Nonparametric Feature Extraction from Dendrograms

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Abstract—We propose feature extraction from dendrograms in a nonparametric way. The commonly used Minimax distance measures correspond to building a dendrogram with single linkage criterion, with defining specific forms of a level function and a distance function over that. Therefore, we extend this method to arbitrary dendrograms. We develop a generalized framework wherein different distance measures can be inferred from different types of dendrograms, level functions and distance functions. Via an appropriate embedding, we compute a vector-based representation of the inferred distances, in order to enable many numerical machine learning algorithms to employ such distances. Then, to address the model selection problem, we study the aggregation of different dendrogram-based distances respectively in solution space and in representation space in the spirit of deep representations. In the first approach, for example for the clustering problem, we build a graph with positive and negative edge weights according to the consistency of the clustering labels of different objects among different solutions, in the context of ensemble methods. Then, we use an efficient variant of correlation clustering to produce the final clusters. In the second approach, we investigate the sequential combination of different distances and features sequentially in the spirit of multi-layered architectures to obtain the final features. Finally, we demonstrate the effectiveness of our approach via several numerical studies.

1. Introduction

Real-world datasets are often complicated and a priori unknown, leading to further enrichment of the basic representation to capture the correct underlying structures and patterns. Kernel methods are commonly used for this purpose [21], [39]. However, their applicability is confined by several limitations [19], [33], [48]. i) Finding the optimal parameter(s) of a kernel function is often nontrivial, in particular in an unsupervised learning task such as clustering where no labeled data is available for cross-validation. ii) The proper values of the parameters usually occur inside a very narrow range that makes cross-validation critical, even in presence of labeled data. iii) Kernels often assume a global structure which does not distinguish between different types of patterns or clusters in the data. To overcome such challenges, some graph-based distance measures have been developed which can be interpreted as nonparametric kernels. In this setup, each object corresponds to a node in a graph, and the edge weights are the pairwise (e.g., Euclidean) distances between the respective objects (nodes).

Then, different methods perform different types of inferences to compute an effective distance measure between the pairs of objects. Link-based methods [4], [50] first compute the path-specific distance of every path between the nodes via summing the edge weights on this path. The final distance is then obtained by summing up the path-specific distances of all paths, and then sum them up. These distances can be computed by inverting the Laplacian of the distance matrix (in the context of Markov diffusion kernel [15], [50]), which, however, would require an $O(n^3)$ runtime, with $n$ the number of objects.

Minimax distance measure is an alternative choice which computes a minimal largest gap among all possible paths between the objects. Several studies demonstrate the superior performance of Minimax distances, even compared to metric learning or link-based measures [12], [14], [18], [24], [25], [26], [31]. Minimax distances have been first employed on clustering problems in two different forms, either as an input in the form of pairwise distance matrix [3], [35], or integrated into different clustering algorithms [13].

The straightforward approach to compute the pairwise Minimax distances is to use an adapted variant of the Floyd-Warshall algorithm, whose runtime is $O(n^3)$ [1]. However, the method in [13] is computationally even more demanding, as its runtime is $O(n^2|E| + n^3 \log n)$ ($|E|$ is the number of edges in the graph). Based on equivalence of Minimax distances over a graph and over any minimum spanning tree constructed on that, [19] proposes to compute first a minimum spanning tree (e.g., using Prim’s algorithm) and then obtain the Minimax distances over that via an efficient dynamic programming algorithm. Then, the runtime of computing pairwise Minimax distances reduces to $O(n^2)$. Several algorithms develop efficient algorithms for $K$-nearest neighbor search with Minimax distances [18], [24], [25].

The method in [24] presents a message passing method similar to the sum-product algorithm [27] to perform $K$-nearest neighbor classification with Minimax distances. Even though it takes $O(n)$ time, it needs computing a minimum spanning tree (MST) in advance that might require $O(n^2)$ runtime. Thereafter, the greedy algorithm in [25] computes the Minimax $K$ nearest neighbors by
space partitioning via a Fibonacci heap whose runtime is $O(\log n + K \log K)$. However, the method is applicable only to Euclidean spaces and where the graph is sparse. Finally, [18] has recently proposed an efficient Minimax $K$-nearest neighbor search method that is applicable to general graphs and distances. Its runtime, similar to the standard method, is linear in any setting. In addition, the method provides an outlier detection mechanism along with performing $K$-nearest neighbor search, all with a linear time. Then, [12], [19], [29], [31], [34], [35], [46], [51] have studied Minimax distances in different classification and kernel estimation tasks.

Minimax distances correspond to building a dendrogram with respect to single linkage criterion and defining a specific form of a level function and a distance function over that. However, in general, dendrograms might be constructed according to different criteria, i.e., the way they define the inter-node distances called linkage. For example, the single linkage criterion [40] defines the linkages as the distance between the nearest members of the nodes. In contrast, the complete linkage criterion [39], [42] defines the distance between two nodes as the distance between their farthest members, which corresponds to the maximum within-node distance of the new node. On the other hand, in average criterion [41] the average of inter-node distances is used as the linkage between two nodes. The Ward method [49] uses the distances between the means of the nodes normalized by a function of the size of the nodes. Therefore, in this paper, we develop a generalized framework to compute different distance measures according to different dendrograms. Moreover, we obtain an embedding of the pairwise dendrogram-based distances into a new vector space such that their squared Euclidean distances in the new space equal to their dendrogram-based distances. This embedding provides to employ dendrogram-based distances with a wide range of different machine learning methods, and yields a rich family of alternative graph-based distances with Minimax distance measure being only a special instantiation.

