Order preserving hierarchical agglomerative clustering of strict posets

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Abstract

We present a method for hierarchical clustering of directed acyclic graphs and other strictly partially ordered data that preserves the data structure. In particular, if we have \( a < b \) in the original data and denote their respective clusters by \([a]\) and \([b]\), we get \([a] < [b]\) in the produced clustering. The clustering uses standard linkage functions, such as single- and complete linkage, and is a generalisation of hierarchical clustering of non-ordered sets.

To achieve this, we define the output from running hierarchical clustering algorithms on strictly ordered data to be partial dendrograms; sub-trees of classical dendrograms with several connected components. We then construct an embedding of partial dendrograms over a set into the family of ultrametrics over the same set. An optimal hierarchical clustering is now defined as follows: Given a collection of partial dendrograms, the optimal clustering is the partial dendrogram corresponding to the ultrametric closest to the original dissimilarity measure, measured in the \( p \)-norm. Thus, the method is a combination of classical hierarchical clustering and ultrametric fitting.

Keywords: Hierarchical clustering, Order preserving clustering, Strict partial order, Partial dendrogram, Unsupervised classification

1 Introduction

Clustering is one of the oldest and most frequently used techniques for exploratory data analysis and unsupervised classification. The toolbox contains a large variety of methods and algorithms, spanning from the initial, but still popular ideas of \( k \)-means [Macqueen, 1967] and hierarchical clustering [Johnson, 1967], to more recent methods, such as density- and model based clustering [Kriegel et al., 2011, Fraley and Raftery, 2002], and semi-supervised methods [Basu et al., 2008], plus a large list of variants. All these methods have one thing in common: they try to extract hidden structure from the data, and make it visible to the analyst. But they also share another feature: if the analysed data is already endowed with some form of structure, the structure is lost in the clustering process; the clustering does not try to retain the structure. This in spite of the fact that strictly partially ordered data, such as directed acyclic graphs, rooted trees and linear orders, are types of data that is more and more commonly analysed by practitioners.

In this paper, we show how to extend clustering to relational data in a way that preserves the relations. In particular, if the input is a set \( X \) equipped with a strict order relation \(<\), and if \( a, b \in X \), we ensure that if \( a < b \), then, after clustering, we will have \([a] <' [b]\). Here, \([a]\) and \([b]\) are the respective clusters containing \( a \) and \( b \), and \(<'\) is an order relation on the clusters naturally induced by \(<\).
1.1 Motivating use case

The motivation for the theory described herein comes from a database of machine parts that are arranged in part-of relations: parts are registered as sub-parts of other parts. Due to historical reasons, there has been incidents of copy-paste of machine designs, and the copies have been given entirely new identifiers with no links to the original design. In hindsight, there is a wish to identify these equivalent machine parts, but telling them apart is hard. Also, the metadata that is available has a tendency of displaying high similarity between a part and its sub-parts, leading to “vertical clustering” in the data.

Since the motivation is to identify equivalent machinery with the aim of replacing one piece of machinery with an equivalent part, and since a part and its sub-parts by no means can be interchanged, it is essential to maintain this parent-child relationship. Moreover, since a part and its sub-part are never equivalent, this is a strict order relation. The set of all machine parts therefore makes up a strictly partially ordered set.

By preserving these relations in the clustering process, we can eliminate the errors due to close resemblance between the part and the sub-part, resulting in improved over all quality of the clustering.

In Section 6, we give a short demonstration of how our method performs on a subset of this data. For the curious reader, it is recommended to skim through this section before proceeding as a further motivation. The section can be read without visiting the foundational material.

1.2 Problem overview

This section presents the research problem on a high level. All terms and concepts used in this section will be properly defined in the main text.

1.2.1 Hierarchical clustering at a glance

From a bird’s-eye view, one may describe hierarchical agglomerative clustering as follows: A clustering of a set $X$ is a partitioning of $X$ into disjoint subsets called clusters. Given a set $X$ together with a notion of (dis-)similarity between the elements of $X$, a hierarchical agglomerative clustering can be obtained as follows:

1. Start by placing each element of $X$ in a separate cluster.

2. Pick the two clusters that are most similar according to the (dis-)similarity measure, and combine them into one cluster by taking their union.

3. If all elements of $X$ are in the same cluster, we are done. Otherwise, go to Step 2 and continue.

The result from this process is a dendrogram; a tree structure showing the sequence of the clustering process. Figure 1 shows a dendrogram over the set $X = \{a, b, c, d, e\}$. The elements of $X$ are the leaf nodes of the dendrogram, and, starting at the bottom, the horizontal bars indicate which elements are joined at which step in the process. The numbers on the y-axis indicate at which dissimilarity level the different clusters were formed.
Figure 1: A dendrogram over the set $X = \{a, b, c, d, e\}$.

It has been shown that the set of dendrograms over a finite set is in a bijective correspondence with the set of ultrametrics over the same set [Carlsson and Memoli, 2010]. An ultrametric is a particular type of metric. From Figure 1 we define the ultrametric distance between two elements to be the minimal height you have to ascend to in order to traverse from one element to the other. For example, the ultrametric distance between elements $c$ and $e$ is 8.0. Dendrograms and ultrametrics play a central role in our theory.

1.2.2 Introducing a strict order relation on $X$

Given a set $X = \{a, b, c, d\}$ where $a < b$ and $c < d$, we can use arrows to denote the order relation, thinking of $X$ as a directed acyclic graph with two connected components. If we want to produce a hierarchical clustering of $X$ as described above, while at the same time maintaining the order relation, our options are depicted in the Hasse diagram in Figure 2.

![Figure 2: Possible hierarchical clusterings over the set $X = \{a, b, c, d\}$ with $a < b$ and $c < d$. Adjacent elements indicate clusters.](image)

Each path in this diagram, starting at the bottom and advancing upwards, represents a hierarchical clustering. But, since we are required to preserve the order relation, we cannot merge any more elements than what we see here. This means that we will never obtain dendrograms like the one in Figure 1 that joins at the top when all elements are placed in a single cluster. Rather, the output of hierarchical agglomerative clustering would take the form of the partial dendrograms of Figure 3.
Figure 3: Partial dendrograms over the set $X = \{a, b, c, d\}$ with $a < b$ and $c < d$. Each partial dendrogram corresponds to a path in Figure 2 starting at the bottom and advancing upwards to the ordered set depicted below the dendrogram.

Moreover, consider the situation where both $(a, d)$ and $(a, c)$ are pairs of minimal dissimilarity. Being mutual exclusive merges, choosing to merge one over the other leads to very different solutions. And it is not at all obvious which of the corresponding partial dendrograms in Figure 3 is the better.

1.3 Outline of our method and contributions

In this section, we provide a high level view of our method, together with our main contributions and results.

1.3.1 An embedding of partial dendrograms into ultrametrics

When we apply hierarchical agglomerative clustering to strictly partially ordered data, the output is partial dendrograms. One of the contributions of this paper is an embedding of partial dendrograms over a set into the family of ultrametrics over the same set. Due to the bijective correspondence between ultrametrics and dendrograms, this also provides an embedding from partial dendrograms into dendrograms.

This embedding is of obvious theoretical interest, since it parallels the bijective correspondence between dendrograms over a set and ultrametrics over the same set. The embedding lifts to the bijection, tying the theories for hierarchical agglomerative clustering for ordered and non-ordered sets together.

But the embedding has value beyond the purely theoretical. The first is that ultrametrics (or metrics) are more suitable as tools for mathematics than are partial dendrograms. Secondly, substantial work has been conducted since Jardine and Sibson [1971] studying hierarchical clustering in the light of the correspondence between dendrograms and ultrametrics. Also, several optimisation based methods for hierarchical clustering use the clustering structure, in terms of dendrograms, as input to the objective function. Our embedding makes it possible to benefit from and participate in all of this. We have therefore laid down extra effort, making sure that this mapping is indeed an embedding (that is, an injective map), and not just any map.

But more importantly, we define our objective function as follows: from a selected list of candidate partial dendrograms, the partial dendrogram representing the best hierarchical clustering is the one that corresponds to the ultrametric that is closest to the original dissimilarity measure when measured in the $p$-norm. This makes our model a variant of ultrametric fitting.
1.3.2 Optimised hierarchical agglomerative clustering

First consider the case of a non ordered set $X$ equipped with a dissimilarity measure. A family of candidate hierarchical clusterings are defined as follows: By running the algorithm for classical hierarchical clustering from Section 1.2.1 we consider every output a candidate solution. In particular, if the algorithm faces two or more equally valid pairs for merging, we simply merge those pairs in every possible order. This generates one candidate solution for each permutation of those connections.

Given the collection of candidate solutions, we define the optimised hierarchical agglomerative clustering to be the dendrogram among the candidate solutions corresponding to the ultrametric closest to the original dissimilarity measure when measured in the $p$-norm.

Due to the way the candidates are generated, this definition is permutation invariant; it is not influenced by the order in which the elements of the set are enumerated. The main characteristics of optimised hierarchical clustering may be summarised as follows:

1. Optimised hierarchical clustering is permutation invariant
2. Classical hierarchical clustering with single linkage is identical to optimised hierarchical clustering with single linkage
3. Optimised hierarchical clustering with complete linkage is NP-hard

As we demonstrate in relation to the proof of Item 3, optimised hierarchical clustering with complete linkage is able to detect maximal cliques in graphs. This is a powerful property, and we take this as part of the evidence that our choice of objective function is reasonable. In some sense, we may say that this is a fulfillment of the idea behind complete linkage.

1.3.3 Order preserving optimised hierarchical agglomerative clustering

Our main result: order preserving hierarchical agglomerative clustering for strictly partially ordered sets extends our model for non-ordered clustering. We copy the process for candidate generation, with the modification that we ensure that every merge leads to an order preserving clustering. Our set of candidates now consists of partial dendrograms. The optimal partial dendrogram is defined as the partial dendrogram corresponding to the ultrametric being closest to the original dissimilarity measure when measured in the $p$-norm. This comparison is possible due to our embedding of partial dendrograms into ultrametrics.

In this way, we end up with order preserving hierarchical clustering that is permutation invariant. For hierarchical clustering of strictly ordered sets, permutation invariance is key: As described in Section 1.2.2, different choices of merges may lead to very different results. Being dependent on the enumeration order of the underlying set would be disastrous.

