Reliable Agglomerative Clustering

Morteza Haghir Chehreghani Department of Computer Science and Engineering Chalmers University of Technology Email: morteza.chehreghani@chalmers.se

Abstract

Standard agglomerative clustering suggests establishing a new *reliable* linkage at every step. However, in order to provide adaptive, density-consistent and flexible solutions, we study extracting all the *reliable* linkages at each step, instead of the smallest one. Such a strategy can be applied with all common criteria for agglomerative hierarchical clustering. We also study that this strategy with the *single* linkage criterion yields a minimum spanning tree algorithm. We perform experiments on several real-world datasets to demonstrate the performance of this strategy compared to the standard alternative.

1 Introduction

Clustering plays an essential role in data processing and management such as text processing, image segmentation, compression, summarization, knowledge management, network analysis, and bioinformatics. The goal of data clustering is to partition the data into groups such that the objects in the same cluster are more similar in some sense, compared to the inter-cluster objects. A category of clustering methods partition the data into K flat clusters via for example optimizing a cost/objective function. Examples of this type of methods are K-means [27], normalized cut [37] and spectral clustering [31, 37], where all produce *flat* clusters without any explicit relation between them. In practice, however, the different clusters often do not carry the same information content, i.e., some are more detailed than the others. Thus, in an exploratory data analysis approach, it is desired to propose the clusters at different levels and resolutions, such that both general and specific information are preserved. In this way, the user has more control to choose the desired resolution or even investigate the clusters at different levels and resolutions. For this reason, hierarchical clustering is often more practical is many applications and situations, where the results are usually presented by a dendrogram. A dendrogram is a tree wherein each node represents a cluster and its final nodes (the nodes connected to only one other node) correspond to the

objects. A node at a higher level includes the combination of the lower-level clusters and the edge weights (and their lengths) represent the inter-cluster distances.

Hierarchical clustering methods, in general, fall into two categories: agglomerative (bottom-up) and divisive (topdown) [28]. Agglomerative algorithms consider each object as a separate cluster, and then combine the clusters in a greedy manner to build larger clusters, until at the end there is only one single cluster. Divisive methods, in an opposite way, start with a single cluster including all objects. Then, at each step, the clusters are divided into two parts to produce finer clusters. Agglomerative methods are more common for hierarchical clustering, and they are usually computationally more efficient than divisive methods [32]. In these approaches, the clusters might be combined or divided according to different criteria, e.g., *single, complete, average, centroid* and *Ward*.

Several methods have been developed to improve the different aspects of these algorithms. [1] studies the locality and outer consistency of agglomerative algorithms in an axiomatic way. The works in [23, 26] consider the statistical significance of hierarchical clustering. [4,9,10,35,36] investigate the optimization aspects of hierarchical clustering and develop several approximate solutions. To provide robustness in pairwise inter-clusters relations, K-Linkage in [44] investigates multiple pairs of distances for each pair of clusters, [2] uses global information for determining the similarities between the clusters, [6] trains a Bayesian network to infer the relations between the items to be clustered, and [5] suggests applying agglomerative methods to small dense subsets of the data instead of the original data. The work in [7] performs the hierarchical clustering on K-nearest neighbor graph where fixing a proper K (and the other hyper-parameters) can be nontrivial as discussed in [42]. The works in [14, 22] might suffer from the same issues. The methods in [13, 20] investigate combining aggolomerative methods with probabilistic models which then yields an extra computational complexity. Finally, [8, 18, 30] develop efficient (and approximate) implementations of aggolomerative methods.

In this paper, we focus on agglomerative hierarchical clus-

tering. We consider that the standard agglomerative algorithms usually select a minimal reliable linkage at each step. We call a linkage between two clusters *reliable* if both clusters are the nearest neighbors of each other. Linkages represent the inter-cluster distances according to a criterion such as single or average distance. A reliable linkage provides the two clusters at its two sides to be consistent and share similar properties. However, in order to be adaptive w.r.t. the data diversity and variability, we investigate extracting at each step all the reliable linkages, instead of the smallest one. This strategy, called reliable agglomerative clustering, enables every object to potentially contribute from the early steps of constructing the dendrogram and, thus, clusters with different shapes and densities can evolve from the beginning. This strategy, similar to the standard agglomerative procedure, can be used with all the common criteria, and it is adaptive to the shape and density of the clusters. A similar idea has been proposed in [3] in an abstract form without further investigations and analysis. We note that this contribution is orthogonal to the aforementioned methods which aim to improve in particular agglomerative clustering, such that any of those improvements can be employed with this strategy too. For example, similar to [5], we may build the dendrogram from the dense subsets of the data or use global information for computing the base pairwise (dis)similarities [2]. We may also apply the feature extraction method in [19] to infer proper unsupervised representations. In the following, inspired by the equivalence of single linkage clustering and the Kruskal's algorithm for computing minimum spanning trees [24], we study that reliable agglomerative clustering with single criterion also yields a minimum spanning tree. We perform extensive experiments on several real-world datasets to demonstrate the performance of this method compared to the standard approach.

The rest of the paper is organized as the following. In the second section we introduce the reliable agglomerative strategy, and in the third section we study the connection to minimum spanning trees. We experimentally investigate *reliable agglomerative clustering* in the next section, and finally, we conclude the paper in the last section.

2 Reliable Agglomerative Clustering

In this section, we describe *reliable agglomerative clustering* and discuss the connection to computing a minimum spanning tree.

