stored data approach* (Anderberg, 1973, § 6.3). In contrast, the second condition has not been given attention yet, but we will see that it affects the validity of algorithms.

We do not aim to present and compare all available clustering algorithms but build upon the existing knowledge and present only the algorithms which we found the best for the given purpose. For reviews and overviews we refer to Rohlf (1982), Murtagh (1983, 1985), Gordon (1987, §3.1), Jain and Dubes (1988, §3.2), Day (1996, §4.2), Hansen and Jaumard (1997). Those facts about alternative algorithms which are necessary to complete the discussion and which are not covered in existing reviews are collected in Section 5.

The paper is structured as follows:

Section 2 contains the definitions for input and output data structures as well as specifications of the distance update formulas and the "primitive" clustering algorithm.

Section 3 is the main section of this paper. We present and discuss three algorithms: our own "generic algorithm", Murtagh's nearest-neighbor-chain algorithm and Rohlf's algorithm based on the minimum spanning tree of a graph. We prove the correctness of these algorithms.

Section 4 discusses the complexity of the algorithms, both as theoretical, asymptotic complexity in Section 4.1 and by use-case performance experiments in Section 4.2. We conclude this section by recommendations on which algorithm is the best one for each distance update scheme, based on the preceding analysis.

Section 5 discusses alternative algorithms, and Section 6 gives a short outlook on extending the context of this paper to vector data instead of dissimilarity input. The paper ends with a brief conclusion in Section 7.

The algorithms in this paper have been implemented in C++ by the author and are available with interfaces to the statistical software R and the programming language Python (van Rossum et al.). This implementation is presented elsewhere (Müllner, 2011).

2 Data structures and the algorithmic definition of SAHN clustering methods

In this section, we recall the common algorithmic (procedural) definition of the SAHN clustering methods which demarcate the scope of this paper. Before we do so, we concretize the setting further by specifying the input and output data structures for the clustering methods. Especially the output data structure has not been specifically considered in earlier works, but nowadays there is a *de facto* standard given by the shared conventions in the most widely used software. Hence, we adopt the setting from practice and specialize our theoretical consideration to the modern standard of the stepwise dendrogram. Later, Section 5 contains an example of how the choice of the output data structure affects the result which algorithms are suitable and/or most efficient.

2.1 Input data structure

The input to the hierarchical clustering algorithms in this paper is always a finite set together with a dissimilarity index (see Hansen and Jaumard, 1997, § 2.1).

Definition. A dissimilarity index on a set S is a map $d: S \times S \to [0, \infty)$ which is reflexive and symmetric, i.e. we have d(x, x) = 0 and d(x, y) = d(y, x) for all $x, y \in S$.

A metric on S is certainly a dissimilarity index. In the scope of this paper, we call the values of d distances in a synonymous manner to dissimilarities, even though they are not required to fulfill the triangle inequalities, and dissimilarities between different elements may be zero.

If the set S has N elements, a dissimilarity index is given by the $\binom{N}{2}$ pairwise dissimilarities. Hence, the input size to the clustering algorithms is $\Theta(N^2)$. Once the primitive clustering algorithm is specified in Section 2.4, it is easy to see that the hierarchical clustering schemes are sensitive to each input value. More precisely, for every input size N and for every index pair $i \neq j$, there are two dissimilarities which differ only at position (i,j) and which produce different output. Hence, all input values must be processed by a clustering algorithm, and therefore the run-time is bounded below by $\Omega(N^2)$.

This bound applies to the general setting when the input is a dissimilarity index. In a different setting, the input could also be given as N points in a normed vector space of dimension D (the "stored data approach", Anderberg, 1973, §6.3). This results in an input size of $\Theta(ND)$, so that the lower bound does not apply for clustering of vector data. See

Section 6 for a discussion to which extent the algorithms in this paper can be used in the "stored data approach".

2.2 Output data structures

The output of a hierarchical clustering procedure is traditionally a dendrogram. The term "dendrogram" has been used with three different meanings: a mathematical object, a data structure and a graphical representation of the former two. In the course of this section, we define a data structure and call it stepwise dendrogram. A graphical representation may be drawn from the data in one of several existing fashions. The graphical representation might lose information (e.g. when two merges happen at the same dissimilarity value), and at the same time contain extra information which is not contained in the data itself (like a linear order of the leaves).

In the older literature, e.g. Sibson (1973), a dendrogram (this time, as a mathematical object) is rigorously defined as a piecewise constant, right-continuous map $D: [0, \infty) \to \mathcal{P}(S)$, where $\mathcal{P}(S)$ denotes the partitions of S, such that

- D(s) is always coarser than or equal to D(t) for s > t,
- D(s) eventually becomes the one-set partition $\{S\}$ for large s.

A dendrogram in this sense with the additional condition that D(0) is the singleton partition is in one-to-one correspondence to an *ultrametric* on S (Johnson, 1967, § I). The ultrametric distance between x and y is given by $\mu(x,y) = \min\{s \geq 0 \mid x \sim y \text{ in } D(s)\}$. Conversely, the partition at level $s \geq 0$ in the dendrogram is given by the equivalence relation $x \sim y \Leftrightarrow \mu(x,y) \leq s$. Sibson's "pointer representation" and "packed representation" (Sibson, 1973, § 4) are examples of data structures which allow the compact representation of a dendrogram or ultrametric.

In the current software, however, the output of a hierarchical clustering procedure is a different data structure which conveys potentially more information. We call this a *stepwise dendrogram*.

Definition. Given a finite set S_0 with cardinality $N = |S_0|$, a stepwise dendrogram is a list of N-1 triples (a_i,b_i,δ_i) $(i=0,\ldots,N-2)$ such that $\delta_i \in [0,\infty)$ and $a_i,b_i \in S_i$, where S_{i+1} is recursively defined as $(S_i \setminus \{a_i,b_i\}) \cup n_i$ and $n_i \notin S \setminus \{a_i,b_i\}$ is a label for a new node.

This has the following interpretation: The set S_0 are the initial data points. In each step, n_i is the new node which is formed by joining the nodes a_i and b_i at the distance δ_i . The order of the nodes within each pair (a_i, b_i) does not matter. The procedure contains N-1 steps, so that the final state is a single node which contains all N initial nodes.

(The mathematical object behind this data structure is a sequence of N+1 distinct, nested partitions from the singleton partition to the one-set partition, together with a nonnegative real number for each partition. We do not need this abstract point of view here, though.)

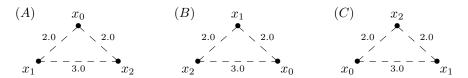
The identity of the new labels n_i is not part of the data structure; instead it is assumed that they are generated according to some rule which is part of the specific data format convention. In view of this, it is customary to label the initial data points and the new nodes by integers. For example, the following schemes are used in software:

- R convention: $S_0 := (-1, \dots, -N)$, new nodes: $(1, \dots, N-1)$
- SciPy convention: $S_0 := (0, ..., N-1)$, new nodes: (N, ..., 2N-2)
- MATLAB convention: $S_0 := (1, ..., N)$, new nodes: (N+1, ..., 2N-1)

We regard a stepwise dendrogram both as an $((N-1)\times 3)$ -matrix or as a list of triples, whichever is more convenient in a given situation.

If the sequence (δ_i) in Section 2.2 is non-decreasing, one says that the stepwise dendrogram does not contain *inversions*, otherwise it does.

In contrast to the first notion of a dendrogram above, a stepwise dendrogram can take inversions into account, which an ordinary dendrogram cannot. Moreover, if more than two nodes are joined at the same distance, the order of the merging steps does matter in a stepwise dendrogram. Consider e.g. the following data sets with three points:



The array

$$\begin{bmatrix} 0, & 1, & 2.0 \\ 2, & 3, & 2.0 \end{bmatrix}$$

is a valid output (SciPy conventions) for single linkage clustering on the data sets (A) and (B) but not for (C). Even more, there is no stepwise dendrogram which is valid for all three data sets simultaneously. On the other hand, the non-stepwise single linkage dendrogram is the same in all cases:

$$D(s) = \begin{cases} \{x_0\}, \{x_1\}, \{x_2\} & \text{if } s < 2 \\ \{x_0, x_1, x_2\} & \text{if } s \ge 2 \end{cases} \quad \text{pictorially:} \quad \begin{vmatrix} & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & & \\ & & \\ & & \\ & & & \\ &$$

Hence, a stepwise dendrogram conveys slightly more information than a non-stepwise dendrogram in the case of *ties* (i.e. when more than one merging step occurs at a certain distance). This must be taken into account when we check the correctness of the algorithms. Although this complicates the proofs in Sections 3.3 and 3.2 and takes away from the simplicity of the underlying ideas, it is not a matter of hairsplitting: E.g. Sibson's SLINK algorithm (Sibson, 1973) for single linkage clustering works flawlessly if all distances are distinct but produces the same output on all data sets (A), (B) and (C). Hence, the output cannot be converted into a stepwise dendrogram. See Section 5 for further details.

2.3 Node labels

The node labels n_i in a stepwise dendrogram may be chosen as unique integers according to one of the schemes described in the last section. In an implementation, when the dissimilarities are stored in a large array in memory, it is preferable if each node label n_i for the joined cluster reuses one of the indices a_i, b_i of its constituents, so that the dissimilarities can be updated in-place. Since the clusters after each row in the dendrogram form a partition of the initial set S_0 , we can identify each cluster not only by its label but also by one of its members. Hence, if the new node label n_i is chosen among a_i, b_i , this is sufficient to reconstruct the partition at every stage of the clustering process, and labels can be converted to any other convention in a postprocessing step. Generating unique labels from cluster representatives takes only $\Theta(N)$ time and memory with a suitable union-find data structure. See Section 3.2 and Figure 5 for details.

