

An objective function for order preserving hierarchical clustering

Daniel Bakkellund

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Abstract

We present an objective function for similarity based hierarchical clustering of partially ordered data that preserves the partial order. That is, if $x \leq y$, and if $[x]$ and $[y]$ are the respective clusters of x and y , then there is an order relation \leq' on the clusters for which $[x] \leq' [y]$. The theory distinguishes itself from existing theories for clustering of ordered data in that the order relation and the similarity are combined into a bi-objective optimisation problem to obtain a hierarchical clustering seeking to satisfy both. In particular, the order relation is weighted in the range $[0, 1]$, and if the similarity and the order relation are not aligned, then order preservation may have to yield in favor of clustering. Finding an optimal solution is NP-hard, so we provide a polynomial time approximation algorithm, with a relative performance guarantee of $O(\log^{3/2}n)$, based on successive applications of directed sparsest cut. We provide a demonstration on a benchmark dataset, showing that our method outperforms existing methods for order preserving hierarchical clustering with significant margin. The theory is an extension of the Dasgupta cost function for divisive hierarchical clustering.

1 Introduction

Clustering is one of the oldest and most popular techniques for exploratory data analysis and classification, and methods for hierarchical clustering dates back almost a century. While clustering methods for graph based and other types of structured data are common, it is also common that the structure is lost during the clustering process; the clustering does not retain the structure of the original data. Alternatively, the methods that do retain the structure of the data are not easily combinable with a general notion of similarity to influence the order of the grouping of elements. In this article, we show how to do order preserving hierarchical clustering for partially ordered data that is equipped with a measure of similarity between elements. The goal is to produce hierarchical clusterings where the clusters themselves are ordered in a way that reflects the original ordering of the data, while simultaneously co-locating similar elements in clusters.

While flat clustering provides partitions that can be considered as classifications of the data, hierarchical clustering provides tree structures over the data, where the leaves are the data points being clustered, and the bifurcations in the trees are where elements are joined into successively larger clusters in the hierarchy. In the context of machine learning, a significant benefit of these trees is that they correspond to ultrametrics (Jardine and Sibson, 1971). This means that in addition to a set of flat classifications of the data, hierarchical clustering yields a distance function on the data, representing the cluster distances. In the industry use case inspiring this work (described below), we are looking for items similar to a given item x_0 . The ultrametric

is perfect for this purpose, allowing the user to explore items contained in successively larger neighbourhoods about x_0 until a suitable element is found.

Now, the data encountered in the mentioned use case is subject to a partial order. From the domain of application, if two distinct elements are comparable, they cannot possibly be equivalent. Moreover, if $x \leq y$, then their respective clusters $[x]$ and $[y]$ should also be comparable in the sense that there should exist a partial order \leq' on the clusters for which $[x] \leq' [y]$.

We therefore require a method for hierarchical clustering that takes the partial order into account. One method for clustering this type of data has previously been described in Bakkelund (2021a). In that work, the partial order is considered as an absolute constraint. This may in some cases lead to difficulties, for example if the partial order itself contains errors. In the current paper, we address this problem by relaxing the partial order and treating it as a non-binary constraint, alongside the similarity.

The method we present is an extension of the model for similarity based hierarchical clustering by Dasgupta (2016), providing an objective function that allows the clustering problem to be solved in terms of optimisation. We introduce an additional component in the objective function; based on the partial order, we provide a function that represents the *level of comparability* of elements. Combining this with the similarity, we can optimise on similarity and comparability simultaneously, obtaining a hierarchical clustering that balances the two objectives.

While several works exist that perform order preserving clustering, and although some of these are also hierarchical in nature (Herrmann et al., 2019), there exists, to the authors' knowledge, no attempts to provide a general definition of the concept. As foundation for the presented theory, we therefore suggest a formal definition of order preserving hierarchical clustering motivated by order theory and classical hierarchical clustering.

Since optimisation turns out to be NP-hard, we also provide a polynomial time approximation algorithm with a relative performance guarantee of $O(\log^{3/2}n)$. We close the paper with a demonstration of the efficacy of the approximation on the benchmark dataset (Bakkelund, 2021b), showing that the provided theory outperforms other methods with a large margin.

The main contributions from this paper can be summarised as follows:

- A formal definition of order preserving hierarchical clustering.
- An objective function for order preserving hierarchical clustering of partially ordered sets equipped with a similarity or dissimilarity.
- A polynomial time algorithm approximating the objective function, with a relative performance guarantee of $O(\log^{3/2}n)$.

1.1 Motivating use case

The theory described in this paper is inspired by an industry database of machine parts. In the database, the machine parts are registered in *part-of* relations, so that a part has a reference to its containing part, according to the design. The result is a family of *part trees* where the nodes in the trees are parts that consist of parts that consist of parts and so on.

Over time, some designs have been copied with small alterations, and due to business reasons, all the parts of the new structure have been given new identifiers, with no reference to where from it was copied. In hindsight, it is desirable to discern which parts are equivalent to which other parts to allow for, for example, spare part interchange. We therefore seek a classification of part types into classes of interchangeable types.

Such a classification has to take into account the part-of relations: As an example, assume that a , b , c and d are machine parts, and that a is a part of b and c is a part of d , as illustrated in

Figure 1.1. Now, if we classify a and c as interchangeable (Figure 1.2), then we also say that a can be a part of d and c can be a part of b . This also implies that a and d can not be interchanged, since you cannot replace a part by a sub-part. Figure 1 presents a selection of classifications of these four elements, together with possible interpretations of what the classifications mean in the domain of part-of relations.

	<p>1. The original data. a is a part of b and c is a part of d.</p>		<p>2. a and c are equivalent, and both can be sub-parts of both b and d, allowing for spare part interchange.</p>
	<p>3. b and d are equivalent, and both contain a and c as sub-parts.</p>		<p>4. a and c are equivalent, and b and d are equivalent. It is likely that one pair is a copy of the other.</p>
	<p>5. b and c are equivalent, and both a and b are sub-parts of d. b and c can be interchanged as spare parts in d.</p>		<p>6. Not a valid clustering since the induced part-of relations are cyclic.</p>

Figure 1: A selection of possible ordered clusterings of the set $\{a, b, c, d\}$. Possible interpretations in terms of the motivating use case are given together with the clusterings. All but 6) are examples of order preserving clusterings. In 6), the part-of relations constitute a cycle, implying that the parts are proper sub-parts of themselves, which is a contradiction.

While each piece of machinery constitutes a tree of machine parts, some part types are used across different types of machinery. As a result, the structure of machine part types and part-of relations make up a directed acyclic graph, or equivalently, a partially ordered set.

In the sought after classification, a cluster should consist of interchangeable parts. But equally important, the clusters should be ordered so that all the parts in the “lesser” cluster can be used as a sub-part of any element of a “greater” cluster. This is depicted in cases 2. and 4. of Figure 1.

This is what brings us to order preserving hierarchical clustering for partial orders—a method that provides us with a hierarchical clustering that preserves the original partial order. As a result, the corresponding ultrametric on the set of parts reflects both the similarities of the parts, as well as the part-of relations. And indeed, as we show in Section 2.3, the more elements that are strictly between two elements in the partial order, the larger the ultrametric distance between the elements in an order preserving hierarchical clustering. This makes perfect sense in the world of machine parts: if one part is deeply buried inside another part, such as a tire valve on a bicycle, there is little chance for the parts to be interchangeable.

Citation graphs. As an alternative, possible application, we briefly mention the classification of research articles. Citation graphs are directed acyclic graphs, and therefore partial orders. If we provide a measure of similarity between articles, and perform order preserving hierarchical clustering based on the similarity and the citation graph, the articles will be grouped not only according to similarity, but also according to order of appearance relative other research: Two related articles that cite the same sources but not each other will be considered to be in a closer relation than the articles and their cited sources. As a result, the articles will be sorted not only according to similarity, but also according to order of appearance relative other research, which is different from appearance in time.

Time series alignment. Another possible application that illustrates the nature of the theory is time series alignment. A time series is a linearly ordered set of events, so that a set of time series is a partially ordered set of events. If we wish to correlate events across time series, but, for some reason, the time stamps across the time series are not fit for this purpose, we can use order preserving clustering as follows: Given a notion of similarity that matches similar events in and across the time series, we can use this to cluster similar events. By adding order preservation, we simultaneously order the classes of events according to their order within the time series. The resulting clusters will therefore consist of similar events that occurred in parallel, and the order on the clusters provides the order of events.

1.2 Related work

The work in this paper extends on the work by Dasgupta (2016). The theory set forth by Dasgupta has been the subject of several publications, whereof Roy and Pokutka (2017), Moseley and Wang (2017), Chatziafratis et al. (2018), Cohen-Addad et al. (2019) are of particular interest with regards to this exposition.

An earlier work on order preserving hierarchical clustering can be found in (Bakkelund, 2021a). Although the topic and aim coincide, the approach is quite different. The method presented there is agglomerative and based on the classical approaches of single-, average-, and complete linkage. Also, the method is developed for strict partial orders, and the order relation is treated as an unbreakable binary constraint.

Similarly to the method we present in this paper, the method by Chatziafratis et al. (2018) extends on Dasgupta’s model in order to incorporate additional constraints from the domain. Their method can be sorted in the category of *clustering with constraints* (Basu et al., 2008; Davidson and Ravi, 2005), where the constraints can be seen as a particular type of structure imposed on the data. As such, this is indeed a variation of what we could call *structure preserving hierarchical clustering*. However, the type of structural constraints do not cover order relations. And, while the constraints in clustering with constraints are provided, for example, by domain experts in order to adjust the clustering, the order relations used in order preserving hierarchical clustering emanate directly from the data. It is the data itself that is ordered, and it is this order relation we wish to preserve.

Carlsson et al. (2014) present a hierarchical clustering regime called *quasi clustering* for asymmetric networks. An asymmetric network is the same as a weighted directed graph, and is covered by what we define as *relaxed order relations* further down. We can therefore say that, at a high level, the methods operate on similar data. However, the method presented by Carlsson et al. is almost opposite of what we define as order preserving: objects are clustered together if there is significant “flow” between the elements. In order preserving clustering, this is exactly when elements are *not* placed together.

A field that does order preserving clustering is that of *acyclic partitioning of graphs*. Given a directed acyclic graph, the goal is to partition the vertices so that the graph that arises when you preserve the edges going between partitions, is also a directed acyclic graph; for an example, see the article by Nossack and Pesch (2014). This is a topic that has been studied intensively with regards to applications ranging from railway planning to parallel processing, compiler theory and VLSI. Hierarchical methods have also been developed of late. While some of the later developments are of a more general nature (Herrmann et al., 2017; Herrmann et al., 2019), a lot of the work focuses on satisfying domain specific constraints and objectives. Also, the methods do not easily combine with a similarity or dissimilarity to support more classical notions of clustering.

Several works has been published on *clustering of ordered data*. We include two classes of methods in this group. The first is that of *comparison based clustering*, where the degree of sim-

ilarity of elements is derived from an order relation. An example is using pairwise comparisons of elements done by users for preference ranking. See the quite recent article by Ghoshdastidar et al. (2019) for more examples and references. In this category, we also find the works of (Janowitz, 2010), providing a wholly order theoretic approach to hierarchical clustering, including the case where the dissimilarity is replaced by a partially ordered set. The other class is that of partitioning a family of ordered sets, so that sets that are similar to each other are co-located in clusters. One example is the work by (Kamishima and Fujiki, 2003), presenting a method for clustering sets containing preference data. Another example of methods in this category is that of clustering of families of time series, such as the model described by Luczak (2016), producing clusters consisting of similar times series.

Whereas all the mentioned work touch upon one or more concepts involved in order preserving hierarchical clustering, none of the methods offer a means to provide hierarchical clusterings where the order relation and the similarity are combined, and where one seeks to find a hierarchical clustering that attempts to satisfy both.

1.3 Layout of the article

Section 1.4 recalls the required background of graph theory, order relations and hierarchical clustering, as well as recalling Dasgupta’s cost function. Section 2 gives a formal definition of order preserving hierarchical clustering, and precisely identifies the binary trees over a set that correspond to order preserving hierarchical clusterings. In Section 3, we introduce our objective function, that extends Dasgupta’s objective to ordered sets. Section 4 provides an investigation of the properties of this model, but looking only at the effect of the order relation by keeping the similarity out of the equation. The combined value function is the topic of Section 5, where we view the clustering problem in terms of bi-objective optimisation. Section 6 describes the polynomial time approximation algorithm, while Section 7 provides a demonstration of the efficacy of the method on data from the machine parts database described in Section 1.1. Section 8 provides a concise summary and presents a short list of future research topics.

1.4 Background

A **graph** is a pair $G = (V, E)$ of vertices and edges. Unless otherwise is specified, we assume that all graphs are directed, and we refer to directed edges as arcs. The graph G is **transitive** if, for every pair of elements $a, b \in V$ for which there is a path from a to b , there is an edge $(a, b) \in E$. A **graph isomorphism** $\theta : G \rightarrow G'$ for graphs $G = (V, E)$ and $G' = (V', E')$ is a bijection $\theta : V \rightarrow V'$ for which $(x, y) \in E \Leftrightarrow (\theta(x), \theta(y)) \in E'$.

For a set X , we write $A \subset X$ if A is a subset of X , proper or not. A **binary relation** on a set X is a subset $E \subset X \times X$. A **partial order** on a set X is a binary relation E on X that is reflexive, antisymmetric and transitive, and in that case we call the pair (X, E) a **partially ordered set**. We usually denote the partially order by \leq , writing $x \leq y$ for $(x, y) \in E$, and $x < y$ to mean $x \leq y \wedge x \neq y$. We write \mathcal{I}_{\leq} to represent the indicator function of the partial order \leq , in which case we have $\mathcal{I}_{\leq}((x, y)) = 1$ if and only of $x \leq y$, and zero otherwise. For subsets $A, B \subset X$, we use the notation $\mathcal{I}_{\leq}(A, B)$ to denote the magnitude

$$\mathcal{I}_{\leq}(A, B) = \sum_{(a,b) \in A \times B} \mathcal{I}_{\leq}((a, b)).$$

We refer to two elements $x, y \in X$ as **comparable** if either $x \leq y$ or $y \leq x$, and a pair of elements that are not comparable are called **incomparable**. A **linear order** is a partial order

in which any two elements are comparable. A **chain** in a partially ordered set (X, \leq) is a subset $Y \subset X$ that is linearly ordered with respect to \leq . Given two partial orders \leq, \leq' on X , we say that \leq' is an **extension** of \leq if $x \leq y \Rightarrow x \leq' y$. If in addition \leq' is a linear order, we call \leq' a **linear extension** of \leq . For two order relations where one is an extension of the other, we say that the orders are **compatible**. The **transitive closure** of a binary relation E on X is the smallest transitive relation on X that extends E .