2.1 A generic view to agglomerative clustering

Data are characterized by a set of *n* objects $\mathbf{O} = \{0, ..., n-1\}$ and a relevant representation. The representation can be for example the vectors in a vector space or the pairwise dissimilarities between the objects. In the former case, the measurements are shown by the $n \times d$ matrix \mathbf{X} , where the i^{th} row (i.e., \mathbf{X}_i) corresponds to the *d* dimensional vector of

the *i*th object. In the latter form, an $n \times n$ matrix **D** represents the pairwise dissimilarities between the objects. A cluster is shown by C_p , which is the set of the object indices that it contains. The function $dist(C_p, C_q)$ denotes the inter-cluster distances that can be defined according to different criteria.

Agglomerative methods follow an iterative procedure where at each step, two clusters (nodes) are combined to build a larger cluster. The procedure continues until there is only one cluster left. The algorithm at each step selects the two clusters that have a minimal distance according to a criterion, i.e., a specific definition of dist(.,.). For example, the *single* linkage criterion [38] defines the distance between two clusters as the distance between the nearest members of the clusters. Opposite to this strategy, the *complete* linkage criterion [25] defines the distance of two clusters as the distance between their farthest members, that corresponds to the maximum within-cluster distance of the new cluster. On the other hand, in *average* criterion [39] the average of inter-cluster distances is used as the distance between the two clusters. Some other methods, e.g., the *centroid* and the median criteria, determine a representative for each cluster and then compute the inter-cluster distances by the distances between the representatives. For example, with the centroid criterion the representatives are the means of the clusters and at each step, the two clusters with closest centroids are combined to construct a larger cluster.

Another category of agglomerative methods aim to optimize a criterion such as *homogeneity*. An important instance is the *Ward* method [43] which aims to minimize the total within-cluster variance at each step. However, this criterion can be written as

$$dist(C_p, C_q) = \sum_{i \in C_p \cup C_q} ||\mathbf{X}_i - \mathbf{m}_{C_p \cup C_q}||^2 - \sum_{i \in C_p} ||\mathbf{X}_i - \mathbf{m}_{C_p}||^2 - \sum_{j \in C_q} ||\mathbf{X}_j - \mathbf{m}_{C_q}||^2 = \frac{|C_p||C_q|}{|C_p| + |C_q|} ||\mathbf{m}_{C_p} - \mathbf{m}_{C_q}||^2,$$

where \mathbf{m}_{C_p} denotes the centroid vector of cluster C_p .

Thus, the *Ward* method also at each step combines the two clusters with a minimal distance, where the inter-cluster distances are defined as the distances between the cluster means normalized by a function of the size of the clusters.

2.2 Reliable agglomerative clustering strategy

We begin with analyzing the performance of the *single* linkage method, in particular on the data with diverse densities. Such an analysis can be applied to the other criteria as well. We first consider the data shown in Figure 1(a), which includes two clusters with different densities. The *single* linkage method starts first from the dense data cloud at the left side (shown by black points) and then performs grouping the members

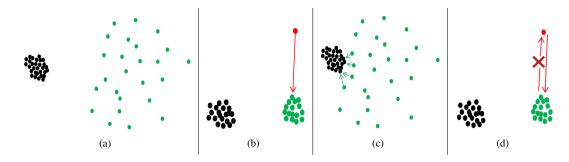


Figure 1: The standard agglomerative clustering is sensitive to data diversity (Fig 1(a)). On the other hand, allowing each object/cluster to connect to its nearest neighbor (regardless of if it happens in the nearest neighborhood of the other side too), can lead to inappropriate results (Fig 1(b) and 1(c)). Therefore, extracting only *reliable* linkages (but all instead of the smallest) avoids such situations (Fig1(d)).

of the cluster at the right side (shown by green points). Such that if we stop the clustering early, then, we will have only the members of the cluster at the left side grouped together. The reason is that picking the smallest inter-cluster distance (linkage) does not necessarily yield contributing every object/cluster to building the dendrogram. In particular, as we saw, this approach is sensitive to the density of the clusters and tends to first extract the densest clusters. One way to overcome this issue and take the variance of clusters into account is to require each object/cluster to participate in building the dendrogram. One might interpret the standard agglomerative strategy for selecting the smallest inter-cluster linkage as i) find the nearest neighbors of the current objects/clusters to obtain the set of potential linkages¹, and ii) then pick the smallest linkage.

Therefore, one way to render contributing many objects/clusters in building the dendrogram is to choose all the linkages instead of the smallest one, which makes the dendrogram grow simultaneously from all the objects. However, allowing all the linkages corresponding to any nearest neighbor might be inappropriate, as it can be sensitive to the presence of outliers or to the clusters which are close but have different densities. Two examples are illustrated in Figures 1(b) and 1(c). If we pick all of the linkages, the red object at the top in Figure 1(b) would establish a linkage to the green cluster (with the closest object of it) at the first level of the dendrogram. However, we know that such a linkage should be established at a higher level, after the members of the green data cloud merge and build their own cluster first. Therefore, this linkage is not a *reliable* linkage, as the two objects at its two sides do not share similar properties and densities. On the other hand, in Figure 1(c), the two green and black clusters are close to each other, such that some objects of the green data cloud choose the members of the black data cloud as the nearest neighbors, instead of choosing from the green data

cloud. This occurs due to the different densities of the clusters. Therefore, one should be careful in choosing any nearest neighbor linkage. In these examples, the objects/clusters at the two sides of a linkage have different properties and densities. In the example of Figures 1(b), the red object is an outlier whose neighborhood is empty, unlike the neighborhood of the object at the other side, which is significantly denser. Thus, the red object establishes a linkage with one of the green objects, but this object selects another object as its nearest neighbor. In Figures 1(c), some of the green objects establish linkage to some of the black objects, which have a different (i.e., higher) densities around. Therefore, the black objects do not select these green objects as their nearest neighbors. This analysis leads to investigate the *reliability* of linkages established by different objects/clusters, defined in Definition 1.