Figure 1 Algorithmic definition of a hierarchical clustering scheme.

```
1: procedure Primitive Clustering(S, d) \triangleright S: node labels, d: pairwise dissimilarities
         N \leftarrow |S|
                                                                                         ▶ Number of input nodes
 2:
         L \leftarrow []
 3:
                                                                                                         ▷ Output list
 4:
         size[x] \leftarrow 1 \text{ for all } x \in S
         for i \leftarrow 0, \ldots, N-2 do
 5:
             (a,b) \leftarrow \operatorname{argmin}_{(S \times S) \setminus \Delta} d
 6:
             Append (a, b, d[a, b]) to L.
 7:
             S \leftarrow S \setminus \{a, b\}
 8:
              Create a new node label n \notin S.
 9:
              Update d with the information
10:
                         d[n, x] = d[x, n] = \text{FORMULA}(d[a, x], d[b, x], d[a, b], size[a], size[b], size[x])
              for all x \in S.
              size[n] \leftarrow size[a] + size[b]
11:
              S \leftarrow S \cup \{n\}
12:
         end for
13:
         return L
                                                     \triangleright the stepwise dendrogram, an ((N-1)\times 3)-matrix
14:
15: end procedure
(As usual, \Delta denotes the diagonal in the Cartesian product S \times S.)
```

2.4 The primitive clustering algorithm

The solution that we expect from a hierarchical clustering algorithm is defined procedurally. All algorithms in this paper are measured against the primitive algorithm in Figure 1. We state it in a detailed form to point out exactly which information about the clusters is maintained: the pairwise dissimilarities and the number of elements in each cluster.

The function FORMULA in line 10 is the distance update formula, which returns the distance from a node x to the newly formed node $a \cup b$ in terms of the dissimilarities between clusters a, b and x and their sizes. The table in Figure 2 lists the formulas for the common distance update methods.

For five of the seven formulas, the distance between clusters does not depend on the order which the clusters were formed by merging. In this case, we also state closed, non-iterative formulas for the cluster dissimilarities in the third row in Figure 2. The distances in the "weighted" and the "median" update scheme depend on the order, so we cannot give non-iterative formulas.

The "centroid" and "median" formulas can produce inversions in the stepwise dendrograms; the other five methods cannot. This can be checked easily: The sequence of dissimilarities at which clusters are merged in Figure 1 cannot decrease if the following condition is fulfilled for all disjoint subsets $I, J, K \subset S_0$:

$$d(I,J) < \min\{d(I,K), d(J,K)\} \Rightarrow d(I,J) < d(I \cup J,K)$$

On the other hand, configurations with inversion in the "centroid" and "median" schemes can be easily produced, e.g. three points near the vertices of an equilateral triangle in \mathbb{R}^2 .

The primitive algorithm takes $\Theta(N^3)$ time since in the *i*-th iteration of N-1 in total, all $\binom{N-1-i}{2} \in \Theta(i^2)$ pairwise distances between the N-i nodes in S are searched.

Note that the stepwise dendrogram from a clustering problem (S, d) is not always uniquely defined, since the minimum in line 6 of the algorithm might be attained for several index

Figure 2 Agglomerative clustering schemes.		
Name	Distance update formula	Cluster dissimilarity
	Formula for $d(I \cup J, K)$	between clusters A and B
single	$\min(d(I,K),d(J,K))$	$\min_{a \in A, b \in B} d[a, b]$
complete	$\max(d(I,K),d(J,K))$	$\max_{a \in A, b \in B} d[a, b]$
average	$\frac{n_I d(I,K) + n_J d(J,K)}{n_I + n_J}$	$\frac{1}{ A B } \sum_{a \in A} \sum_{b \in B} d[a, b]$
weighted	$\frac{d(I,K) + d(J,K)}{2}$	
Ward	$\sqrt{\frac{(n_I + n_K)d(I, K) + (n_J + n_K)d(J, K) - n_Kd(I, J)}{n_I + n_J + n_K}}$	$\sqrt{\frac{2 A B }{ A + B }} \cdot \ \vec{c}_A - \vec{c}_B\ _2$
centroid	$\sqrt{\frac{n_{I}d(I,K) + n_{J}d(J,K)}{n_{I} + n_{J}} - \frac{n_{I}n_{J}d(I,J)}{(n_{I} + n_{J})^{2}}}$	$\ \vec{c}_A - \vec{c}_B\ _2$
median	$\sqrt{\frac{d(I,K)}{2} + \frac{d(J,K)}{2} - \frac{d(I,J)}{4}}$	$\ \vec{w}_A - \vec{w}_B\ _2$

Legend: Let I, J be two clusters joined into a new cluster, and let K be any other cluster. Denote by n_I, n_J and n_K the sizes of (i.e. number of elements in) clusters I, J, K, respectively.

The update formulas for the "Ward", "centroid" and "median" methods assume that the input points are given as vectors in Euclidean space with the Euclidean distance as dissimilarity measure. The expression \vec{c}_X denotes the centroid of a cluster X. The point \vec{w}_X is defined iteratively and depends on the clustering steps: If the cluster L is formed by joining I and J, we define \vec{w}_L as the midpoint $\frac{1}{2}(\vec{w}_I + \vec{w}_J)$.

All these formulas can be subsumed (for squared Euclidean distances in the three latter cases) under a single formula

$$d(I \cup J, K) := \alpha_I d(I, K) + \alpha_J d(J, K) + \beta d(I, J) + \gamma |d(I, K) - d(J, K)|,$$

where the coefficients $\alpha_I, \alpha_J, \beta$ may depend on the number of elements in the clusters I, J and K. For example, $\alpha_I = \alpha_J = \frac{1}{2}, \beta = 0, \gamma = -\frac{1}{2}$ gives the single linkage formula. All clustering methods which use this formula are combined under the name "flexible" in this paper, as introduced by Lance and Williams (1967).

References: Lance and Williams (1967), Kaufman and Rousseeuw (1990, §5.5.1)

pairs. We consider every possible output of PRIMITIVE_CLUSTERING under any choices of minima as a valid output.

3 Algorithms

In the main section of this paper, we present three algorithms which are the most efficient ones for the task of SAHN clustering with the stored matrix approach. Two of the algorithms were described previously: The nearest-neighbor chain ("NN-chain") algorithm by Murtagh (1985, page 86), and an algorithm by Rohlf (1973), which we call "MST-algorithm" here since it is based on Prim's algorithm for the minimum spanning tree of a graph. Both algorithms were presented by the respective authors, but for different reasons each one still lacks a correctness proof. Sections 3.2 and 3.3 state the algorithms in a way which is suitable for modern standard input and output structures and supply the proofs of correctness.

The third algorithm in Section 3.1 is a new development based on Anderberg's idea to maintain a list of nearest neighbors for each node Anderberg (1973, pages 135–136). While we do not show that the worst-case behavior of our algorithm is better than the $O(N^3)$ worst-case complexity of Anderberg's algorithm, the new algorithm is for all inputs at least equally fast, and we show by experiments in Section 4.2 that the new algorithm is considerably faster in practice since it cures Anderberg's algorithm from its worst-case behavior at random input.

As we saw in the last section, the solution to a hierarchical clustering task does not have a simple, self-contained specification but is defined as the outcome of the "primitive" clustering algorithm. The situation is complicated by the fact that the primitive clustering algorithm itself is not completely specified: if a minimum inside the algorithm is attained at more than one place, a choice must be made. We do not require that ties are broken in a specific way; instead we consider any output of the primitive algorithm under any choices as a valid solution. Each of the "advanced" algorithms is considered correct if it always returns one of the possible outputs of the primitive algorithm.

3.1 The generic clustering algorithm

The most generally usable algorithm is described in this section. We call it GENERIC_LINKAGE since it can be used with any distance update formula. It is the only algorithm among the three in this paper which can deal with inversions in the dendrogram. Consequentially, the "centroid" and "median" methods must use this algorithm.

The algorithm is presented in Figure 3. It is a sophistication of the primitive clustering algorithm and of Anderberg's approach (Anderberg, 1973, pages 135–136). Briefly, candidates for nearest neighbors of clusters are cached in a priority queue to speed up the repeated minimum searches in line 6 of PRIMITIVE CLUSTERING.

For the pseudocode in Figure 3, we assume that the set S are integer indices from 0 to N-1. This is the way in which it may be done in an implementation, and it makes the description easier than for an abstract index set S. In particular, we rely on an order of the index set (see e.g. line 6: the index ranges over all y > x).

There are two levels of sophistication from the primitive clustering algorithm to our generic clustering algorithm. In a first step, one can maintain a list of nearest neighbors for each cluster. For the sake of speed, it is enough to search for the nearest neighbors of a node x only among the nodes with higher index y > x. Since the dissimilarity index is symmetric, this list will still contain a pair of closest nodes. The list of nearest neighbors speeds up the global minimum search in the i-th step from $\binom{N-i-1}{2}$ comparisons to N-i-1 comparisons at the beginning of each iteration. However, the list of nearest neighbors must be maintained: if the