A map $h : (X, \leq) \rightarrow (Y, \leq')$ between partially ordered sets is said to be **order preserving** if $x \leq y \Rightarrow h(x) \leq' h(y)$. Notice that a composition of order preserving maps is also order preserving. See (Schröder, 2003) for a general introduction to order theory.

A (flat) **clustering** of a set X is a partition $\mathcal{C} = \{C_i\}_{i=1}^k$ of X into disjoint subsets. We do not consider overlapping clusters; every clustering is a partition and corresponds to an equivalence relation \sim on X . A **cluster** is a block in the partition, equivalently, an equivalence class under the equivalence relation. We employ the usual bracket notation for equivalence classes based on representatives, writing $[x]_{\mathcal{C}}$ for the cluster of x in the clustering \mathcal{C} , possibly leaving out the subscript if there is no risk of ambiguity. For every clustering \mathcal{C} of X , the unique map $q : X \rightarrow \mathcal{C}$ defined by $q(x) = [x]_{\mathcal{C}}$, sending an element to its cluster, is called the **quotient map** of \mathcal{C} .

Starting with a non-empty, finite set X , a **split** of X is a partition (A, B) of X into two non-empty, disjoint subsets. Each of these sets may again be split, giving rise to a hierarchical decomposition of X that can be drawn as a tree, where every node has its split components as children until no more splits can be made. This process produces a binary tree that has the set X at the root, and the **singleton sets** $\{\{x\} \mid x \in X\}$ as leaf nodes, and defines a **hierarchical clustering** of X .

We consider every split (A, B) to be *oriented*, meaning that the split (A, B) is considered to be different from the split (B, A) . We refer to this concept as **oriented splits**, and the trees as **oriented trees**. If a node in a tree splits into (A, B) , we refer to A as the **left child**, and B as the **right child** of the parent node.

We denote the set of all oriented binary trees over X that can be generated according to the above procedure by $\mathfrak{B}(X)$. And, for a tree $T \in \mathfrak{B}(X)$, if S is a node in T that splits into (A, B) , we denote this by writing $S \xrightarrow{T} (A, B)$.

Notice that for $T \in \mathfrak{B}(X)$, every node S in T is a subset of X . Let $x \vee y$ denote the smallest node in T , considered as a subset of X , containing both x and y , and let $T[x \vee y]$ be the subtree of T rooted at $x \vee y$.

In particular, $T[x \vee y]$ is the smallest subtree rooted at an internal node containing both $\{x\}$ and $\{y\}$ as leafs. Finally, we write $|T[x \vee y]|$ to denote **the number of leaf nodes** of $T[x \vee y]$, noting that this number coincides with the cardinality of the root node of $T[x \vee y]$, namely $|x \vee y|$. An example of a hierarchical clustering is depicted in Figure 2.

An **ultrametric** on X is a metric d on X for which

$$d(x, z) \leq \max\{d(x, y), d(y, z)\} \quad \forall x, y, z \in X.$$

We refer to the above equation as **the ultrametric inequality**, and note that it implies the triangle inequality. The set of all ultrametrics over X is denoted $\mathcal{U}(X)$.

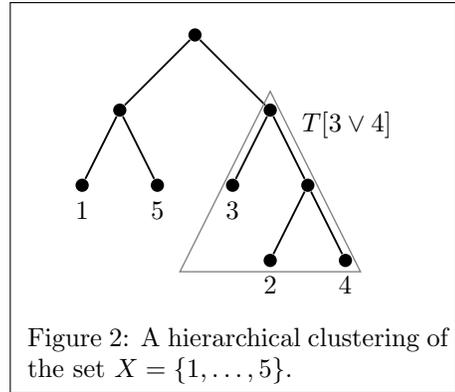


Figure 2: A hierarchical clustering of the set $X = \{1, \dots, 5\}$.

Given a binary tree $T \in \mathfrak{B}(X)$, Roy and Pokutta (2017) show that the map $\mathfrak{U}_X : \mathfrak{B}(X) \rightarrow \mathcal{U}(X)$ given by

$$\mathfrak{U}_X(T)(x, y) = |T[x \vee y]| - 1 \quad (1)$$

is an embedding for non-ordered trees. That is, every non-ordered binary tree over X maps to a unique ultrametric over X via \mathfrak{U}_X . Unless there is any chance of ambiguity, we denote the ultrametric $\mathfrak{U}_X(T)$ by u_T .

Given an ultrametric u on X , for every $t \in \mathbb{R}_+$, the relation \sim_t given by $x \sim_t y \Leftrightarrow u(x, y) \leq t$ is an equivalence relation on X , and provides us with a flat clustering of X . (See Carlsson and Mémoli (2010) or Jardine and Sibson (1971) for details.) When we refer to the clustering of an equivalence relation \sim_t in the context of a tree $T \in \mathfrak{B}(X)$, unless otherwise is stated, this is always in relation to the ultrametric u_T . In particular, for $T \in \mathfrak{B}(X)$, **the flat clusterings provided by T** are the clusterings defined by the equivalence relations $\{\sim_t \mid t \in \mathbb{R}_+\}$. For example, considering the tree in Figure 2 and the ultrametric u_T , the corresponding flat clusterings are presented in Table 1.

Clustering	Equivalence relations
$\{1\}, \{2\}, \{3\}, \{4\}, \{5\}$	$\{\sim_t \mid t \in [0, 1)\}$
$\{1, 5\}, \{2, 4\}, \{3\}$	$\{\sim_t \mid t \in [1, 2)\}$
$\{1, 5\}, \{2, 3, 4\}$	$\{\sim_t \mid t \in [2, 4)\}$
$\{1, 2, 3, 4, 5\}$	$\{\sim_t \mid t \in [4, \infty)\}$

Table 1: The flat clusterings of the tree in Figure 2. The clusters are listed in the left hand side column, and the sets of equivalence relations generating the clusterings are presented on the right.

1.4.1 The Dasgupta cost model

A **similarity** on a set X is a symmetric function $s : X \times X \rightarrow [0, 1]$. Given a similarity s on X , the **Dasgupta cost function** is the function $\text{cost}_s : \mathfrak{B}(X) \rightarrow \mathbb{R}_+$ defined as

$$\text{cost}_s(T) = \sum_{\{x, y\}} |T[x \vee y]| s(x, y), \quad (2)$$

where the sum is over all distinct pairs of elements of X . The optimisation problem is to find a tree $T \in \mathfrak{B}(X)$ minimising (2). For a list of desirable properties of optimal trees under this model, please consult the references given in the related work section.

Dasgupta defines similarity measures to have codomain all of \mathbb{R}_+ , but since minimising (2) is invariant with respect to positive scaling of s , and since X is finite, the above definition implies no loss of generality.

Dual formulation. The dual formulation of Dasgupta’s cost function allows us to solve the optimisation by maximisation. The motivation for introducing the dual is that when we introduce order relations, it is easier to discuss the optimisation problem in the context of maximisation.

Define the dual of s to be the function $s_d : X \times X \rightarrow [0, 1]$ given by

$$s_d(x, y) = 1 - s(x, y), \quad (3)$$

and define the **value function** $\text{val}_{s_d} : \mathfrak{B}(X) \rightarrow \mathbb{R}_+$ by

$$\text{val}_{s_d} = \sum_{\{x, y\}} |T[x \vee y]| s_d(x, y).$$

As of (Dasgupta, 2016, §4.1) any binary tree over X maximising val_{s_d} is a tree that minimises cost_s .

2 Order preserving hierarchical clustering

The contributions from this section are two-fold: first, we provide a formal definition of order preserving hierarchical clustering. Second, we define a class of binary trees called *order preserving trees*, and prove that these trees are exactly the oriented binary trees over X that correspond to order preserving hierarchical clusterings.

Towards the end of the section, we present a result describing how the partial order is reflected in the ultrametric u_T of an order preserving tree T ; that the more elements there are between two elements in the partial order, the more different they are under the ultrametric.

2.1 Formal definition

We start by recalling the order theoretical notion of an order preserving flat clustering, and then provide an extended definition that includes hierarchical clustering.

The next two definitions and following theorem can be found in (Blyth, 2005, §3.1). We recall them here for completeness, and also to rephrase the concepts in the context of clustering. We start by defining what it means for a flat clustering to be order preserving.

Definition 1. Let (X, \leq) be a partially ordered set, and let \mathcal{C} be a clustering of X . We say that the clustering \mathcal{C} is **order preserving (with respect to \leq)** if there exists a partial order \leq' on \mathcal{C} so that

$$x \leq y \Rightarrow [x]_{\mathcal{C}} \leq' [y]_{\mathcal{C}}.$$

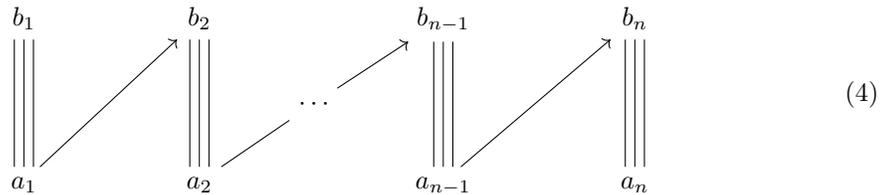
The next definition and theorem classify exactly the order preserving clusterings for a partially ordered set.

Definition 2. Let (X, \leq) be an ordered set, and let $\mathcal{C} = \{C_i\}_{i=1}^k$ be a clustering of X . Let E be the binary relation on \mathcal{C} satisfying

$$(C_i, C_j) \in E \Leftrightarrow \exists x, y \in X : x \leq y \wedge x \in C_i \wedge y \in C_j.$$

We define **the induced relation on \mathcal{C}** , denoted \leq' , to be the transitive closure of E .

An instructive illustration of what the induced relation looks like, is that of a **\mathcal{C} -fence** (Blyth, 2005), or just fence, for short:



Triple lines indicate elements in the same cluster, and the arrows represent comparability in (X, \leq) . The fence allows traversal from b_1 to a_n along arrows and through clusters, in which case we say that the fence **links** b_1 to a_n . The induced relation \leq' has the property that $x \leq' y$ if and only if there exists a \mathcal{C} -fence linking x to y .

Theorem 3 ((Blyth, 2005, Thm.3.1)). *Let (X, \leq) be an ordered set, and let \mathcal{C} be a clustering of X . Then the following two statements are equivalent:*

1. *The induced relation \leq' is a partial order on \mathcal{C} .*
2. *The quotient map $p : (X, \leq) \rightarrow (\mathcal{C}, \leq')$ is order preserving.*

Notice that Item 2 of the theorem implies that \mathcal{C} is an order preserving flat clustering. Our task now, is to define what it means for a hierarchical clustering to be order preserving. We start by recalling the definition of a hierarchical clustering, and then propose an extension that includes order preservation.

For two clusterings $\mathcal{C} = \{C_i\}_{i=1}^m$ and $\mathcal{D} = \{D_j\}_{j=1}^n$ of X , we say that \mathcal{C} is a **refinement** of \mathcal{D} if, for every $C_i \in \mathcal{C}$, there is a $D_j \in \mathcal{D}$ so that $C_i \subset D_j$. If this is the case, then the map $q : \mathcal{C} \rightarrow \mathcal{D}$ defined by $q(C) = D \Leftrightarrow C \subset D$ is also a quotient map. We denote the refinement relation by $\mathcal{C} \sqsubset \mathcal{D}$, and refer to the map q as **the quotient map induced by the refinement**.

A hierarchical clustering over X is, thus, a sequence $\{\mathcal{C}_i\}_{i=0}^k$ of clusterings of X for which

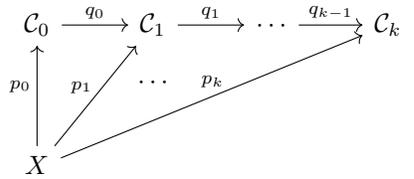
$$\mathcal{C}_0 \sqsubset \cdots \sqsubset \mathcal{C}_k. \tag{5}$$

A sequence $\{\mathcal{C}_i\}_{i=0}^k$ satisfying (5) corresponds to a *persistent set* as of Carlsson and Mémoli (2013). If we require that we have $\mathcal{C}_k = \{X\}$, the sequence corresponds to a *dendrogram* in the nomenclature of Jardine and Sibson (1971), and, recalling the singleton partition $S(X) = \cup_{x \in X} \{\{x\}\}$, if $\mathcal{C}_0 = S(X)$, the sequence corresponds to a *definite dendrogram*, also according to Jardine and Sibson. All of the mentioned concepts define hierarchical clustering in the classical sense.

We now have the following observation.

Theorem 4. *Given a partially ordered set (X, \leq) and a hierarchical clustering $\mathcal{H} = \{\mathcal{C}_i\}_{i=0}^k$ of X , then the following statements are equivalent:*

1. *All quotient maps $p_i : X \rightarrow \mathcal{C}_i$, for $0 \leq i \leq k$, are order preserving with respect to \leq ;*
2. *All quotient maps $q_i : \mathcal{C}_i \rightarrow \mathcal{C}_{i+1}$ for $0 \leq i \leq k - 1$, induced by the refinements, are order preserving with respect to the induced order relations;*
3. *The following diagram is commutative and all quotient maps are order preserving:*



Before presenting the proof, we suggest the following definition:

Definition 5. Given a partially ordered set (X, \leq) , **an order preserving hierarchical clustering of X with respect to \leq** is a hierarchical clustering of X satisfying any and all of the statements of Theorem 4.

Proof of Theorem 4. We start by proving the equivalence of of statements 1 and 2. Assume first that the quotient maps $p_i : X \rightarrow \mathcal{C}_i$ are order preserving. If we can show that for every $A, B \in \mathcal{C}_i$ we have $A \leq'_i B \Rightarrow q_i(A) \leq'_{i+1} q_i(B)$, we are done.

Since $A \leq'_i B$, there are elements $a \in A$ and $b \in B$ that are linked via a \mathcal{C}_i -fence. Now, \mathcal{C}_i is a refinement of \mathcal{C}_{i+1} , so every pair of co-clustered elements in \mathcal{C}_i are also co-clustered in \mathcal{C}_{i+1} . Since this implies that all in-cluster links in fences are maintained, there is also a \mathcal{C}_{i+1} -fence linking a and b , and we must therefore have $A \leq'_{i+1} B$. Since p_{i+1} is order preserving, \leq'_{i+1} is an order relation on \mathcal{C}_{i+1} , so according to Theorem 3, q_i is order preserving too.

Now assume that all the q_i are order preserving. Since the maps p_i must be quotient maps sending elements to their clusters, there is only one possible definition of these maps; namely

$$p_i = q_{i-1} \circ \dots \circ q_0 \circ p_0.$$

Since p_0 is order preserving, the result follows by induction on i , as all maps on the right hand side are order preserving, and since a composition of order preserving maps is an order preserving map.