Definition 1. A linkage between two clusters C_p and C_q is 'reliable' if and only if both clusters are nearest neighbors of each other, i.e., $C_q \in nn(C_p)$ and $C_p \in nn(C_q)$, where $nn(C_p)$ returns the nearest clusters of cluster C_p .²

Note that a cluster might have several nearest neighbors, i.e., $|nn(C_p)| \ge 1$.

Therefore, instead of establishing the linkage(s) from every cluster/object, we select only a subset that are *reliable*. Such an approach provides the clusters at the two sides of a linkage to share consistent neighborhood and densities. Thus, merging them to build a larger cluster becomes meaningful. Then, it avoids non-robust linkages, for example merging the outlier objects at the lowest levels (Figure 1(d)). Proposition 1 indicates that a linkage with a minimal length is *reliable*, i.e., the standard agglomerative strategy which combines only the nearest clusters at each step performs reliable selections.

Proposition 1. Given a set of clusters $\{C_i\}$ and the respective linkages between them, a linkage with minimal length (called e^*) is a 'reliable' linkage.

¹The nearest neighbors are defined according to the dist(.,.) function, which can encode any criterion (e.g., *single*, *complete*, *average*, *centroid* and *Ward*).

²A cluster may include only one single object, i.e., each object is a cluster at the lowest level of the dendrogram.

Proof sketch. We denote the clusters at the two sides of e^* respectively C_p and C_q . Since e^* has a minimal length among all linkages, thus, it will also be the smallest linkage connected to C_p and the same for C_q . Therefore, C_p is the nearest neighbor of C_q and C_q is the nearest neighbor of C_p , which makes the corresponding linkage (i.e., e^*) reliable.

However, a minimal linkage is *not* the only *reliable* linkage, in particular when the data contain clusters with diverse densities, as demonstrated in Figure 1(a). Thus, in order to build the dendrogram in a density-aware and adaptive way, at each level we may select *all* the linkages that are *reliable*. Thereby, this strategy at each step first finds *all the reliable* linkages, and then combines the respective clusters to build a larger cluster at a higher level. Algorithm 1 describes the procedure in detail providing an implementation of the high-level method in [3].

Algorithm 1 Reliable Agglomerative Clustering.

Require: Objects and the measurements.

Ensure: List of the clusters at different levels stored in *Cluster_List*.

Cluster_List.
1: $l = 0$ // l specifies the current level
2: for all $i \in \mathbf{O}$ do
3: $Cluster_List[l].add(\{i\})$
4: end for
5: while $ Cluster_List[l] > 1$ do
$6: min_dist = []$
7: for $0 \le p < Cluster_List[l] $ do
8: $min_dist.add(min_{0 \le q < Cluster_List[l] , q \ne p})$
$dist(Cluster_List[l][p],Cluster_List[l][q]))$
9: end for
10: Initialize matrix \mathcal{G} by 0 .
11: for $p, q \in \{0,, Cluster_List[l] - 1\}, p \neq q$ do
12: if $dist(Cluster_List[l][p], Cluster_List[l][q])$
$min_dist[p]$ and
$dist(Cluster_List[l][p],Cluster_List[l][q])$
min_dist[q] then
13: $\mathcal{G}[p,q] = 1$
14: $\mathcal{G}[q,p] = 1$
15: end if
16: end for
{Extract the connected components of \mathcal{G} }:
17: $CC = connected_components(\mathcal{G}).$
18: for all $cc \in CC$ do
19: $new_cluster = Cluster_List[l][cc]$
20: $Cluster_List[l+1].add(new_cluster)$
21: end for
22: l = l + 1
23: end while
24: return Cluster_List

In this algorithm, $Cluster_List$ is used to store the clusters at different levels, such that $Cluster_List[l][p]$ gives the

 p^{th} cluster at the level l. The variable l indicates the current level while building the dendrogram. At the beginning, each individual object constitutes a separate cluster at level 0. Next, the distance of each cluster at the current level l(stored in *Cluster List*[l]) to its nearest neighbor is computed and stored in *min dist*. Function dist(,) computes the intercluster distance between the two input clusters, according to a predefined criterion, e.g., *single*, *complete* and so on. Then, in graph $\mathcal{G} \in \{0,1\}^{|Cluster_List[l]| \times |Cluster_List[l]|}$ (whose nodes represent the cluster indices at Cluster_List[level]) an edge is established if and only if the two respective clusters are nearest neighbors of each other (i.e., the linkage is reliable). Note that a cluster might have several nearest neighbors, i.e., several clusters might have the same (smallest) distance from that. At the next step, the connected components of the graph G are extracted, where each of them represents a new cluster at a higher level. Thus, the clusters at the same connected components are combined to build a new single cluster at the higher level. This procedure (i.e., finding the nearest neighbors and combining them to build new higher-level clusters) continues until only one cluster is left at the highest level.