Then, we encounter a model selection problem which asks for the choice of the appropriate distance measure (and dendrogram). Therefore, we first study the aggregation of different distance measures in the solution space in the context of model averaging and ensemble methods. Assuming, e.g., the different distance measures are used for an unsupervised clustering task, we build a graph with positive and negative edge weights based on the (dis)agreement of the respective nodes among different clustering solutions. Then, we develop an efficient variant of correlation clustering to obtain the final ensemble solution. Second, several recent studies demonstrate the superior performance of deep representation learning models that extract complex features via aggregating representations at different levels. Such models are highly over-parameterized and thus require huge amounts of training data to infer the parameters. However, unsupervised representation learning is expected to become far more important in longer term, as human and animal learning is mainly unsupervised [30]. Thereby, with the possibility of having access to a wide range of alternative feature extraction models, we investigate a nonparametric design of multi layer deep approach in an unsupervised manner (in representation space, instead of solution space) which does not require inferring or fixing any critical parameter. Finally, we experimentally validate the effectiveness of our approach on several standard real-word datasets from UCI data repository.

2. Feature Extraction from Dendrograms

In this section, we first introduce the setup for computing distance measures from dendrograms, and then, based on the relation between Minimax distances and single linkage agglomerative clustering, we propose a generalized approach to extract features from dendrograms.

2.1. Pairwise distances over dendrograms

We are given a dataset of $n$ objects $O = \{1, ..., n\}$ and the corresponding measurements. The measurements can be for example the vectors in a feature space or the pairwise distances between the objects. In the former case, the measurements are shown by the $n \times d$ matrix $Y$, wherein the $i^{th}$ row (i.e., $Y_i$) specifies the $d$ dimensional vector of the $i^{th}$ object. In the latter form, an $n \times n$ matrix $X$ represents the pairwise distances between the objects. Then, we might show the data by graph $G(O, X)$, wherein $O$ is the set of its vertices and $X$ represents the edge weights. Note that the former is a specific form of the latter representation, where the pairwise distances are computed according to (squared) Euclidean distances.

A dendrogram $D$ is defined as a rooted ordered tree such that,

1) each node $v$ in $D$ includes a non-empty subset of the objects, i.e., $v \subset O, |v| > 0, \forall v \in D$, and
2) the overlapping nodes are ordered, i.e., $\forall u, v \in D, u \cap v \neq \emptyset$, then either $u \subseteq v$ or $v \subseteq u$.

The latter condition implies that between every two overlapping nodes an ancestor-descendant relation holds, i.e., $u \subseteq v$ indicates $v$ is an ancestor of $u$, and $u$ is a descendant of $v$.

The nodes at the lowest level (called the final nodes) are the singleton objects, i.e., node $v$ is a final node if and only if $|v| = 1$. A node at a higher level contains the union of the objects of its children (direct descendants). The root of a dendrogram is defined as the node at the highest level (which has the maximum size), i.e., all other nodes are its descendants. $\text{linkage}(v)$ returns the distance between the children of $v$ based on the criterion used to compute the dendrogram. For the simplicity of explanation, we assume each node has only two children. Then, the level of node $v$, i.e., $\text{level}(v)$ is determined by $\max(\text{level}(c_l), \text{level}(c_r)) + 1$, where $c_l$ and $c_r$ indicate the two child nodes of $v$. For the final nodes, the $\text{level}()$ function returns 0. Every connected subtree of $D$ whose final nodes contain only singleton objects from $O$ constitutes a dendrogram on this set. We use $D^D$ to refer to the set of all (sub)dendrograms derived in this form from $D$. 

Note that in an agglomerative method we always have $\text{linkage}(v) \geq \max(\text{linkage}(c_l, c_r))$. In particular, we usually expect $\text{linkage}(v) > \max(\text{linkage}(c_l, c_r))$, unless there are ties for example in the case of single linkage method, where then the new combination does not yield a higher level node. Rather, the new node has effectively three children instead of two, where two of them are combined to make an intermediate node. Without loss of generality and for the sake of simplicity of presentation, we assume that ties do not occur, i.e., we always have

$$\text{level}(v) = \max(\text{level}(c_l, c_r)) + 1. \quad (1)$$

We consider a generalized variant of the $\text{level}()$ function over a dendrogram $D$. Any function $f(v)$ that satisfies the following conditions is a generalized level function.

1. $f(v) = 0$ if and only if $v \in O, |v| = 1$.
2. $f(v) > f(u)$ if and only if $v$ is an ancestor of $u$.