Finally, the diagram commutes due to the above definition of the p_i , and the maps are all order preserving if and only of both statements 1 and 2 hold. \square

2.2 Order preserving binary trees

We now define order preserving binary trees and show that these trees are exactly the binary trees that correspond to order preserving hierarchical clusterings.

All the concepts on binary trees given in this section extend straight forwardly to the class of all oriented trees over X , regardless of the arity of the splits. However since the rest of the paper deals exclusively with binary trees, we have chosen to stick to binary trees also for this part.

Recall that for a split (A, B) , the order of the components is significant; the split is ordered.

Definition 6. Let (X, \leq) be a partially ordered set. A split (A, B) of X is **order preserving (with respect to \leq)** if

$$x \leq y \Rightarrow (y, x) \notin A \times B \quad \forall x, y \in X. \quad (6)$$

An **order preserving tree** is a tree in which every split is order preserving.

The idea is that, in an order preserving split there are no “reversals” of ordered pairs; the order of the elements shall coincide with the order of the sets they reside in. For example, if $x \leq y$, we can have $(x, y) \in A \times B$, $x, y \in A$ or $x, y \in B$. The only illegal constellation is that of equation (6).

Recalling the indicator function \mathcal{I}_{\leq} of the partial order, we could replace equation (6) by requiring that $\mathcal{I}_{\leq}(B, A) = 0$, a statement that is equivalent to that of Definition 6.

Notice that if we draw a tree $T \in \mathfrak{B}(X)$ on a piece of paper, with the root at the top and the leaves at the bottom, since all splits are oriented, the tree induces a unique linear ordering on the leaves as they appear from left to right. We write \leq_T to denote this ordering, and refer to \leq_T as **the linear order on X induced by T** .

For an order preserving tree, the order \leq_T is a linear extension of the partial order:

Lemma 7. *If (X, \leq) is a partially ordered set, then $T \in \mathfrak{B}(X)$ is an order preserving tree with respect to \leq if and only if*

$$x \leq y \Rightarrow x \leq_T y \quad \forall x, y \in X.$$

Proof. Assume first that T is order preserving, and pick $x, y \in X$ for which $x \leq y$. Let $S = x \vee y$ and $S \dashrightarrow(A, B)$, so that x and y end up in different split components of S . Since T is order preserving, we must have $x \in A$ and $y \in B$, but this means that $x \leq_T y$ too, so the implication holds.

For the opposite direction, let $S \dashrightarrow(A, B)$ be a split in T . Furthermore, let $a, b \in X$ be comparable, and let a and b end up in different components in the split of S ; that is: $a \leq b$, and $a \vee b = S$. Due to the assumption $a \leq b \Rightarrow a \leq_T b$, we get $a \in A$ and $b \in B$. Since this covers all comparable pairs across A and B , the split $S \dashrightarrow(A, B)$ is order preserving. \square

Recall that for a tree $T \in \mathfrak{B}(X)$ and a non-negative real number t , there is a flat clustering \mathcal{C}_t of X defined by the equivalence relation \sim_t (Section 1.4). For every flat clustering under a tree T , the relation \leq_T also induces an order on the clusters:

Lemma 8. *For a partially ordered set (X, \leq) , let $T \in \mathfrak{B}(X)$ and $u_T = \mathfrak{U}_X(T)$. If $t \in \mathbb{R}_+$, and if $\mathcal{C}_t = \{C_i\}_{i=1}^k$ are the clusters of \sim_t , then the enumeration on the clusters can be chosen so that*

$$x \leq_T y \wedge x \in C_i \wedge y \in C_j \Rightarrow i \leq j \quad \forall x, y \in X. \quad (7)$$

Proof. We prove this by induction. Let $\{t_1 > \dots > t_m\}$ be a maximal set of real numbers so that each equivalence relation \sim_{t_i} is distinct for $1 \leq i \leq m$. Clearly, the statement holds for t_1 , where there is only one cluster. Assume that the statement holds for t_k when $k \geq 1$, and consider the case t_{k+1} . Let C_i, C_j be distinct clusters under $\sim_{t_{k+1}}$. If there is a cluster C under \sim_{t_k} for which $C \dashrightarrow(C_i, C_j)$, then the split defines an ordering of C_i and C_j that is compatible with \leq_T . If no such C exists, then C_i and C_j are subsets of distinct clusters under \sim_{t_k} . Due to the induction hypothesis, these equivalence classes are already ordered compatibly with \leq_T , and this order propagates to C_i and C_j , maintaining compatibility. \square

We accept the risk of using \leq_T also to denote the relation on the clusters, writing $C_i \leq_T C_j$.

Remark 9. *In order theoretic jargon, Lemma 8 implies that all the clusters are convex with respect to \leq_T ; if $x, z \in C_i$ and $x \leq_T y \leq_T z$, then $y \in C_i$ too.*

We are now ready to state the main result of this section.

Theorem 10. *Let (X, \leq) be a partially ordered set, and let $T \in \mathfrak{B}(X)$. Then T is an order preserving tree with respect to \leq if and only if the hierarchical clustering corresponding to T is an order preserving hierarchical clustering of X with respect to \leq .*

Proof. Recall that the hierarchical clustering corresponding to T is the sequence of clusters $\mathcal{H} = \{C_i\}_{i=0}^k$ corresponding to the equivalence relations \sim_t under u_T .

Assume that T is order preserving, and let $\mathcal{C} = \{C_i\}_{i=1}^m$ be a flat clustering in \mathcal{H} . We shall show that \mathcal{C} is an order preserving clustering, implying that the quotient map $p : X \rightarrow \mathcal{C}$ is order preserving, where after the theorem follows from Theorem 4.

By combining Lemmas 7 and 8, we can enumerate the clusters of \mathcal{C} according to \leq_T so that $C_1 \leq_T \dots \leq_T C_m$, and moreover, $x \leq y \Rightarrow [x]_{\mathcal{C}} \leq_T [y]_{\mathcal{C}}$. Let \leq' be the induced relation on \mathcal{C} (Definition 2). Then $x \leq y \Rightarrow [x]_{\mathcal{C}} \leq' [y]_{\mathcal{C}}$. But this means that the linear order \leq_T on \mathcal{C} is an extension of \leq' , so \leq' must be a partial order on \mathcal{C} .

For the only-if part, let \mathcal{H} be the clustering corresponding to T , and assume that \mathcal{H} is an order preserving hierarchical clustering of X with respect to \leq . In particular, we have $C_0 = S(X)$ as an order preserving clustering, and since \leq_0 has \leq_T as a linear extension, it follows that \leq_T is a linear extension also of \leq . According to Lemma 7, this means that T is order preserving with respect to \leq . \square

Now we know that we are looking for order preserving trees. What remains is simply to devise a method to identify the best of them. Before we close the section, we present a result that links order preserving trees to ultrametrics, and shows how the partial order is reflected in the ultrametric distances.

2.3 Order preserving trees and ultrametric distances

We now demonstrate that for an order preserving tree $T \in \mathfrak{B}(X)$ over a partially ordered set (X, \leq) , given the ultrametric $u_T = \mathfrak{U}_X(T)$, the distance between two elements $u_T(x, y)$ is bounded below by the number of elements strictly between x and y in \leq .

For an ordered set (X, \leq) and $x, y \in X$, define the function $\text{jmp} : X \times X \rightarrow \mathbb{N}$ so that $x \leq y$, then $\text{jmp}(x, y)$ is one less than the cardinality of a maximal chain having x as minimal element and y as maximal element, and zero if $x \not\leq y$. The magnitude of $\text{jmp}(x, y)$ is equal to the maximal number of “jumps” one would have to make, jumping one element at the time, starting at x and stopping at y , when jumping only in the direction of strictly larger elements. We define the **ordered separation** of $x, y \in X$ to be the magnitude

$$\text{sep}(x, y) = \max\{\text{jmp}(x, y), \text{jmp}(y, x)\}.$$

Notice that $\text{sep}(x, y) = 0$ if and only if either $x = y$, or x and y are incomparable.

Theorem 11. *Let (X, \leq) be a partially ordered set, let $T \in \mathfrak{B}(X)$ be order preserving with respect to \leq , and let $\{x_i\}_{i=1}^n$ be the enumeration of elements of X corresponding to the order \leq_T so that $i \leq j \Leftrightarrow x_i \leq_T x_j$. Let $u_T = \mathfrak{U}_X(T)$. Then*

$$u_T(x_i, x_j) \geq |i - j| \geq \text{sep}(x_i, x_j).$$

Proof. The right hand side inequality follows from the fact that every element between x_i and x_j under \leq , must also be between x_i and x_j under \leq_T , due to Lemma 7. The left hand side inequality follows from the definition of u_T , namely $u_T(x_i, x_j) = |T[x_i \vee x_j]| - 1$, and the fact that every leaf between x_i and x_j under \leq_T must be a leaf of $T[x_i \vee x_j]$. To see why this must be true, it is sufficient to consider the planar drawing of T , and realising that every element between x_i and x_j must join either x_i or x_j before x_i and x_j are joined. \square

This essentially tells us that the more elements that lie between two elements, the more different they are under an ultrametric that corresponds to an order preserving tree. Our choice of ultrametric definition makes the result easily quantifiable, but the observation holds for all ultrametrics. The intuition behind this is straight forward: The more elements that are between two elements in the partial order, the more elements there are between the elements in \leq_T . And for any ultrametric (equivalently, dendrogram) that is based on an order preserving tree, this means that the more elements there are between two elements in the partial order, the higher in the tree (or dendrogram) they join, leading to a higher ultrametric distance.

Looking back at the motivating industry use case, where we have parts that consists of parts that consists of parts and so on, Theorem 11 simply reflects the fact that the more nested levels of composition there is between two parts, the less similar they are.

3 An objective function for trees over ordered data

The remainder of the paper is devoted to the task of devising a method for identifying “good” order preserving trees. In this section, we define our representation of ordered data, and present

a value function for binary trees that incorporates the idea of order preservation. The value function extends the cost function of Dasgupta, and as we show in the next section, it is a realisation of order preserving hierarchical clustering in the sense that it correctly identifies order preserving trees when the data is partially ordered.

In the continuation, we shall treat the order relation as a stochastic object. Let the function $\omega : X \times X \rightarrow [0, 1]$ represent a family of random binary relations E on X , where $(x, y) \in E$ with probability $\omega(x, y)$. We refer to ω as a **relaxed binary relation** on X .

Example 1. If (X, \leq) is a partially ordered set, and if $0 \leq q < p \leq 1$, we can define

$$\omega(x, y) = \begin{cases} p & \text{if } x \leq y, \\ q & \text{otherwise.} \end{cases}$$

Then ω is a relaxed binary relation. Moreover, for any random relation E in the family of relations represented by ω , recalling the indicator function \mathcal{I}_E of E , the expected value of \mathcal{I}_E is $\mathbb{E}(\mathcal{I}_E(x, y)) = \omega(x, y)$. However, we cannot in general expect E to be a partial order on X .

To remind ourselves that we are working with ordered sets, we shall mostly refer to ω as a **relaxed order**, keeping in mind that it is the same thing as a relaxed binary relation.

Next, define **the antisymmetrisation of ω** as the function $g : X \times X \rightarrow [-1, 1]$, given by

$$g(x, y) = \omega(x, y) - \omega(y, x). \tag{8}$$

As the name suggests, the function is antisymmetric, and it computes the *signed net comparability* between x and y . We see that $g(x, y)$ takes on a large positive value if there is strong evidence for $x < y$, and a large negative value if there is strong evidence for $x > y$. Moreover, if the comparability is ambiguous, with $\omega(x, y)$ and $\omega(y, x)$ being very similar, $g(x, y)$ will take on a value close to zero.

To see why this is useful, consider Example 1, and assume that q and p are very close in magnitudes. For a random binary relation E represented by ω , the probability of $(x, y) \in E$ is very close to the probability of $(y, x) \in E$. If we are producing a split (A, B) of X and trying to decide where to place x and y in order to make the split order preserving (Definition 6), it makes little sense to strongly favour one placement over the other in this situation. The close to zero value of $g(x, y)$ effectively reduces the significance of this choice. The function g can be used for hierarchical clustering on its own without any similarity, and the properties of g is the subject of study of Section 4.

However, to achieve order preserving hierarchical clustering, we must combine g with a similarity. Define an **ordered similarity space** to be a triple (X, s, ω) , where X is a set, s is a similarity, and ω is a relaxed order on X . For a given (X, s, ω) , recall the similarity dual s_d from (3). Let **the split value function** $f : X \times X \rightarrow [-1, 2]$ be defined as

$$f(x, y) = s_d(x, y) + g(x, y). \tag{9}$$

This function will attain its maximal value on (x, y) if both $s_d(x, y)$ and $g(x, y)$ are maximal, meaning that x and y are considered to be both highly dissimilar and we have $x < y$ with high confidence; both being evidence for splitting x and y into separate clusters.

On the other hand, the function will attain its minimal value on (x, y) only if $g(x, y)$ has a large negative value. Since s_d is symmetric and g is antisymmetric, this means that by swapping the arguments, $f(y, x)$ will attain a large positive value, again being evidence for splitting the elements apart.

And finally, if the elements are not comparable, then $g(x, y)$ is close to zero, and if the elements are not dissimilar, then s_d is close to zero, so f is close to zero if there is little evidence for splitting the elements apart.

Definition 12. Given (X, s, ω) and a tree $T \in \mathfrak{B}(X)$, the **value of T under (X, s, ω)** is given by the function $\text{val}_f : \mathfrak{B}(X) \rightarrow \mathbb{R}$, defined as

$$\text{val}_f(T) = \sum_{x \leq_T y} |T[x \vee y]| f(x, y), \quad (10)$$

where the iteration order is dictated by the linear order \leq_T induced by T . Furthermore, an **optimal hierarchical clustering of (X, s, ω)** is a binary tree $T^* \in \mathfrak{B}(X)$ for which

$$\text{val}_f(T^*) = \max_{T \in \mathfrak{B}(X)} \text{val}_f(T).$$

The multiplier $|T[x \vee y]|$ of val_f encourages pairs of elements for which $f(x, y)$ attains a large positive value to be split apart close to the root of the tree. Looking back at the discussion preceding the definition, this means that elements that are strongly indicated to belong to different clusters will be split apart close to the root.

But the maximisation also favors an orientation on elements: If ω is as in Example 1, and if $x < y$, then $g(x, y) > 0$ and $g(y, x) < 0$. This intuitively suggests that a tree $T \in \mathfrak{B}(X)$ for which $x \leq_T y$ will have higher value compared to if $y \leq_T x$, and therefore suggests that a maximal tree will be order preserving, as of Lemma 7; a property that will be proven formally in Section 4.