Figure 3 The generic clustering algorithm.

```
1: procedure Generic Linkage(N, d)
                                                                \triangleright N: input size, d: pairwise dissimilarities
         S \leftarrow (0, \dots, N-1)
 2:
         L \leftarrow []
                                                                                                      ▷ Output list
 3:
         size[x] \leftarrow 1 \text{ for all } x \in S
 4:
         for x in S \setminus \{N-1\} do
                                                                   ▷ Generate the list of nearest neighbors.
 5:
             n\_nghbr[x] \leftarrow \operatorname{argmin}_{y>x} d[x,y]
 6:
 7:
             mindist[x] \leftarrow d[x, n\_nghbr[x]]
         end for
 8:
         Q \leftarrow \text{(priority queue of indices in } S \setminus \{N-1\}, \text{ keys are in } mindist)
 9:
         for i \leftarrow 1, \ldots, N-1 do
                                                                                                      ▶ Main loop.
10:
             a \leftarrow (\text{minimal element of } Q)
11:
             b \leftarrow n \quad nqhbr[a]
12:
             \delta \leftarrow mindist[a]
13:
             while \delta \neq d[a,b] do
                                                       ▶ Recalculation of nearest neighbors, if necessary.
14:
                  n\_nghbr[a] \leftarrow \operatorname{argmin}_{x>a} d[a,x]
15:
                  Update mindist and Q with (a, d[a, n\_nghbr[a]])
16:
                  a \leftarrow (\text{minimal element of } Q)
17:
                 b \leftarrow n\_nghbr[a]
18:
                  \delta \leftarrow mindist[a]
19:
             end while
20:
             Remove the minimal element a from Q.
21:
             Append (a, b, \delta) to L.
                                                                         ▶ Merge the pairs of nearest nodes.
22:
             size[b] \leftarrow size[a] + size[b]
                                                                 \triangleright Re-use b as the index for the new node.
23:
             S \leftarrow S \setminus \{a\}
24:
             for x in S \setminus \{b\} do
                                                                                ▶ Update the distance matrix.
25:
                  d[x,b] \leftarrow d[b,x] \leftarrow \text{Formula}(d[a,x],d[b,x],d[a,b],\textit{size}[a],\textit{size}[b],\textit{size}[x])
26:
27:
             end for
             for x in S such that x < a do
                                                               ▶ Update candidates for nearest neighbors.
28:
                 if n nghbr[x] = a then
                                                                                 ▶ Deferred search; no nearest
29:
                      n\_nghbr[x] \leftarrow b
                                                                                ▷ neighbors are searched here.
30:
                  end if
31:
             end for
32:
             for x in S such that x < b do
33:
                  if d[x,b] < mindist[x] then
34:
                      n \quad nghbr[x] \leftarrow b
35:
                      Update mindist and Q with (x, d[x, b])
                                                                                     ▶ Preserve a lower bound.
36:
                  end if
37:
             end for
38:
             n\_nghbr[b] \leftarrow \operatorname{argmin}_{x>b} d[b,x]
39:
             Update mindist and Q with (b, d[b, n \ nghbr[b]])
40:
         end for
41:
         {\bf return}\ L
                                                  \triangleright The stepwise dendrogram, an ((N-1)\times 3)-matrix.
42:
43: end procedure
```

nearest neighbor of a node x is one of the clusters a, b which are joined, then it is sometimes necessary to search again for the nearest neighbor of x among all nodes y > x. Altogether, this reduces the best-case complexity of the clustering algorithm from $\Theta(N^3)$ to $\Theta(N^2)$, while the worst case complexity remains $O(N^3)$. This is the method that Anderberg suggested in (Anderberg, 1973, pages 135–136).

On a second level, one can try to avoid or delay the nearest neighbor searches as long as possible. Here is what the algorithm Generic_Linkage does: It maintains a list n_nghbr of **candidates** for nearest neighbors, together with a list mindist of **lower bounds** for the distance to the true nearest neighbor. If the distance $d[x, n_nghbr[x]]$ is equal to mindist[x], we know that we have the true nearest neighbor, since we found a realization of the lower bound; otherwise the algorithm must search for the nearest neighbor of x again.

To further speed up the minimum searches, we also make the array mindist into a priority queue, so that the current minimum can be found quickly. We require a priority queue Q with a minimal set of methods as in the list below. This can be implemented conveniently by a binary heap (see Cormen et al., 2009, Chapter 6). We state the complexity of each operation by the complexity for a binary heap.

- QUEUE(v): Generate a new queue from a vector v of length |v| = N. Return: an object Q. Complexity: O(N).
- Q.Argmin: Return the index to a minimal value of v. Complexity: O(1).
- Q.Remove_Min: Remove the minimal element from the queue. Complexity: $O(\log N)$.
- Q.UPDATE(i, x): Assign $v[i] \leftarrow x$ and update the queue accordingly. Complexity: $O(\log N)$.

We can now describe the GENERIC_LINKAGE algorithm step by step: Lines 5 to 8 search the nearest neighbor and the closest distance for each point x among all points y > x. This takes $O(N^2)$ time. In line 9, we generate a priority queue from the list of nearest neighbors and minimal distances.

The main loop is from line 10 to the end of the algorithm. In each step, the list L for a stepwise dendrogram is extended by one row, in the same way as the primitive clustering algorithm does.

Lines 11 to 20 find a current pair of closest nodes. A candidate for this is the minimal index in the queue (assigned to a), and its candidate for the nearest neighbor $b := n_nghbr[a]$. If the lower bound mindist[a] is equal to the actual dissimilarity d[a,b], then we are sure that we have a pair of closest nodes and their distance. Otherwise, the candidates for the nearest neighbor and the minimal distance are not the true values, and we find the true values for $n_nghbr[a]$ and mindist[a] in line 15 in O(N) time. We repeat this process and extract the minimum among all lower bounds from the queue until we find a valid minimal entry in the queue and therefore the actual closest pair of points.

This procedure is the performance bottleneck of the algorithm. The algorithm might be forced to update the nearest neighbor O(N) times with an effort of O(N) for each of the O(N) iterations, so the worst-case performance is bounded by $O(N^3)$. In practice, the inner loop from lines 14 to 20 is executed less often, which results in faster performance.

Lines 22 to 27 are nearly the same as in the primitive clustering algorithm. The only difference is that we specialize from an arbitrary label for the new node to re-using the index b for the joined node. The index a becomes invalid, and we replace any nearest-neighbor reference to a by a reference to the new cluster b in lines 28 to 32. Note that the array n_nghbr contains only candidates for the nearest neighbors, so we could have written any

valid index here; however, for the single linkage method, it makes sense to choose b: if the nearest neighbor of a node was at index a, it is now at b, which represents the join $a \cup b$.

The remaining code in the main loop ensures that the array n_nghbr still contains lower bounds on the distances to the nearest neighbors. If the distance from the new cluster x to a cluster b < x is smaller than the old bound for b, we record the new smallest distance and the new nearest neighbor in lines 34 to 37.

Lines 39 and 40 finally find the nearest neighbor of the new cluster and record it in the arrays n_nghbr and mindist and the queue Q

The main idea behind this approach is that invalidated nearest neighbors are not recomputed immediately. Suppose that the nearest neighbor of a node x is far away from x compared to the global closed pair of nodes. Then it does not matter that we do not know the nearest neighbor of x, as long as we have a lower bound on the distance to the nearest neighbor. The candidate for the nearest neighbor might remain invalid, and the true distance might remain unknown for many iterations, until the lower bound for the nearest-neighbor distance has reached the top of the queue Q. By then, the set of nodes S might be much smaller since many of them were already merged, and the algorithm might have avoided many unnecessary repeated nearest-neighbor searches for x in the meantime.

This concludes the discussion of our generic clustering algorithm; for the performance see Section 4. Our explanation of how the minimum search is improved also proves the correctness of the algorithm: Indeed, in the same way as the primitive algorithm does, the Generic_Linkage algorithm finds a pair of globally closest nodes in each iteration. Hence the output is always the same as from the primitive algorithm (or more precisely: one of several valid possibilities if the closest pair of nodes is not unique in some iteration).

3.2 The nearest-neighbor-chain algorithm

In this section, we present and prove correctness of the nearest-neighbor-chain algorithm (shortly: NN-chain algorithm), which was described by Murtagh (1985, page 86). This algorithm can be used for the "single", "complete", "average", "weighted" and "Ward" methods.

The NN-chain algorithm is presented in Figure 4 as NN-CHAIN-LINKAGE. It consists of the core algorithm NN-CHAIN-CORE and two postprocessing steps. Because of the postprocessing, we call the output of NN-CHAIN-CORE an unsorted dendrogram. The unsorted dendrogram must first be sorted row-wise, with the dissimilarities in the third column as the sorting key. In order to correctly deal with merging steps which happen at the same dissimilarity, it is crucial that a stable sorting algorithm is employed, i.e. one which preserves the relative order of elements with equal sorting keys. At this point, the first two columns of the output array L contain the label of a member of the respective cluster, but not the unique label of the node itself. The second postprocessing step is to generate correct node labels from cluster representatives. This can be done in $\Theta(N)$ time with a union-find data structure. Since this is a standard technique, we do not discuss it here but state an algorithm in Figure 5 for the sake of completeness. It generates integer node labels according to the convention in SciPy but can easily be adapted to follow any convention.

We prove the correctness of the NN-chain algorithm in this paper for two reasons:

- We make sure that the algorithm resolves ties correctly, which was not in the scope of earlier literature.
- Murtagh claims (Murtagh, 1984, page 111), (Murtagh, 1985, bottom of page 86) that the NN-chain algorithm works for any distance update scheme which fulfills a certain "reducibility property"

$$d(I,J) \le \min\{d(I,K), d(J,K)\} \quad \Rightarrow \quad \min\{d(I,K), d(J,K)\} \le d(I \cup J,K) \tag{1}$$

for all disjoint nodes I, J, K at any stage of the clustering (Murtagh, 1984, § 3), (Murtagh, 1985, § 3.5). This is false. We give a correct proof which also shows the limitations of the algorithm. In Murtagh's papers (Murtagh, 1984, 1985), it is not taken into account that the dissimilarity between clusters may depend on the order of clustering steps; on the other hand, it is explicitly said that the algorithm works for the "weighted" scheme, in which dissimilarities depend on the order of the steps.

Since there is no published proof for the NN-chain algorithm but claims which go beyond what the algorithm can truly do, it is necessary to establish the correctness by a strict proof:

Theorem 1. Fix a distance update formula. For any sequence of merging steps and any four disjoint clusters I, J, K, L resulting from these steps, require two properties from the distance update formula:

- It fulfills the reducibility property (1).
- The distance $d(I \cup J, K \cup L)$ is independent of whether (I, J) are merged first and then (K, L) or the other way round.