It is obvious that the basic function $\text{level}()$ satisfies these conditions. We use $v^*_ij$ to denote the node at the lowest level which contains both $i$ and $j$, i.e.,

$$v^*_ij = \arg\min_{v \in D} f(v) \quad \text{s.t.} \ i, j \in v. \quad (2)$$

Given dendrogram $D$, each node $v \in D$ represents the root of a dendrogram $D' \in D^D$. Thereby, the dendrogram $D'$ inherits the properties of its root node, i.e., $f(D') = \max_{v \in D} f(v)$ and $\text{linkage}(D') = \max_{v \in D} \text{linkage}(v)$, since the root node has the maximum linkage and level among the nodes of $D'$. In this paper, we investigate inferring pairwise distances from a dendrogram computed according to an arbitrary criterion, i.e., beyond single linkage criterion. Moreover, our framework allows one to define the level function in a very flexible and diverse way. For this purpose, we consider the following generic distance measure over dendrogram $D$, where $D_{ij}$ indicates the pairwise dendrogram-based distance between the pair of objects (final nodes) $i, j \in O$.

$$D_{ij} = \min_{i, j \in D'} f(D') \quad \text{s.t.} \ i, j \in D', \text{ and } D' \in D^D. \quad (3)$$

The level function $f(v)$ and the distance matrix $D^D$ provide distinguishing outliers at different levels. The outlier objects do not occur in the nearest neighborhood of many other clusters or objects. Thus, they join the other nodes of the dendrogram only at higher levels. Hence, the probability of object $i$ being an outlier is proportional to the level at which it joins to other objects/clusters. Therefore, such objects will have a large dendrogram-based distance from the other objects.

2.2. Minimax distances and single linkage agglomeration

We first study the relation between Minimax distances and single linkage agglomerative method. In particular, we elaborate that given the pairwise dissimilarity matrix $X$, the pairwise Minimax distance between objects $i$ and $j$ is equivalent to $D^D_{ij}$ where the dendrogram is produced with single linkage criterion and $D^D_{ij}$ is defined by

$$D_{ij} = \min \text{linkage}(D') \quad \text{s.t.} \ i, j \in D' \text{ and } D' \in D^D, \quad (4)$$

i.e., $f(D')$ in Eq. 3 is replaced by $\text{linkage}(D')$.

**Theorem 1.** For each pair of objects $i, j \in O$, their Minimax distance measure over graph $G(O, X)$ is equivalent to their pairwise distance $D_{ij}^M$ defined in Eq. 4 where the dendrogram $D$ is obtained according to single linkage agglomerative method.

**proof** It can be shown that the pairwise Minimax distances over an arbitrary graph are equivalent to pairwise Minimax distances over ‘any’ minimum spanning tree computed from the graph. The proof is similar to the maximum capacity problem[22] problem. Thereby, the Minimax distances are obtained by

$$D_{i,j}^{MM} = \min_{r \in R_{i,j}(G)} \left\{ \max_{1 \leq l \leq |r|-1} X_{r(l)r(l+1)} \right\} \quad (5)$$

where $r_{ij}$ indicates the (only) route between $i$ and $j$, i.e., to obtain Minimax distances $D_{i,j}^{MM}$, we select the maximal edge weight on the only route between $i$ and $j$ over the minimum spanning tree.

On the other hand, single linkage method and the Kruskal’s minimum spanning tree algorithm are equivalent[16]. Thus, dendrogram $D$ represents the pairwise Minimax distances. Now, we only need to show that the Minimax distances in Eq. 5 equal the distances defined in Eq. 3 of the main text, i.e., $D_{ij}$ is the largest edge weight on the route between $i$ and $j$ in the hierarchy.

Given $i, j, \text{ let } D^* = \arg\min_{i, j \in D'} \text{linkage}(D') \quad \text{s.t.} \ i, j \in D' \text{ and } D' \in D^D$. Then, $D^*$ represents a minimum spanning subtree, which includes a route between $i, j$ (because the root node of $D^*$ contains both $i, j$) and it is consistent with a complete minimum spanning on all the objects. On the other hand, we know that for each pair of nodes $u, v \in D^*$ which have direct or indirect parent-child relation, we have, $\text{linkage}(u) \geq \text{linkage}(v)$ iff $f(u) \geq f(v)$. This indicates that the linkage of the node root of $D^*$ represents the maximal edge weight on the route between $i$ and $j$ induced by the dendrogram $D$. Thus, $D_{ij}$ defined in Eq. 3 of the main text represents $D_{ij}^{MM}$ and the proof is complete.

Notice that the Minimax distances in Eq. 5 are obtained by replacing $f(D')$ with $\text{linkage}(D')$ in the generic form of Eq. 5.

2.3. Vector-based representation of dendrogram-based distances

The generic distance measure defined in Eq. 5 yields an $n \times n$ matrix of pairwise dendrogram-based distances.
between objects. However, a lot of machine learning algorithms perform on a vector-based representation of the objects, instead of the pairwise distances. For instance, mixture density estimation methods such as Gaussian Mixture Models (GMMs) fall in this category. Vectors constitute the most basic form of data representation, since they provide a bijective map between the objects and the measurements, such that a wide range of numerical machine learning methods can be employed with them. Moreover, feature selection is more straightforward with this representation. Thereby, we compute an embedding of the objects into a new space, such that their pairwise squared Euclidean distances in the new space equal to their pairwise distances obtained from the dendrogram. For this purpose, we first investigate the feasibility of this kind of embedding. Theorem 2 verifies the existence of an \( L_2^2 \) embedding for the general distance measure defined in Eq. 3.