There is an alternative formulation of (10) which we will make occasional use of. Recall that every node in a tree $T \in \mathfrak{B}(X)$ is a subset of X , and an internal node $S \in T$ splits according to $S \stackrel{T}{\rightarrow} (A, B)$. If we define $f(A, B) = \sum_{(a,b) \in A \times B} f(a, b)$, we can formulate val_f as

$$\text{val}_f(T) = \sum_{S \stackrel{T}{\rightarrow} (A, B)} |S| f(A, B),$$

where the sum is over all the splits $S \stackrel{T}{\rightarrow} (A, B)$ in T .

4 Properties of g

In this section, we study the value function

$$\text{val}_g(T) = \sum_{x \leq_T y} |T[x \vee y]| g(x, y), \quad (11)$$

where we only take into account the order relation, ignoring the similarity. The first part, Section 4.1, is concerned with the behaviour on ideal inputs. That is, we show that when ω is a binary partial order, then the optimal trees under val_g are order preserving. Next, in Section 4.2, we turn to relaxed orders, and present a quantitative analysis of val_g , showing that the efficacy of val_g with respect to order preservation is in the same class as Dasgupta's model is with respect to clustering. Finally, Section 4.3 presents a worked example, showing how (11) can be used to analyse migration patterns between states.

4.1 Optimality on partially ordered data

The goal of this section is to show that if (X, \leq) is a partially ordered set, and if we define $\omega = \mathcal{I}_{\leq}$, then the optimal trees under val_g are order preserving. This is important, for it shows that when the input is well formed, then order preserving hierarchical clustering works as intended. Therefore, in what follows, let that $\omega = \mathcal{I}_{\leq}$.

Before we embark on the main theorem, we introduce some new tools. For a partially ordered set (X, \leq) and a tree $T \in \mathfrak{B}(X)$, every pair of elements in X are evaluated in val_g according to how they are ordered under \leq_T . We define **the T -symmetrisation of g** to be the function $\gamma_T : X \times X \rightarrow \mathbb{R}$, defined as

$$\gamma_T(x, y) = \begin{cases} g(x, y) & \text{if } x \leq_T y, \\ g(y, x) & \text{otherwise.} \end{cases}$$

That is, γ_T is a symmetric function that computes the value under g consistent with the orientation on the arguments induced by T .

Moreover, given a partially ordered set (X, \leq) and a tree $T \in \mathfrak{B}(X)$, we define **the cluster graph over (X, \leq) and T** to be the weighted undirected complete graph $G_T = (X, E, \nu)$, where the weight function is given by

$$\nu(x, y) = |T[x \vee y]| \gamma_T(x, y).$$

That is, every edge (x, y) in G_T has a weight that corresponds to the value of the pair $\{x, y\}$ in $\text{val}_g(T)$. The T -symmetrisation ensures that the orientation induced by T is adhered to. The following lemma points up the purpose of the above construction; it allows us to replace the formula for the value val_g of a tree by a sum over the edge weights of the cluster graph.

Lemma 13. *If $G_T = (X, E, \nu)$ is the cluster graph over (X, \leq) and T , then*

$$\text{val}_g(T) = \sum_{e \in E} \nu(e).$$

Proof. Every distinct pair $\{x, y\} \in X \times X$ is summed over exactly once, and since γ_T ensures that the pair is associated with the value under g corresponding to the orientation induced by T , the lemma holds. \square

The next lemma allows us to manipulate the cluster graph in a controlled manner. Recall that for a tree $T \in \mathfrak{B}(X)$ with $T = (V, E)$, every node $S \in V$ is a subset of X , and every edge $e \in E$ is a subset inclusion.

Lemma 14. *Let $\phi : X \rightarrow X$ be a bijection, and let $T = (V, E)$ be a binary tree over X . Then there exists a binary tree $T' = (V', E')$ over X that is isomorphic to T , and where the isomorphism $\phi_T : V \rightarrow V'$ is given by*

$$\phi_T(S) = \{\phi(x) \mid x \in S\}.$$

In particular, for all $x, y \in X$, we have

$$|T[x \vee y]| = |T'[\phi(x) \vee \phi(y)]|. \quad (12)$$

Proof. The set V is a subset of the power set of X , and the map ϕ_T is the mapping from the power set of X to itself induced by ϕ , restricted to V . Since ϕ is a bijection, the map $\phi_T : V \rightarrow V'$ is also a bijection. Moreover, since ϕ_T preserves subset inclusion, it follows that the tree structure is preserved under ϕ_T . Thus, T' is a well-defined binary tree over X , and is isomorphic to T . Equation (12) follows since ϕ_T preserves cardinalities. \square

Given ϕ and T from Lemma 14, the tree T' is necessarily unique. We refer to T' as **the tree induced by T and ϕ** .

We are now ready to state our theorem, telling us that for a partially ordered set, the optimal trees under val_g are order preserving:

Theorem 15. *If (X, \leq) is a partially ordered set and $T \in \mathfrak{B}(X)$ is not order preserving, then there exists a bijection $\phi : X \rightarrow X$ so that the tree T' induced by T and ϕ is order preserving and has strictly higher value than T . In particular, the optimal trees over X are order preserving.*

Proof. If T is not order preserving, we can pick distinct $a, b \in X$ for which $a \leq b$ and $b \leq_T a$. Let σ be the permutation on X swapping a and b , and leaving all other elements fixed, and let T' be the tree induced by T and σ . We shall show that $\text{val}_g(T) < \text{val}_g(T')$.

Let $G_T = (X, E, \nu)$ be the cluster graph over (X, \leq) and T , and let $G_{T'} = (X, E, \nu')$ be the cluster graph over (X, \leq) and T' . We claim that both of the following holds:

$$\exists e \in E : \nu'(e) > \nu(e), \quad (13)$$

$$\forall e \in E : \nu'(e) \geq \nu(e). \quad (14)$$

If so, according to Lemma 13, T' has a strictly higher value than T . We may then repeat the process of permuting elements and generating induced trees of strictly higher value until we reach an order preserving tree. Since a sequence of permutations is a bijection, it follows that the order preserving tree is induced by T and this sequence of permutations.

To prove the claim, since no element outside the subtree $T[a \vee b]$ is affected by the permutation, we can assume that a and b are joined at the root of T , without loss of generality.

To prove (13), notice that

$$\nu(a, b) = |X|\gamma_T(a, b) = -|X| < |X| = |X|\gamma_{T'}(a, b) = \nu_\sigma(a, b).$$

To prove (14), we partition the edges E into five disjoint sets:

$$\begin{aligned} E_1 &= \{(x, y) \in E \mid x, y \neq a, b\} & E_4 &= \{(a, x) \in E \mid a \leq x \wedge b \not\leq x\} \\ E_2 &= \{(x, a) \in E \mid x \leq a\} & E_5 &= \{(x, b) \in E \mid x \not\leq a \wedge x \leq b\} \\ E_3 &= \{(b, x) \in E \mid b \leq x\} \end{aligned} \quad (15)$$

Case E_1 : Since all edges in E_1 are between fixed points under σ , there are no changes of the edge weights.

Case E_2 : Let $(x, a) \in E_2$. Then $x \leq a \leq y$, since \leq is transitive. From Lemma 14, and since $\gamma_T(x, a) = \gamma_{T'}(x, b)$ and $\gamma_T(x, b) = \gamma_{T'}(x, a)$, we get

$$\begin{aligned} \nu(x, a) &= |T[x \vee a]|\gamma_T(x, a) = |T'[\sigma(x) \vee \sigma(b)]|\gamma_{T'}(x, b) = \nu'(x, b), \\ \nu(x, b) &= |T[x \vee b]|\gamma_T(x, b) = |T'[\sigma(x) \vee \sigma(a)]|\gamma_{T'}(x, a) = \nu'(x, a). \end{aligned}$$

Hence, the edge weights are merely swapped around by σ . Case E_3 is proven by a symmetric argument.

Case E_4 : Let X split into (A, B) at the root of T so that $b \in A$ and $a \in B$, and let $(a, x) \in E_4$. Now, if $x \in A$, then $\nu(a, x) = -|X|$, which is the lowest possible value, so $\nu'(a, x) \geq \nu(a, x)$. And if $x \in B$, then $\nu'(x, a) = |X|$, which is the largest possible value, so also in this case, $\nu'(a, x) \geq \nu(a, x)$.

A symmetric argument covers case E_5 . □

Recalling the random family of graphs over a partially ordered set given in Example 1, the following corollary states that in expectation, the trees of maximal value are order preserving.

Corollary 16. *Let (X, \leq) be a partially ordered set, and let $G = (V, E)$ be a graph according to the random family of Example 1. If we define $\omega = \mathcal{I}_E$, and if T is a non-order preserving tree with respect to \leq , then there exists an order preserving tree $T' \in \mathfrak{B}(X)$ with $\text{Eval}_g(T') > \text{Eval}_g(T)$.*

Proof. First, for $\alpha > 0$, because $\text{val}_{\alpha g} = \alpha \text{val}_g$, the optimal trees under $\text{val}_{\alpha g}$ coincide with the optimal trees under val_g . Hence, optimisation under val_g is invariant to positive scaling of g .

Second, given (X, ω) , the optimal trees under val_g are invariant with respect to a large class of affine transformations of ω . This is because if $\alpha, \beta \in \mathbb{R}$ with $\alpha > 0$, and if we define $\omega' = \alpha\omega + \beta$, we get

$$g'(x, y) = \omega'(x, y) - \omega'(y, x) = \alpha\omega(x, y) + \beta - \alpha\omega(y, x) - \beta = \alpha g(x, y).$$

Now, given ω from Example 1, and defining $\omega' = \frac{1}{p-q}(\omega - q)$, we get $\omega' = \mathcal{I}_{\leq}$. That is, the optimal trees under val_g for $\omega = \mathcal{I}_{\leq}$ coincide with the optimal trees under val_g for ω as given in Example 1. Since the latter is the expected value of ω for a graph from the random family, the corollary follows. \square

4.2 Efficacy on planted partial orders

In this section, we provide quantitative results on the difference in order preservation between optimal trees and suboptimal trees for a simple class of partial orders. The analysis parallels the analysis provided in (Dasgupta, 2016), and we show that our model partitions partially ordered input with power comparable to how Dasgupta’s model partitions cliques.

For the duration of this section, we fix $|X| = n$ even.

4.2.1 Background

Dasgupta (2016, §3.3.2) provides a demonstration of the power of the model on *simple planted partitions*. Given a set X , a **simple planted partition** consists of a division of X into two equally sized blocks of $\frac{n}{2}$ elements, together with two numbers p, q where $0 < q < p < 1$. This gives rise to a stochastic family of undirected graphs $G = (X, E)$ over X defined by

$$\Pr((x, y) \in E) = \begin{cases} p & \text{if } x \text{ and } y \text{ belong to the same block,} \\ q & \text{otherwise.} \end{cases}$$

Dasgupta then introduces the notion of an **ϵ -good tree** as a tree that at some point has a node that splits into two blocks that approximates the planted partition so well that no more than $\epsilon \frac{n}{2}$ vertices end up in the “wrong” block.

Now, an undirected graph $G = (X, E)$ gives rise to a similarity on X in the obvious way; namely $s(x, y) = \mathcal{I}_E(x, y)$. Dasgupta proceeds by showing, (Dasgupta, 2016, Theorem 9), that if G is drawn at random from the above family, and T is a tree that is optimal with respect to cost_s , then at most an $O(\sqrt{(\log n)/n})$ fraction of the points are placed in the wrong cluster.

Although the simple planted partition model may seem very simple, it captures the ability of the hierarchical clustering to separate the two cliques. Moreover, the simplicity allows us to provide quantified statements.

4.2.2 Bounding the number of reversed pairs for planted bipartite partial orders

We start by defining our notion of a planted partial order.

Definition 17. Let X be a set, (A^*, B^*) a split of X into equally large blocks, and p, q real numbers for which $0 \leq q < p \leq 1$. Let \leq^* denote the smallest partial order on X satisfying $(x, y) \in A^* \times B^* \Rightarrow x \leq^* y$, and let Γ denote the stochastic family of directed graphs $G = (X, E)$ for which

$$\Pr((x, y) \in E) = \begin{cases} p & \text{if } x \leq^* y, \\ q & \text{otherwise.} \end{cases}$$

We refer to the partially ordered set (X, \leq^*) as the **planted bipartite partial order** defined by X, A^*, B^*, p and q .

Notice that if $G = (X, E)$ is drawn from Γ , then G gives rise to a relaxed order on X defined by $\omega_G = \mathcal{I}_{\leq}$. In particular, we have $\mathbb{E}[\omega_G(x, y)] = \Pr((x, y) \in E)$, so that if we have $g(x, y) = \omega_G(x, y) - \omega_G(y, x)$, we get

$$\mathbb{E}g(x, y) = \begin{cases} p - q & \text{if } x <^* y, \\ q - p & \text{if } y <^* x, \\ 0 & \text{otherwise.} \end{cases} \quad (16)$$

As a consequence, any tree that splits into (A^*, B^*) at the root is of maximal expected value.

The next definition serves to define the quality of a binary tree in terms of order preservation. For a partially ordered set (X, \leq) , we write $[\leq]$ to denote the number of comparable pairs of distinct elements under \leq ; that is $[\leq] = |\{(x, y) \in X \times X \mid x < y\}|$.

Definition 18. Let (X, \leq) be a partial order, and let $\delta \in [0, \frac{1}{2}]$. A tree $T \in \mathfrak{B}(X)$ is **δ -good (with respect to \leq)** if, for every split (A, B) in T , we have

$$\frac{\mathcal{I}_{\leq}(B, A)}{[\leq]} \leq \delta.$$

That is, the fraction of reversed pairs over the split against the total number of comparable pairs in (X, \leq) is no larger than δ .

Clearly, a tree is order preserving if and only if it is 0-good. Also, for the bipartite planted partial order, any tree that splits into (A^*, B^*) at the root is 0-good with respect to \leq^* .

The first result of this section shows that if we define our value function based on a random graph from Γ , then there is a significant difference in expected value between an optimal tree and one that is not δ -good.