Then the algorithm NN-CHAIN-LINKAGE produces valid stepwise dendrograms for the given method.

Proposition 2. The "single", "complete", "average", "weighted" and "Ward" distance update formulas fulfill the requirements of Theorem 1.

Proof of Theorem 1. We prove the theorem by induction in the size of the input set S. The induction start is trivial since a dendrogram for a one-point set is empty.

We call two nodes $a, b \in S$ reciprocal nearest neighbors ("pairwise nearest neighbors" in the terminology of Murtagh, 1985) if the distance d[a, b] is minimal among all distances from a to points in S, and also minimal among all distances from b:

$$d[a,b] = \min_{\substack{x \in S \\ x \neq a}} d[a,x] = \min_{\substack{x \in S \\ x \neq b}} d[b,x].$$

Every finite set S with at least two elements has at least one pair of reciprocal nearest neighbors, namely a pair which realizes the global minimum distance.

The list *chain* is in the algorithm constructed in a way such that every element is a nearest neighbor of its predecessor. If *chain* ends in $[\ldots, b, a, b]$, we know that a and b are reciprocal nearest neighbors. The main idea behind the algorithm is that reciprocal nearest neighbors a, b always contribute a row (a, b, d[a, b]) to the stepwise dendrogram, even if they are not discovered in ascending order of dissimilarities.

¹For example, consider the distance update formula $d(I \cup J, K) := d(I, K) + d(J, K) + d(I, J)$. This formula fulfills the reducibility condition. Consider the following distance matrix between five points in the first column below. The Primitive_clustering algorithm produces the correct stepwise dendrogram in the middle column. However, if the point A is chosen first in line 7 of NN-chain-core, the algorithm outputs the incorrect dendrogram in the right column.

Figure 4 The nearest-neighbor clustering algorithm.

```
1: procedure NN-CHAIN-LINKAGE(S, d)
                                                             \triangleright S: node labels, d: pairwise dissimilarities
         L \leftarrow \text{NN-chain-core}(N, d)
 2:
        Stably sort L with respect to the third column.
 3:
        L \leftarrow \text{Label}(L)
                                                       ▶ Find node labels from cluster representatives.
 4:
 5:
        return L
 6: end procedure
 1: procedure NN-CHAIN-CORE(S, d)
                                                             \triangleright S: node labels, d: pairwise dissimilarities
         S \leftarrow (0, \dots, N-1)
 2:
 3:
         chain = []
        size[x] \leftarrow 1 \text{ for all } x \in S
 4:
        while |S| > 1 do
 5:
 6:
            if length(chain) \leq 3 then
 7:
                 a \leftarrow (\text{any element of } S)
                                                                                                     \triangleright E.g. S[0]
 8:
                 chain \leftarrow [a]
                 b \leftarrow (\text{any element of } S \setminus \{a\})
                                                                                                     \triangleright E.g. S[1]
 9:
10:
             else
                 a \leftarrow chain[-4]
11:
12:
                 b \leftarrow chain[-3]
                 Remove chain[-1], chain[-2] and chain[-3]
                                                                                      \triangleright Cut the tail (x, y, x).
13:
             end if
14:
             repeat
15:
                 c \leftarrow \operatorname{argmin}_{x \neq a} d[x, a] with preference for b
16:
                 a, b \leftarrow c, a
17:
                 Append a to chain
18:
             until length(chain) \geq 3 and a = chain[-3]
                                                                                          \triangleright a, b are reciprocal
19:
             Append (a, b, d[a, b]) to L
                                                                                          ▷ nearest neighbors.
20:
             Remove a, b from S
21:
22:
             n \leftarrow \text{(new node label)}
             size[n] \leftarrow size[a] + size[b]
23:
24:
             Update d with the information
                       d[n,x] = d[x,n] = \text{FORMULA}(d[a,x],d[b,x],d[a,b],size[a],size[b],size[x])
             for all x \in S.
             S \leftarrow S \cup \{n\}
25:
        end while
26:
        return L
                                                                                  ▷ an unsorted dendrogram
27:
28: end procedure
(We use the Python index notation: chain[-2] is the second-to-last element in the list chain.)
```

Figure 5 A union-find data structure suited for the output conversion.

```
1: procedure Label(L)
       L' \leftarrow []
2:
       N \leftarrow \text{(number of rows in } L) + 1
                                                                          ▶ Number of initial nodes.
3:
       U \leftarrow \text{new Union-Find}(N)
4:
 5:
       for (a, b, \delta) in L do
           Append (U.Efficient-Find(a), U.Efficient-Find(b), \delta) to L'
 6:
7:
       end for
8:
       return L'
9:
10: end procedure
11: class Union-Find
12:
       method Constructor(N)
                                                                 \triangleright N is the number of data points.
           parent \leftarrow \text{new int}[2N-1]
13:
           parent[0, \dots, 2N-2] \leftarrow None
14:
           nextlabel \leftarrow N
                                                        \triangleright SciPy convention: new labels start at N
15:
       end method
16:
17:
       method Union(m, n)
           parent[m] = nextlabel
18:
           parent[n] = nextlabel
19:
           nextlabel \leftarrow nextlabel + 1
                                           ▷ SciPy convention: number new labels consecutively
20:
21:
       end method
       method FIND(n)
                                              \triangleright This works but the search process is not efficient.
22:
           while parent[n] is not None do
23:
               n \leftarrow parent[n]
24:
25:
           end while
           return n
26:
       end method
27:
       method Efficient-Find(n)
                                                                   > This speeds up repeated calls.
28:
29:
           p \leftarrow n
30:
           while parent[n] is not None do
               n \leftarrow parent[n]
31:
           end while
32:
           while parent[p] \neq n do
33:
               p, parent[p] \leftarrow parent[p], n
34:
           end while
35:
           return n
36:
       end method
37:
38: end class
```

Lines 15 to 19 in NN-CHAIN-CORE clearly find reciprocal nearest neighbors (a,b) in S. One important detail is that the index b is preferred in the argmin search in line 16, if the minimum is attained at several indices and b realizes the minimum. This can be respected in an implementation with no effort, and it ensures that reciprocal nearest neighbors are indeed found. That is, the list chain never contains a cycle of length > 2, and a $chain = [\dots, b, a]$ with reciprocal nearest neighbors at the end will always be extended by b, never with an element $c \neq b$ which coincidentally has the same distance to a.

After line 19, the chain ends in (b, a, b). The nodes a and b are then joined, and the internal variables are updated as usual.

We now show that the remaining iterations produce the same output as if the algorithm had started with the set $S' := (S \setminus \{a,b\}) \cup \{n\}$, where n is the new node label and the distance array d and the *size* array are updated accordingly.

The only data which could potentially be corrupted is that the list chain could not contain successive nearest neighbors any more, since the new node n could have become the nearest neighbor of a node in the list.

At the beginning of the next iteration, the last elements (b, a, b) are removed from *chain*. The list *chain* then clearly does not contain a or b at any place any more, since any occurrence of a or b in the list would have led to an earlier pair of reciprocal nearest neighbors, before (b, a, b) was appended to the list. Hence, *chain* contains only nodes which really are in S. Let e, f be two successive entries in *chain*, i.e. f is a nearest neighbor of e. Then we know

$$d[e, f] \le d[e, a] \qquad \qquad d[a, b] \le d[a, e]$$

$$d[e, f] \le d[e, b] \qquad \qquad d[a, b] \le d[b, e]$$

Together with the reducibility property (1) (for I=a, J=b, K=e), this implies $d[e,f] \le d[e,n]$. Hence, f is still the nearest neighbor of e, which proves our assertion.

We can therefore be sure that the remaining iterations of NN-CHAIN-CORE produce the same output as if the algorithm would be run freshly on S'. By the inductive assumption, this produces a valid stepwise dendrogram for the set S' with N-1 nodes. Proposition 3 carries out the remainder of the proof, as it shows that the first line (a,b,d[a,b]) of the unsorted dendrogram, when it is sorted into the right place in the dendrogram for the nodes in S', is a valid stepwise dendrogram for the original set S with N nodes.

Proposition 3. Let (S,d) be a set with dissimilarities (|S| > 1). Fix a distance update formula which fulfills the requirements in Theorem 1. Let a,b be two distinct nodes in S which are reciprocal nearest neighbors.

Define S' as $(S \setminus \{a,b\}) \cup \{n\}$, where the label n represents the union $a \cup b$. Let d' be the updated dissimilarity matrix for S', according to the chosen formula. Let $L' = ((a_i, b_i, \delta_i)_{i=0,...,m})$ be a stepwise dendrogram for S'. Let j be the index such that all $\delta_i < d[a,b]$ for all i < j and $\delta_i \geq d[a,b]$ for all $i \geq j$. That is, j is the index where the new row (a,b,d[a,b]) should be inserted to preserve the sorting order, giving d[a,b] priority over potentially equal sorting keys. Then the array L, which we define as

$$\rightarrow \begin{bmatrix}
a_0 & b_0 & \delta_0 \\
... & & & \\
a_{j-1} & b_{j-1} & \delta_{j-1} \\
a & b & d[a,b] \\
a_j & b_j & \delta_j \\
... & & \\
a_m & b_m & \delta_m
\end{bmatrix}
\leftarrow$$

is a stepwise dendrogram for (S, d).

Proof. Since a and b are reciprocal nearest neighbors at the beginning, the reducibility property (1) guarantees that they stay nearest neighbors after any number of merging steps between other reciprocal nearest neighbors. Hence, the first j steps in a dendrogram for S cannot contain a or b, since these steps all happen at merging dissimilarities smaller than d[a,b]. This is the point where we must require that the sorting in line 3 of NN-CHAIN-LINKAGE is stable.

Moreover, the first j rows of L cannot contain a reference to n: Again by the reducibility property, dissimilarities between n and any other node are at least as big as d[a, b]. Therefore, the first j rows of L are correct for a dendrogram for S.