Notice that the several improvements developed for the standard strategy can be applied to this strategy as well. The computational complexity of this strategy is similar to the complexity of the standard variant. Both strategies establish in total n - 1 linkages. For this, they compute the inter-cluster distances (linkages) according to a priori fixed criterion, and for each selected linkage, they merge the respective clusters and update the new inter-cluster linkages. Therefore, the operations and the computations are similar, whereas the choice of specific linkages and/or the order might differ which can lead to different dendrograms. Selecting all reliable linkages, instead of the smallest one, may reduce the overall number of steps, but it might need more merges at each step. However, as mentioned, the total number of merges is the same for both strategies.

On the other hand, as mentioned, an important computational advantage of the reliable strategy is the possibility of *early stopping*. It builds and develops several clusters simultaneously, whereas the standard approach develops fewer clusters at the same time. Thus, if we stop at early/intermediate steps, it is more likely that we obtain good representatives of different clusters. But, with the standard strategy, it could happen that only a few clusters are developed and the rest have not even been started yet. This might happen in particular when the clusters have diverse densities and shapes. Therefore, early-stopping, to reduce the computational time, can be more effective with *reliable agglomerative clustering*. For example, the early clusters can be exposed to the user to select only the interesting and relevant ones to develop further.

Algorithm 1 enables every object to *potentially* participate in building the dendrogram from the beginning, depending on having a reliable linkage. In other words, establishing and selecting a linkage and therefore growth of a cluster depends

_

only on the relation of an object/cluster to its neighbors, independent of the relations of the other object/clusters with each other. However, this is not the case for the standard agglomerative clustering. Thus, if we stop the algorithm early, then, we will possibly have representatives of many clusters which correspond to the denser and more important (informative) parts. On the other hand, the outlier objects do not occur in the nearest neighborhood of many other clusters or objects. Thus, they join the other parts of the dendrogram only at the higher levels. Thereby, Algorithm 1 can be employed to provide a systematic way to separate structure from noise and outlier objects at different resolutions. The probability of object ibeing an outlier is proportional to the level at which the object joins to the other objects/clusters, i.e.,

$$\Pr[i \in outlier] \propto l^*(i)$$

where $l^*(i)$ specifies the level at which object *i* joins to one of the other clusters/objects for the first time. The higher $l^*(i)$ is, the larger the outlier probability is. We postpone the detail to future work.

We may parametrize this strategy by a parameter such as α which specifies the ratio of the (smallest) *reliable* linkages to be established at each step. A value close to zero then corresponds to the standard variant, whereas $\alpha = 1$ will be equal to the reliable strategy described in Algorithm1. In this way, we can provide even a richer family of alternative strategies for performing agglomerative clustering.

3 Reliable Minimum Spanning Trees

Minimum spanning trees (MSTs) are used in several applications such as transportation, computer and telecommunication networks [17], image segmentation [12], taxonomy learning [38] and power systems [29]. It is known that the *single* linkage method is equivalent to the Kruskal's algorithm [24] for computing a minimum spanning tree [16]. Consistently, we study that Algorithm 1 with the *single* criterion also yields a minimum spanning tree (Theorem 1), which then its construction is adaptive w.r.t. the diverse density of the underlying data.

Before proving Theorem 1, we first introduce some notations. Consider a forest (collection) of trees $\{T_0, T_1, ...\}$. The distance (the edge weight) between the two trees T_p and T_q is computed according to the *single* criterion, i.e.,

$$\Delta_{pq} = \min_{i \in T_p} \min_{j \in T_q} \mathbf{D}_{ij}$$

The nearest tree from tree T_p , i.e. T_p^* , is obtained via $T_p^* = \arg \min_{T_q} \Delta pq, q \neq p$. Moreover, e_p^* shows the edge corresponds to the nearest tree from T_p , i.e.,

$$e_p^* = \arg\min_{e \in E} \Delta_{pq}, q \neq p$$
,

where E is the set of all current inter-tree edges.

Theorem 1. *The dendrogram generated by Algorithm 1 with the single linkage criterion computes a minimum spanning tree.*

Proof sketch. Consider a forest of trees T_0, T_1, \dots . According to the connectivity condition of the final minimum spanning tree, every tree T_p should be connected via an edge to the rest of the MST. This edge should be e_p^* , i.e., an edge (linkage) with minimal weight among the edges of T_p , to keep the spanning tree minimal. Otherwise, if a larger edge is selected, then, the resultant spanning tree will have a larger total weight (i.e., a contradiction occurs). The linkage suggested by Algorithm 1 (with the *single* criterion) satisfies this condition: The selected linkage is the smallest linkage connected to both T_p and T_p^* (the tree at the other side).

Hence, at the beginning, we consider each object as a separate tree, where all must belong to the final minimum spanning tree. Then, according to the aforementioned argument and based on induction, the edges selected at each step belong to the final MST. Thus, the final tree will be a minimum spanning tree.

In this context, the generalized greedy algorithm [15] provides a general framework for computing minimum spanning trees, by showing that the edge e_{p*} is a consistent choice with a final minimum spanning tree. Thereby, a greedy MST algorithm, at each step, i) picks T_p and T_p^* , i.e., two candidate trees where at least one is the nearest neighbor of the other, ii) combines them via the smallest edge e_p^* to build a larger tree, and iii) removes the selected trees T_p and T_p^* . The procedure continues until only a single tree with *n* nodes remains, which is a MST.