Lemma 19. *Let $G = (X, E)$ be drawn from Γ , and define $g(x, y) = \mathcal{I}_E(x, y) - \mathcal{I}_E(y, x)$. If T^* is a tree that splits X into (A^*, B^*) at the root, and if T is a tree that is not δ -good with respect to \leq^* , then*

$$\text{Eval}_g(T^*) > \mathbb{E}\text{Eval}_g(T) + (n + 2)(p - q)\delta \frac{n^2}{4}.$$

Proof. Since T is not δ -good, there is a split (A, B) in T where $\mathcal{I}_{\leq^*}(B, A)/[\leq^*] > \delta$. By construction, we have $[\leq^*] = |A^*||B^*| = \frac{n^2}{4}$, and since the split (A, B) involves reversed pairs,

we must have $|A \cup B| \geq 2$. Hence, the reversed pairs contribute negatively in the split with magnitude

$$(p - q)|A \cup B|\mathcal{I}_{\leq^*}(B, A) > |A \cup B|(p - q)\delta[\leq^*] \geq 2(p - q)\delta[\leq^*] = 2(p - q)\delta\frac{n^2}{4}.$$

Moreover, the pairs contributing to $\mathcal{I}_{\leq^*}(B, A)$ fail to contribute positively to the value of the root split by a magnitude

$$|X|(p - q)\mathcal{I}_{\leq^*}(B, A) \geq n(p - q)\delta[\leq^*] = n(p - q)\delta\frac{n^2}{4}.$$

Adding the magnitudes yields the statement of the lemma. \square

The above result is on the expected value $\mathbb{E}\text{val}_g(T)$. The next result bounds the difference between $\mathbb{E}\text{val}_g(T)$ and $\text{val}_g(T)$.

Lemma 20. *Let $G = (X, E)$ be a random graph from Γ , let $g(x, y) = \mathcal{I}_E(x, y) - \mathcal{I}_E(y, x)$, and pick $\varepsilon \in (0, 1)$. Then we have, for any $T \in \mathfrak{B}(X)$, with probability $1 - \varepsilon$,*

$$|\text{val}_g(T) - \mathbb{E}\text{val}_g(T)| < n^2\sqrt{2n \ln 2n + \ln \frac{2}{\varepsilon}}.$$

Proof. The proof is identical to that of (Dasgupta, 2016, Lemma 8) with one modification: If, for every pair $x <_T y$ of elements in X , we consider the functions $g(x, y)$ to be separate independent random variables, then the magnitude of change of $\text{val}_g(T)$ is bounded by $2n$ whenever only one of these random variables are allowed to change. This because $g \in [-1, 1]$. The result now follows from an application of McDiarmid's inequality and Dasgupta's proof. \square

We now combine the two above lemmas, showing that for a random graph drawn from the family corresponding to the bipartite planted partial order, that a tree that is optimal with respect to that graph has an upper bound on the fraction of reversed pairs given by $O(\sqrt{(\log n)/n})$.

Theorem 21. *Let $G = (X, E)$ be a random graph from Γ , let $g(x, y) = \mathcal{I}_E(x, y) - \mathcal{I}_E(y, x)$, and pick $\varepsilon \in (0, 1)$. If T is an optimal tree for val_g , then T is δ -good with respect to \leq^* with probability $1 - \varepsilon$ for*

$$\delta = \frac{8}{p - q}\sqrt{\frac{2 \ln 2n}{n} + \frac{1}{n^2} \ln \frac{2}{\varepsilon}}.$$

Proof. Let T^* be a tree that splits into (A^*, B^*) at the root. Since $\text{val}_g(T) \geq \text{val}_g(T^*)$, we can deduce that

$$\begin{aligned} \mathbb{E}\text{val}_g(T^*) - \mathbb{E}\text{val}_g(T) &= \mathbb{E}\text{val}_g(T^*) - \text{val}_g(T^*) + \text{val}_g(T^*) - \mathbb{E}\text{val}_g(T) \\ &\leq \mathbb{E}\text{val}_g(T^*) - \text{val}_g(T^*) + \text{val}_g(T) - \mathbb{E}\text{val}_g(T) \\ &\leq |\mathbb{E}\text{val}_g(T^*) - \text{val}_g(T^*)| + |\text{val}_g(T) - \mathbb{E}\text{val}_g(T)| \\ &\leq 2n^2\sqrt{2n \ln 2n + \frac{2}{\varepsilon}} \end{aligned}$$

with probability $1 - \varepsilon$. Hence, we have

$$\mathbb{E}\text{val}_g(T^*) \leq \mathbb{E}\text{val}_g(T) + 2n^2\sqrt{2n \ln 2n + \frac{2}{\varepsilon}}$$

with probability $1 - \varepsilon$ too.

Now, if T is not δ -good, Lemma 19 yields

$$\mathbb{E} \text{val}_g(T) + (n + 2)(p - q)\delta[<^*] \leq \mathbb{E} \text{val}_g(T) + 2n^2 \sqrt{2n \ln 2n + \frac{2}{\varepsilon}},$$

giving us

$$\delta \leq \frac{2n^2 \sqrt{2n \ln 2n + \frac{2}{\varepsilon}}}{(n + 2)(p - q)[<^*]} < \frac{2n^2 \sqrt{2n \ln 2n + \frac{2}{\varepsilon}}}{(p - q)\frac{n^3}{4}} = \frac{8}{p - q} \sqrt{\frac{2 \ln 2n}{n} + \frac{1}{n^2} \ln \frac{2}{\varepsilon}}.$$

□

On the number of comparable pairs in the bipartite planted partial order. By construction, the number of comparable pairs between A^* and B^* in the planted partial order is $\frac{n^2}{4}$, which is as high as it can be. An interesting question is to how many pairs we need in order to be able to separate the two blocks. Re-tracing the steps in the above calculations while letting $[<^*]$ denote the number of comparable pairs between the blocks, gives us a fraction of reversed pairs of $O((n^2/[<^*])\sqrt{\log(n)/n})$. Indeed, if we choose to have as few comparable pairs as possible while still separating the two blocks, we can manage with $[<^*] = \frac{n}{2}$. This yields an asymptotic fraction of $O(\sqrt{n \log n})$ reversed pairs.

For the fraction of reversed arcs to diminish as $n \rightarrow \infty$, we need $[<^*] = \Omega(n^2)$ ¹. This can be achieved, for example, by having all points in a fixed fraction α of the elements of A^* being related to all points of an equally large fraction of B^* , while the remaining pairs of points are related to exactly one point in the other set. This yields

$$[<^*] = \alpha^2 n^2 / 4 + (1 - \alpha)n/2 = \Omega(n^2)$$

for any choice of $\alpha > 0$.

4.3 A worked example – migration between states

This section presents a worked example, analysing migration flow between states in the USA. The purpose of the example is to get a hold on how order preserving hierarchical clustering with val_g behaves on data that is not partially ordered, but that has a directed nature. As the example shows, the produced hierarchical clustering is similar to what can be obtained by applying other methods already in use for hierarchical clustering, such as `MAXDICT` (Feige and Goemans, 1995) and `DIRECTEDSPARSESTCUT` (Chuzhoy and Khanna, 2006). However, for these methods, it is not obvious how to combine them with a similarity.

The states being subject to this analysis, and the migration data, is presented in Table 2. The values are obtained from <http://www.census.gov>, and represent migration data between US states in the year 2011.

We let the function ω represent the flow of people moving from one state to another in the course of one year. The hierarchical clustering proceeds by splitting the set of states in two, providing the two blocks of states having maximal net flow of migrants from one block to the other. Then these blocks will be split accordingly, and so on, until only single states remain.

The result of the hierarchical clustering of this data is presented in Figure 3. We see that the first state to be split off is California, indicating that the largest flow of migration is *from*

¹Where Ω is according to Knuth (1976)

		1	2	3	4	5	6	7
1: Arizona	1	—	0.064	0.006	0.018	0.014	0.012	0.022
2: California	2	0.089	—	0.016	0.072	0.061	0.033	0.069
3: Idaho	3	0.004	0.009	—	0.007	0.011	0.014	0.020
4: Nevada	4	0.016	0.065	0.006	—	0.013	0.008	0.009
5: Oregon	5	0.008	0.033	0.013	0.003	—	0.004	0.052
6: Utah	6	0.019	0.016	0.011	0.006	0.006	—	0.009
7: Washington	7	0.025	0.065	0.016	0.008	0.039	0.009	—

Table 2: Migration data normalised so that the total migration sums to one. The table displays the migration magnitudes in “from row to column”-fashion.

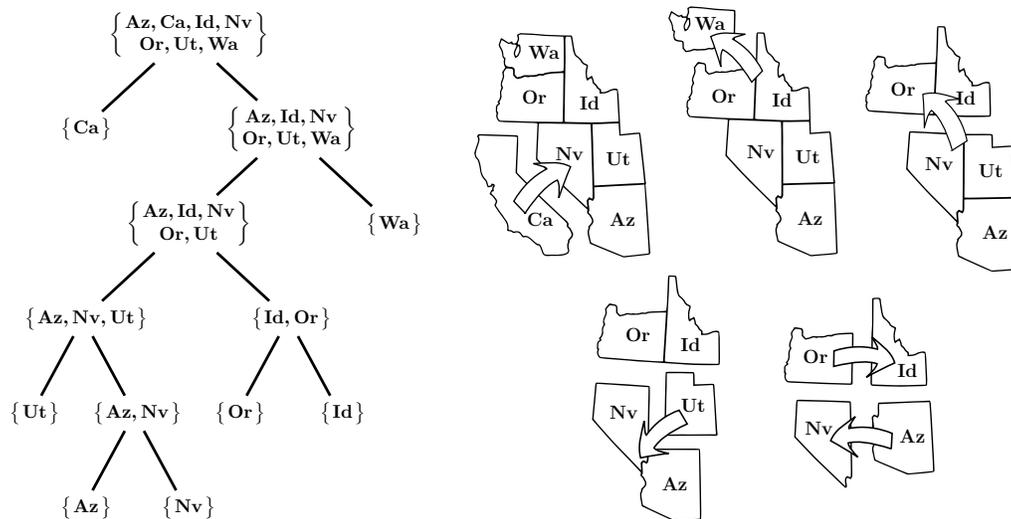


Figure 3: Figure showing the result of the clustering of the migration data. The binary tree is displayed to the left, and the sequence of splits of the states are shown to the right. The arrows on the splits indicate the direction of net migration.

California *to* all the other states. Second, Washington is split off from the remaining states, and the orientation (arrow) tells us that the net flow of migration is from Arizona, Idaho, Oregon, Nevada and Utah to Washington. Third, Oregon and Idaho is split off from Nevada, Utah and Arizona, with net migration from the latter group to the former, and so on. The linear order on the states induced by the binary tree is

$$\text{Ca} \leq_T \text{Ut} \leq_T \text{Az} \leq_T \text{Nv} \leq_T \text{Or} \leq_T \text{Id} \leq_T \text{Wa},$$

indicating the general direction of net migration flow.

5 Properties of $f = s_d + g$

We now turn to study the interplay between the two components of the objective function f as defined in (9), namely the dissimilarity s_d , and the antisymmetrisation g of the relaxed order relation.

We start by looking at an example, showing how we can use order preserving hierarchical clustering to recover the ancestral tree of former U.S. president John F. Kennedy. The example illustrates how the dissimilarity and the order relation combine to successfully recover the ancestral tree in a situation where neither objective could have managed alone.

The example also shows us that the two objectives must be balanced in order to achieve both good clustering and good order preservation. This is the topic of the second part of the section, where we consider the problem of finding the Pareto optimal trees in the context of bi-objective optimisation. We show that due to the linearity of the objectives, we can recover the entire Pareto front by studying the convex combinations of s_d and g .

5.1 Analysing the JFK ancestral tree

We will now illustrate how the dissimilarity and the order relation combine to successfully recover the ancestral tree of John F. Kennedy in a situation where neither of the objectives can do this alone. The idea is to cluster the individuals in the tree so that closely related individuals are grouped together, while at the same time keeping the generations apart. The dissimilarity is derived from name differences, and the order relation is based on the ancestor-descendant relations among the individuals. The ancestral tree is depicted in Figure 4, and the dissimilarities are listed in Table 3.

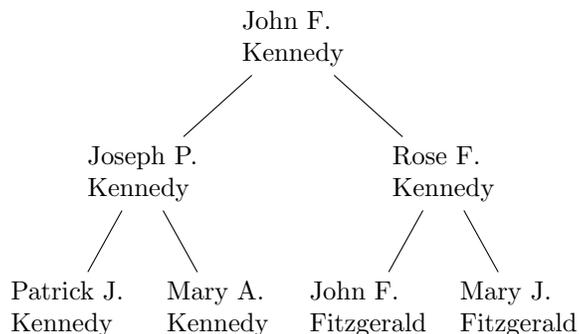


Figure 4: John F. Kennedy’s ancestral tree, two generations back.

1: John F. Kennedy		2	3	4	5	6	7
2: Joseph P. Kennedy	1	0.29	0.31	0.53	0.53	0.50	0.63
3: Rose F. Kennedy	2		0.40	0.50	0.59	0.62	0.73
4: Patrick J. Kennedy	3			0.61	0.53	0.65	0.70
5: Mary A. Kennedy	4				0.44	0.50	0.47
6: John F. Fitzgerald	5					0.65	0.56
7: Mary J. Fitzgerald	6						0.28

Table 3: Dissimilarities of names in the ancestral tree. On the left are mappings from individuals to indices, and on the right is the table of name dissimilarities, rounded to two decimal places. The dissimilarities correspond to the Jaccard distances between the names.

Notice that, in the ancestral tree, the Kennedy name is present throughout, and in particular across the generations, yielding high similarities between descendant- and ancestor names. Due to this, attempting to cluster using only the dissimilarity will cause descendants and ancestors to be placed in the same cluster, rather than keeping the generations apart.

On the other hand, defining ω so that $\omega(x, y) = 1$ if and only if x is a descendant of y (and zero otherwise), this will keep generations apart, but w holds no information about how to identify groups of individuals within the same generation.

If we combine the two objectives as in $f = s_d + g$, the corresponding optimal hierarchical clustering is presented in Figure 5. We see that the generations are nicely split apart, and the grandparents are nicely grouped together, as we wished for. Hence, by combining the dissimilarity and the order relation, the result turns out correctly.

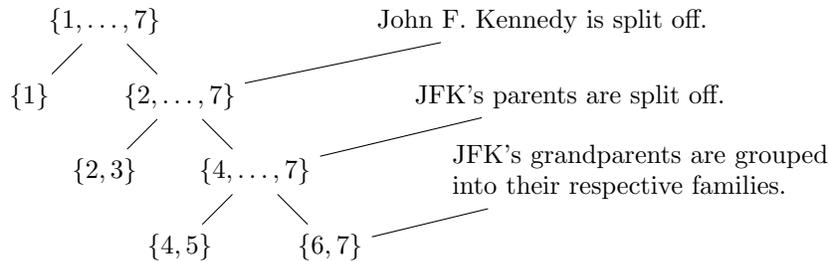


Figure 5: The optimal hierarchical clustering of the Kennedy family tree. We have left out the final splits into leaf nodes.