After j steps, we know that no inter-cluster distances in $S \setminus \{a, b\}$ are smaller than d[a, b]. Also, d[a, b] is minimal among all distances from a and b, so the row (a, b, d[a, b]) is a valid next row in L.

After this step, we claim that the situation is the same in both settings: The sets S' after j steps and the set S after j+1 steps, including the last one merging a and b into a new cluster n, are clearly equal as partitions of the original set. It is required to check that also the dissimilarities are the same in both settings. This is where we need the second condition in Theorem 1:

The row (a,b,d[a,b]) on top of the array L' differs from the dendrogram L by j transpositions, where (a,b,d[a,b]) is moved one step downwards. Each transposition happens between two pairs (a,b) and (a_i,b_i) , where all four nodes are distinct, as shown above. The dissimilarity from a distinct fifth node x to the join $a \cup b$ does not depend on the merging of a_i and b_i since there is no way in which dissimilarities to a_i and b_i enter the distance update formula FORMULA(d[a,x],d[b,x],d[a,b],size[a],size[b],size[x]). The symmetric statement holds for the dissimilarity $d[x,a_i\cup b_i]$. The nodes a,b,a_i,b_i are deleted after the two steps, so dissimilarities like $d[a,a_i\cup b_i]$ can be neglected. The only dissimilarity between active nodes which could be altered by the transposition is $d[a\cup b,a_i\cup b_i]$. It is exactly the second condition in Theorem 1 that this dissimilarity is independent of the order of merging steps. This finishes the proof of Theorem 1.

We still have to prove that the requirements of Theorem 1 are fulfilled by the "single", "complete", "average", "weighted" and "Ward" schemes:

Proof of Proposition 2. It is easy and straightforward to check from the table in Figure 2 that the distance update schemes in question fulfill the reducibility property. Moreover, the table also conveys that the dissimilarities between clusters in the "single", "complete" and "average" schemes do not depend on the order of the merging steps.

For Ward's scheme, the global dissimilarity expression in the third column in Figure 2 applies only if the dissimilarity matrix consists of Euclidean distances between vectors (which is the prevalent setting for Ward's method). For a general argument, note that the global cluster dissimilarity for Ward's method can also be expressed by a slightly more complicated expression:

$$d(A,B) = \sqrt{\frac{1}{|A| + |B|} \left(2 \sum_{a \in A} \sum_{b \in B} d(a,b)^2 - \frac{|B|}{|A|} \sum_{a \in A} \sum_{a' \in A} d(a,a')^2 - \frac{|A|}{|B|} \sum_{b \in B} \sum_{b' \in B} d(b,b')^2 \right)}$$

This formula can be proved inductively from the recursive distance update formula for Ward's method, hence it holds independently of whether the data is Euclidean or not. This proves that the dissimilarities in Ward's scheme are also independent of the order of merging steps.

Dissimilarities in the "weighted" scheme, however, do in general depend on the order of merging steps. However, the dissimilarity between joined nodes $I \cup J$ and $K \cup L$ is always the

Figure 6 The single linkage algorithm.

```
1: procedure MST-LINKAGE(S, d)
                                                                  \triangleright S: node labels, d: pairwise dissimilarities
         L \leftarrow \text{MST-LINKAGE-CORE}(S, d)
 3:
         Stably sort L with respect to the third column.
 4:
         L \leftarrow \text{Label}(L)
                                                            ▶ Find node labels from cluster representatives.
         return L
 5:
 6: end procedure
    procedure MST-LINKAGE-CORE(S_0, d)
                                                                 \triangleright S_0: node labels, d: pairwise dissimilarities
         L \leftarrow []
 2:
 3:
         c \leftarrow \text{(any element of } S_0\text{)}
                                                                                                     \triangleright c: current node
         D_0[s] \leftarrow \infty \text{ for } s \in S_0 \setminus \{c\}
 4:
         for i in (1, ..., |S_0| - 1) do
 5:
              S_i \leftarrow S_{i-1} \setminus \{c\}
 6:
              for s in S_i do
 7:
                  D_i[s] \leftarrow \min\{D_{i-1}[s], d[s, c]\}
 8:
              end for
 9:
              n \leftarrow \operatorname{argmin}_{s \in S_i} D_i[s]
10:
                                                                                                         \triangleright n: new node
              Append (c, n, D_i[n]) to L
11:
              c \leftarrow n
12:
         end for
13:
         return L
                                                                                         ⊳ an unsorted dendrogram
14:
15: end procedure
```

mean dissimilarity $\frac{1}{4}(d[I,K]+d[I,L]+d[J,K]+d[J,L])$, independent of the order of steps, and this is all that is required for Proposition 2.

3.3 The single linkage algorithm

In this section, we present and prove correctness of a fast algorithm for single linkage clustering. Gower and Ross (1969) observed that a single linkage dendrogram can be obtained from a minimum spanning tree (MST) of the weighted graph which is given by the complete graph on the singleton set S with the dissimilarities as edge weights. The algorithm here was originally described by Rohlf (1973) and is based on Prim's algorithm for the MST (see Cormen et al., 2009, § 23.2).

The single linkage algorithm MST-LINKAGE is given in Figure 6. In the same way as the NN-chain algorithm, it consists of a core algorithm MST-LINKAGE-CORE and two postprocessing steps. The output structure of the core algorithm is again an unsorted list of clustering steps with node representatives instead of unique labels. As will be proved, exactly the same postprocessing steps can be used as for the NN-chain algorithm.

Rohlf's algorithm in its original version is a full Prim's algorithm and maintains enough data to generate the MST. He also mentions a possible simplification which does not do enough bookkeeping to generate an MST but enough for single linkage clustering. It is this simplification that is discussed in this paper. We prove the correctness of this algorithm for two reasons:

• Since the algorithm MST-LINKAGE-CORE does not generate enough information to reconstruct a minimum spanning tree, one cannot refer to the short proof of Prim's algo-

rithm in any easy way to establish the correctness of MST-LINKAGE.

• Like for the NN-chain algorithm in the last section, it is not clear a priori that the algorithm resolves ties correctly. A third algorithm can serve as a warning here (see Section 5 for more details): There is an other fast algorithm for single linkage clustering, Sibson's SLINK algorithm (Sibson, 1973). More or less by coincidence, all three algorithms NN-CHAIN-CORE, MST-LINKAGE-CORE and SLINK generate output which can be processed by exactly the same two steps: sorting followed by LABEL. In case of the SLINK algorithm this works fine if all dissimilarities are distinct but produces wrong stepwise dendrograms in situations when two merging dissimilarities are equal. There is nothing wrong with the SLINK algorithm, however. Sibson supplied a proof for the SLINK algorithm in his paper (Sibson, 1973), but it is written for a (non-stepwise) dendrogram as the output structure, not for a stepwise dendrogram. Hence, the additional information which is contained in a stepwise dendrogram in the case of ties is not provided by all, otherwise correct algorithms.

This should be taken as a warning that ties demand more from an algorithm and must be explicitly taken into account when we prove the correctness of the MST-LINKAGE algorithm below.

Theorem 4. The algorithm MST-LINKAGE yields an output which can also be generated by Primitive clustering.

We do not explicitly refer to Prim's algorithm in the following, and we make the proof self-contained, since the algorithm does not collect enough information to construct a minimum spanning tree. There are unmistakable similarities, of course, and the author got most of the ideas for this proof from Prim's algorithm (see Cormen et al., 2009, § 23.2).

Let us first make two observations about the algorithm MST-LINKAGE.

(a) Starting with the full initial set S_0 , the algorithm MST-LINKAGE-CORE chooses a "current node" c in each step and removes it from the current set S_i in every iteration. Let $S_i^c := S_0 \setminus S_i$ be the complement of the current set S_i . Then $D_i[s]$ $(s \in S_i)$ is the distance from S_i^c to s, i.e.

$$D_i[s] = \min_{t \in S_i^c} d[s, t].$$

(b) Let L be the output of MST-LINKAGE-CORE(S,d). The 2i entries in the first two columns and the first i rows contain only i+1 distinct elements of S, since the second entry in one row is the first entry in the next row.

We prove Theorem 4 by the following stronger variant:

Theorem 5. Let L be the output of MST-LINKAGE-CORE(S,d). For all n < |S|, the first n rows of L are an unsorted single linkage dendrogram for the n+1 points of S in this list (see Observation (b)).

Proof. We proceed by induction. After the first iteration, the list L contains one triple (a_0, b_0, δ_0) . $\delta_0 = D_1[b_0]$ is clearly the dissimilarity $d[a_0, b_0]$, since the array D_1 contains the dissimilarities to a_0 after the first iteration (Observation (a)).

Let $(a_0, b_0, \delta_0), \ldots, (a_n, b_n, \delta_n)$ be the first n+1 rows of L. We sort the rows with a stable sorting algorithm as specified in MST-LINKAGE. We leave the postprocessing step LABEL out of our scope and work with the representatives a_i , b_i for the rest of the proof.

Let $s(0), \ldots, s(n)$ be the stably sorted indices (i.e. $\delta_{s(i)} \leq \delta_{s(i+1)}$ for all i and s(i) < s(i+1) if $\delta_{s(i)} = \delta_{s(i+1)}$). Let k be the sorted index of the last row n. Altogether, we have a sorted matrix

$$\rightarrow \begin{bmatrix} a_{s(0)} & b_{s(0)} & \delta_{s(0)} \\ \dots & & & & \\ a_{s(k-1)} & b_{s(k-1)} & \delta_{s(k-1)} \\ a_{s(k)} & b_{s(k)} & \delta_{s(k)} \\ a_{s(k+1)} & b_{s(k+1)} & \delta_{s(k+1)} \\ \dots & & & \\ a_{s(n)} & b_{s(n)} & \delta_{s(n)} \end{bmatrix} \leftarrow$$

The new row is at the index k, i.e. $(a_{s(k)}, b_{s(k)}, \delta_{s(k)}) = (a_n, b_n, \delta_n)$. The matrix without the k-th row is a valid stepwise, single linkage dendrogram for the points a_0, \ldots, a_n , by the induction hypothesis. (Recall that $b_i = a_{i+1}$.) Our goal is to show that the matrix with its k-th row inserted yields a valid single linkage dendrogram on the points a_0, \ldots, a_n, b_n .