1.3.4 Main contributions

Our main contributions may thus be summarised as follows:

- Theory and algorithms for order preserving hierarchical agglomerative clustering for strict posets.
- Optimised hierarchical agglomerative clustering for non-ordered sets; a hierarchical clustering methodology very close to classical hierarchical clustering, but that is permutation invariant.
- A general framework for order preserving ultrametric fitting of strict partial orders equipped with a dissimilarity measure.
1.4 Related work

Hierarchical agglomerative clustering is described in a plethora of books and articles, and we shall not try to give a comprehensive account of the material here. For an introduction to the subject, we can recommend [Jain and Dubes, 1988 §3.2].

1.4.1 Clustering of ordered data

There are quite a few articles presenting clustering of orders, whereof we can mainly split the works in two.

The first variant is clustering of sets where the (dis)similarity measure is replaced by information about whether one pair of elements is more similar than another pair of elements, for example based on user preferences. This is sometimes referred to as comparison based clustering. See the recent article by Ghoshdastidar et al. [2019] for an example and references. In this category, we also find the works of Janowitz [2010], providing a wholly order theoretic description of hierarchical clustering, including the case where the dissimilarity measure is replaced by a partially ordered set.

The second variant is to partition a family of ordered sets, so that similarly ordered sets are associated with each other. Examples include the paper by Kamishima and Fujiki [2003], where they develop a variation of $k$-means, called $k$-$\sigma$-means, for clustering preference data, each list of preferences being a totally ordered set. Other examples in this category include clustering of times series, identifying which times series are alike [Luczak, 2010].

Our method differs from all of these examples in that we cluster elements inside one ordered set through the use of a (dis)similarity measure, while maintaining the original orders of elements.

1.4.2 Clustering to detect order

Another variant is the detection of order relations in data through clustering: In Carlsson et al. [2014], it is demonstrated how hierarchical agglomerative quasi-clustering can be used to deduce a partial order of “net flow” from an asymmetric network.

In this category, it is also worth mentioning dynamic time warping. This is a method for aligning time series, and can be considered as clustering across two time series that is indeed order preserving. See [Luczak, 2010] for further references on this.

1.4.3 Acyclic graph partitioning problems

The problem of order preserving hierarchical agglomerative clustering of strict partial orders can be said to belong to the family of acyclic graph partitioning problems [Herrmann et al., 2017]. If we consider the strict partial order to be a directed acyclic graph (DAG), the task is to partition the vertices into groups so that the groups together with the arrows still makes up a DAG.

Graph partitioning has received a substantial attention from researchers, especially within computer science, over the last 50 years. Two important fields of application of this theory are VLSI and parallel execution.

For VLSI, short for Very Large Scale Integration, the problem can be formulated as follows: Given a set of micro processors, the wires that connect them, and a set of circuit boards, how do you best place the processors on the circuit boards in order to optimise a given objective function? Typically, a part of the objective function is to minimise the wire length. But other features may also be part of the optimisation, such as the amount or volume of traffic between certain processors etc. [Markov et al., 2015]
For parallel processing, the input data is a set of tasks to be executed. The tasks are organised as a DAG, where predecessors must be executed before descendants. Given a finite number of processors, the problem is to group the tasks so that they can be run group-wise on a processor, or running groups in parallel on different processors, in order to execute all tasks as quickly as possible. Typically additional information available is memory requirements, expected execution times for the tasks, etc. [Buluç et al., 2016]

It is not difficult to understand why both areas have received attention, being essential in the development of modern computers. The development of theory and methods has been both successful and abundant, and a large array of techniques are available, both academic and commercially.

Although both problems do indeed perform clustering of strict partial orders, their solutions are not directly transferable to exploratory data analysis. Mostly because they have very specific constraints and objectives originating from their respective problem domains.

The method we propose in this paper has as input a strict partial order (equivalently; a DAG) together with an arbitrary dissimilarity measure. We then use the classical linkage functions single-, average-, and complete linkage to suggest clusterings of the vertices from the input dataset, while preserving the original order relation.

Our method therefore places itself firmly in the family of acyclic graph partitioning methodologies, but with different motivation, objective and solution, compared to existing methods.

1.4.4 Hierarchical clustering as an optimisation problem

Several publications aim at solving hierarchical clustering in terms of optimisation. However, due to the procedural nature of classical hierarchical clustering, combined with the linkage functions, pinning down an objective function may be an impossible task. Especially since classical hierarchical clustering is not even well defined for complete linkage in the presence of tied connections. This leads to a general abandonment of linkage functions in optimisation based hierarchical clustering.

Quite commonly, optimisation based hierarchical clustering is done in terms of ultrametric fitting. That is, it aims to find an ultrametric that is as close to the original dissimilarity measure as possible, perhaps adding some additional constraints [Gilpin et al., 2013; Chierchia and Perrot, 2019]. It is well known that solving single linkage hierarchical clustering is equivalent to finding the so called maximal sub-dominant ultrametric. That is; the ultrametric that is pointwise maximal among all ultrametrics not exceeding the original dissimilarity [Rammal et al., 1986]. But for the other linkage functions, there is no equivalent result.

Optimisation based hierarchical clustering therefore generally present alternative definitions of hierarchical clustering. Quite often based on objective functions that originate from some particular domain. Exceptions from this are, for example, Ward’s method [Ward, 1963], where the topology of the clusters are the focus of the objective, and also the recent addition by Dasgupta [2016], where the optimisation aims towards topological properties of the generated dendrogram.

Although our method is, eventually, based on ultrametric fitting, we optimise over a very particular set of dendrograms. Namely the dendrograms that can be generated through classical hierarchical clustering with linkage functions. It is therefore reasonable to claim that our method places itself between classical hierarchical clustering and optimised models.

1.5 Organisation of the remainder of this paper

Section 2 provides the necessary background material. We start by recalling strict and non-strict partial order relations and equivalence relations. Thereafter, we revisit classical hierarchical
agglomerative clustering, recalling central concepts such as dissimilarity measures, ultrametrics and dendrograms.

In Section 3 we tackle the problem of order preservation during clustering: We define what we mean by order preservation, and classify exactly the clusterings that are order preserving. We also provide concise necessary and sufficient conditions for an hierarchical agglomerative clustering algorithm to be order preserving.

In Section 4 we define partial dendrograms, and develop the embedding of partial dendrograms over an ordered set into the family of ultrametrics over the same set.

Our main results are given in Section 5. First, we define optimised hierarchical agglomerative clustering for non-ordered sets. We then generalise this to order preserving hierarchical agglomerative clustering for strict partial orders. We also provide some main characteristics of both methods.

Section 6 provides a demonstration, where we apply order preserving hierarchal agglomerative clustering to a part of the real-world data described in Section 1.1. Section 7 closes the article with some concluding remarks, and a list of future work topics.

2 Background

In this section we recall basic background material. We start by recollecting the required order-theoretical tools together with equivalence relations, before recalling classical hierarchical clustering.

2.1 Relations

Definition 1. A relation $R$ on a set $X$ is a subset $R \subseteq X \times X$, and we say that $x$ and $y$ are related if $(x, y) \in R$. The short hand notation $aRb$ is equivalent to writing $(a, b) \in R$.

2.1.1 Strict and non-strict partial orders

A strict partial order on a set $X$ is a relation $S$ on $X$ that is irreflexive and transitive. Recall that, an irreflexive and transitive relation is also anti-symmetric. A strictly partially ordered set, or a strict poset, is a pair $(X, S)$, where $X$ is a set and $S$ is a strict partial order on $X$. We commonly denote a strict partial order by the symbol $<$. On the other hand a partial order on $X$ is a relation $P$ on $X$ that is reflexive, asymmetric and transitive, and the pair $(X, P)$ is called a partially ordered set, or a poset. The usual notation for a partial order is $\leq$.

We shall just refer to strict and non-strict partial orders as orders, unless there is any need for disambiguation: If $R$ is an order on $X$, we say that $a, b \in X$ are comparable if either $(a, b) \in R$ or $(b, a) \in R$. And, if every pair of elements in $X$ are comparable, we call $X$ totally ordered. A totally ordered subset of an ordered set is called a chain, and a subset where no two elements are comparable is called an antichain. We denote non-comparability by $a \perp b$. That is, for any elements $a, b$ in an antichain, we have $a \perp b$.

A cycle in a relation $E$ on a set $X$ is a sequence in $E$ on the form $(a, b_1), (b_1, b_2), \ldots, (b_n, a)$. The transitive closure of $E$ is the minimal set $\overline{E}$ for which the following holds: If there is a sequence of pairs $(a_1, a_2), (a_2, a_3), \ldots, (a_{n-1}, a_n)$ in $E$, then $(a_1, a_n) \in \overline{E}$.

Let $(X, E)$ be an ordered set. An element $x_0 \in X$ is a minimal element if there is no element $y \in X - \{x_0\}$ for which $(y, x_0) \in E$. Dually, $y_0$ is a maximal element if there is no $x \in X - \{y_0\}$ for which $(y_0, x) \in E$. If $(X, E)$ has a unique minimal element, then this is called
the bottom element or the least element, and a unique maximal element is called the top element or the greatest element.

Finally, a map \( f : (X, <_X) \to (Y, <_Y) \) is order preserving if \( a <_X b \Rightarrow f(a) <_Y f(b) \), and if \( f \) is a set isomorphism for which \( f^{-1} \) is also order preserving, we say that \( f \) is an order isomorphism, and that the sets \((X, <_X)\) and \((Y, <_Y)\) are order isomorphic, writing \((X, <_X) \cong (Y, <_Y)\).

2.1.2 Partitions and equivalence relations

A partition of \( X \) is a collection of disjoint subsets of \( X \), the union of which is \( X \). That is; a clustering of \( X \) is a partition of \( X \). The family of all partitions of \( X \), denoted \( \mathcal{P}(X) \), has a natural partial order defined by partition-refinement: If \( A = \{A_i\}_i \) and \( B = \{B_j\}_j \) are partitions of \( X \), we say that \( A \) is a refinement of \( B \), writing \( A \subseteq B \), if, for every \( A_i \in A \) there exists a \( B_j \in B \) such that \( A_i \subseteq B_j \). The sets of a partition are referred to as blocks.