Looking back at our motivating use case (Section 1.1), the database of machinery exhibits the exact same tendency: The high similarity between parts and sub-parts makes clustering difficult, but we can mitigate this problem by taking the part-of relation into account.

5.2 Balancing clustering against order preservation

In the above example, the dissimilarity s_d and the order relation ω are, in a sense, competing: the dissimilarity wants to place similar elements together, in spite of them being in different generations, and the order relation tries to keep the generations apart. In the field of operations research, this is termed a *bi-objective optimisation problem*, having two distinct objectives where ideally both shall be optimised for. Multi-objective optimisation is a thoroughly studied area of

research, and several methods exist to approach this class of problems. See, for example, the survey by [Marler and Arora \(2004\)](#) for an overview.

The material presented in this section are known results and ideas within multiobjective optimisation, and the authors make no claim to originality in the below exposition. However, we choose to present the concepts for the sake of completeness, and also to show how order preserving hierarchical clustering can be addressed as a bi-objective optimisation problem.

We have chosen to focus on *Pareto optimality* ([Zadeh, 1963](#)) in the context of bi-objective maximisation. In order to do that, for an ordered similarity space (X, s, ω) , we decompose val_f into its sum components val_{s_d} and val_g :

Definition 22. Let (X, s, ω) be an ordered similarity space. For trees $T, T' \in \mathfrak{B}(X)$ we say that T is **Pareto dominated** by T' if

1. $\text{val}_\theta(T') \geq \text{val}_\theta(T)$ for $\theta \in \{s_d, g\}$, and
2. for at least one objective val_θ we have $\text{val}_\theta(T') > \text{val}_\theta(T)$.

A solution is **Pareto optimal** if there are no solutions dominating it, and the family of all Pareto optimal solutions is referred to as the **Pareto front**.

Thus, a Pareto optimal solution has the property that for any other candidate solution, at least one objective will deteriorate. An illustration of the Pareto front is given in Figure 6.

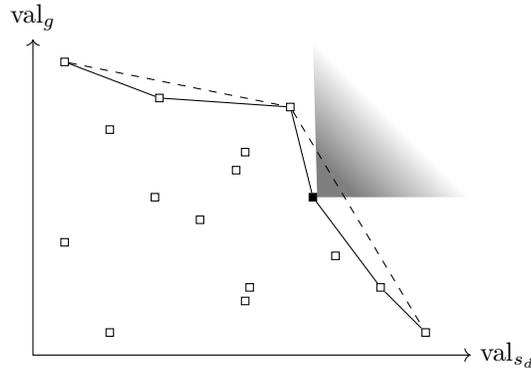


Figure 6: The Pareto front of a bi-objective optimisation problem with objectives $(\text{val}_{s_d}, \text{val}_g)$. The squares are the different candidate solutions, and the solid line connects the candidates at the Pareto front. The shaded wedge illustrates why the black square belongs on the Pareto front: there are no solutions above or to the right of this point. The dashed line indicates the convex hull of the Pareto front.

To identify the Pareto front for a bi-objective optimisation problem, the naive approach is to identify the optimal solutions for all linear combinations $\gamma \text{val}_{s_d} + \delta \text{val}_g$ for $\gamma, \delta > 0$.² However, as the following definition and lemma shows, in our case, we can limit the study to convex combinations of the objectives. This is a general property that follows from the linearity of the objectives, and is not particular for our case. We still choose to write it out, since it provides insight into the structure of the problem, and also points to possible ways of attacking the problem of tracing out the Pareto front. We start by introducing a new value function val_α , which is a convex combination of the two objectives.

²More efficient methods exist, such as ([Kim and de Weck, 2005](#)).

Definition 23. Given (X, s, ω) and $\alpha \in [0, 1]$, define $\text{val}_\alpha : \mathfrak{B}(X) \rightarrow \mathbb{R}$ as

$$\text{val}_\alpha(T) = \sum_{x \leq_T y} |T[x \vee y]| [\alpha s_d(x, y) + (1 - \alpha)g(x, y)]. \quad (17)$$

Notice that due to the linearity of val_{s_d} and val_g , we have

$$\text{val}_\alpha(T) = \alpha \text{val}_{s_d}(T) + (1 - \alpha) \text{val}_g(T).$$

Optimising a linear combination $\gamma \text{val}_{s_d} + \delta \text{val}_g$ can be replaced by optimising val_α for a suitable value of α :

Lemma 24. For $\gamma, \delta > 0$, let $\alpha = \frac{\gamma}{\gamma + \delta}$. Then $T \in \mathfrak{B}(X)$ maximises val_α if and only if T also maximises $\gamma \text{val}_{s_d} + \delta \text{val}_g$.

Proof. For a fixed $\beta > 0$, a tree that maximises $\text{val}_{s_d} + \text{val}_g$ also maximises $\beta(\text{val}_{s_d} + \text{val}_g)$. And since

$$\frac{1}{\gamma + \delta} (\gamma \text{val}_{s_d} + \delta \text{val}_g) = \frac{\gamma}{\gamma + \delta} \text{val}_{s_d} + \frac{\delta}{\gamma + \delta} \text{val}_g = \alpha \text{val}_{s_d} + (1 - \alpha) \text{val}_g,$$

and since $0 \leq \frac{\gamma}{\gamma + \delta}, \frac{\delta}{\gamma + \delta} \leq 1$ and $\frac{\gamma}{\gamma + \delta} + \frac{\delta}{\gamma + \delta} = 1$, the lemma holds. \square

According to the above Lemma, the Pareto front is convex in the sense that all Pareto optimal solutions are located on the convex hull indicated by the dashed line in Figure 6. Also, this means that if $0 \leq \beta \leq \beta' \leq 1$ and val_β and $\text{val}_{\beta'}$ have the same optimal trees, then optimisation of val_α is constant for $\alpha \in [\beta, \beta']$. This is useful, since it gives a well defined basis on which to apply, for example, binary search to explore the Pareto front.

The objective val_α has the property that $\text{val}_{\alpha=0} = \text{val}_g$, optimising only with respect to the order relation, and $\text{val}_{\alpha=1} = \text{val}_{s_d}$, optimising only with respect to the similarity. Part of the optimisation problem is thus to find an $\alpha \in [0, 1]$ providing the best balance between the objectives given the current context. For multi-objective optimisation in general, there is no canonical best solution on the Pareto front, and therefore no canonically best α for val_α . A significant amount of research has focused on the topic of aiding the domain expert in identifying the best solution; see Miettinen's book (Miettinen, 1998, pp. 131–213) for an overview.

While we believe it is doable to produce a theorem along the lines of Theorem 21 also in the presence of both a similarity and an order relation, we consider this to be a major task, and postpone this for future research.

5.3 A note on idempotency

A function $h : X \rightarrow X$ is **idempotent** if $h \circ h = h$. Jardine and Sibson (1971) define a clustering method as *appropriate* if it is idempotent. This is considered to be a key feature of any clustering methodology. Cohen-Addad et al. (2019) show that Dasgupta's model is appropriate, and the below theorem shows that this still holds for order preserving hierarchical clustering. An important difference is, of course, that we must pass along the induced order relation for the second invocation. Notice that for a normalised ultrametric u_T on X , the function $1 - u_T$ is a similarity on X .

Theorem 25. Assume that (X, s, ω) has T as an optimal tree under val_f , and let u_T be the normalised ultrametric corresponding to T . Then $(X, 1 - u_T, \leq_T)$ has T as an optimal tree under val_f . That is; val_f is appropriate.

Proof. Since Dasgupta’s model is appropriate, clustering the similarity space $(X, 1 - u_T)$ without any order relation will yield a binary tree T' that reproduces u_T under val_{u_T} . This tree may not be order preserving, but it is isomorphic to T , and this tree isomorphism must necessarily be a pairwise swapping of elements so that the isomorphism is induced by T' and these swaps. Hence, according to Theorem 15, T has at least the value of T' under val_f . \square

The following corollary expresses the same result in from a different angle: if we do not care about the induced order relation but only about the ultrametric, we can omit the order relation all together, given that we have a suitable similarity.

Corollary 26. *For every ordered similarity space (X, s, ω) , if T is an optimal tree with respect to val_f , then there exists a similarity s' on X for which T' is an optimal tree of $\text{val}_{s'}$ and where $u_{T'} = u_T$.*

6 Approximation

From Dasgupta (2016), we know that the optimisation problem over val_f is NP-hard. In this section, we present a polynomial time approximation algorithm with a relative performance guarantee of $O(\log^{3/2} n)$. This result is similar to that presented in (Dasgupta, 2016), a result that has been improved upon in subsequent papers (Charikar and Chatziafratis, 2017; Cohen-Addad et al., 2019; Roy and Pokutta, 2017). In this paper, we present the simpler $O(\log^{3/2} n)$ approximation, leaving possible improvements for future work.

The algorithm presented by Dasgupta is based on successive applications of SPARSESTCUT (Leighton and Rao, 1999) to generate a binary tree that approximates the optimal tree. There exists a directed equivalent to SPARSESTCUT called DIRECTEDSPARSESTCUT (Chuzhoy and Khanna, 2006), which we shall use for our approximation. To get there, we must first establish a dual to our optimisation problem, allowing us to solve the optimisation as a minimisation problem.

Although the different cut models are defined on graphs, there is no real difference between cuts and the concept we have called splits. The difference lies in that a split focuses on *splitting a set*, whereas the cut focuses on *cutting edges or arcs spanned by the split*. Moreover, every (possibly relaxed) relation $\omega : X \times X \rightarrow [0, 1]$ corresponds to a complete directed weighted graph with ω as weight function. We shall therefore use both splits and cuts in what follows.

Definition 27. Given a complete directed weighted graph over X with weight function ν , the **directed cut density** of a split (A, B) of X is the magnitude

$$\frac{\nu(A, B)}{|A||B|} = \frac{\sum_{a,b} \nu(a, b)}{|A||B|}.$$

In particular, a **directed sparsest cut** is a split of minimal cut density, taken over all possible binary splits (A, B) of X .

Notice that, just as for splits in trees, a directed cut is oriented, in the sense that (A, B) may have a different cut density than (B, A) .

Also notice that, for an undirected graph, the weight function is symmetric, so that the cut densities of (A, B) and (B, A) coincide. In this case, we simply drop the prefix *directed*, and refer to (A, B) as a possibly **sparsest cut**.

6.1 Duality

We introduce the dual to val_f , namely cost_{f_d} , and show that maximisation under val_f is equivalent to minimisation under cost_{f_d} . We start by showing that there is a dual function to g , denoted g_d , that allows us to maximise val_g by minimising cost_{g_d} . Thereafter, we combine cost_{g_d} with the non-dual cost_s of Dasgupta to make up cost_{f_d} .

For an ordered set (X, ω) , we define the **dual of the antisymmetrisation** of ω to be the function

$$g_d(x, y) = 1 - g(x, y). \quad (18)$$

Notice that $g = 1 - g_d$, meaning that the two functions are each others duals. Notice also that $g_d : X \times X \rightarrow [0, 2]$, so we have eliminated the negative coefficients in the optimisation problem.

Lemma 28. *Let (X, ω) be given, and let g_d be the dual of the antisymmetrisation of ω . Then the function $\text{cost}_{g_d} : \mathfrak{B}(X) \rightarrow \mathbb{R}_+$ defined as*

$$\text{cost}_{g_d}(T) = \sum_{x \leq_T y} |T[x \vee y]| g_d(x, y) \quad (19)$$

is dual to val_g in the sense that any tree that is a maximiser of val_g is a minimiser of cost_{g_d} .

Proof. Recalling (Dasgupta, 2016, Theorem 3), stating that

$$\sum_{x \leq_T y} |T[x \vee y]| = \frac{|X|^3 - |X|}{3}$$

for all trees $T \in \mathfrak{B}(X)$, this yields

$$\begin{aligned} \text{cost}_{g_d}(T) &= \sum_{x \leq_T y} |T[x \vee y]| (1 - g(x, y)) \\ &= \sum_{x \leq_T y} |T[x \vee y]| - \sum_{x \leq_T y} |T[x \vee y]| g(x, y) \\ &= \frac{|X|^3 - |X|}{3} - \text{val}_g(T). \end{aligned}$$

Hence, any tree that maximises val_g is a tree that minimises cost_{g_d} . \square

For an ordered similarity space (X, s, ω) , recalling the split value function $f = s_d + g$, we define the **dual split value function** $f_d : X \times X \rightarrow [0, 3]$ as

$$f_d(x, y) = 2 - f(x, y).$$

Theorem 29. *Given (X, s, ω) where s is a similarity and ω is a relaxed order, the maximisation problem of Definition 12 can be solved by minimising*

$$\text{cost}_{f_d}(T) = \sum_{x \leq_T y} |T[x \vee y]| f_d(x, y).$$

Proof. Since $f_d = 2 - f = (1 - s_d) + (1 - g) = s + g_d$, it follows that $\text{cost}_{f_d} = \text{cost}_s + \text{cost}_{g_d}$. If we let $M = \frac{|X|^3 - |X|}{3}$, we have

$$2M - \text{cost}_{f_d} = (M - \text{cost}_s) + (M - \text{cost}_{g_d}) = \text{val}_{s_d} + \text{val}_g = \text{val}_f.$$

Hence, a tree that is a maximiser of val_f is a minimiser of cost_{f_d} . \square

A remark on the dual of the antisymmetrisation. In Dasgupta’s model, the similarity s is defined in terms of an undirected graph with weight function s , and the dual $s_d = 1 - s$ is also a graph. Indeed, if s has unit weights, then s_d is the graph with complementary edge set. However, in the ordered setting, we have a directed weighted graph with weight function ω , and with antisymmetrisation $g(x, y) = \omega(x, y) - \omega(y, x)$. The dual of the antisymmetrisation $g_d = 1 - g$ is dual to g , but does not correspond to an antisymmetrisation of a relaxed order or weight function, since g_d itself is not antisymmetric. It is the dual graph to the complete graph over X with weight function g , but what this dual graph represents is not obvious.

Since the dual formulation lacks a clear intuitive interpretation, we have chosen to stick to the maximisation problem for the main part of this paper.

6.2 Approximation algorithm

This section describes our approximation algorithm, and provides an analysis of its relative performance guarantee. In the algorithm, we assume the existence of a *cut approximation function*; that is, a function that takes as arguments a vertex set and a weight function, and produces an approximation of an optimal cut that comes with a relative performance guarantee. For example, given a similarity space (X, s) , if θ is an approximation of SPARSESTCUT with a relative performance guarantee α_θ and if $\theta(X, s) = (A, B)$, then $s(A, B)/(|A||B|)$ is no more than a factor α_θ off from a true sparsest cut of (X, s) .