First step: rows 0 to k-1. The distance δ_n is the minimal distance from b_n to any of the points a_0, \ldots, a_n . Therefore, the dendrograms for the sets $S^- := \{a_0, \ldots, a_n\}$ and $S^+ := S^- \cup \{b_n\}$ have the same first k steps, when all the inter-cluster distances are smaller than or equal to δ_n . (If the distance δ_n occurs more than once, i.e. when $\delta_{s(k-1)} = \delta_n$, we assume by stable sorting that the node pairs which do not contain b_n are chosen first.)

Therefore, the first k rows are a possible output of PRIMITIVE_CLUSTERING in the first k steps. After this step, we have the same partial clusters in S^+ as in the smaller data set, plus a singleton $\{b_n\}$.

Second step: row k. The distance δ_n from b_n to some point a_0, \ldots, a_n is clearly the smallest inter-cluster distance at this point, since all other inter-cluster distances are at least $\delta_{s(k+1)}$, which is greater than $\delta_{s(k)} = \delta_n$. Since the output row is (a_n, b_n, δ_n) , it remains to check that the distance δ_n is realized as the distance from b_n to a point in the cluster of a_n , i.e. that a_n is in a cluster with distance δ_n to b_n .

The clusters mentioned in the last sentence refer to the partition of S^+ which is generated by the relations $a_{s(0)} \sim b_{s(0)}, \ldots, a_{s(k-1)} \sim b_{s(k-1)}$. Since we have $b_i = a_{i+1}$, the partition of S^+ consists of contiguous chains in the original order of points $a_0, a_1, \ldots, a_n, b_n$.

The diagram below visualizes a possible partition after k steps.

$$(a_0 \quad a_1 \quad a_2) (a_3) (a_4 \quad a_5) \quad \dots \quad (\dots \quad a_m \quad \dots \quad a_n) (b_n)$$

In this particular example, the distances δ_0 , δ_1 and δ_4 are among the first k smallest, while δ_2 , δ_3 and δ_5 come later in the sorted order.

Let δ_n be realized as the distance between b_n and a_m for some $m \leq n$. Then the dissimilarities between consecutive points in the sequence a_m , $b_m = a_{m+1}$, $b_{m+1} = a_{m+2}$, ..., $b_{n-1} = a_n$ must be less than or equal to δ_n ; otherwise b_n and the dissimilarity $\delta_n = d[b_n, a_m]$ would have been chosen first over these other dissimilarities in one of the first k steps. Since the dissimilarities of all pairs (a_i, b_i) in this chain are not more than δ_n , they are contained in the first k sorted triples. Hence, a_m and a_n have been joined into a cluster in the first k steps, and a_n is a valid representative of the cluster that also contains a_m .

Note that the argument in the last paragraph is the point where we need that the sorting in line 3 of MST-LINKAGE is stable. Otherwise it could not be guaranteed that a_m and a_n have been joined into a cluster before b_n is added.

Third step: rows k+1 to n. Here is the situation after row k: We have the same clusters in S^+ as after k steps in the smaller data set S, except that the last cluster (the one which

contains a_n) additionally contains the point b_n . In a diagram:

$$(a_0 \quad a_1 \quad a_2)(a_3)(a_4 \quad a_5) \quad \dots \quad (\dots \quad a_m \quad \dots \quad a_n \quad b_n)$$

The inter-cluster distances in S^+ from the cluster with b_n to the other clusters might be smaller than without the point b_n in S^- . We show, however, that this does not affect the remaining clustering steps:

In each step r > k, we have the following situation for some $x \le y \le s(k)$. The point b_n might or might not be in the same cluster as $b_{s(r)}$.

Let the distance $\delta_{s(r)}$ be realized as the distance from $b_{s(r)}$ to a_y . From Observation (a) and line 10 in MST-LINKAGE-CORE, we know that this distance is minimal among the distances from $X := \{a_0, \ldots, a_{s(r)}\}$ to all other points in $S_0 \setminus X$. In particular, the distance from X to $b_n \in S_0 \setminus X$ is not smaller than $\delta_{s(r)}$.

This proves that the addition of b_n in step k does not change the single linkage clustering in any later step r > k. This completes the inductive proof of Theorem 5

4 Performance

In this section, we compare the performance of the algorithms and give recommendations on which algorithm to choose for which clustering method. We compare both the theoretical, asymptotic worst-case performance, and the use-case performance on a range of synthetic random data sets.

4.1 Asymptotic worst-case performance

Let N denote the problem size, which is in this case the number of input data points. The input size is $\binom{N}{2} \in \Theta(N^2)$.

The asymptotic run-time complexity of MST-LINKAGE-CORE is obviously $\Theta(N^2)$, since there are two nested levels of loops in the algorithm (line 8 and implicitly line 10). The run-time complexity of the NN-CHAIN-CORE algorithm is also $\Theta(N^2)$ (Murtagh, 1985, page 86). Postprocessing is the same for both algorithms and is less complex, namely $O(N \log N)$ for sorting and $\Theta(N)$ for LABEL, so the overall complexity is $\Theta(N^2)$. This is optimal (in the asymptotic sense): the lower bound is also quadratic since all $\Theta(N^2)$ input values must be processed.

The NN-chain algorithm needs a writable working copy of the input array to store intermediate dissimilarities and otherwise only $\Theta(N)$ additional memory.

The generic algorithm has a best-case time complexity of $\Theta(N^2)$, but without deeper analysis, the worst-case complexity is $O(N^3)$. The bottleneck is line 15 in Generic_Linkage: In O(N) iterations, this line might be executed up to O(N) times and does a minimum search over O(N) elements, which gives a total upper bound of $O(N^3)$. This applies for all clustering schemes except single linkage, where the loop starting at line 14 is never executed and thus the worst-case performance is $\Theta(N^2)$. The memory requirements for the generic algorithm are similar to the NN-chain algorithm: a working copy of the dissimilarity array and additionally only $\Theta(N)$ temporary memory.

In contrast, the MST algorithm does not write to the input array d. All other temporary variables are of size O(N). Hence, MST-LINKAGE requires no working copy of the input

array and hence only half as much memory as GENERIC_LINKAGE and NN-CHAIN-LINKAGE asymptotically.

Anderberg's algorithm (Anderberg, 1973, pages 135–136) has the same asymptotic bounds as our generic algorithm. The performance bottleneck are again the repeated minimum searches among the updated dissimilarities. Since the generic algorithm defers minimum searches to a later point in the algorithm (if they need to be performed at all, by then), there are at least as many minimum searches among at least as many elements in Anderberg's algorithm as in the generic algorithm. The only point where the generic algorithm could be slower is the maintenance of the priority queue with nearest neighbor candidates, since this does not exist in Anderberg's algorithm. The bottleneck here are potentially up to $O(N^2)$ updates of a queue in line 36 of Generic_Linkage. In the implementation in the next section, the queue is realized by a binary heap, so an update takes $O(\log N)$ time. This could potentially amount to $O(N^2 \log N)$ operations for maintenance of the priority queue. However, a reasonable estimate is that the saved minimum searches in most cases save more time than the maintenance of the queue with O(N) elements costs, and hence there is a good reason to believe that the generic algorithm is at least as fast as Anderberg's algorithm.

Note that the maintenance effort of the priority queue can be easily reduced to $O(N^2)$ instead of $O(N^2 \log N)$ worst case:

- A different priority queue structure can be chosen, where the "decrease-key" operation takes only O(1) time. (Note that the bottleneck operation in line 36 of GENERIC_LINK-AGE never increases the nearest-neighbor distance, only decreases it.) The author did not test a different structure since a binary heap convinces by its simple implementation.
- Changed keys (minimal distances) need not be updated in the priority queue immediately. Instead, the entire queue might be resorted/regenerated at the beginning of every iteration. This takes N-1 times O(N) time with a binary heap. Although this lowers the theoretical complexity for the maintenance of the binary queue, it effectively slowed down the algorithms in practice by a small margin. The reason is, of course, that the number and complexity of updates of the priority queue did by far not reach their theoretical upper bound in our test data sets (see below). Altogether, the maintenance of the priority queue, as proposed in Figure 3 seems quite optimal from the practical perspective.

4.2 Use-case performance

In addition to the theoretical, asymptotic and worst-case considerations, we also measured the practical performance of the algorithms. Figure 7 shows the run-time of the algorithms for a number of synthetic test data sets (for details see below). The solid lines are the average over the data sets. (The graphs labeled "Day-Edelsbrunner" are discussed in Section 5.) The lightly colored bands show the range from minimum to maximum time over all data sets for a given number of points.

The following observations can be made:

- For single linkage clustering, the MST-algorithm is clearly the fastest one. Together with the fact that it has only half the memory requirements of the other algorithms (if the input array is to be preserved), and thus allows the processing of larger data sets, the MST-algorithm is clearly the best choice for single linkage clustering.
- For the clustering schemes without inversions (all except "centroid" and "median"), the generic algorithm, the NN-chain algorithm and Anderberg's algorithm have very similar performance.