Partitions are intimately related to the concept of equivalence relations: An equivalence relation \( \mathcal{R} \) on \( X \) that is reflexive, symmetric and transitive. Let the family of all equivalence relations over a set \( X \) be denoted by \( \mathcal{R}(X) \). If \( \mathcal{R} \in \mathcal{R}(X) \) and \( (x, y) \in \mathcal{R} \), we say that \( x \) and \( y \) are equivalent, writing \( x \sim y \). The maximal set of elements equivalent to \( x \in X \) is called the equivalence class of \( x \), and is denoted \([x] \). \( \mathcal{R}(X) \) is also partially ordered, but by subset inclusion: that is, for \( \mathcal{R}, \mathcal{I} \in \mathcal{R}(X) \), we say that \( \mathcal{R} \) is less than or equal to \( \mathcal{I} \) if and only if \( \mathcal{R} \subseteq \mathcal{I} \).

The quotient of \( X \) modulo \( \mathcal{R} \), denoted \( X/\mathcal{R} \), is the set of equivalence classes of \( X \) under \( \mathcal{R} \). Notice that \([x] \) is an element of \( X/\mathcal{R} \), but a subset of \( X \).

Since the equivalence classes are subsets of \( X \) that together cover \( X \), \( X/\mathcal{R} \) is a partition of \( X \). Indeed, the family of partitions of \( X \) is in a one-to-one correspondence with the equivalence relations of \( X \): if \( A \in \mathcal{P}(X) \), then there exists a unique \( \mathcal{R} \in \mathcal{R}(X) \) for which \( A = X/\mathcal{R} \). Moreover, the correspondence is order preserving; for \( A = X/\mathcal{R} \) and \( B = X/\mathcal{I} \), we have

\[
A \subseteq B \Leftrightarrow \mathcal{R} \subseteq \mathcal{I}.
\]

Both \( \mathcal{P}(X) \) and \( \mathcal{R}(X) \) have top- and bottom elements: The least element of \( \mathcal{P}(X) \) is the singleton partition \( S(X) \), where each element is in an equivalence class by itself: \( S(X) = \{\{x\} \mid x \in X\} \). The singleton partition corresponds to the diagonal equivalence relation, given by \( \Delta(X) = \{(x, x) \mid x \in X\} \), which is the least element of \( \mathcal{R}(X) \). The greatest element of \( \mathcal{P}(X) \) is the trivial partition, \( \{X\} \), corresponding to the equivalence relation \( X \times X \), where all elements are equivalent. That is

\[
S(X) = X/\Delta(X) \quad \text{and} \quad \{X\} = X/(X \times X).
\]

If \( \mathcal{A} \) and \( \mathcal{B} \) are partitions of \( X \) with \( \mathcal{A} \) being a refinement of \( \mathcal{B} \), we say that \( \mathcal{A} \) is finer than \( \mathcal{B} \), and that \( \mathcal{B} \) is coarser than \( \mathcal{A} \). We use the exact same terminology for the corresponding equivalence relations \( \mathcal{A} \trianglelefteq \mathcal{B} \in \mathcal{R}(X) \), having \( \mathcal{A} \subseteq \mathcal{B} \).

For a subset \( A \subseteq X \), let the notation \( X/A \) denote the partition of \( X \) where all of \( A \) is one equivalence class, and the rest of \( X \) remains as singletons. Formally, this corresponds to the equivalence relation \( \mathcal{A} = \Delta(X) \cup (A \times A) \). And finally, the quotient map corresponding to an equivalence relation \( \mathcal{R} \in \mathcal{R}(X) \) is the unique map \( q_{\mathcal{R}} : X \to X/\mathcal{R} \) defined as \( q_{\mathcal{R}}(x) = [x] \). That is, \( q_{\mathcal{R}} \) sends each element to its equivalence class.

Definition 2. A clustering of a set \( X \) is a partition of \( X \), and a hierarchical clustering is a chain in \( \mathcal{P}(X) \) containing both the bottom and top elements. A cluster in a clustering is a block in the partition.
Alternatively, a clustering of $X$ is an equivalence relation $R \in \mathcal{R}(X)$, and a hierarchical clustering is a chain in $\mathcal{R}(X)$ containing both the bottom- and top elements of $\mathcal{R}(X)$. A cluster is, then, an equivalence class in $X/R$.

We will refer to clusters as equivalence classes, clusters or blocks depending on the context, all terms being frequently used in clustering literature.

**Example 1.** For the three-element space $X = \{a, b, c\}$, the lattice of partitions takes the form of the below Hasse diagram.

$$
n = \{\{a, b, c\}\} \quad \mathcal{P}(X) : \quad \{\{a, b\}, \{c\}\} \quad \{\{a\}, \{b, c\}\} \quad \{\{a\}, \{b\}, \{c\}\}
n
The elements in bold make up a chain in $\mathcal{P}(X)$ that contains both the bottom- and top elements, and therefore also constitutes a hierarchical clustering of the elements in $X$.

### 2.2 Classical hierarchical clustering

In this section, we recall classical hierarchical clustering in terms of Jardine and Sibson [1971]. Our theory builds directly on the theory for classical hierarchical clustering, so we provide a fair bit of detail: We start by recalling the formal definition of a dendrogram, before recalling dissimilarity measures and ultrametrics. Thereafter, we recall linkage functions, and at the end of the section, we tie all the concepts together and provide a description of the classical hierarchical agglomerative clustering algorithm.

#### 2.2.1 Dendrograms

Hierarchical clustering outputs dendrograms. But the graphical tree structure depicted in Figure 1 is not well-suited for formal deduction. In this section, we recall the definition of dendrogram due to Jardine and Sibson [1971] for this purpose. For the remainder of the text, let $\mathbb{R}_+$ denote the non-negative reals.

**Definition 3.** Let $\mathbb{R}_+$ be equipped with the usual total order $\leq$, and let $\mathcal{P}(X)$ be partially ordered by partition refinement. A **dendrogram** over a finite set $X$ is an order preserving map $\theta : \mathbb{R}_+ \rightarrow \mathcal{P}(X)$ for which

- **D1.** $\theta(0) = S(X)$, the least element of $\mathcal{P}(X)$.
- **D2.** $\exists t_0 > 0$ s.t. $\theta(t_0) = \{X\}$, the greatest element of $\mathcal{P}(X)$,
- **D3.** $\forall t \in \mathbb{R}_+ \exists \varepsilon > 0$ s.t. $\theta(t) = \theta(t + \varepsilon)$.

Axiom D3 ensures that the dendrogram is piecewise constant on intervals on the form $[t, t')$, as illustrated in the following example.

**Example 2.** Below, we see a graphical dendrogram over the set $X = \{a, b, c, d, e\}$ on the left hand side, and the corresponding definition of $\theta : \mathbb{R}_+ \rightarrow \mathcal{P}(X)$ on the right.
We will use the term dendrogram to denote both the graphical and the functional representation. If \( \text{im}(\theta) = \{ B_i \}_{i=0}^n \), we assume that the enumeration is compatible with the order relation on \( \mathcal{P}(X) \); in other words, that \( \{ B_i \}_{i=0}^n \) is a chain in \( \mathcal{P}(X) \). We denote the family of all dendrograms over \( X \) by \( \mathcal{D}(X) \).

### 2.2.2 Dissimilarity measures and ultrametrics

As pointed out in Section 1.2.1 in order to produce a hierarchical agglomerative clustering, we need a notion of (dis-)similarity, or “distance” between elements: A **dissimilarity measure** on a set \( X \) is a function \( d : X \times X \to \mathbb{R}_+ \), satisfying

\[
d1. \forall x \in X : d(x, x) = 0,
\]

\[
d2. \forall x, y \in X : d(x, y) = d(y, x).
\]

If \( d \) additionally satisfies

\[
d3. \forall x, y, z \in X : d(x, z) \leq \max\{d(x, y), d(y, z)\},
\]

we call \( d \) an **ultrametric**. The pair \((X, d)\) is correspondingly called a **dissimilarity space** or an **ultrametric space**. The family of all dissimilarity measures over \( X \) is denoted by \( \mathcal{M}(X) \), and the family of all ultrametrics by \( \mathcal{U}(X) \).

**Example 3** (Ultrametric). Property \( d3 \) is referred to as the **ultrametric inequality**, and is a strengthening of the usual triangle inequality. In an ultrametric space \((X, u)\), **every triple of points is arranged in an isosceles triangle**: Let \( a, b, c \in X \), and let the pair \( a, b \) be of minimal distance such that \( u(a, b) \leq \min\{u(a, c), u(b, c)\} \). The ultrametric inequality gives us

\[
u(a, c) \leq \max\{u(a, b), u(b, c)\} = u(b, c) \quad \Rightarrow \quad u(a, c) = u(b, c).
\]

In general, \((X, u)\) is not Euclidean. However, the discrete metric is an ultrametric, so any set of equidistant points in \( \mathbb{R}^n \) makes an Euclidean, ultrametric subspace of \( \mathbb{R}^n \). Ultrametrics show up in many different contexts, such as \( p \)-Adic number theory [Holm, 2001], infinite trees [Hughes, 2004], numerical taxonomy [Sneath and Sokal, 1973] and also within physics [Rammal et al., 1980], just to cite a few. For hierarchical clustering, ultrametrics are relevant because the dendrograms over a set are in a bijective relation to the ultrametrics over the same set [Carlsson and Mémoli, 2010].

We shall also need the following terms, which apply to any dissimilarity space: The **diameter** of \((X, d)\) is given by the maximal inter-point distance:

\[
diam(X, d) = \max\{d(x, y) \mid x, y \in X\}.
\]

And the **separation** of \((X, d)\) is the minimal inter point distance:

\[
sep(X, d) = \min\{d(x, y) \mid x, y \in X \land x \neq y\}.
\]
2.2.3 Classical hierarchical clustering

Before we define classical hierarchical clustering, we need to recall linkage functions:

**Definition 4.** Given a set \(X\), a family \(\mathcal{L}\) of **linkage functions** on \(X\) is a set of maps
\[
\ell_Q : Q \times Q \times \mathcal{M}(X) \rightarrow \mathbb{R}_+ \quad \text{for } Q \in \mathcal{P}(X)
\]
so that for each partition \(Q \in \mathcal{P}(X)\) and dissimilarity measure \(d \in \mathcal{M}(X)\), the map \(\ell_Q(-, -, d) : Q \times Q \rightarrow \mathbb{R}_+\) is a dissimilarity measure on \(Q\).