For our approximation algorithm, we need an approximation of DIRECTEDSPARSESTCUT. The currently best known approximation algorithm, provided by Agarwal et al. (2005), has a relative performance guarantee of $O(\sqrt{\log n})$. The structure of our algorithm is like to that provided by Dasgupta, but where Dasgupta requires a SPARSESTCUT approximation, we require an approximation of DIRECTEDSPARSESTCUT. Also, we must pay explicit attention, keeping track of the left- and right splits, whereas in Dasgupta’s algorithm, this is not a required invariant.

Definition 30. Let (X, E) be a complete directed weighted graph with weight function f_d , and let θ be an approximation algorithm of DIRECTEDSPARSESTCUT. The following algorithm produces the approximate order preserving hierarchical clustering of (X, f_d) .

```

procedure MAKE TREE( $X, f_d$ )
  if  $|X| = 1$  then
    return  $X$ 
  else
    Let  $(A, B)$  be the cut approximation returned by  $\theta(X, f_d)$ 
    Let LEFT TREE be the tree returned by MAKE TREE( $A, f_d$ )
    Let RIGHT TREE be the tree returned by MAKE TREE( $B, f_d$ )
    return (LEFT TREE, RIGHT TREE)
  end if
end procedure

```

Given an approximation of DIRECTEDSPARSESTCUT with an approximation guarantee of $O(\sqrt{\log n})$, according to the following theorem, the above algorithm produces a binary tree that has a cost that is no higher than a factor $O(\log^{3/2} n)$ of an optimal tree.

Theorem 31. Given (X, s, ω) , let T^* be a tree minimising cost_{f_d} , and let T be the tree returned by the algorithm of Definition 30, using a cut approximation function for DIRECTEDSPARSESTCUT with a relative performance guarantee of α_θ . Then

$$\text{cost}_{f_d}(T) \leq \frac{27\alpha_\theta \log n}{2} \text{cost}_{f_d}(T^*).$$

Proof (sketch). Since a DIRECTEDSPARSESTCUT is equivalent to a SPARSESTCUT for an undirected graph, the theorem is a generalisation of (Dasgupta, 2016, Theorem 12). The proof of Dasgupta’s Theorem 12 requires the existence of a split with a particular bound of the cut density, provided by (Dasgupta, 2016, Lemma 11). By replacing Dasgupta’s Lemma 11 with our Lemma 32 (below), proving Theorem 31 amounts to reproducing the steps in the proof of (Dasgupta, 2016, Theorem 12), just keeping in mind that we have to treat every split as an oriented split. We therefore provide the required split, and refer to (Dasgupta, 2016) for details regarding the proof of the theorem. \square

Lemma 32. *Given (X, s, ω) , for every binary tree $T \in \mathfrak{B}(X)$, there exists a split (A, B) of X for which*

$$\frac{f_d(A, B)}{|A||B|} \leq \frac{27}{2n^3} \text{cost}_{f_d}(T).$$

Proof. The key is to control the cardinalities of the components of the split (A, B) , while at the same time making sure that the split is ordered according to the order induced by the tree.

For a tree $T \in \mathfrak{B}(X)$, we define a **maximum cardinality path** to be a path in T starting at the root, and for every node, the next node on the path is a child of the current node of maximal cardinality. Based on a maximum cardinality path $\{N_i\}_{i=1}^m$, we can create the required split over the following steps:

1. Construct two sequences $\{\mathcal{L}_i\}_{i=1}^{m-1}$ and $\{\mathcal{R}_i\}_{i=1}^{m-1}$ of subsets of X as follows: For $1 \leq i \leq m-1$, let $\ell(N_i)$ and $r(N_i)$ be the left and right children of N_i , respectively. Now, if $|\ell(N_i)| < |r(N_i)|$, set $\mathcal{L}_i = \ell(N_i)$ and $\mathcal{R}_i = \emptyset$, otherwise set $\mathcal{L}_i = \emptyset$ and $\mathcal{R}_i = r(N_i)$. We refer to these sets as the *i -th left split-off* and *i -th right split-off*, respectively.
2. Define the set sequences $\{\mathcal{A}_k\}_{k=1}^{m-1}$ and $\{\mathcal{B}_k\}_{k=1}^{m-1}$ as

$$\mathcal{A}_k = \bigcup_{i=1}^k \mathcal{L}_i \qquad \mathcal{B}_k = \bigcup_{i=1}^k \mathcal{R}_i.$$

We refer to \mathcal{A}_k as *the k -th accumulated left split-off*, and \mathcal{B}_k as *the k -th accumulated right split-off*.

3. Let K be the smallest natural number for which $\max\{|\mathcal{A}_K|, |\mathcal{B}_K|\} \geq n/3$.
4. Finally, if $|\mathcal{A}_K| \geq n/3$, set $A = \mathcal{A}_K$ and $B = X - A$. Otherwise, set $B = \mathcal{B}_K$ and $A = X - B$.

We refer to (A, B) as a **balanced T -split**, and call $\{N_i\}_{i=1}^K$ **the head sequence** of the balanced T -split. The key points to take away from this construction are the following:

- b1. $|N_K| \geq \frac{n}{3}$,
- b2. $(a, b) \in A \times B \Rightarrow a \leq_T b$,
- b3. $\cup_{i=1}^K \ell(N_i) = A$ and $\cup_{i=1}^K r(N_i) = B$.

We prove each property in turn:

b1: Since $\max\{|\mathcal{A}_{K-1}|, |\mathcal{B}_{K-1}|\} < \frac{n}{3}$, and since, by construction, $X = N_K \cup \mathcal{A}_{K-1} \cup \mathcal{B}_{K-1}$, and since these sets are disjoint, it follows that $|N_K| \geq \frac{n}{3}$.

b2: Notice that the \mathcal{L}_i and \mathcal{R}_i are left- and right children of the head sequence elements. If x is the leaf of the maximum cardinality path, this means that $a \in \mathcal{L}_i \Rightarrow a \leq_T x$, and likewise,

$b \in \mathcal{R}_i \Rightarrow x \leq_T b$, so $(\mathcal{A}_K, \mathcal{B}_K)$ is order preserving with respect to \leq_T . Now, if $|\mathcal{A}_K| \geq \frac{n}{3}$, this means that $A = \mathcal{A}_K$ and $B = \mathcal{B}_K \cup r(N_K)$, which again means that (A, B) is order preserving with respect to \leq_T . A symmetric argument covers the case $|\mathcal{B}_K| \geq \frac{n}{3}$.

b3: If $|\mathcal{A}_K| \geq \frac{n}{3}$, then $\mathcal{R}_K = \emptyset$, so

$$\begin{aligned} A &= \bigcup_{i=1}^K \mathcal{L}_i = \bigcup_{i=1}^K \ell(N_i), \\ B &= \left(\bigcup_{i=1}^K \mathcal{R}_i \right) \cup r(N_K) = \left(\bigcup_{i=1}^{K-1} r(N_i) \right) \cup r(N_K). \end{aligned}$$

And again, a symmetric argument attests **b3** for $|\mathcal{B}_K| \geq \frac{n}{3}$.

That proves the properties of the balanced T -split, and we are now in position to prove the statement of the lemma: Let (A, B) be a balanced T -split, and let $\{N_i\}_{i=1}^K$ be the head sequence of the split. Then

$$\text{cost}_{f_d}(T) \geq \sum_{i=1}^K |N_i| f_d(\ell(N_i), r(N_i)) \geq \sum_{i=1}^K \frac{n}{3} f_d(\ell(N_i), r(N_i)) \geq \frac{n}{3} f_d(A, B).$$

From this, we deduce that

$$\frac{f_d(A, B)}{|A||B|} < \frac{3}{n} \cdot \frac{\text{cost}_{f_d}(T)}{(2n/3)(n/3)} = \frac{27}{2n^3} \text{cost}_{f_d}(T).$$

□

Recovering intuition—DirectedDensestCut: While the dual of the antisymmetrisation defies intuitive interpretation, we can recover our intuitive understanding of the approximation as follows. Assume that (A, B) is a sparsest cut under f_d . Since

$$\frac{f_d(A, B)}{|A||B|} = \frac{\sum_{A \times B} 2 - f(a, b)}{|A||B|} = \frac{2|A||B| - f(A, B)}{|A||B|} = 2 - \frac{f(A, B)}{|A||B|},$$

it follows that (A, B) is a maximiser of $f(A, B)/(|A||B|)$. It seems natural to call a cut that maximises $f(A, B)/(|A||B|)$ a **directed densest cut (under f)**. From what the authors can see, this cut is not previously mentioned in the literature³, but one may still assume the existence of an approximation algorithm for DIRECTEDDENSESTCUT. It is thus clear that the above approximation algorithm of cost_{f_d} is equivalent to successive applications of a DIRECTEDDENSESTCUT approximation to approximate a maximal tree under val_f .

7 Demonstration

In this section, we demonstrate the efficacy of the theory in recovering copy-paste relations from the machine parts dataset described in Section 1.1.

The demonstration makes use of the approximation scheme describe in Section 6. As mentioned, there exist good approximations of DIRECTEDSPARSESTCUT. However, as we discuss further in Section 8, the availability of open implementations of these approximations is scarce, so for the demonstration, we have settled on optimal DIRECTEDSPARSESTCUT. The downside is that the algorithm cannot deal with sets of much more than 20 elements and still terminate in reasonable time. But, as we show below, the small sample sizes still suffice to provide a valuable demonstration. For industrial applications, a proper DIRECTEDSPARSESTCUT approximation will be required.

³The literature on graph cuts is very abundant, and the cut may very well be described under a different name or in a different context without the authors being aware of this.

7.1 A model for planted partitions over machine parts data

The dataset we use is described in detail in the data article (Bakkelund, 2021b), and is the same dataset that was used for the demonstration in (Bakkelund, 2021a). The data article is backed by an open source implementation⁴ that produces planted partitions simulating the copy paste mechanism described in Section 1.1.

In brief, the planted partitions are generated as follows: First, a sample X_0 of size n is drawn from the original data, giving us an ordered similarity space (X_0, s_0, \leq_0) . We then duplicate (X_0, \leq_0) a total of m times. These duplications represent the copy-paste relations. We denote the copies by (X_j, \leq_j) for $1 \leq j \leq m$, and enumerate the sets as $X_j = \{x_1^j, \dots, x_n^j\}$ for $0 \leq j \leq m$. This means that, for $1 \leq i \leq n$ we have that x_i^j and x_i^k are copies of each other whenever $j \neq k$. Now, set $X = \cup_{j=0, \dots, m} X_j$, and let the order relation \leq on X be the union of the \leq_j , so that (X, \leq) is a partially ordered set. To define the similarity $s : X \times X \rightarrow [0, 1]$, we proceed as follows: If x and y are in the same copy-paste component, then their similarity is the same as in the original component. And, if they are in different copy-paste components, then their similarity is that of the original similarity minus a stochastic value. Concretely, let $\mathcal{N}(\mu, \sigma^2)$ be the normal distribution located at μ with scale σ^2 , and let $Y \sim \mathcal{N}(\mu, \sigma^2)$. We then define

$$s(x_p^i, x_q^j) = \begin{cases} s_0(x_p^0, x_q^0) & \text{if } i = j, \\ s_0(x_p^0, x_q^0) - Y & \text{otherwise,} \end{cases} \quad (20)$$

applying rejection sampling to ensure $s(x_p^i, x_q^j) \in [0, 1]$. In this way, the internal cohesion in the copy-paste components are maintained, while the coupling between the copy-paste related items is reduced as μ and σ^2 increase.

The above process leaves us with two pieces of data:

1. The ordered similarity space (X, \leq, s) to be clustered;
2. The hidden clustering (planted partition) representing the copy-paste relations, given by the clusters $C_i = \{x_i^j\}_{j=0}^m$ for $1 \leq i \leq n$.

7.2 Measures of clustering quality

To evaluate the quality of a binary tree $T \in \mathfrak{B}(X)$ relative a planted partition, we follow the method of (Bakkelund, 2021a, Sections 8 and 9), applying the following measures of clustering quality:

Adjusted Rand index. Adjusted Rand indices are some of the most popular measures of clustering quality, and the one-sided Rand indices are good indicators of the success in recovering planted partitions. To report to which degree the methods can recover the planted clustering, we use the one-sided adjusted Rand index (ARI) assuming that the candidate clustering is drawn from the family of all possible clusterings over the set (Gates and Ahn, 2017).

Element wise adjusted order Rand index. Bakkelund (2021a, §8.2.2) introduces a quality measure to determine to which degree the induced order relation between two different clusterings of the same ordered set coincide. We use this quality measure, \bar{o} ARI, to decide to which degree the reported clustering has an induced order relation that coincides with the induced order relation of the planted partition.

⁴<https://pypi.org/project/machine-parts-pp/>

Loops. This quality measure computes the fraction of elements of X participating in cycles in the induced relation of the clustering. While simple, it pins down the error in order preservation for a clustering. For easier comparison alongside the other measures, we report on $1 - \text{fraction}$, so that $\text{loops} = 1$ if there are no cycles, and $\text{loops} = 0$ if all elements participate in a cycle. The loops measure is described in detail in (Bakkelund, 2021a, §9.3).

Given a planted partition $\{C_j\}_j$ over X and a tree $T \in \mathfrak{B}(X)$, to compute the quality of T with respect to the above measures, we start by identifying the flat clustering of T with the highest ARI,⁵ and then proceed to compute the other quality measures for this flat clustering.

Although this puts a higher emphasis on ARI compared to the other measures, we would like to emphasise that both $\bar{\text{ARI}}$ and loops are central measures for order preserving clustering, and in particular for applications where order preservation is key.

7.3 Methods evaluated in the demonstration

To demonstrate the method described in this paper, we use the approximation method from Section 6 to approximate a good tree for val_α using optimal DIRECTEDSPARSESTCUT. We denote this method by $\widehat{\text{val}}_\alpha$.

For comparison, we run a selection of other methods on the same problem instances. From (Bakkelund, 2021a), we know that the method provided by that article⁶ is currently best in class for this type of problems. This method is denoted by $\mathcal{HC}_{30,\varepsilon}^{<\mathcal{CL}}$, representing a 30-fold approximation using complete linkage (Bakkelund, 2021a, Definition 14).

Also, to compensate for the lack of hierarchical clustering methods that support do-not-cluster constraints, Bakkelund (2021a, §9.2) presents a method termed *simulated constrained clustering* based on the following trick. The initial similarity is modified so that every pair of comparable elements have similarity zero. As demonstrated there, when used with classical hierarchical clustering and complete linkage, this provides a significant improvement on the results, compared to just classical hierarchical clustering and complete linkage without the trick. We do the same here, modifying the similarity and approximating a good tree using Dasgupta’s method and no order relation. We denote the method by $\widehat{\text{val}}_1^0$, since $\alpha = 1$ means we ignore the order relation, and the zero indicates that all comparable elements have zero similarity. As we demonstrate below, the trick has a significant effect, but it does not compete with the objective function where both the similarity and the order relation are taken into account.