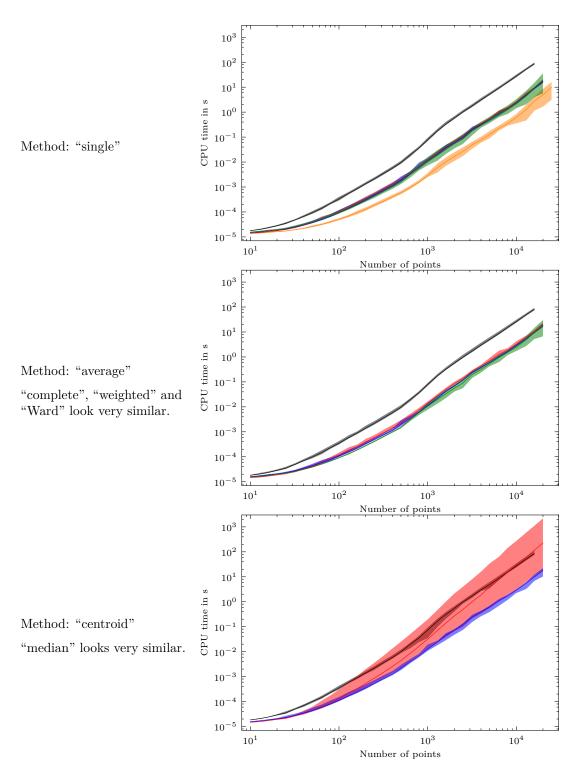


Figure 7: Performance of several SAHN clustering algorithms. Legend: ■ Generic algorithm (Figure 3), ■ Anderberg (1973, pages 135–136), ■ NN-chain algorithm (Figure 4), ■ MST-algorithm (Figure 6), ■ Day and Edelsbrunner (1984, Table 5).

The NN-chain algorithm is the only one with guaranteed $O(N^2)$ performance here. We can conclude that the good worst-case performance can be had here without any cut-backs to the use-case performance.

• For the "centroid" and "median" methods, we see a very clear disadvantage to Anderberg's algorithm. Here, the worst case cubic time complexity occurs already in the random test data sets. This happens with great regularity, over the full range of input sizes. Our Generic_linkage algorithm, on the other hand, does not suffer from this weakness: Even though the theoretical worst-case bounds are the same, the complexity does not raise above the quadratic behavior in our range of test data sets. Hence, we have grounds to assume that Generic_linkage is much faster in practice.

4.3 Conclusions

Based on the theoretical considerations and use-case tests, we can therefore recommend algorithms for the various distance update schemes as follows:

- "single" linkage clustering: The MST-algorithm is the best, with respect to worst-case complexity, use-case performance and memory requirements.
- "complete", "average", "weighted", "ward": The NN-chain algorithm is preferred, since it guarantees $O(N^2)$ worst case complexity without any disadvantage to practical performance and memory requirements.
- "centroid", "median": The generic clustering algorithm is the best choice, since it can handle inversions in the dendrogram and the performance exhibits quadratic complexity in all observed cases.

Of course, the timings in the use-case tests depend on implementation, compiler optimizations, machine architecture and the choice of data sets. Nevertheless, the differences between the algorithms are very clear here, and the comparison was performed with careful implementations in the identical environment.

The test setup was as follows: All algorithms were implemented in C++ with an interface to Python (van Rossum et al.) and the scientific computing package NumPy (Num) to handle the input and output of arrays. The test data sets are samples from mixtures of multivariate Gaussian distributions with unity covariance matrix in various dimensions (2, 3, 10, 200) with various numbers of modes $(1, 5, [\sqrt{N}])$, ranging from N = 10 upwards until memory was exhausted (N = 20000 except for single linkage). The centers of the Gaussian distributions are also distributed by a Gaussian distribution. Moreover, for the methods for which it makes sense (single, complete, average, weighted: the "combinatorial" methods), we also generated 10 test sets per number of input points with a uniform distribution of dissimilarities.

The timings were obtained on a PC with an Intel dual-core CPU T7500 with 2.2 GHz clock speed and 4GB of RAM and no swap space. The operating system was Ubuntu 11.04 64-bit, Python version: 2.7.1, NumPy version: 1.5.1, compiler: GNU C++ compiler, version 4.5.2. Only one core of the two available CPU cores was used in all computations.

5 Alternative algorithms

The MST algorithm has the key features that it (1) needs no working copy of the $\Theta(N^2)$ input array and only $\Theta(N)$ working memory, (2) is fast since it reads every input dissimilarity only once and otherwise deals only with $\Theta(N)$ memory. There is a second algorithm with these

characteristics, Sibson's SLINK algorithm (Sibson, 1973). It is based on the insight that a single linkage dendrogram for N+1 points can be computed from the dendrogram of the first N points plus a single row of distances $(d[N,0],\ldots,d[N,N-1])$. In this fashion, the SLINK algorithm even reads the input dissimilarities in a fixed order, which can be an advantage over the MST algorithm if the favorable input order can be realized in an application, or if dissimilarities do not fit into random-access memory and are read from disk.

However, there is one important difference: even though the output data format looks deceptively similar to the MST algorithm (the output can be converted to a stepwise dendrogram by exactly the same process: sorting with respect to dissimilarities and a union-find procedure to generate node labels from cluster representatives), the SLINK algorithm cannot handle ties. This is definite, since e.g. the output in the example situation on page 5 is the same in all three cases, and hence no postprocessing can recover the different stepwise dendrograms.

There is an easy way out by specifying a secondary order

$$d(i,j) \prec d(k,l) \quad :\Longleftrightarrow \quad \begin{cases} d(i,j) < d(k,l) & \text{if this holds,} \\ Ni+j < Nk+l & \text{if } d(i,j) = d(k,l) \end{cases}$$

to make all dissimilarities artificially distinct. In terms of performance, the extra comparisons put a slight disadvantage on the SLINK algorithm, according to the author's experiments. However, the difference is not much, and the effect on timings may be compensated or even reversed in a different software environment or when the input order of dissimilarities is in favor of SLINK. Hence, the SLINK algorithm is a perfectly fine tool, as long as care is taken to make all dissimilarities unique.

The same idea of generating a dendrogram inductively is the basis of an algorithm by Defays (1977). This paper is mostly cited as a fast algorithm for complete linkage clustering. However, it definitely is not an algorithm for complete linkage clustering, as the complete linkage method is commonly defined, in this paper and identically elsewhere.

An algorithm which is interesting from the theoretical point of view is given by Day and Edelsbrunner (1984, Table 5). It uses N priority queues for the nearest neighbor of each point. By doing so, the authors achieve a worst-case time complexity of $O(N^2 \log N)$, which is better than the existing bound $O(N^3)$ for the schemes where the NN-chain algorithm cannot be applied. The overhead for maintaining a priority queue for each point, however, slows the algorithm down in practice. The performance measurements in Figure 7 include the Day-Edelsbrunner algorithm. Day and Edelsbrunner write their algorithm in general terms, for any choice of priority queue structure. We implemented the algorithm for the measurements in this paper with binary heaps, since these have a fixed structure and thus require the least additional memory. But even so, the priority queues need additional memory of order $\Theta(N^2)$ for their bookkeeping, which can also be seen in the graphs since they stop at fewer points, within the given memory size of the test. The graphs show that even if the Day-Edelsbrunner algorithm gives the currently best asymptotic worst-case bound for the "centroid" and "median" methods, it is inefficient for practical purposes.

Křivánek (1990, §II) suggested to put all $\binom{N}{2}$ dissimilarity values into an (a,b)-tree data structure. He claims that this enables hierarchical clustering to be implemented in $O(N^2)$ time. Křivánek's conceptually very simple algorithm relies on the fact that m insertions into an (a,b)-tree can be done in O(m) amortized time. This is only true when the positions, where the elements should be inserted into the tree, are known. Searching for these positions takes $O(\log N)$ time per element, however. (See Mehlhorn and Tsakalidis (1990, §2.1.2) for an accessible discussion of amortized complexity for (2,4)-trees; Huddleston and Mehlhorn (1982) introduce and discuss (a,b)-trees in general.) Křivánek did not give any details of his

analysis, but based on his short remarks, the author cannot see how Křivánek's algorithm achieves $O(N^2)$ worst-case performance for SAHN clustering.

6 Extension to vector data

If the input to a SAHN clustering algorithm is not the array of pairwise dissimilarities but N points in a D-dimensional real vector space, the lower bound $\Omega(N^2)$ on time complexity does not hold any more. Since much of the time in an SAHN clustering scheme is spent on nearest-neighbor searches, algorithms and data structures for fast nearest-neighbor searches can potentially be useful. The situation is not trivial, however, since (1) in the "combinatorial" methods (e.g. single, complete, average, weighted linkage) the inter-cluster distances are not simply defined as distances between special points like cluster centers, and (2) even in the "geometric" methods (the Ward, centroid and median schemes), points are removed and new centers added with the same frequency as pairs of closest points are searched, so a dynamic nearest-neighbor algorithm is needed, which handles the removal and insertion of points efficiently.

Moreover, all known fast nearest-neighbor algorithms lose their advantage over exhaustive search with increasing dimensionality. Additionally, algorithms will likely work for one metric in \mathbb{R}^D but not universally. Since this paper is concerned with the general situation, we do not go further into the analysis of the "stored data approach" (Anderberg, 1973, § 6.3). We only list at this point what can be achieved with the algorithms from this paper. This will likely be the best solution for high-dimensional data or general-purpose algorithms, but there are better solutions for low-dimensional data outside the scope of this paper. The suggestions below are at least helpful to process large data sets since memory requirements are of class $\Theta(ND)$, but they do not overcome their $\Omega(N^2)$ lower bound on time complexity.