Different algorithms, e.g. Kruskal's and Prim's [33], differ only in the way they pick the candidate trees at each step. Kruskal's, at each step, picks a pair of trees that have a minimal distance among all pairs of trees. However, Prim's produces the MST via growing only one tree, say T_0 , by iteratively attaching a singleton tree which has minimal distance to that, until it contains all the singleton trees.

Algorithm 1 with the *single* criterion yields an alternative viewpoint on the construction of MSTs. According to the *generalized greedy algorithm*, to combine two candidate trees, it is sufficient that one of them occurs in the nearest neighborhood of the other. However, Algorithm 1 requires that both trees mutually occur insides the nearest neighborhood of each other. As shown, e.g. in Figures 1(b) and 1(c), such a strategy yields a robust and adaptive minimum spanning tree. In summary,

I. the standard agglomerative method, in a very strict way, selects only one *reliable* linkage at each step, the one which has a minimal length (weight).

II. On the other hand, the *generalized greedy algorithm* for MST construction allows one to select any edge which occurs inside the nearest neighbors of one of the trees, regardless of being *reliable* or not (which might not be robust).

III. Algorithm 1 follows an intermediate strategy. It suggests to select all the *reliable* linkages (edges) which yields adaptation and flexibility (compared to the former approach) and robustness (compared to the latter approach).

IV. Parameterization of Algorithm 1 (by α , as discussed before) can lead to an even larger family of different (*reliable*) minimum spanning tree algorithms.

We note that the final MST obtained by Algorithm 1 could be the same as the Kruskal's MST. However, the order of selecting the edges differs. Thus, in particular, if we stop early constructing the MST, then the available solution could be different.

4 Experiments

We experimentally evaluate the performance of the reliable agglomerative strategy on a variety of real-world datasets and compare it against the standard approach. In these datasets, each object (i.e., document, image, etc) is represented by a vector according to the respective features. For the text documents, we use the tf-idf vectors. We compute the pairwise dissimilarities between the objects according to squared Euclidean distance measure.

Data The first datasets are selected from the UCI data repository [11].

- 1. *Ecoli*: contains the information of 336 protein localization sites in 7 categories.
- 2. *Hayes Roth*: is related to a study on human subjects which contains 160 instances and 3 classes.
- 3. *Iris*: contains the information of 150 iris plants grouped in 3 classes.
- 4. *Lung Cancer*: includes 3 types of 32 instances of pathological lung cancer.
- 5. *Perfume*: consists of odors of 20 different perfumes (classes), where there are in total 560 measurements.
- Seeds: includes 210 measurements of geometrical properties of kernels belonging to different varieties of wheat.
- 7. *Wine*: contains 178 measurements of a chemical analysis of different types of wines.

We also use the three main subsets of 20-newsgroup data collection:

1. COMP: a subset of 1,955 documents in five groups: 'comp.graphics', 'comp.windows.x', 'comp.os.mswindows.misc', 'comp.sys.ibm.pc.hardware', 'comp.sys.mac.hardware'.

- REC: a subset of 1,590 documents in four groups related to race and sports: 'rec.autos', 'rec.motorcycles', 'rec.sport.baseball', 'rec.sport.hockey'.
- 3. *SCI*: a subset of 1,579 documents in four groups related to science: '*sci.crypt*', '*sci.electronics*', '*sci.med*', '*sci.space*'.

In addition, we investigate the performance of different strategies on real datasets collected by a document processing corporation. The original dataset (called *Real I*) contains the vectors of 675 scanned documents each represented in a 4,096 dimensional space. This dataset contains 56 clusters which several of them have only one or few documents. Then, by removing the clusters with only one or two documents, we obtain a new dataset, called *Real II* (634 documents). Finally, we obtain *Real III* by keeping the clusters that have at least 5 documents (592 documents).

Evaluation To investigate the quality of a dendrogram, cophenetic correlation [40] is sometimes employed specially in biostatistics which measures the correlation between the dendrogram and the base dissimilarities between the objects. However, this evaluation measure has several issues, e.g. i) it considers only the direct distances and discards the manifolds or the elongated structures, and ii) its value is very sensitive to the way the inter-cluster distances are computed. For example, the two single and Ward criteria might lead to the same dendrograms, but their cophenetic correlation could significantly differ, since they compute different types of distances between the clusters (which constitute the elements of a dendrogram). However, in our experiments, we have access to the groundtruth, i.e. to the true labels of the objects. Thus, we may use early stopping up to K clusters or eliminate the last K - 1linkages from a dendrogram to produce K clusters. There exist more involved methods to convert a dendrogram into a set of K clusters, but they require fixing critical parameters in advance which finding their correct values is non-trivial in an unsupervised setting such as clustering. With both strategies, ties might occur when producing exactly K clusters. We tackle the problem in the same way as the common implementations do, e.g. we break the ties according to the order (index) of the clusters, where all other tricks are applicable to both approaches as well. Moreover, we observe such ties usually occur at the lower levels of the dendrogram, i.e., for a very large K. For a rather small K, which is the case in many clustering problems, such ties are very rare. In real data it does not often happen that many real clusters are mutually the nearest neighbors of each other. Having multiple reliable linkages to establish occurs at the low or intermediate levels. Thus, at the higher level, where we remove the linkages, ties are not common.