**Theorem 2.** Given the dendrogram \( D \) computed on the input data \( Y \) or \( X \), the matrix of pairwise distances \( D^2 \) obtained via Eq. 3 induces an \( L_2^2 \) embedding, such that there exists a new vector space for the set of objects \( O \) wherein the pairwise squared Euclidean distances equal to \( D^2 \)'s in the original data space.

**Proof.** First, we show that the matrix \( D^2 \) yields an *ultrametric*. The conditions to be satisfied are:

1. \( \forall i, j : D^2_{ij} = 0 \) if and only if \( i = j \). We investigate each of the conditions separately. i) First, if \( i = j \), then \( D_{ii}^2 = \min f(i) = 0 \). ii) If \( D_{ij}^2 = 0 \), then \( v^*_i = i = j \), because \( f(v) = 0 \) if and only if \( v \in O \). On the other hand, \( \forall i \neq j, X_{ij} > 0, i.e., f(v^*_i) > 0 \) if \( i \neq j \).
2. \( \forall i, j : D^2_{ij} = 0 \). We have, \( \forall v, f(v) = 0 \). Thus, \( D' \in D^2, \min f(D') \geq 0, i.e., D_{ij}^2 \geq 0 \).
3. \( \forall i, j : D^2_{ij} = D^2_{ji} \). We have, \( D^2 = \{ \min f(D) \text{ s.t. } i, j \in D', \text{ and } D' \in D^2 \} = \{ \min f(D) \text{ s.t. } i, j \in D', \text{ and } D' \in D^2 \} = D^2_{ij} \).
4. \( \forall i, j, k : D^2_{ij} \leq \max(D^2_{ik}, D^2_{kj}) \). We first investigate \( D^2_{ij} \) where we consider the two following cases: i) If \( D^2_{ij} \leq D^2_{ik} \) (Figure 1(a)), then \( D^2_{ik} \) does not yield a contradiction. ii) If \( D^2_{ij} > D^2_{ik} \), then \( i \) and \( j \) join earlier than \( i \) and \( j \), i.e., \( f(v^*_{ij}) > f(v^*_{ik}) \) (Figure 1(b)). In this case, we have \( f(v^*_{ij}) = f(v^*_{ik}) \) and \( f(v^*_{ij}) = f(v^*_{kj}) \). Thus, we will have \( f(v^*_{ij}) = f(v^*_{kj}) \), i.e., \( D^2_{ij} \leq \max(D^2_{ik}, D^2_{kj}) \).

On the other hand, one can show that an *ultrametric* induces an \( L_2^2 \) embedding [9]. Therefore, \( D^2 \) represents the pairwise squared Euclidean distances in a new vector space.

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1. Note that \( X \) is not required to induce a *metric*, i.e., the triangle inequality might fail.

2. In [46], this method has been used to obtain an \( L_2^2 \) embedding for the general distance measure defined in Eq. 3.
colors. However, the intra-cluster Minimax distances for the members of the blue cluster are considerably large compared to the intra-cluster Minimax distances of the black cluster, or even the inter-cluster Minimax distances. Thereby, a clustering algorithm might split the blue cluster, instead of performing a cut on the boundary of the two clusters. According to Proposition 1, the Minimax distance between objects $i$ and $j$ seeks for a linkage with maximal weight on the path between them in the dendrogram. However, the absolute value of a linkage might be biased in a way that it does not precisely reflect the real coherence of the two nodes compared to the other nodes/objects. Thereby, in order to be more adaptive with respect to the diverse densities of the underlying structures, we will investigate the following choice in our experiments.

$$D_{ij}^D = \min_{D'} \text{level}(D') \text{ s.t. } i, j \in D', \text{ and } D' \in D^D.$$  \hfill (7)

Note that our analysis is generic and can be applied to any definition of dendrogram-based distance measure and to any choice of $f$ defined in Eq. [3]. It only needs to satisfy the aforementioned conditions for generalized level functions.

3. Aggregation of Multiple Choices

3.1. Aggregation in solution space

As discussed earlier, a dendrogram can be constructed in several ways according to different criteria. Moreover, the choice of a level function and a distance function over a dendrogram renders another degree of freedom. Therefore, choosing the right method constitutes a model selection question. Let us assume such distances and features are used later in a clustering task, which is the most common unsupervised learning problem. Then, we address this problem via an ensemble method in the context of model averaging.