- The MST algorithm for single linkage can compute distances on-the-fly. Since every pairwise dissimilarity is read in only once, there is no performance penalty compared to first computing the whole dissimilarity matrix and then applying the MST algorithm. Quite the contrary, computing pairwise distances in-process can result in faster execution since much less memory must be reserved and accessed. The MST algorithm is suitable for any dissimilarity measure which can be computed from vector representations (that is, all scale types are possible, e.g. \mathbb{R} -valued measurements, binary sequences and categorical data).
- The NN-chain algorithm is suitable for the "Ward" scheme, since inter-cluster distances can be defined by means of centroids as in Figure 2. The initial inter-point dissimilarities must be Euclidean distances (which is anyway the only setting in which Ward linkage describes a meaningful procedure).
- The generic algorithm is suitable for the "Ward", "centroid" and "median" scheme on Euclidean data. There is a simpler variant of the Generic_linkage algorithm in Section 6, which works even faster in this setting. The principle of the algorithm Generic_linkage_variant is the same: each array entry mindist[x] maintains a lower bound on all dissimilarities d[x,y] for nodes with label y>x. The Generic_linkage algorithm is designed to work efficiently with a large array of pairwise dissimilarities. For this purpose, the join of two nodes a and b re-uses the label b, which facilitates in-place updating of the dissimilarity array in an implementation. The Generic_linkage_variant algorithm, in contrast, generates a unique new label for each new node, which is smaller than all existing labels. Since the new label is at the beginning of the (ordered) list of

Figure 8 The generic clustering algorithm (variant).

```
1: procedure Generic Linkage variant(N, d)
    d is either an array or a function which computes dissimilarities from cluster centers.
    (Lines 2 to 13 are the same as in Generic Linkage.)
        for x in S \setminus \{N-1\} do
            while b \notin S do
14:
                                                  ▶ Recalculation of nearest neighbors, if necessary.
21:
            end while
            Remove a and b from Q.
22:
23:
            Append (a, b, \delta) to L.
            Create a new label n \leftarrow -i
24:
            size[n] \leftarrow size[a] + size[b]
25:
            S \leftarrow (S \setminus \{a, b\}) \cup \{n\}
26:
            for x in S \setminus \{n\} do
                                                                   ▷ Extend the distance information.
27:
                d[x, n] \leftarrow d[n, x] \leftarrow \text{FORMULA}(d[a, x], d[b, x], d[a, b], size[a], size[b], size[x])
28:
            end for
29:
    or
            Compute the cluster center for n as in Figure 2.
27:
            n\_nghbr[n] \leftarrow \operatorname{argmin}_{x>n} d[n,x]
30:
            Insert (n, d[n, n \ nghbr[n]]) into mindist and Q
31:
        end for
32:
33:
        return L
34: end procedure
```

nodes and not somewhere in the middle, the bookkeeping of nearest neighbor candidates and minimal distances is simpler in Generic_Linkage_variant: in particular, the two loops in lines 28–38 of Generic_Linkage can be disposed of entirely. Moreover, experiments show that Generic_Linkage_variant needs much less recalculations of nearest neighbors in some data sets. However, both algorithms are similar, and which one is faster in an implementation seems to depend strongly on the actual data structures and their memory layout.

Another issue which is not in the focus of this paper is that of parallel algorithms. For the "stored matrix approach", this has a good reason since the balance of memory requirements versus computational complexity does not make it seem worthwhile to attempt parallelization with current hardware. This changes for vector data, when the available memory is not the limiting factor and the run-time is pushed up by bigger data sets. In high-dimensional vector spaces, the advanced clustering algorithms in this paper require little time compared to the computation of inter-cluster distances. Hence, parallelizing the nearest-neighbor searches with their inherent distance computations appears a fruitful and easy way of sharing the workload. The situation becomes less clear for low-dimensional data, however.

7 Conclusion

Among the algorithms for sequential, agglomerative, hierarchic, nonoverlapping (SAHN) clustering on data with a dissimilarity index, three current algorithms are most efficient: Rohlf's algorithm MST-LINKAGE for single linkage clustering, Murtagh's algorithm NN-CHAIN-LINKAGE for the "complete", "average", "weighted" and "Ward" schemes, and the author's GENERIC_LINKAGE algorithm for the "centroid" and "median" schemes and the "flexible" family. The last algorithm can also be used for an arbitrary distance update formula. There is even a simpler variant GENERIC_LINKAGE_VARIANT, which seems to require less internal calculations, while the original algorithm is optimized for in-place updating of a dissimilarity array as input. The GENERIC_LINKAGE algorithm and its variant are new; the other two algorithms were described before, but for the first time they are proved to be correct.

Acknowledgments

This work was funded by the National Science Foundation grant DMS-0905823 and the Air Force Office of Scientific Research grant FA9550-09-1-0643.

References

- NumPy: Scientific computing tools for Python. Available at http://numpy.scipy.org/.
- Michael R. Anderberg. Cluster analysis for applications. Academic Press, New York, 1973. ISBN 0120576503.
- Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, and Clifford Stein. *Introduction to Algorithms*. MIT Press, 3rd edition, 2009.
- William H. E. Day. Complexity theory: an introduction for practitioners of classification. In Clustering and classification, pages 199–233. World Scientific Publishing, River Edge, NJ, 1996.
- William H. E. Day and Herbert Edelsbrunner. Efficient algorithms for agglomerative hierarchical clustering methods. *Journal of Classification*, 1(1):7–24, 1984. doi: 10.1007/BF01890115.
- Daniel Defays. An efficient algorithm for a complete link method. The Computer Journal, 20 (4):364–366, 1977. doi: 10.1093/comjnl/20.4.364.
- Damian Eads. *Hierarchical clustering* (scipy.cluster.hierarchy), 2007. Package for SciPy version 0.9.0. Available at http://www.scipy.org.
- Brian S. Everitt, Sabine Landau, Morven Leese, and Daniel Stahl. *Cluster Analysis*. John Wiley & Sons, 5th edition, 2011. doi: 10.1002/9780470977811.
- Allan D. Gordon. A review of hierarchical classification. *Journal of the Royal Statistical Society. Series A (General)*, 150(2):119–137, 1987. doi: 10.2307/2981629.
- John C. Gower and G. J. S. Ross. Minimum spanning trees and single linkage cluster analysis. Journal of the Royal Statistical Society. Series C (Applied Statistics), 18(1):54–64, 1969. doi: 10.2307/2346439.

- Pierre Hansen and Brigitte Jaumard. Cluster analysis and mathematical programming. *Mathematical Programming*, 79(1–3):191–215, 1997. doi: 10.1007/BF02614317.
- Scott Huddleston and Kurt Mehlhorn. A new data structure for representing sorted lists. *Acta Informatica*, 17(2):157–184, 1982. doi: 10.1007/BF00288968.
- Anil K. Jain and Richard C. Dubes. Algorithms for Clustering Data. Prentice Hall, Englewood Cliffs, NJ, 1988.
- Stephen C. Johnson. Hierarchical clustering schemes. *Psychometrika*, 32(3):241–254, 1967. doi: 10.1007/BF02289588.
- Eric Jones, Travis Oliphant, Pearu Peterson, et al. SciPy: Open source scientific tools for Python, 2001. http://www.scipy.org.
- Leonard Kaufman and Peter J. Rousseeuw. Finding groups in data: An introduction to cluster analysis. John Wiley & Sons, New York, 1990. doi: 10.1002/9780470316801.
- Mirko Křivánek. Connected admissible hierarchical clustering. KAM series, (90-189), 1990. Department of Applied Mathematics, Charles University, Prague (CZ). Available at http://kam.mff.cuni.cz/~kamserie/serie/clanky/1990/s189.pdf.
- G. N. Lance and W. T. Williams. A general theory of classificatory sorting strategies. *Computer Journal*, 9(4):373–380, 1967. doi: 10.1093/comjnl/9.4.373.
- Kurt Mehlhorn and Athanasios Tsakalidis. Data structures. In *Handbook of theoretical computer science*, Vol. A, pages 301–341. Elsevier, Amsterdam, 1990. Available at http://www.mpi-sb.mpg.de/~mehlhorn/ftp/DataStructures.pdf.
- Fionn Murtagh. A survey of recent advances in hierarchical clustering algorithms. *Computer Journal*, 26(4):354–359, 1983. doi: 10.1093/comjnl/26.4.354.
- Fionn Murtagh. Complexities of hierarchic clustering algorithms: State of the art. Computational Statistics Quarterly, 1(2):101-113, 1984. Available at http://thames.cs.rhul.ac.uk/~fionn/old-articles/complexities/.
- Fionn Murtagh. Multidimensional clustering algorithms, volume 4 of Compstat Lectures. Physica-Verlag, Würzburg/Wien, 1985. ISBN 3-7051-0008-4. Available at http://www.classification-society.org/csna/mda-sw/.
- Daniel Müllner. fastcluster: Fast hierarchical, agglomerative clustering routines for R and Python. *Preprint*, 2011. Will be available at http://math.stanford.edu/~muellner.
- R Development Core Team. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria, 2011. http://www.R-project.org.
- F. James Rohlf. Hierarchical clustering using the minimum spanning tree. *Comput. Journal*, 16:93-95, 1973. Available at http://life.bio.sunysb.edu/ee/rohlf/reprints.html.
- F. James Rohlf. Single-link clustering algorithms. In P.R. Krishnaiah and L.N. Kanal, editors, Classification Pattern Recognition and Reduction of Dimensionality, volume 2 of Handbook of Statistics, pages 267–284. Elsevier, 1982. doi: 10.1016/S0169-7161(82)02015-X.
- R. Sibson. SLINK: an optimally efficient algorithm for the single-link cluster method. *Comput. Journal*, 16:30–34, 1973. doi: 10.1093/comjnl/16.1.30.

Peter H. A. Sneath and Robert R. Sokal. *Numerical taxonomy*. W. H. Freeman, San Francisco, 1973.

The MathWorks, Inc. MATLAB, 2011. http://www.mathworks.com.

Guido van Rossum et al. Python programming language. Available at http://www.python.org.

Wolfram Research, Inc. Mathematica, 2010. http://www.wolfram.com.

Daniel Müllner Stanford University Department of Mathematics 450 Serra Mall, Building 380 Stanford, CA 94305

E-mail: muellner@math.stanford.edu http://math.stanford.edu/~muellner