Let \((X, d)\) be a dissimilarity space with \(Q \in \mathcal{P}(X)\), and let \(p, q \in Q\). We will commit to the following abuse of notation: for a family of linkage functions \(\mathcal{L}\), we will write \(\mathcal{L}(p, q, d)\) for the dissimilarity between \(p\) and \(q\) assigned by the unique dissimilarity measure \(\ell_Q(-, -, d)\). We will, also somewhat misleading, refer to the family \(\mathcal{L}\) as a linkage function.

**Definition 5.** For a dissimilarity space \((X, d)\), let \(Q \in \mathcal{P}(X)\) and recall that \(p, q \in Q\) are subsets of \(X\), since they are blocks of \(Q\). The classical linkage functions are defined as follows:

- **Single linkage** : \(\mathcal{SL}(p, q, d) = \min_{x \in p} \min_{y \in q} d(x, y)\).
- **Complete linkage** : \(\mathcal{CL}(p, q, d) = \max_{x \in p} \max_{y \in q} d(x, y)\).
- **Average linkage** : \(\mathcal{AL}(q, p, d) = \frac{\sum_{x \in p} \sum_{y \in q} d(x, y)}{|p| \cdot |q|}\).

**Definition 6 (Classical HC).** Given a dissimilarity space \((X, d)\) and a linkage function \(\mathcal{L}\), if we follow the procedure outlined in Section 1.2.1, using \(\mathcal{L}\) as the “notion of dissimilarity”, the result is a chain of partitions \(\{Q_i\}_{i=1}^{|X|-1}\) together with the dissimilarities \(\{\rho_i\}_{i=1}^{|X|-1}\) at which the partitions were formed. The sequence of pairs \(Q = \{(Q_i, \rho_i)\}_{i=1}^{|X|-1}\) maps to a dendrogram \(\theta_Q\) as follows:
\[
\theta_Q(x) = \max_{i \in \mathbb{N}| \rho_i \leq x} Q_i.
\]

We define a **classical hierarchical clustering of \((X, d)\)** using \(\mathcal{L}\) to be a dendrogram
\[
\mathcal{HC}^\mathcal{L}(X, d) = \theta_Q
\]
on obtained through this procedure.

The question of when \(\mathcal{HC}^\mathcal{L}(X, d)\) is well defined is captured in the following lemma:

**Lemma 7.** The sequence \(\{(Q_i, \rho_i)\}_{i=1}^{|X|-1}\) maps to a dendrogram via (1) if and only if
\[
\text{sep}(Q_i, \mathcal{L}) \leq \text{sep}(Q_{i+1}, \mathcal{L}) \quad \text{for } 0 \leq i < |X| - 1.
\]
(2)

Otherwise, the \(\rho_i\) will not make up a monotone sequence, and the resulting function \(\theta_Q\) will not be an order preserving map. Although all of \(\mathcal{SL}, \mathcal{AL}\) and \(\mathcal{CL}\) satisfy (2), it is fully possible to define linkage functions that do not.

At any point during the clustering process, if we encounter a partition \(Q \in \mathcal{P}(X)\) with two distinct pairs of elements \((p_1, q_1), (p_2, q_2) \in Q \times Q\) for which
\[
\mathcal{L}(p_1, q_1, d) = \mathcal{L}(p_2, q_2, d) = \text{sep}(Q, \mathcal{L}),
\]
we say that the two connections are **tied**, since they are both eligible candidates for the next merge. It is well known that \(\mathcal{HC}^{\mathcal{SL}}\) is invariant with respect to the order of resolution of ties, a property referred to as being **permutation invariant**, since the order of enumeration of elements will not affect the output of the clustering process. On the other hand, both \(\mathcal{HC}^{\mathcal{AL}}\) and \(\mathcal{HC}^{\mathcal{CL}}\) are sensitive to enumeration order [Jardine and Sibson 1971].
2.2.4 Dendrograms and ultrametrics

It has been long known that dendrograms map to ultrametrics [Jardine and Sibson, 1971]:
\[ \Psi_X : \mathcal{D}(X) \rightarrow \mathcal{U}(X). \]

In [Carlsson and Mémoli, 2010] the map \( \Psi_X \) is shown to be a bijection. If \( \theta \in \mathcal{D}(X) \), the map is defined as
\[ \Psi_X(\theta)(x, y) = \min\{ t \in \mathbb{R}_+ \mid \exists B \in \theta(t) : x, y \in B \}. \] (3)

That is, the ultrametric distance is the least real number \( t \) for which \( \theta \) maps to a partition where \( x \) and \( y \) are in the same block. The minimisation is well defined due to Axiom D3. The ultrametric can be read from the diagrammatic representation of the dendrogram as the minimum height you have to ascend to in order to traverse from one element to the other following the paths in the tree.

3 Order preserving clustering

In this section, we determine what it means for an equivalence relation to be order preserving with regards to a strict partial order. Some of the material presented here is already known, and can be found in articles on acyclic graph partitioning, for example [Herrmann et al., 2017]. In most of these works, one is usually content by stating that the resultant graph shall be acyclic. We proceed further to establish precise conditions that are necessary and sufficient for a hierarchical agglomerative clustering algorithm to be order preserving.

3.1 Order preserving equivalence relations

Having established what we mean by a clustering (Definition 2), we can start the discussion of what constitutes an order preserving clustering of a strict poset \((X, <)\). If \( \mathcal{R} \) is an equivalence relation on \( X \) with quotient map \( q : X \rightarrow X/\mathcal{R} \), we have already established, in Section 1.1, that we require
\[ \forall x, y \in X : x < y \Rightarrow q(x) <' q(y). \]

That is, we are looking for a particular class of equivalence relations; namely those that preserve the structure of the strict partial order—in other words, the equivalence relations for which the quotient map is order preserving.

Given an ordered set \((X, E)\), there is a particular relation induced on the quotient set \( X/\mathcal{R} \) for any equivalence relation \( \mathcal{R} \in \mathcal{R}(X) \) [Blyth, 2003, §3.1]:

**Definition 8.** Given an ordered set \((X, E)\) and an equivalence relation \( \mathcal{R} \in \mathcal{R}(X) \), first define the relation \( S_0 \) on \( X \) by
\[ ([a], [b]) \in S_0 \iff \exists x, y \in X : a \sim x \land b \sim y \land (x, y) \in E. \] (4)

The transitive closure of \( S_0 \) is called the relation on \( X/\mathcal{R} \) induced by \( E \). We denote this relation by \( S \).

**Example 4.** An instructive illustration of what the relation \( S_0 \) looks like for an ordered set \((X, <)\) under the equivalence relation \( \mathcal{R} \) is that of an \( \mathcal{R} \)-fence [Blyth, 2003, or just fence, for short:
There exists an order on \( X / \mathcal{R} \) that is transitive by construction, 2. Since a non-cyclic set is irreflexive, and since \( S \) is a strict partial order, and assume that \( q \exists a, b \in X \): \( a \sim x \land b \sim y \land (b', a') \in E \).

But, since \( ([x], [y]) \in S_0 \), we also have

\[
\exists a, b \in X : a \sim x \land b \sim y \land (a, b) \in E.
\]

This yields \( a \sim a' \) and \( b \sim b' \), so we have

\[
(q_\mathcal{R}(a), q_\mathcal{R}(b)) \in S_0 \land q_\mathcal{R}(b) = q_\mathcal{R}(b') \land (q_\mathcal{R}(b'), q_\mathcal{R}(a')) \in S_0.
\]

But, since we have both \( q_\mathcal{R}(a) = q_\mathcal{R}(a') \) and \( (a, b) \in E \), this contradicts the fact that \( q_\mathcal{R} \) is order preserving, so our assumption that both \( ([x], [y]) \) and \( ([y], [x]) \) are elements of \( S_0 \) must be wrong. Hence, if \( q_\mathcal{R} \) is order preserving, there are no cycles in \( S_0 \), and \( S \) is a strict partial order on \( X / \mathcal{R} \). This shows that 3 \( \Rightarrow 1 \).

Finally, let \( S \) be a strict partial order, and assume that \( q_\mathcal{R} \) is not order preserving. Then, there exists \( x, y \in X \) where \( (x, y) \in E \) and for which at least one of \( ([x], [y]) \notin S \) or \( ([y], [x]) \in S \) holds. Now, \( ([x], [y]) \in S \) by Definition 10. Therefore, \( ([y], [x]) \in S \) implies that \( S \) has a cycle, contradicting the fact that \( S \) is a strict partial order. \( \square \)

**Definition 10.** Let \( (X, E) \) be an ordered set. An equivalence relation \( \mathcal{R} \in \mathcal{R}(X) \) is regular if there exists an order on \( X / \mathcal{R} \) for which the quotient map is order preserving. We denote the set of all regular equivalence relations over an ordered set \( (X, <) \) by \( \mathcal{R}(X, <) \). Likewise, the family of all regular partitions of \( (X, <) \) is denoted \( \mathcal{P}(X, <) \).

In general, for an ordered set \( (X, <) \) and a regular equivalence relation \( \mathcal{R} \in \mathcal{R}(X, <) \), we will denote the induced order relation by \( <' \).
3.2 The structure of regular equivalence relations

In this section, we establish a sufficient and necessary condition for an agglomerative clustering algorithm to be order preserving. To help in the proof, we employ the concept of crowns [Blyth, 2005]:

If \((X, <)\) is a strict poset and the induced order on \(X/R\) contains a cycle, then this corresponds to the existence of an \(\mathcal{R}\)-crown:

\[
\begin{array}{c}
\quad b_1 \\
a_1 \\
\quad b_2 \\
a_2 \\
\quad \ddots \\
a_{n-1} \\
\quad b_n \\
a_n \\
\end{array}
\]

That is; the \(\mathcal{R}\)-crown is a “circular” \(\mathcal{R}\)-fence.

Recall that, if \(A \subseteq X\), \(X/A\) denotes the quotient for which the quotient map \(q_A : X \to X/A\) sends all of \(A\) to a point, and is the identity otherwise. That is, for every \(x, y \in X\), we have

\[
q_A(x) = q_A(y) \iff x, y \in A.
\]

**Theorem 11.** If \(A \subseteq X\) for a strictly ordered set \((X, <)\), the quotient map \(q_A : X \to X/A\) is order preserving if and only if \(A\) is an antichain in \((X, <)\).

**Proof.** If \(A\) is not an antichain, then \(X/A\) places comparable elements in the same equivalence class, so \(q_A\) is not order preserving.