We follow a two-step procedure to compute an aggregated clustering that represents a given set of clustering solutions (where, e.g., each solution is the result of a particular dendrogram and then a clustering algorithm). First, we construct a graph whose vertices represent the objects and its edge weights can be any integer number (i.e., positive, negative or zero), depending how often the respective vertices appear at the same cluster among the $M$ different clustering solutions. More specifically, we initialize the edge weights by zero. Then, for each clustering solution $c^m \in \{1, \ldots, K\}^n, 1 \leq m \leq M$ (each obtained from a different dendrogram-based representation), we compute a co-clustering matrix whose $(i, j)^{th}$ entry is $+1$ if $c^m_i = c^m_j$, and it is $-1$ otherwise ($K$ indicates the number of clusters). Finally, we sum up the co-clustering matrices to obtain $S^c$. Algorithm 1 describes the procedure in detail.

**Algorithm 1** Aggregation of $M$ clustering solution by correlation clustering.

**Require:** A set of $M$ clustering solutions $c^m, 1 \leq m \leq M$ on the same set of objects $O$.

**Ensure:** An ensemble clustering solution $c^e$.

1. for $i \in O$ do
2. for $j \in O$ do
3. $S^e_{ij} = 0$
4. end for
5. end for
6. for $1 \leq m \leq M$ do
7. for $i \in O$ do
8. for $j \in O$ do
9. if $c^m_i = c^m_j$ then
10. $S^e_{ij} = S^e_{ij} + 1$
11. else
12. $S^e_{ij} = S^e_{ij} - 1$
13. end if
14. end for
15. end for
16. end for
17. Apply Correlation Clustering on $S^e$ to obtain final clustering solution $c^e$.
18. return $c^e$.

Given the graph with positive and negative edge weights, we use correlation clustering [2] to partition it into $K$ clusters. This model computes a partitioning that minimizes the disagreements, i.e., sum of the inter-cluster positive edge weights plus sum of the intra-cluster negative edge weights should be minimal. The cost function for a fixed number of clusters $K$ is written by [2], [20]

$$R(c, S^e) = \frac{1}{2} \sum_{k=1}^{K} \sum_{i,j \in O_k} (|S^e_{ij} - S^e_{ij}|) + \frac{1}{2} \sum_{k=1}^{K} \sum_{k'=k+1}^{K} \sum_{i \in O_k} \sum_{j \in O_{k'}} (|S^e_{ij} + S^e_{ij}|),$$  \hfill (8)

where $O_k$ indicates the objects of the $k^{th}$ cluster, i.e., $\forall i : i \in O_k \text{ iff } c_i = k$.

This ensemble clustering method yields a consistent aggregation of the clustering solutions obtained from different representations, i.e., in the case of $M = 1$ the optimal solution of Eq. [8] does not change the given clustering solution of this single representation.

Efficient optimization of correlation clustering cost function. Finding the optimal solution of the cost function in Eq. [8] is NP-hard [2], [8] and even APX-hard [8]. Therefore, we develop a local search method which computes a local
minimum of the cost function. The good performance of such a greedy strategy is well studied for different clustering models, e.g., K-means [32], kernel K-means [38] and in particular several graph partitioning methods [10], [11].

We begin with a random clustering solution and then we iteratively assign each object to the cluster that yields a maximal reduction in the cost function. We repeat this procedure until no further improvement is achieved, i.e., a local optimal solution is found.

At each step of the aforementioned procedure, one needs to investigate the costs of assigning every object to each of the clusters. The cost function is quadratic, thus, a single evaluation might take $O(n^2)$. Thereby, if the local search converges after $t$ steps, the total runtime will be $O(tn^3)$. However, we do not need to recalculate the cost function for each individual evaluation. Let $R(c, S^c)$ denote the cost of clustering solution $c$, wherein the cluster label of object $i$ is $k$. To obtain a more efficient cost function evaluation, we first consider the contribution of object $i$ in $R(c, S^c)$, i.e., $R_i(c, S^c)$, which is written by

$$R_i(c, S^c) = \frac{1}{2} \sum_{j \in O_k} (|S^c_{ij} - S^c_{ij}|^2 + \frac{1}{2} \sum_{q=1, q \neq k \in O_k} \sum_{j \in O_q} (|S^c_{ij} + S^c_{ij}|).$$

(9)

Then, the cost of the clustering solution $c'$ being identical to $c$ except for the object $i$ which is assigned to cluster $k' \neq k$, i.e., $R(c', S')$ is computed by

$$R(c', S') = R(c, S') - R_i(c, S^c) + R_i(c', S^c),$$

(10)

where $R(c, S')$ is already known and $R_i(c, S^c)$ and $R_i(c', S^c)$ both require an $O(n)$ runtime. Thus, we evaluate the cost function $8$ only once for the initial random clustering. Then, iteratively and until the convergence, we compute the costs of assigning objects to different clusters via Eq. 10 and assign them to the clusters that yields a minimal cost. The total runtime is then $O(tn^3)$.