We compare the true and the computed clusters according to three criteria:

	single		complete		average		centroid		Ward	
dataset	stnd	rlbl	stnd	rlbl	stnd	rlbl	stnd	rlbl	stnd	rlbl
Ecoli	0.0564	0.0564	0.6235	0.6235	0.5907	0.6812	0.0462	0.0383	0.5473	0.5445
Hayes Roth	0.0161	0.2336	0.0354	0.2338	0.1629	0.2338	0.0000	0.0030	0.0249	0.0808
Iris	0.5821	0.5821	0.6963	0.6963	0.6301	0.6301	0.7934	0.7934	0.7578	0.7578
Lung Cancer	0.0149	0.0149	0.1537	0.2070	0.0239	0.1413	0.0000	0.0000	0.1766	0.1684
Perfume	0.7024	0.7024	0.7332	0.7332	0.7601	0.7595	0.7544	0.7664	0.8246	0.8246
Seeds	0.0283	0.0283	0.6029	0.6029	0.6083	0.7055	0.6034	0.6140	0.7243	0.7243
Wine	0.0237	0.0237	0.4307	0.4307	0.3223	0.3452	0.3251	0.3251	0.4097	0.4097
СОМР	0.0604	0.0604	0.1459	0.1459	0.0453	0.1611	0.0312	0.0341	0.1021	0.1140
REC	0.0228	0.0402	0.1793	0.1793	0.0330	0.2375	0.0161	0.0315	0.2574	0.2574
SCI	0.0617	0.0617	0.0823	0.0823	0.0387	0.1557	0.0339	0.0651	0.1997	0.3042
Real I	0.5782	0.5782	0.7114	0.7114	0.7813	0.8237	0.0785	0.0670	0.5976	0.7546
Real II	0.5711	0.5711	0.7430	0.7430	0.7704	0.8130	0.0458	0.0268	0.6542	0.8274
Real III	0.5389	0.5389	0.7581	0.7581	0.7209	0.7733	0.0132	0.0145	0.7156	0.8697

Table 1: Performance of standard (stnd) and reliable (rlbl) agglomerative strategies w.r.t. Mutual Information. The reliable strategy often yields the improvment of the results.

Table 2: Performance of standard (stnd) and reliable (rlbl) strategies with different criteria w.r.t. Rand score, where the reliable strategy usually gives superior results.

	single		complete		average		centroid		Ward	
dataset	stnd	rlbl	stnd	rlbl	stnd	rlbl	stnd	rlbl	stnd	rlbl
Ecoli	0.0386	0.0386	0.6908	0.6908	0.6974	0.7509	0.0297	0.0252	0.4686	0.3914
Hayes Roth	0.0185	0.2086	0.0327	0.2451	0.1620	0.2451	0.0000	0.0058	0.0496	0.1073
Iris	0.5638	0.5638	0.6423	0.6423	0.5659	0.5659	0.7592	0.7592	0.7312	0.7312
Lung Cancer	0.0371	0.0371	0.2809	0.3533	0.1327	0.1170	0.0000	0.0000	0.3388	0.1698
Perfume	0.4667	0.4667	0.5096	0.5096	0.5651	0.5600	0.5600	0.5749	0.6590	0.6590
Seeds	0.0025	0.0025	0.5461	0.5461	0.5543	0.7320	0.5664	0.5626	0.7132	0.7132
Wine	0.0054	0.0054	0.3708	0.3708	0.2926	0.3204	0.3266	0.3266	0.3684	0.3684
СОМР	0.0531	0.0531	0.1331	0.1331	0.0040	0.1459	0.0119	0.0138	0.0290	0.0296
REC	0.0262	0.0742	0.0905	0.0905	0.0025	0.2266	0.0014	0.0052	0.2162	0.2162
SCI	0.0884	0.0884	0.0108	0.0108	0.0034	0.0782	0.0493	0.0588	0.0908	0.1688
Real I	0.4296	0.4296	0.4133	0.4133	0.4687	0.5699	0.0401	0.0403	0.2649	0.4969
Real II	0.4409	0.4409	0.4142	0.4142	0.5581	0.6685	0.0283	0.0198	0.3193	0.6176
Real III	0.4235	0.4235	0.4414	0.4414	0.6850	0.6443	0.0123	0.0151	0.4101	0.7042

- 1. Normalized Mutual Information [41], which measures the mutual information between the true and the estimated solutions.
- 2. Normalized Rand score [21], which computes the similarity between the two solutions.
- 3. V-measure [34], which obtains the harmonic mean of homogeneity and completeness.

We compute the normalized variant of these measures, such that they yield zero for randomly estimated solutions and thereby any positive score indicates a (partially) consistent

solution.

Results Tables 1, 2 and 3 show the performance scores in order w.r.t. Normalized Mutual Information, Normalized Rand score and V-measure, where the best results for each dataset are bolded. We observe that on different datasets, the reliable agglomeration strategy always contributes to the best results. In most cases, it improves significantly the best results of the standard strategy, and in fewer cases it yields consistent results with that. Moreover, in few cases it could happen that for a non-optimal criterion, the reliable variant yields (slightly) worse results. However, such a criterion is not the best choice