Assume \(A\) is an antichain. If \(q_A\) is not order preserving, then there is a cycle in \((X/A, <')\), and since we have only one non-singleton equivalence class, there must exist a crown on the form

\[
\begin{array}{c}
b \\
\quad A \\
c \\
\end{array}
\]

But this means we have \(a, a' \in A\) for which \(b < a\) and \(a' < c\), but since \(c < b\), this implies \(a' < a\), contradicting the fact that \(A\) is an antichain.

Since a composition of order preserving maps is order preserving, this also applies to a composition of quotient maps for a chain of regular equivalence relations \(\mathcal{R}_1 \subseteq \cdots \subseteq \mathcal{R}_n\). Combining this with Theorem 11 we get the following:

**Given a strictly ordered set, a hierarchical agglomerative clustering algorithm will be order preserving if a pair of non-comparable elements are merged at each iteration.**

We close the section with an observation about the family of all hierarchical clusterings over a strict poset:

**Theorem 12.** For a strictly ordered set \((X, <)\), the set \(\mathcal{P}(X, <)\) of regular partitions over \((X, <)\) has \(S(X)\) as its least element. Unless \(<\) is the empty order, there is no greatest element.

**Proof.** \(S(X)\) is always a regular partition, so \(S(X) \in \mathcal{P}(X, <)\). And since \(S(X)\) is a refinement of every partition of \(X\), \(S(X)\) is the least element of \(\mathcal{P}(X, <)\).

If the order relation is not empty, then there are at least two elements that are comparable, and, according to Theorem 11 they cannot be in the same equivalence class. Hence, there is no greatest element.
The situation of Theorem 12 is depicted in Figure 2 and has already been discussed in Section 1.2.2. In the case of tied connections that represent mutually exclusive merges, choosing to merge one connection over the other may lead to very different results. We therefore need a strategy to select one of these solutions over the others. This will be the main focus of Sections 4 and 5.

4 Partial dendrograms

In this section, we construct the embedding of partial dendrograms into ultrametrics. Let an ordered dissimilarity space be denoted by \((X, <, d_X)\). We generally assume that the order relation is non-empty, meaning that there are comparable elements in \((X, <)\). Recall that \(P(X, <)\) is the set of all regular partitions over \((X, <)\); that is, the partitions for which the quotient map is order preserving.

Example 5. Recall the Hasse diagram of regular partitions of the set \(X = \{a, b, c, d\}\) equipped with the order relation \(a < b, c < d\) depicted in Figure 2. Assume that we equip \(X\) with the dissimilarity measure

\[
\begin{array}{ccc}
a & b & c & d \\
\hline 
a & 2.0 & 1.0 & 1.3 \\
b & & 1.0 & 1.5 \\
c & & & 2.0 \\
\end{array}
\]  

For the usual agglomerative hierarchical clustering algorithms, the maximal chains in \(P(X, <)\) will correspond to the partial dendrograms in Figure 4.

![Partial Dendrograms](image)

Figure 4: The partial dendrograms corresponding to the maximal chains in the Hasse diagram of Figure 2. The levels in the dendrograms are given by the dissimilarity \(d_X\) in (5). The corresponding maximal partitions are displayed below each dendrogram.

A significant difference from non-ordered sets is that there is no greatest element \(\{X\}\) in \(P(X, <)\). As a consequence, there are no dendrograms \(\theta : \mathbb{R}_+ \to P(X, <)\), so we have to provide an alternative:

Definition 13. Let \(\mathbb{R}_+\) be equipped with the usual total order \(\leq\), and let \(P(X, <)\) be partially ordered by partition refinement. A **partial dendrogram** over \((X, <)\) is an order preserving map \(\theta : \mathbb{R}_+ \to P(X, <)\) satisfying

- \(P1. \ \theta(0) = S(X)\), the least element of \(P(X, <)\).
- \(P2. \ \forall t \in \mathbb{R}_+ \ \exists \varepsilon > 0 \ s.t. \ \theta(t) = \theta(t + \varepsilon)\).

We will let \(\theta(\infty)\) denote the maximal partition in the image of \(\theta\), and denote the family of all partial dendrograms over \((X, <)\) by \(\mathcal{PD}(X, <)\).
Remark 14. If the order relation is non-empty, we have $\mathcal{PD}(X, <) \cap \mathcal{D}(X) = \emptyset$.

The only difference between a partial dendrogram, and the definition of dendrogram given in Definition 3, is that we do not any longer require a greatest element to be in the image of $\theta$. However, since $\mathcal{P}(X, <)$ is finite, a partial dendrogram $\theta \in \mathcal{PD}(X, <)$ is eventually constant; that is, there exists a positive real number $t_0$ for which

$$t \geq t_0 \Rightarrow \theta(t) = \theta(\infty).$$

Partial dendrograms are clearly a generalisation of dendrograms. To distinguish between the two, we will occasionally refer to the non-partial dendrograms as complete dendrograms. As before, we will use the term partial dendrogram to address both the diagrammatic- and functional representations.

Example 6. The partial dendrogram $\theta : \mathbb{R}_+ \rightarrow \mathcal{P}(X, <)$ corresponding to the right hand side diagram in Figure 4 is defined as follows:

$$\theta(x) = \begin{cases} \{\{a\}, \{b\}, \{c\}, \{d\} \} & \text{for } x \in [0.0, 1.0) \\ \{\{a, c\}, \{b\}, \{d\} \} & \text{for } x \in [1.0, 1.5) \\ \{\{a, c\}, \{b, d\} \} & \text{for } x \in [1.5, \infty) \end{cases}$$

4.1 Mapping partial dendrograms to dendrograms

We will now demonstrate, on a high level, how we can construct an ultrametric from a partial dendrogram in a well defined manner. Looking at the partial dendrograms of Example 5 each connected component in the partial dendrograms is a complete dendrogram over its leaf nodes. Since complete dendrograms map to ultrametrics, each connected component gives rise to an ultrametric on the subset of $X$ constituted by its leaf nodes:

Example 7. Recalling that any singleton $\{x\}$ is a trivial ultrametric space with ultrametric $d_{\{x\}} : (x, x) \rightarrow 0$, the center diagram of Figure 4 provides the following ultrametrics for the subsets $\{a, d\}$, $\{b\}$ and $\{c\}$ of $X$:

$$d_{\{a, d\}}(x, y) = \begin{cases} 0 & \text{if } x = y, \\ 1.3 & \text{otherwise} \end{cases} \quad d_{\{b\}} = 0 \quad d_{\{c\}} = 0.$$

For a disjoint family of ultrametric spaces we have the following classical result:

Lemma 15. Given a family of bounded, disjoint ultrametric spaces $\{(X_j, d_j)\}_{j=1}^n$ together with a positive real number $K \geq \max_j \{\text{diam}(X_j, d_j)\}$, the map

$$d_U : \bigcup_j X_j \times \bigcup_j X_j \rightarrow \mathbb{R}_+$$

given by

$$d_U(x, y) = \begin{cases} d_j(x, y) & \text{if } \exists j : x, y \in X_j, \\ K & \text{otherwise} \end{cases}$$

is an ultrametric on $\bigcup_j X_j$. \hfill 17
Restricting \( K \) to be strictly positive makes the above construction work even when each \((X_j, d_j)\) is a trivial ultrametric space, in which case \( d_j \) becomes the discrete metric on \( \bigcup_j X \).

Turning back to partial dendrograms, assume \( \theta \in PD(X, \prec) \), and that the partition \( \theta(\infty) \) is given by \( B = \{B_j\}_{j=1}^m \). That is; the number of connected components in the partial dendrogram of \( \theta \) is \( m \): one connected component for each block in the coarsest partition.

Let \( d_X|_{B_j} \) be the restriction of \( d_X \) to \( B_j \times B_j \), and, likewise, let \( \prec|_{B_j} \) be the order relation induced on \( B_j \) by \( \prec \). Each space \((B_j, \prec|_{B_j}, d_X|_{B_j})\) is an ordered dissimilarity subspace of \((X, \prec, d_X)\), and each \( B_j \) has a complete dendrogram over all of its points. Since complete dendrograms correspond to ultrametrics, each connected component in the partial dendrogram of \( X \) corresponds to an ultrametric space \((B_j, d_{u_j})\). Furthermore, since the \( \{(B_j, d_{u_j})\}_{j=1}^m \) make up a disjoint family of ultrametric spaces covering \( X \), we can use Lemma 15 to define an ultrametric on all of \( X \) as follows:

Pick a \( K \geq \max_j \{diam(B_j, d_{u_j})\} \), and define \( u_\theta : X \times X \rightarrow \mathbb{R}_+ \) by

\[
    u_\theta(x, y) = \begin{cases} 
        d_{u_j}(x, y) & \text{if } \exists j : x, y \in B_j, \\
        K & \text{otherwise.}
    \end{cases}
\]

(6)

**Example 8.** An illustration of how this construction turns out in the case of the partial dendrograms of Example 5 is provided in Figure 5.

![Figure 5: “Completed” dendrograms corresponding to the partial dendrograms of Example 5, using \( \varepsilon = 2.0 \). The completions are marked by the dashed lines.](image)

### 4.2 Ultrametric Completions

We will now formalise the above construction in terms of a function from partial dendrograms to complete dendrograms. We will also present necessary and sufficient conditions for this function to be injective. Injectivity is not strictly required for the theory to work, but it significantly increases the discriminative power of the theory. Without injectivity, the families of optimal solutions may include clusterings of rather appalling quality. An example is provided towards the end of the section.

We define the **diameter** of a partial dendrogram \( \theta \) to be the number

\[
    diam(\theta) = \sup \{ x \in \mathbb{R}_+ | \theta(x) \neq \theta(\infty) \}.
\]

**Definition 16.** Given an ordered space \((X, \prec)\) and a positive real number \( \varepsilon \), we define the **ultrametric completion on** \( \varepsilon \) to be the map \( U_\varepsilon : PD(X, \prec) \rightarrow U(X) \) for which

\[
    U_\varepsilon : \theta \mapsto u_\theta,
\]

where \( u_\theta \) is defined as in (6), setting \( K = diam(\theta) + \varepsilon \).
From the discussion in Section 4.1, we know that this is well-defined, but we want a concrete function describing the mapping. We already have the map $\Psi_X : D(X) \rightarrow U(X)$ from (2), mapping dendrograms to ultrametrics. We therefore seek a map

$$\kappa_\varepsilon : \mathcal{PD}(X, <) \rightarrow D(X)$$

making the following diagram commute:

$$\begin{array}{ccc}
D(X) & \xrightarrow{\Psi_X} & U(X) \\
\kappa_\varepsilon \downarrow & & \downarrow U_\varepsilon \\
\mathcal{PD}(X, <) & & \\
\end{array}$$

Seeing that $\kappa_\varepsilon$ must map partial dendrograms to complete dendrograms, a quick glance at Figure 5 suggests the following definition:

$$\kappa_\varepsilon(\theta)(x) = \begin{cases} 
\theta(x) & \text{for } x < \text{diam}(\theta) + \varepsilon \\
\{X\} & \text{otherwise.}
\end{cases}$$

It is straightforward to check that $\kappa_\varepsilon(\theta)$ is a complete dendrogram.