3.2. Aggregation in representation space

In this section, instead of an ensemble-based approach in the solution space, we describe the aggregation of different (dendrogram-based) distances in the representation space, independent of what the next task will be. The embedding phase of our general-purpose framework not only enables us to employ any numerical machine learning algorithm, but also provides an amenable way to successively combine different representations. In this approach, the features extracted from a dendrogram (e.g., single linkage) are used to build another dendrogram according to the same or a different criterion (e.g., average linkage), in order to yield more complex features. The degree of freedom (richness of the function class) can increase by the choice of a different level or distance function over dendrograms. Such a framework leads to a nonparametric deep architecture wherein a cascade of multiple layers of nonparametric information processing units are deployed for feature transformation and extraction. The output of each layer is a set of features, which can be fed into another layer as input. Note that in this architecture any other (nonparametric) unit can be employed at the layers, beyond the dendrogram-based feature extraction units. Each layer (dendrogram) extracts a particular type of features in the space of data representation.

4. Experiments

We empirically investigate the performance of dendrogram-based representations on different datasets and demonstrate the usefulness of this approach to extract suitable features. Our methods are parameter-free. Thus, to fully benefit from this property, we consider an unsupervised representation learning strategy, such that no free parameter is involved in inferring the new features. Thereby, we apply our methods to clustering and density estimation problems, for which parametric feature extraction methods might be inappropriate, due to lack of labeled data for cross validation (to estimate the parameters). In particular, after extracting the new features, we apply the following algorithms to obtain a clustering solution: i) Gaussian Mixture Model (GMM), ii) K-means, and iii) spectral clustering. In the case of GMM, after computing the assignment probabilities, we assign each object to the cluster (distribution) with a maximal probability. We run each method and as well as correlation clustering (to obtain the ensemble solution) 100 times and pick a solution with the smallest cost or negative log-likelihood.

Data. We perform our experiments on the following datasets selected randomly from the UCI data repository:

1. **Lung Cancer**: Each instance contains 56 attributes and is categorized as cancer or non-cancer.
2. **One-Hundred Plant**: Contains leaf samples for 100 plant species for each 16 samples with 64 features (1,600 samples in total with 100 clusters).
3. **Perfume**: Contains 560 instances (odors) of 20 different perfumes measured by a handheld odor meter.
4. **Statlog (Australian Credit Approval)**: Includes credit card data (described with 14 attributes) of 690 users.
5. **Vertebral Column**: Contains information of 6 biomechanical features of 310 patients categorized according to their status.

In these datasets, the objects and as well as the features extracted from different dendrograms are represented by vectors. Thus, to obtain the pairwise distances, we compute the squared Euclidean distances between the respective vectors. Some clustering algorithms such as spectral clustering require pairwise similarities as input, instead of a vector-based representation. Therefore, as proposed in [17], we convert the pairwise distances $X$ (or $D^{D^2}$, if

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4. Consistently, for correlation clustering we observe a better performance with the local search method compared to the different approximation schemes such as those proposed in [7], [8].

5. Game-theoretic clustering methods such as [5] or other probabilistic approaches such as [6] are applicable with our features too.

6. We observe similar results on several other datasets.
obtained from a dendrogram) to a similarity matrix \( S \) via \( S_{ij} = \max(X) - X_{ij} + \min(X) \), where the \( \max(.) \) and \( \min(.) \) operations return the maximal and minimal elements of the given matrix. Note that an alternative transformation is an exponential function in the form of \( S_{ij} = \exp(-\frac{X_{ij}}{\sigma}) \), which requires fixing the free parameter \( \sigma \) in advance. However, in particular in unsupervised learning, this task is nontrivial and the appropriate values of \( \sigma \) occur in a very narrow range [48].

**Evaluation.** The ground truth solutions of these datasets are available. Therefore, we can quantitatively measure the performance of each method by comparing the estimated and the true cluster labels. For each estimated clustering solution, we compute three commonly used quality measures: i) adjusted Mutual Information [47], that gives the mutual information between the two estimated and true solutions, ii) adjusted Rand score [23], that computes the similarity between them, and iii) V-measure [36], that gives the harmonic mean of homogeneity and completeness. We compute the adjusted variants of these criteria, i.e., they yield zero for random solutions.

**Results.** Table 1 shows the results on different datasets. Each block row represents a separate UCI dataset (in order, Lung Cancer, One-Hundred Plant, Perfume, Statlog and Vertebral Column). For each dataset, we investigate the different feature extraction methods (base, PCA, LSA and those obtained by different dendrograms) with three different clustering algorithms. The goal of studying the three clustering algorithms is to demonstrate that our feature extraction methods can be used with various forms of clustering algorithms and are not limited to a specific algorithm. In this way, we investigate one probabilistic clustering model (GMM), one which uses vector-based representation (K-means) and another that is applied to pairwise relations (spectral clustering). The three evaluation criteria that we use are the most common criteria for evaluating clustering methods. The results of the ensemble method are shown in blue. For each clustering algorithm and each evaluation measure, the best result is bolded among the different feature extraction methods.

The base method indicates performing the GMM, K-means or spectral clustering on the original vectors without inferring any new features. We also investigate Principal Component Analysis (PCA) and Latent Semantic Analysis (LSA) as two other baselines. Different dendrogram-based feature extraction methods are specified by the name of the criterion used to build the dendrogram. The ensemble method refers to the aggregation of the different solutions and then performing correlation clustering. According to the equivalence of single linkage method and Minimax distances, this method can be seen as another baseline which also constitutes a special instantiation of the dendrogram-based feature extraction methodology. Note that the superior performance of Minimax distances (single linkage features) over methods such as metric learning or link-based methods has been demonstrated in previous works [18], [19], [24], [25] (see for example Figure 1 in [25]).