	single		complete		average		centroid		Ward	
dataset	stnd	rlbl	stnd	rlbl	stnd	rlbl	stnd	rlbl	stnd	rlbl
Ecoli	0.1355	0.1355	0.6789	0.6789	0.6683	0.7115	0.1008	0.0819	0.6123	0.5658
Hayes Roth	0.0579	0.3472	0.0556	0.3010	0.2164	0.3010	0.0000	0.0203	0.0412	0.0995
Iris	0.7175	0.7175	0.7221	0.7221	0.7046	0.7046	0.8057	0.8057	0.7701	0.7701
Lung Cancer	0.0287	0.0287	0.1810	0.2303	0.0742	0.1743	0.0000	0.0000	0.2140	0.2030
Perfume	0.8117	0.8117	0.8251	0.8251	0.8437	0.8417	0.8380	0.8442	0.8796	0.8796
Seeds	0.0663	0.0663	0.6152	0.6152	0.6204	0.7094	0.6150	0.6260	0.7309	0.7309
Wine	0.0615	0.0615	0.4423	0.4423	0.4049	0.3920	0.4277	0.4277	0.4161	0.4161
СОМР	0.0351	0.0351	0.1857	0.1857	0.0754	0.1922	0.0515	0.0558	0.1323	0.1468
REC	0.0307	0.0614	0.2310	0.2310	0.0609	0.2737	0.0308	0.0569	0.3124	0.3124
SCI	0.0518	0.0518	0.1337	0.1337	0.0714	0.2005	0.0270	0.0339	0.2546	0.3407
Real I	0.7708	0.7708	0.8484	0.8484	0.8409	0.8714	0.2181	0.2016	0.7932	0.8421
Real II	0.7570	0.7570	0.8221	0.8221	0.8361	0.8725	0.1384	0.0925	0.8023	0.8614
Real III	0.7197	0.7197	0.8155	0.8155	0.8427	0.8408	0.0510	0.0594	0.8238	0.8951

Table 3: Performance of standard (stnd) and reliable (rlbl) strategies w.r.t. V-measure. The reliable strategy provides better results compared to the standard variant.

and the respective scores are not high compared to the alternatives. For example, on Real I and Real II with the centroid criterion, the standard strategy yields slightly better scores than the reliable strategy. However, the centroid criterion is not the best option and yields anyway very low scores. With a more appropriate criterion (e.g. average and Ward), the reliable strategy gives significantly higher scores. Note that the different evaluation measures are often consistent, but in some cases they might disagree. For example, on the Seeds dataset, Normalized Mutual Information suggests the Ward criterion as the best option, but Normalized Rand score selects the average criterion, although Ward still yields high scores. Finally, it is notable that we observe similar experimental runtimes for the two strategies, as they perform similar operations. For example, on the COMP dataset and with the single criterion, the runtimes of the standard and reliable strategies are 0.9135 and 0.9208 seconds. With the average criterion, the runtimes respectively are 0.5338 and 0.5326 seconds.

5 Conclusion

We investigated an adaptive and density-consistent strategy for agglomerative clustering, wherein at each step we establish all the *reliable* linkages, instead of establishing only the smallest one (consistent with the high-level method in [3]). The two clusters connected by a *reliable* linkage share similar properties, such that they select each other as a nearest neighbor. This strategy enables the dendrogram to be adaptive w.r.t. the diverse densities of different clusters and supports early stopping the clustering procedure. In the following, we studied how *reliable agglomerative clustering* with the *single* criterion can be used to produce a minimum spanning tree. Finally, we performed experiments on several real-world datasets to investigate the performance of the reliable agglomerative strategy.

Acknowledgement. This work was partially done at Xerox Research Centre Europe (XRCE).

References

- [1] Margareta Ackerman and Shai Ben-David. A characterization of linkage-based hierarchical clustering. *Journal of Machine Learning Research*, 17:1–17, 2016.
- [2] Maria-Florina Balcan, Yingyu Liang, and Pramod Gupta. Robust hierarchical clustering. J. Mach. Learn. Res., 15(1):3831–3871, 2014.
- [3] Michel Bruynooghe. Méthodes nouvelles en classification automatique de données taxinomiques nombreuses. *Statistique et analyse des données*, 2(3):24–42, 1977.
- [4] Moses Charikar and Vaggos Chatziafratis. Approximate hierarchical clustering via sparsest cut and spreading metrics. In *Proceedings of the Twenty-Eighth Annual* ACM-SIAM Symposium on Discrete Algorithms, SODA '17, pages 841–854, 2017.
- [5] Morteza Haghir Chehreghani, Hassan Abolhassani, and Mostafa Haghir Chehreghani. Improving density-based methods for hierarchical clustering of web pages. *Data Knowl. Eng.*, 67(1):30–50, 2008.
- [6] Morteza Haghir Chehreghani, Mostafa Haghir Chehreghani, and Hassan Abolhassani. Probabilis-

tic heuristics for hierarchical web data clustering. *Computational Intelligence*, 28(2):209–233, 2012.