**Theorem 17.** $\Psi_X \circ \kappa_\varepsilon = U_\varepsilon$. That is; the diagram in (7) commutes.

**Proof.** Assume first that $\theta \in \mathcal{PD}(X, <)$ is a proper partial dendrogram, and that $\text{im}(\theta) = \{B_i\}_{i=0}^n$. Let the coarsest partition in the image of $\theta$ be given by $B_n = \{B_i\}_{i=1}^n$. That is, each block $B_j$ corresponds to a connected component in the partial dendrogram. Pick a block $B \in B_n$ and assume $x, y \in B$.

If

$$k = \min \{ i \in \mathbb{N} : \exists B' \in B_i : B = B' \},$$

then $B_k$ is the finest partition containing all of $B$ in one block. Since $B \subseteq X$, the partitions

$$B_i^B = \{ B \cap B' : B' \in B_i \}$$

for $1 \leq i \leq k$

constitute a chain in $\mathcal{P}(B)$ containing both $S(B)$ and $\{B\}$. Hence, we can construct a complete dendrogram over $B$ by defining

$$\theta_B(x) = \{ B \cap B' : B' \in \theta(x) \}.$$ (8)

This is exactly the complete dendrogram corresponding to the connected component of the tree over $X$ having the elements of $B$ as leaf nodes. By Definition 10,

$$x, y \in B \Rightarrow U_\varepsilon(\theta)(x, y) = \Psi_B(\theta_B)(x, y).$$ (9)

Due to (8), we have

$$x, y \in B \Rightarrow \left( \exists B \in \theta_B(x) : x, y \in B \iff \exists B' \in \theta(x) : x, y \in B' \right)$$

$$\Rightarrow \min \{ t \in \mathbb{R}_+ : \exists B \in \theta_B(t) : x, y \in B \} = \min \{ t \in \mathbb{R}_+ : \exists B' \in \theta(t) : x, y \in B' \}.$$
Hence, by the definition of $\Psi_X$ in (3) we conclude that

$$x, y \in B \Rightarrow \Psi_B(\theta_B)(x, y) = (\Psi_X \circ \kappa_\varepsilon)(\theta)(x, y).$$

Combining this with (9), we get that whenever $x, y \in B$, we have $\Psi_X \circ \kappa_\varepsilon = \Upsilon_\varepsilon$.

On the other side, let $x \in B_i$ and $y \in B_j$ with $i \neq j$. By definition, we have $\Upsilon_\varepsilon(\theta)(x, y) = \text{diam}(\theta) + \varepsilon$. And, since there is no block in $\theta(\infty)$ containing both $x$ and $y$, we find that the minimal partition in $\text{im}(\kappa_\varepsilon(\theta))$ containing $x$ and $y$ in one block is $\{X\}$. But this means that $\Psi_X(\kappa_\varepsilon(\theta))(x, y) = \text{diam}(\theta) + \varepsilon$, so $\Psi_X \circ \kappa_\varepsilon = \Upsilon_\varepsilon$ holds in this case too.

Finally, if $\theta$ is a complete dendrogram, we have $\kappa_\varepsilon(\theta) = \theta$, so $\Psi_X \circ \kappa_\varepsilon = \Psi_X(\theta)$. But since $\theta(\infty) = \{X\}$, it follows that $\Upsilon_\varepsilon(\theta)$ maps exactly to the ultrametric over $X$ defined by $\Psi_X(\theta)$.

**Theorem 18.** Given a strict poset $(X, \prec)$ with a non-empty order relation and a positive real number $\varepsilon$, the map

$$\Upsilon_\varepsilon : \mathcal{PD}(X, \prec) \longrightarrow \mathcal{U}(X)$$

is injective.

**Proof.** Since $\Upsilon_\varepsilon = \Psi_K \circ \kappa_\varepsilon$ and $\Psi_X$ is a bijection, injectivity follows if $\kappa_\varepsilon$ is injective. Assume that $\kappa_\varepsilon(\theta) = \kappa_\varepsilon(\theta')$. Then, for every $x < \text{diam}(\theta) + \varepsilon$, we have

$$\kappa_\varepsilon(\theta)(x) = \kappa_\varepsilon(\theta')(x) \iff \theta(x) = \theta'(x).$$

**Example 9.** If $\varepsilon$ is not chosen to be strictly positive, the map $\Upsilon_\varepsilon$ will not necessarily be injective. Let $\varepsilon = 0$ and consider the two partial dendrograms

Both are mapped to the following dendrogram via $\kappa_0$:

This demonstrates what we mean by *reduced discriminative power* in the case of a non-injective completion. Since the partial dendrograms exhibit distinctively different information, it is desirable that the methodology distinguishes between them.

**5 Hierarchical clustering of ordered sets**

In this section, we define order preserving hierarchical agglomerative clustering for strict posets. To achieve this, we first suggest a new definition of hierarchical clustering of non-ordered dissimilarity spaces in terms of optimisation. We then proceed by generalising this definition to also include ordered dissimilarity spaces.
5.1 Optimised hierarchical clustering

Recall the definition of classical hierarchical clustering $HC^L$ (Definition 6). If we resolve tied connections by picking a random minimal dissimilarity pair, the way it is specified, $HC^L$ becomes a non-deterministic algorithm: It may produce different dendrograms for the same input in the presence of ties, depending on which tied pair is selected. And, moreover, it is capable of producing any dendrogram than can be produced by any possible tie resolution strategy:

**Definition 19.** Given a dissimilarity space $(X, d)$ and a linkage function $L$, let $D^L(X, d)$ be the set of all possible outputs from $HC^L(X, d)$.

Recall that a dissimilarity measure $d$ over a finite set $X$ can be described as an $|X| \times |X|$ real matrix $[d_{i,j}]$. Hence, we can compute the $p$-norm of a dissimilarity measure, and for an ultrametric $u \in \mathcal{U}(X)$, we can compute the pointwise difference

$$||u - d||_p = \sqrt[p]{\sum_{x,y \in X} |u(x, y) - d(x, y)|^p}. \quad (10)$$

We suggest the following definition:

**Definition 20.** Given a dissimilarity space $(X, d)$ and a linkage function $L$, the optimised hierarchical agglomerative clustering over $(X, d)$ using $L$ is given by

$$HC^L_{opt}(X, d) = \arg\min_{\theta \in D^L(X, d)} \|\Psi_X(\theta) - d\|_p. \quad (11)$$

That is; optimised hierarchical agglomerative clustering picks the dendrogram among all dendrograms that can be generated by $HC^L(X, d)$ that is closest to the original dissimilarity measure. In the tradition of ultrametric fitting, this is the right choice of candidate.

Since $D^L(X, d)$ contains all dendrograms generated over all possible permutations of enumerations of $X$, the below theorem follows directly from Definition 20:

**Theorem 21.** $HC^L_{opt}$ is permutation invariant. That is, the order of enumeration of the elements of the set $X$ does not affect the output from $HC^L_{opt}(X, d)$.

Also, since $SL$ is permutation invariant, we always have $|D^{SL}(X, d)| = 1$, yielding

**Theorem 22.** $HC^{SL}_{opt}(X, d) = HC^{SL}(X, d)$.

Since $HC^{AC}$ and $HC^{CL}$ are not permutation invariant, we have no corresponding result in these cases. For complete linkage, however, we have the following theorem. First, notice that due to the definition of complete linkage (Definition 5), if $\theta$ is a solution to $HC^{CL}_{opt}(X, d)$ and $u = \Psi_X(\theta)$ is the corresponding ultrametric, then

$$u(x, y) \geq d(x, y) \quad \forall x, y \in X.$$

Hence, in the case of complete linkage we can reformulate (11) as follows:

$$HC^{CL}_{opt}(X, d) = \arg\min_{\theta \in D^{CL}(X, d)} \|\Psi_X(\theta)\|_p. \quad (12)$$

To see why this is the case, notice that if $u, u' \in \mathcal{M}(X)$ and both $d \leq u$ and $d \leq u'$ pointwise, then we can produce two non-negative functions $\delta, \delta'$ on $X \times X$ so that $u = d + \delta$ and $u' = d + \delta'$. In particular, we have $u - d = \delta$, from which we deduce

$$||u - d||_p \leq ||u' - d|| \iff ||\delta||_p \leq ||\delta'||_p \iff \|d + \delta\|_p \leq \|d + \delta'\|_p \iff \|u\|_p \leq \|u'\|_p.$$
Theorem 23. Solving $\mathcal{H}_{\text{opt}}(X, d)$ is NP-hard.

Proof. Let $G = (V, E)$ be an undirected graph with vertices $V$ and edges $E \subseteq V \times V$. Recall the clique problem: Given a positive integer $K < |V|$, is there a clique in $G$ of size at least $K$? Equivalently: is there a set $V' \subseteq V$ with $|V'| \geq K$ for which $V' \times V' \subseteq E$? This is a known NP-hard problem [Karp, 1972].

To reduce clique to $\mathcal{H}_{\text{opt}}$, define a dissimilarity measure on $V$ as follows:

$$d(v, v') = \begin{cases} 1 & \text{if } (v, v') \in E, \\ 2 & \text{otherwise.} \end{cases}$$

(13)

Then $(V, d)$ is a dissimilarity space. Let $\theta$ be a solution of $\mathcal{H}_{\text{opt}}(V, d)$, and set $b = \Psi_V(\theta)$.