Finally, we also compare with classical hierarchical clustering with complete linkage,⁷ denoting this method by $\mathcal{HC}^{\mathcal{CL}}$.

7.4 Reporting on mean values

In the below plots, we present the mean values of the different methods’ performance. What we do not show is the variance, which is very large. This is as expected, and is due to the small sample sizes. In the experiments, we see that the variance is equally large for the method from (Bakkelund, 2021a), but we know that this variance drops dramatically with increased sample size. We have no reason to believe that the case is different for the method we present here.

7.5 Execution and results

A number of experiments were run with different parameter settings and on different parts of the dataset. While the magnitudes of the quality measures varied between the different

⁵We employed the `clusim python` library, version 0.4, to compute the ARI.

⁶We employed the `ophac python` library version 0.4.5 for this demonstration.

⁷We employed `scipy.cluster.hierarchy` from `scipy` version 1.7.1.

parameter settings, the trend was the same in all cases. Even the order of the methods with respect to quality of results hardly changed between experiments. We have picked a subset of the experiments, presented in Table 4, to represent the overall observations. For each parameter set in Table 4, we ran 50 experiments,⁸ where each experiment can be outlined as

1. Create a planted partition based on the given parameters according to the above procedure;
2. Run each of the methods on the generated partially ordered similarity space;
3. Evaluate the output of each method according to the listed quality measures.

The mean values reported in the below plots are the means over these 50 executions.

par.	range	default	explanation
cc	6	6	connected component no. to draw from
n	5	5	size of drawn sample
m	4	4	number of copies to make
α	$0 \cdots 1$	best	weight of order relation vs similarity
σ^2	$0.05 \cdots 0.4$	0.15	variance of subtracted noise
μ	$0.0 \cdots 0.4$	0.075	location of subtracted noise
d_{\min}	1.0	1.0	minimum average degree of the drawn sample

Table 4: Parameters for the presented experiments. If the range column contains more than one value, this means that we present plots where this parameter varies over the specified range. In that case, all other parameters are set to the value in the default column. Notice that for α , we have no default value, but present the result for the α with the best mean ARI value.

7.5.1 Varying α

Figure 7 shows the effect of varying α through $[0, 1]$. Recall that for $\alpha = 0$, it is only the order relation that determines the tree. The abrupt change for arbitrary small $\alpha > 0$ is due to tie resolution; in the experiment, the order relation is binary, all relations having the same weight. This may in some cases lead to several equally valued, optimal binary trees. As soon as we introduce the similarity, the ties are broken, and the number of viable solutions drops. Additionally, since the similarity contains information identifying good trees, the average quality increases. But, as $\alpha \rightarrow 1$, the information provided by the order relation is gradually phased out, and the quality of the clustering decreases until it reaches the value on the right end of the plot.

Notice that for $\alpha = 1$, the ARI, $\bar{\text{ARI}}$ and loops values are those that would be obtained for the Dasgupta objective function, since $\widehat{\text{val}}_1 = \widehat{\text{val}}_{s_d}$. From the plot, we see that for ARI, the Dasgupta objective function outperforms $\mathcal{HC}_{30,\varepsilon}^{<\mathcal{CL}}$ with a small margin, even though $\widehat{\text{val}}_{s_d}$ does not take the order relation into account.

It is also interesting to notice that $\widehat{\text{val}}_1^0$, that neither uses the order relation, outperforms $\mathcal{HC}_{30,\varepsilon}^{<\mathcal{CL}}$ with significant margin with respect to ARI; an observation that is consistent through all the experiments we have done. We choose to conclude that these observations merely underline the significance of the Dasgupta objective function.

The loops measure deserves a separate comment. First, we note that $\mathcal{HC}_{30,\varepsilon}^{<\mathcal{CL}}$ has zero loops, which is also guaranteed by that method. Second, from Theorem 15, we know that $\text{val}_{\alpha=0}$, has

⁸We ran tests with 200 experiments for a small selection of parameter sets. Seeing that the observations remained unchanged, we concluded that 50 experiments was sufficient for this demonstration.

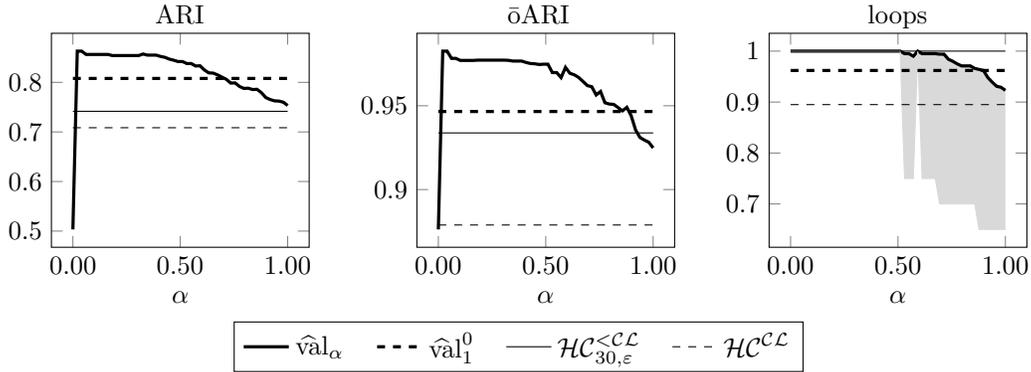


Figure 7: The mean performance of $\widehat{\text{val}}_\alpha$ for different values of α , plotted together with the mean values of the other methods. Notice that the other methods are constant with respect to α , explaining the horizontal plot lines. The bottom of the shaded region indicates the minimum observed value of the loops measure for $\widehat{\text{val}}_\alpha$.

no loops for an optimal tree. But what we see from the plots is that even the approximation $\widehat{\text{val}}_\alpha$ returns nothing but loop-free trees for α significantly larger than zero. This is a very promising observation, indicating that $\widehat{\text{val}}_\alpha$ can be used for applications where loops are unacceptable, such as classic use cases requiring acyclic partitioning of graphs. We note that further research is required to establish for which $\alpha > 0$ and under which assumptions on the order relation and the similarity such a guarantee can be set forth.

It should also be mentioned that for all the experiments, the best results were obtained for values of α close to zero. An open question is to whether this would also be the case for a weighted partial order without uniform weights.

7.5.2 Varying the variance

Figure 8 shows the effect of varying σ^2 through $[0.05, 0.4]$; that is, the variance of the noise added to the copy-paste similarities in (20). While each point in the plot of $\widehat{\text{val}}_\alpha$ corresponds to the optimal value over all $\alpha \in [0, 1]$, from what we see across the experiments, more or less equally good results would be obtained by simply fixing $\alpha = 0.1$ or some other low value (see the comment at the end of Section 7.5.1).

As can be expected, all methods degrade in quality of the result when the variance in the similarities increases, but $\widehat{\text{val}}_\alpha$ is clearly less affected by this than the other methods. Notice in particular that $\widehat{\text{val}}_\alpha$ seems to be less affected by increase in variance than $\widehat{\text{val}}_1^0$, although they are based on very much the same optimisation principles. At first, one may think that this is because the order relation is not modified by the noise, and this information is available to $\widehat{\text{val}}_\alpha$, but not to $\widehat{\text{val}}_1^0$. However, the order relation is utilised by $\mathcal{HC}_{30,\epsilon}^{<CL}$, and this method degrades just as severely as $\widehat{\text{val}}_1^0$ when the variance increases. One possible explanation is that it is the combined objective function, utilising both the Dasgupta objective and the antisymmetrisation of the order relation (8) that causes $\widehat{\text{val}}_\alpha$ to outperform the other methods.

Notice also that $\widehat{\text{val}}_\alpha$ performs perfectly with respect to loops, regardless of the increasing noise variance.

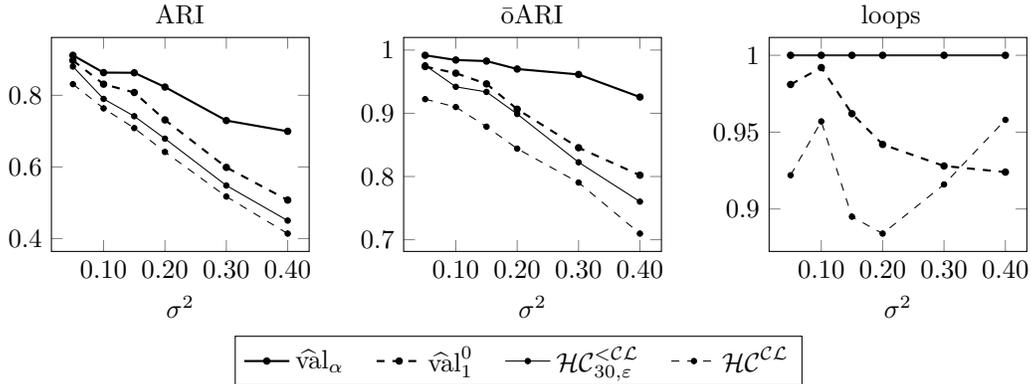


Figure 8: The mean performances of the different methods for varying σ^2 . The markers indicate for which values of σ^2 the experiments were conducted, and the other parameters are according to the default values of Table 4. For $\widehat{\text{val}}_\alpha$, each point in the plot corresponds to the optimal value over all $\alpha \in [0, 1]$. Notice that for the loops-plots, the plot for $\mathcal{HC}_{30,\varepsilon}^{<C L}$ coincides with the plot of $\widehat{\text{val}}_\alpha$. All trees returned by $\widehat{\text{val}}_\alpha$ were loop-free for the chosen α , hence, compared to Figure 7, there is no visible gray region in the plot.

7.5.3 Varying translation magnitude

Figure 9 shows the effect of varying μ through $[0, 0.4]$; that is, the location of the noise added to copy-paste similarities. As before, we present the result for the optimal α for $\widehat{\text{val}}_\alpha$.

We see that all methods, $\widehat{\text{val}}_\alpha$ included, are equally affected by increasing translation of similarities, but that $\widehat{\text{val}}_\alpha$ performs consistently better than all the other methods throughout all the experiments.

Also in this case, given a tree T approximated by $\widehat{\text{val}}_\alpha$, the flat clustering with the best ARI is loop-free in every experiment.

8 Summary and future work

We have defined the concept of order preserving hierarchical clustering and classified the binary trees over a set that correspond to order preserving hierarchical clusterings. We have introduced the concept of a *relaxed order relation*, where the relations are weighted over $[0, 1]$, presented an objective function for hierarchical clustering of relaxed orders, and proven several beneficial properties of this function. In particular, whenever the relaxed order relation is a uniformly weighted partial order relation, an optimal tree is always order preserving. We have discussed the method in terms of bi-objective optimisation, where the order relation and the similarity are convexly combined, and provided an efficient basis on which to explore the Pareto front. We have provided a polynomial time approximation algorithm for the model, with a proven relative performance guarantee of at least $O(\log^{3/2} n)$, and, finally, we have demonstrated the method on the machine parts dataset, showing that our method outperforms existing methods with significant margin.

The following future research topics have been mentioned in the paper:

- Theorem 21 gives a probability bound for order preservation quality for val_g , just as (Dasgupta, 2016, Theorem 9) gives a probability bound for clustering quality for val_{s_d} .

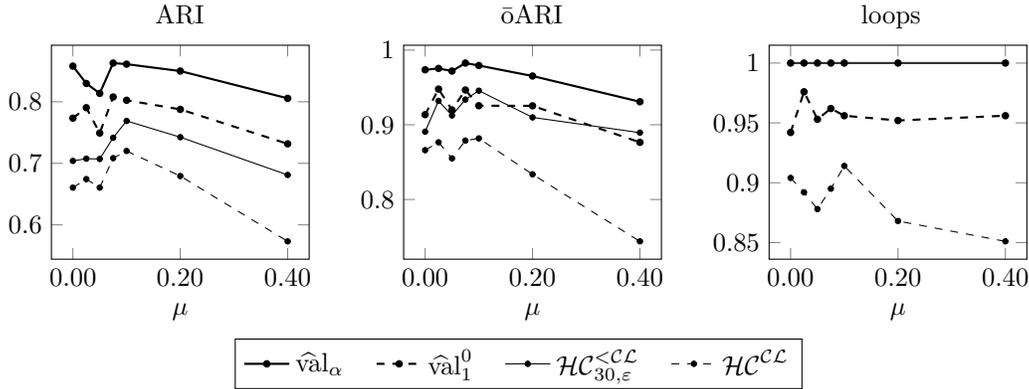


Figure 9: The mean performances of the different methods for varying μ . The markers indicate for which values of μ the experiments were conducted, and the other parameters are according to the default values of Table 4. For $\widehat{\text{val}}_\alpha$, each point in the plot corresponds to the optimal value over all $\alpha \in [0, 1]$. Notice that for the loops-plots, the plot for $\mathcal{HC}_{30,\epsilon}^{<C L}$ coincides with the plot of $\widehat{\text{val}}_\alpha$. All trees returned by $\widehat{\text{val}}_\alpha$ were loop-free for the chosen α , hence, compared to Figure 7, there is no visible gray region in the plot.

We suggest to establish a probability bound for the combined order preservation- and clustering quality for val_α .

- According to Theorem 15, if the order relation is a partial order, then the optimal trees for val_g are order preserving. It follows that the same result holds for val_α when $\alpha = 0$. However, from the demonstration in Section 7.5.1, we see that the approximation $\widehat{\text{val}}_\alpha$ provides trees that are order preserving for α significantly larger than 0. For applications, a result that that can provide an order preservation guarantee for non-zero α would be of great value. It would allow the optimisation to take both the order relation and the similarity into account, and at the same time guarantee order preservation.
- The approximation bound $O(\log^{3/2} n)$ of $\widehat{\text{val}}_\alpha$ (Theorem 31) can most likely be improved, in the same manner that has been achieved for the Dasgupta objective function approximation.

Additionally, at the start of Section 7, we mentioned the lack of available implementations of approximations of DIRECTEDSPARSESTCUT. When trying to locate openly available implementations of such algorithms, we found none. A complicating factor is that the theory behind the DIRECTEDSPARSESTCUT approximations is far from trivial, so implementing one’s own is not generally achievable unless already an expert in semidefinite programming. And finally, there are no known non-trivial approximations of DIRECTEDSPARSESTCUT that provide useful cuts. We therefore suggest a call for action within operations research to make available realisations of the existing approximation theories for DIRECTEDSPARSESTCUT, at least for the scientific community, and for not-unreasonably-small datasets.

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