- [7] K. Chidananda Gowda and G. Krishna. Agglomerative clustering using the concept of mutual nearest neighbourhood. *Pattern Recognition*, 10(2):105–112, 1978.
- [8] Michael Cochez and Hao Mou. Twister tries: Approximate hierarchical agglomerative clustering for average distance in linear time. In *SIGMOD '15*, pages 505–517, 2015.
- [9] Vincent Cohen-Addad, Varun Kanade, and Frederik Mallmann-Trenn. Hierarchical clustering beyond the worst-case. In *NIPS* '17, pages 6201–6209. 2017.
- [10] Sanjoy Dasgupta. A cost function for similarity-based hierarchical clustering. In STOC '16, pages 118–127, 2016.
- [11] Dheeru Dua and Casey Graff. UCI machine learning repository, 2017.
- [12] Pedro F. Felzenszwalb and Daniel P. Huttenlocher. Efficient graph-based image segmentation. *Int. J. Comput. Vision*, 59(2):167–181, 2004.
- [13] Chris Fraley and Adrian E Raftery. Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association*, 97:611–631, 2002.
- [14] Pasi Fränti, Olli Virmajoki, and Ville Hautamäki. Fast agglomerative clustering using a k-nearest neighbor graph. *IEEE Trans. Pattern Anal. Mach. Intell.*, 28(11):1875–1881, 2006.
- [15] H N Gabow, Z Galil, T Spencer, and R E Tarjan. Efficient algorithms for finding minimum spanning trees in undirected and directed graphs. *Combinatorica*, 6(2):109–122, 1986.
- [16] 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), 1969.
- [17] R. L. Graham and Pavol Hell. On the history of the minimum spanning tree problem. *IEEE Ann. Hist. Comput.*, 7(1):43–57, 1985.
- [18] Yan Gu, Yong He, Kayvon Fatahalian, and Guy Blelloch. Efficient bvh construction via approximate agglomerative clustering. In *Proceedings of the 5th High-Performance Graphics Conference*, HPG '13, pages 81– 88, 2013.

- [19] Morteza Haghir Chehreghani and Mostafa Haghir Chehreghani. Learning representations from dendrograms. *Mach. Learn.*, 109(9-10):1779–1802, 2020.
- [20] Nicholas A. Heard. Iterative reclassification in agglomerative clustering. *Journal of Computational and Graphical Statistics*, 20(4):920–936, 2012.
- [21] L. Hubert and P. Arabie. Comparing partitions. *Journal* of classification, 2(1):193–218, 1985.
- [22] George Karypis, Eui-Hong Han, and Vipin Kumar. Chameleon: Hierarchical clustering using dynamic modeling. *Computer*, 32(8):68–75, 1999.
- [23] Patrick K. Kimes, Yufeng Liu, David Neil Hayes, and James Stephen Marron. Statistical significance for hierarchical clustering. *Biometrics*, 73(3):811–821, 2017.
- [24] Joseph B. Kruskal. On the Shortest Spanning Subtree of a Graph and the Traveling Salesman Problem. In *Proceedings of the American Mathematical Society*, 7, 1956.
- [25] G. N. Lance and W. T. Williams. A general theory of classificatory sorting strategies. *The Computer Journal*, 9(4):373–380, 1967.
- [26] Mark A. Levenstien, Yaning Yang, and Jurg Ott. Statistical significance for hierarchical clustering in genetic association and microarray expression studies. *BMC Bioinformatics*, 4(1), 2003.
- [27] J. MacQueen. Some methods for classification and analysis of multivariate observations. In 5th Berkeley Symposium on Mathematical Statistics and Probability, pages 281–297, 1967.
- [28] Oded Maimon and Lior Rokach. *Data Mining and Knowledge Discovery Handbook*. 2005.
- [29] H. Mori and S. Tsuzuki. A fast method for topological observability analysis using a minimum spanning tree technique. *IEEE Trans. Power Systems*, 6:491–500, 1991.
- [30] Daniel Mullner. Modern hierarchical, agglomerative clustering algorithms. *CoRR*, abs/1109.2378, 2011.
- [31] Andrew Y. Ng, Michael I. Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. In *NIPS* '01, pages 849–856, 2001.
- [32] J. Podani. Introduction to the exploration of multivariate biological data. Backhuys Publishers, 2000.
- [33] Robert C. Prim. Shortest connection networks and some generalizations. *The Bell Systems Technical Journal*, 36(6):1389–1401, 1957.

- [34] Andrew Rosenberg and Julia Hirschberg. V-measure: A conditional entropy-based external cluster evaluation measure. In *EMNLP-CoNLL*, pages 410–420. ACL, 2007.
- [35] Aurko Roy and Sebastian Pokutta. Hierarchical clustering via spreading metrics. In *NIPS* '16, pages 2324– 2332, 2016.
- [36] Aurko Roy and Sebastian Pokutta. Hierarchical clustering via spreading metrics. *J. Mach. Learn. Res.*, 18(1):3077–3111, 2017.
- [37] Jianbo Shi and Jitendra Malik. Normalized cuts and image segmentation. *IEEE Trans. Pattern Anal. Mach. Intell.*, 22(8):888–905, 2000.
- [38] Peter Henry Andrews Sneath. The application of computers to taxonomy. *Journal of General Microbiology*, 17:201–226, 1957.
- [39] R. R. Sokal and C. D. Michener. A statistical method for evaluating systematic relationships. *University of Kansas Science Bulletin*, 38:1409–1438, 1958.

- [40] R. R. Sokal and F. J. Rohlf. The comparison of dendrograms by objective methods. *Taxon*, 11(2):33–40, 1962.
- [41] Nguyen Xuan Vinh, Julien Epps, and James Bailey. Information theoretic measures for clusterings comparison: Variants, properties, normalization and correction for chance. J. Mach. Learn. Res., 11:2837–2854, 2010.
- [42] Ulrike von Luxburg. A tutorial on spectral clustering. *Statistics and Computing*, 17(4):395–416, 2007.
- [43] Joe H. Ward. Hierarchical grouping to optimize an objective function. *Journal of the American Statistical Association*, 58(301):236–244, 1963.
- [44] Pelin Yildirim and Derya Birant. K-linkage: A new agglomerative approach for hierarchical clustering. 17:77– 88, 2017.