An intrinsic property of $\mathcal{CL}$ is that if two blocks $p, q \in Q_i$ are merged, then

$$\forall v, v' \in p \cup q : d(v, v') \leq \mathcal{CL}(p, q, d).$$

And since we have $d(v, v') = 1 \iff (v, v') \in E$, it means that for a subset $V' \subseteq V$, we have that

$$\forall v, v' \in V' : b(v, v') = 1 \iff V' \text{ is a clique in } G.$$

(14)

It follows that a largest possible cluster at proximity level 1 is a maximal clique in $G$.

We claim that minimising the norm is equivalent to producing a maximal cluster at proximity level 1: Let $b$ be the $|V| \times |V|$ distance matrix $[b_{i,j}]$. Due to the definition of $\mathcal{CL}$, we have $b(v, v') \in \{0, 1, 2\}$. If $\theta(1) = \{V_i\}_{i=1}^s$, then these are exactly the blocks that are subsets of cliques, so each $V_i$ contributes with $|V_i|(|V_i| - 1)$ ones in $[b_{i,j}]$.

Having more ones reduces the norm of $b$. Let $V_j$ be of maximal cardinality in $\{V_i\}_{i=1}^s$. Assume first that $V_j$ has at least two elements more than the next to largest block, and let $|V_j| = P$.

Removing one element from $V_j$ reduces the number of ones in the dissimilarity matrix by $P(P-1) - (P-1)(P-2) = 2(P-1)$. Let the next to largest block have $Q$ elements. Transferring the element to this block then increases the number of ones by $(Q+1)Q - Q(Q-1) = 2Q$. Since $Q < P - 1$, this means that the total number of ones is reduced by moving an element from the largest block to any of the smaller blocks. Hence, achieving the largest possible number of ones implies maximising the size of the largest block.

If now, $V_j$ only has one element more than the next to largest block, moving an element as above corresponds to keeping the number of ones. Since each $V_i$ for $1 \leq i \leq s$ is a subset of a clique in $G$, the maximal number of ones is achieved by producing a block $V_j$ that contains exactly a maximal clique of $G$.

Therefore, if $I_{\{1\}}(x)$ is the indicator function for the set $\{1\}$, the size of a maximal clique in $G$ can be computed as

$$\max_{1 \leq i \leq |V|} \left\{ \sum_{j=1}^{|V_i|} I_{\{1\}}(b_{i,j}) \right\};$$

counting the maximal number of row-wise ones in $[b_{i,j}]$ in $O(N^2)$ time. We therefore conclude that $\mathcal{H}_{\text{opt}}$ is NP-hard.

The computational hardness of $\mathcal{H}_{\text{opt}}$ is directly connected to the presence of tied connections: every encounter of $n$ tied connections leads to $n!$ new candidate solutions.

Since neither $\mathcal{H}_{\text{opt}}$ is permutation invariant, it is strongly believed that this is also NP-hard, although that remains to be proven.
5.1.1 A comment on equivalent solutions of $HC_{opt}^L$

We cannot, in general, expect the mapping $\theta \mapsto \|\Psi_X(\theta) - d\|_p$ to be injective, meaning that the answer to (11) may not be unique. Now, $HC^L$, by construction, and $HC_{opt}^{SL}$, by Theorem 22, have unique solutions for every input $(X, d)$. But both $HC_{opt}^L$ and $HC_{opt}^{CL}$ may have more than one solution, each solution being optimal.

This is actually a strength of $HC_{opt}^L$, over classical $HC^L$: Imagine that you, as an analyst, are trying to reveal social network structures from data using hierarchical clustering. Receiving more than one output from $HC_{opt}^L$ simply tells you that there is more than one optimal way of grouping people. And for an analyst, this may be highly valuable information.

The fact that $HC_{opt}^L$ may return more than one result poses a formal problem, since it is not returning dendrograms, but rather sets of dendrograms: Given a set $X$, denote the power set of $X$ by $\mathcal{P}(X)$. We shall consider $HC_{opt}^L(X, -)$ to be the function

$$HC_{opt}^L(X, -) : \mathcal{M}(X) \rightarrow \mathcal{P}(\mathcal{D}(X)),$$

mapping a dissimilarity measure over $X$ to a set of dendrograms over $X$.

5.2 Hierarchical clustering of ordered sets

We are now ready to embark the specification of order preserving hierarchical clustering of ordered sets. For an ordered set $(X, \prec)$, recall that non-comparability of $a, b \in X$ is denoted $a \perp b$. We introduce the non-comparable separation of $(X, \prec, d)$, defined as

$$\text{sep}_\perp(X, \prec, d) = \min_{x, y \in X} \{ d(x, y) \mid x \neq y \land x \perp y \}.$$  

Consider the following modification of classical hierarchical clustering. The only difference is that for each iteration, we check that there are elements that actually can be merged while preserving the order relation: according to Theorem 11, merging a pair of non-comparable elements produces a regular quotient.

Let $(X, \prec, d)$ be given together with a linkage function $\mathcal{L}$.

1. Start by setting $Q_0 = S(X)$, and endow $Q_0$ with the induced order relation $\prec_0$.
2. Among the pairs of non-comparable clusters, pick a pair of minimal dissimilarity according to $\mathcal{L}$, and combine them into one cluster by taking their union.
3. Endow the new clustering with the induced order relation.
4. If all elements of $X$ are in the same cluster, or if all clusters are comparable, we are done. Otherwise, go to Step 2 and continue.

The procedure results in a chain of ordered partitions $\{(Q_i, \prec_i, \rho_i)\}_{i=0}^m$ together with the dissimilarities $\{\rho_i\}_{i=0}^m$ at which the partitions were formed. And the sequence of pairs $Q = \{(Q_i, \rho_i)\}_{i=0}^m$ maps to a partial dendrogram through (1) if the following lemma is satisfied:

**Lemma 24.** The sequence of pairs $\{(Q_i, \rho_i)\}_{i=0}^m$ maps to a partial dendrogram through application of (1) if and only if

$$\text{sep}_\perp(Q_i, \prec_i, \mathcal{L}) \leq \text{sep}_\perp(Q_{i+1}, \prec_{i+1}, \mathcal{L}).$$
Since the singleton partition \(Q_0\) maps to a partial dendrogram, the algorithm will produce a partial dendrogram for any ordered dissimilarity space, and since there can be at most \(|X| - 1\) merges, the procedure always terminates.

As for classical hierarchical clustering, the procedure is non-deterministic in the sense that given a set of tied pairs, we select a random pair for the next merge. Hence, the procedure is able to produce all possible partial dendrograms for all possible tie resolution strategies:

**Definition 25.** Given an ordered dissimilarity space \((X, <, d)\) and a linkage function \(L\), let the set of all possible outputs from the above procedure be denoted by \(D^L(X, <, d)\).

The set \(D^L(X, <, d)\) differs from \(D^L(X, d)\) in two important ways:

- \(D^L(X, <, d)\) contains partial dendrograms, not dendrograms
- The cardinality of \(D^L(X, <, d)\) is at least that of \(D^L(X, d)\), and often higher, due to mutually exclusive merges and the “dead ends” in \(P(X, <)\) (see Figure 2).

Even for single linkage we have \(|D^{SL}(X, <, d)| > 1\) if there are mutually exclusive tied connections.

In the spirit of optimised hierarchical clustering, we suggest the following definition:

**Definition 26.** Given an ordered dissimilarity space \((X, <, d)\), together with a linkage function \(L\) and \(\varepsilon > 0\). An order preserving hierarchical agglomerative clustering using \(L\) and \(\varepsilon\) is given by

\[
\text{HC}^{<L, \varepsilon}(X, <, d) = \arg \min_{\theta \in D^L(X, <, d)} \|\mathcal{U}_\varepsilon(\theta) - d\|_p.
\]

**Theorem 27.** If the order relation is empty, then order preserving optimised hierarchical clustering and optimised hierarchical clustering coincide:

\[
\text{HC}^{<L, \varepsilon}(X, \emptyset, d) = \text{HC}^L_{opt}(X, d).
\]

**Proof.** First, notice that

\[
\forall (Q, <_Q) \in P(X, \emptyset) : \text{sep}_{<}(Q, <_Q, L) = \text{sep}(Q, L),
\]

where \(<_Q\) denotes the (trivial) induced order. Hence, we have \(D^L(X, \emptyset, d) = D^L(X, d)\). Since \(U_{\varepsilon}|_D(X) = \Psi_X\), the result follows.

**5.2.1 On the choice of \(\varepsilon\)**

In \(\text{HC}^{<L, \varepsilon}(X, <, d)\) we identify the elements from \(D^L(X, <, d)\) that are closest to the dissimilarity measure \(d\) when measured in the \(p\)-norm. Since \(\mathcal{U}_{\varepsilon} : PD(X, <) \to U(X)\) is injective, \(\mathcal{U}_{\varepsilon}\) induces a relation \(\preceq_{d, \varepsilon}\) on \(PD(X, <)\) defined by

\[
\theta \preceq_{d, \varepsilon} \theta' \iff \|\mathcal{U}_{\varepsilon}(\theta) - d\|_p \leq \|\mathcal{U}_{\varepsilon}(\theta') - d\|_p,
\]

and the optimisation finds the minimal elements under this order.

The choice of \(\varepsilon\) may affect the ordering of dendrograms under \(\preceq_{d, \varepsilon}\). We will show this by providing an alternative formula for \(\|u - d\|_p\) that better expresses the effect of the choice of \(\varepsilon\).
in the ultrametric completion: Assume that $\theta$ is a partial dendrogram over $(X, \prec)$, and let $\theta(\infty) = \{B_i\}_{i=1}^n$. Furthermore, let $n_i = |B_i|$ for $1 \leq i \leq m$ be the cardinalities of the blocks, and let the corresponding ultrametric be given by $u = U_{\epsilon}(\theta)$. The sum in the standard formula for $\|u - d\|_p$ given by (16) can be split in two: the intra-block differences and the inter-block differences. The \textbf{intra-block differences} are independent of $\epsilon$, and are given by

$$\alpha = \sum_{i=1}^m \sum_{x, y \in B_i} |u(x, y) - d(x, y)|^p. \quad (16)$$

On the other hand, for every \textbf{inter-block pair} $(x, y)$, we have $u(x, y) = \text{diam}(\theta) + \epsilon$, so the \textbf{inter-block differences}, that are dependent on $\epsilon$, can be computed as

$$\beta_\epsilon = \sum_{(x, y) \in B_i \times B_j} |\text{diam}(\theta) + \epsilon - d(x, y)|^p. \quad (17)$$

We can now write $\|u - d\|_p = \sqrt[N]{\alpha + \beta_\epsilon}$. If we think of $u$ as an approximation of $d$, and saying that $|X| = N$, the mean $p$-th error of this approximation can be expressed as a function of $\epsilon$:

$$E_d(\epsilon|\theta, p) = \frac{1}{N} \|u - d\|_p^p = \frac{\alpha}{N} + \frac{1}{N} \sum_{(x, y) \in B_i \times B_j, i \neq j} |\text{diam}(\theta) + \epsilon - d(x, y)|^p.$$ 

\textbf{Notice that the} minimisation in (15) \textbf{exactly identifies the partial dendrograms of minimal mean $p$-th error.}

Moreover, $X$ being finite means that $d$ is bounded, so $E_d(\epsilon|\theta, p) \to \infty$ when $\epsilon \to \infty$. Hence, $E_d(\epsilon|\theta, p)$ has at least one global minimum on $[0, \infty)$.