We interpret the results of Table 1 as follows. For each dataset (block row) and each clustering algorithm, we investigate whether some of the dendrogram-based features (i.e., single, complete, average or Ward) perform better (according to the three evaluation criteria) than the baseline methods (base, PCA and LSA). If so, then we conclude our framework provides a rich and diverse family of non-parametric feature extraction methods wherein some instances yield more suitable features for the data at hand. Thus, a user has more freedom and options to choose the correct features. However, the user might not have sufficient information to choose the correct features (dendrograms), thus, we propose to use the ensemble variant, in the context of averaging (aggregating) multiple learners.

According to the results reported in Table 1, we observe: i) extracting features from dendrograms yields better representations that improve the evaluation scores of the final clusters. The dendrogram might be built in different ways which correspond to computing different types of features. In particular, we observe the features extracted via complete linkage, average linkage and Ward linkage often lead to very good results. Single linkage (Minimax) features are more suitable for low-dimensional data wherein connectivity paths still exists. However, in higher dimensions, the other methods might perform better due to robustness and flexibility. ii) The ensemble method works well in particular compared to the baselines and most of the dendrogram-based approaches. Note that the ensemble method is more than just averaging the results. It can be interpreted as obtaining a good (strong) learner from a set of weaker learners. Thereby, in several cases, the ensemble method performs even better than all the other alternatives.

Aggregation of representations. As a side study, we investigate the sequential aggregation of different dendrogram-based features in representation space, i.e., we consider the combination of every two such feature extractors. For this purpose, we first compute a dendrogram and extract the respective features. Then, we use these features to compute a second dendrogram from which we obtain a new set of features. Finally, we apply a clustering method (GMM, K-means and spectral clustering) and evaluate the results w.r.t. Mutual Information, Rand score and V-measure.

We observe for most of the datasets, aggregation of different features either improves the results or preserves the accuracy of the results as same as the first representation. However, aggregation of the clustering solutions usually yields more significant changes (improvements) compared to the aggregating the representations. One of the significant changes happens on the Perfume dataset. See the results in Tables 2 and 3, where respectively GMM, K-means and spectral clustering have been applied to the final features to produce the clusters. The first and the second dendrograms
are indicated by the rows and the columns, respectively (where S refers to single, C to complete, A to average, and W to Ward, the different ways of obtaining the features). These results should be compared with the block row in Table 1 that corresponds to the Perfume dataset (the third block row). We observe that over this dataset, feature aggregation often improves the results for different clustering methods. However, as mentioned before, such an aggregation is usually less significant (on other datasets).

We observe that on this dataset, the W-S combination (extracting the features first via Ward and then via single linkages) consistently yields the best results, among all different combinations. In Table 5, we compare these results with the best feature extractor for the perfume dataset, which is based on the Ward linkage. Single linkage even though does not yield very good results itself, but improves the Ward features the most. According to Table 5 except spectral clustering, using the single linkage features helps the clustering algorithm to produce better results. However, the best result is obtained with GMM for which combining Ward with any option is helpful.

| METHOD   | GMM | K-MEANS | SPECTRAL CLUSTERING |
|----------|-----|---------|---------------------|
|          | M.I. | RAND | V.M. | M.I. | RAND | V.M. | M.I. | RAND | V.M. |
| BASE     | 0.1684 | 0.1698 | 0.2030 | 0.1997 | 0.2294 | 0.2356 | 0.1197 | 0.1294 | 0.1356 |
| PCA      | 0.1170 | 0.1170 | 0.1743 | 0.1962 | 0.2362 | 0.2430 | 0.0609 | 0.0678 | 0.0890 |
| LSA      | 0.1702 | 0.2162 | 0.2730 | 0.1962 | 0.2362 | 0.2430 | 0.0728 | 0.0419 | 0.0606 |
| SINGLE   | 0.1677 | 0.2316 | 0.1892 | 0.1525 | 0.2636 | 0.2425 | 0.1016 | 0.1316 | 0.1282 |
| COMPLETE | 0.1537 | 0.2809 | 0.1810 | 0.1537 | 0.2809 | 0.1810 | 0.1537 | 0.2809 | 0.1810 |
| AVERAGE  | 0.1475 | 0.2253 | 0.1795 | 0.2070 | 0.3533 | 0.2303 | 0.1239 | 0.1327 | 0.0742 |
| WARD     | 0.1766 | 0.3388 | 0.2140 | 0.1766 | 0.3388 | 0.2140 | 0.1766 | 0.3388 | 0.2140 |
| ENSEMBLE | 0.2659 | 0.4345 | 0.2957 | 0.2659 | 0.4345 | 0.2957 | 0.2659 | 0.4345 | 0.2957 |

| METHOD   | BASE | PCA | LSA | SINGLE | COMPLETE | AVERAGE | WARD | ENSEMBLE |
|----------|------|-----|-----|--------|----------|---------|------|----------|
|          | 0.4834 | 0.2195 | 0.6867 | 0.6765 | 0.4844 | 0.8138 | 0.6386 | 0.2185 |
|          | 0.4510 | 0.2070 | 0.6791 | 0.6571 | 0.4580 | 0.8024 | 0.4704 | 0.2507 |
|          | 0.4745 | 0.2942 | 0.7121 | 0.6593 | 0.4794 | 0.8034 | 0.4225 | 0.2185 |
| SINGLE   | 0.4841 | 0.2426 | 0.6915 | 0.4809 | 0.2354 | 0.6884 | 0.4922 | 0.2625 |
| COMPLETE | 0.6381 | 0.4459 | 0.7893 | 0.6377 | 0.4427 | 0.7893 | 0.6377 | 0.4456 |
| AVERAGE  | 0.6975 | 0.5336 | 0.8258 | 0.6885 | 0.5176 | 0.8211 | 0.6788 | 0.5051 |
| WARD     | 0.6914 | 0.5249 | 0.8207 | 0.6852 | 0.5158 | 0.8174 | 0.6876 | 0.5151 |
| ENSEMBLE | 0.6990 | 0.5408 | 0.8251 | 0.6925 | 0.5362 | 0.8218 | 0.6836 | 0.5197 |

| METHOD   | BASE | PCA | LSA | SINGLE | COMPLETE | AVERAGE | WARD | ENSEMBLE |
|----------|------|-----|-----|--------|----------|---------|------|----------|
|          | 0.8350 | 0.6783 | 0.8944 | 0.8555 | 0.7243 | 0.8974 | 0.2353 | 0.3981 |
|          | 0.8916 | 0.7051 | 0.9159 | 0.8174 | 0.7430 | 0.8731 | 0.7933 | 0.6890 |
|          | 0.7853 | 0.5912 | 0.8485 | 0.7982 | 0.6237 | 0.8625 | 0.8038 | 0.6049 |
| SINGLE   | 0.8975 | 0.7924 | 0.9178 | 0.8967 | 0.7939 | 0.9245 | 0.8943 | 0.7960 |
| COMPLETE | 0.8941 | 0.7842 | 0.9169 | 0.8752 | 0.7474 | 0.9025 | 0.8632 | 0.7197 |
| AVERAGE  | 0.9054 | 0.8193 | 0.9229 | 0.9116 | 0.8288 | 0.9298 | 0.9041 | 0.8088 |
| WARD     | 0.9390 | 0.8831 | 0.9516 | 0.9348 | 0.8729 | 0.9491 | 0.9348 | 0.8729 |

TABLE 1: PERMANENCE OF DIFFERENT REPRESENTATIONS AND CLUSTERING METHODS ON DIFFERENT UCI DATASETS. THE FIVE BLOCK ROWS CORRESPOND TO THE FIVE DATASETS, RESPECTIVELY TO Lung Cancer, One-Hundred Plant, Perfume, Statlog and Vertebral Column. The results of the ENSEMBLE METHOD ARE SHOWN IN BLUE. FOR EACH CLUSTERING ALGORITHM AND EACH EVALUATION MEASURE, THE BEST RESULT IS BOLDED AMONG THE DIFFERENT FEATURE EXTRACTION METHODS.
5. Conclusion

Based on the correspondence of the Minimax distances to building a single linkage dendrogram, we proposed a generic framework to compute distance measures from different dendrograms in a nonparametric way. Then, we developed an embedding to extract vector-based features for such distances. This property extends the applicability to a wide range of machine learning algorithms. Then, we studied the aggregation of different dendrogram-based features in solution space and representation space. First, based on the consistency of the cluster labels of different objects, we build a graph with positive and negative edge weights and then apply correlation clustering to obtain the final clusters. In the second approach, in the spirit of deep learning models, we apply different dendrogram-based features sequentially, such that the input of the next layer is the output of the current one, and then we apply the particular (clustering) algorithm to the final features. Such a generalization, also advocates the extension of Minimax objectives in many other domains such as game theory and convergence rate analysis. Our experiments on several datasets revealed the effectiveness of the proposed methods.

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TABLE 5. COMPARISON OF WAR(D(W) AND WAR-DING( W-S) FEATURES ON THE PERFUME DATASET. PERFORMING SINGLE LINKAGE ON THE WAR FEATURES IMPROVES THE FINAL CLUSTERING.

| METHOD | M.I. | RAND | V.M. | M.I. | RAND | V.M. | SPECTRAL CLUSTERING | M.I. | RAND | V.M. |
|--------|------|------|------|------|------|------|----------------------|------|------|------|
| W      | 0.9390 | 0.8831 | 0.9546 | 0.9348 | 0.8729 | 0.9491 |                     | 0.9348 | 0.8729 | 0.9491 |
| W-S    | 0.9612 | 0.9360 | 0.9667 | 0.9481 | 0.8963 | 0.9603 |                     | 0.9217 | 0.8368 | 0.9426 |

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