\textbf{Theorem 28. Different choices of $\epsilon$ may result in different orders on the dendrograms.}

\textbf{Proof.} Let $\theta_1$ be a partial dendrogram over $(X, \prec, d)$, and let $\{\epsilon_i\}_{i=1}^n$ be the set of strictly positive global minima of $E_d(\epsilon|\theta_1, p)$, assuming $n \geq 1$. Then $\theta_1$ is a minimal element in $(\mathcal{PD}(X, \prec), \preceq_{\epsilon_i, p})$ for $1 \leq i \leq n$. Assume that there exists a partial dendrogram $\theta_2 \in \mathcal{PD}(X, \prec)$ that is not minimal in $(\mathcal{PD}(X, \prec), \preceq_{\epsilon_i, p})$ for any of the $\epsilon_i$, so that $\theta_1 \prec_{\epsilon_i, p} \theta_2$. Assume further that there is an $\epsilon' > 0$ that is a global minimum of $E_d(\epsilon|\theta_2, p)$ so that $\theta_2$ is minimal in $(\mathcal{PD}(X, \prec), \preceq_{\epsilon', p})$. Since $\epsilon' \neq \epsilon_i$ for $1 \leq i \leq n$, we get $\theta_2 \prec_{\epsilon', p} \theta_1$. \hfill $\square$

The question now is which value to pick for $\epsilon$. From the formula for $E_d(\epsilon|\theta, p)$, we see that \textbf{when $\epsilon$ becomes large, the inter-block differences dominate the approximation error. For increasing $\epsilon$, having low error eventually equals having few inter-block pairs}. \textbf{Alternatively: the intra-block differences have insignificant influence on the approximation error for large $\epsilon$.}

The effect of this is that, when $\epsilon$ increases, the partial dendrograms close to $d$ will be those that have a low number of inter-block pairs, regardless of the quality of the intra-block approximations of $d$. From the standpoint of ultrametric fitting, this is intuitively wrong. Also, it will lead to clusterings where as many elements as possible are placed in one large cluster, since this is the most effective method for reducing the number of inter-block pairs.

On the other side, a low value of $\epsilon$ will move the weight towards improving the approximation of the intra-block distances. Again from the standpoint of ultrametric fitting, this is the right thing to do. Also, since the inter-block distances are between non-mergeable pairs, one may claim that these differences should be given less attention in the ultrametric fitting.

This points towards selecting a low value for $\epsilon$. In the process of choosing, we have the following result at our aid:
Theorem 29. For any finite ordered dissimilarity space \((X, <, d)\) and linkage function \(\mathcal{L}\), there exists an \(\varepsilon_0 > 0\) for which

\[ \varepsilon, \varepsilon' \in (0, \varepsilon_0) \Rightarrow (D^\varepsilon(X, <, d), \preceq_{d, \varepsilon}) \approx (D^{\varepsilon'}(X, <, d), \preceq_{d, \varepsilon'}). \]

That is: all \(\varepsilon \in (0, \varepsilon_0)\) induce the same order on the partial dendrograms.

Proof. Since \(X\) is finite, \(D^\varepsilon(X, <, d)\) is also finite. And according to \(E_d(\varepsilon|\theta, p)\), if the cardinality of \(D^\varepsilon(X, <, d)\) is \(n\), there are at most \(pn\) positive values of \(\varepsilon\) that are distinct global minima of partial dendrograms in \(D^\varepsilon(X, <, d)\). But this means there is a finite set of \(\varepsilon\) for which the order on \((D^\varepsilon(X, <), \preceq_{\varepsilon, \theta})\) changes. And since all these values are strictly positive, they have a strictly positive lower bound. \(\square\)

It is, of course, possible to play with different values of \(\varepsilon\) to obtain different results. But, since \(\varepsilon + \text{diam}(\theta)\) is an upper bound of the partial dendrogram to begin with, we generally advise as follows:

**We suggest to use a value of \(\varepsilon\) that is as small as possible.**

5.3 Idempotency of \(\mathcal{H}_\text{opt}^{<, \varepsilon}\)

A detailed axiomatic analysis along the lines of for example [Ackerman and Ben-David, 2016] is beyond the scope of this paper, and is considered for future work. We still include a proof of idempotency of \(\mathcal{H}_\text{opt}^{<, \varepsilon}\), since this is an essential property of classical hierarchical clustering.

A function \(f\) is **idempotent** if \(f \circ f = f\). For classical hierarchical clustering, the set of ultrametrics \(U(X) \subseteq M(X)\) over a set \(X\) are fixed points under the map

\[(\Psi_X \circ \mathcal{H}_\text{L}(X, -)) : M(X) \to U(X).\]

In particular, if \(u = \Psi_X \circ \mathcal{H}_\text{L}(X, d)\) for some \(d \in M(X)\), since \(u \in U(X)\), this yields \(u = \Psi_X \circ \mathcal{H}_\text{L}(X, u)\). This property is what [Jardine and Sibson, 1971] refers to as **appropriateness**, being the first of a set of conditions expected fulfilled by clustering methods.

This property does necessarily depend on the linkage function. We say that \(\mathcal{L}\) is a **convex linkage function** if we always have

\[ \mathcal{S} \mathcal{L}(p, q, d) \leq \mathcal{L}(p, q, d) \leq \mathcal{C} \mathcal{L}(p, q, d). \]

Now, if \(u\) is an ultrametric on \(X\), the ultrametric inequality yields

\[ u(a, b) = \text{sep}(X, u) \Rightarrow \forall c \in X : u(a, c) = u(b, c). \]

So if \(\mathcal{L}\) is a convex linkage function and \(u(a, b) = \text{sep}(X, u)\), we have

\[ \mathcal{L}({a, b}, \{c\}) = \mathcal{L}({a}, \{c\}) = \mathcal{L}({b}, \{c\}) \quad \forall c \neq a, b. \]

This is to say that a convex linkage function preserves the structure of the original ultrametric when minimal dissimilarity elements are merged. As a result, we get that \(D^\varepsilon(X, u)\) contains exactly one element, namely the dendrogram that corresponds to the ultrametric.

**Theorem 30.** For a convex linkage function \(\mathcal{L}\), an ultrametric \(u \in U(X)\) and \(\theta = \Psi_X^{-1}(u)\), we have \(\mathcal{H}_\text{opt}^{<, \varepsilon}(X, u) = \{\theta\}\).
Hence, all of $U(X)$ are fixed points under $\Psi_X \circ HC^L_{opt}(X, -)$ whenever $L$ is convex.

For ordered spaces, the case is different. It is easy to construct an ordered ultrametric space $(X, <, u)$ for which $u(a, b) = \text{sep}(X, u)$ and $a < b$, in which case the ultrametric cannot be reproduced. Hence, all of $U(X)$ cannot be fixed points under $U \circ HC^{<L}_{opt, \varepsilon}(X, <, -)$, but the mapping is still idempotent:

**Theorem 31 (Idempotency).** For an ordered dissimilarity space $(X, <, d)$ and a convex linkage function $L$, if $\theta \in HC^{<L}_{opt, \varepsilon}(X, <, d)$ and $U_{\varepsilon}(\theta) = u$, then $HC^{<L}_{opt, \varepsilon}(X, <, u) = \{\theta\}$.

**Proof.** Let $\theta(\infty) = \{B_i\}_{i=1}^m$. Then each $B_i$ is an antichain in $(X, <)$, so we have

$$\forall x, y \in B_i : \text{sep}(B_i, u|B_i) = \text{sep}_L(B_i, u|B_i) \quad \text{for} \quad 1 \leq i \leq m.$$ 

Since $\varepsilon > 0$, we also have

$$x, y \in B_i \Rightarrow u(x, y) < \text{diam}(X, u) \quad \text{for} \quad 1 \leq i \leq m.$$ 

And, lastly, since every pair of comparable elements are in pairwise different blocks, we have

$$x < y \lor y < x \Rightarrow u(x, y) = \text{diam}(X, u).$$ 

Now, since $L$ is convex, based on the discussion before Theorem 30 the intra-block structure of every block will be preserved. And, since every inter-block dissimilarity is accompanied by comparability across blocks, the procedure for generation of $D^L(X, <, d)$ will exactly reproduce the intra-block structure of all blocks and then halt. Hence, $D^L(X, <, d) = \{\theta\}$. 

### 6 Applying $HC^{<L}_{opt, \varepsilon}$ to real data

This section demonstrates order preserving hierarchical agglomerative clustering for a small subset of the data described in Section 1.1. Due to confidentiality, the data is anonymised. It is recommended to revisit Section 1.1 to refresh ones mind regarding the origin and nature of the data. As a courtesy to the reader who skipped directly here from Section 1.1, please note that the method $HC^{<L}_{opt, \varepsilon}$ refers to order preserving hierarchical clustering, whereas $HC_{opt}$ refers to non-order preserving hierarchical clustering.

Figure 6 shows a small (13 element) subset of the data, together with their strict partial order, represented as a DAG. Each node represents a type of machinery, and the edges represent “part-of” relations that are extracted from the assembly metadata. For two elements $a, b$ in the DAG, we say that $a < b$ if there exists a directed path from $a$ to $b$. The numbers of the vertices correspond to the indices of the dissimilarity measure in Table 1.

The dissimilarity measure we have used is shown in Table 1. It is obtained from an ongoing project in the company owning the data. The project aims to use supervised machine learning to predict which pieces of equipment are equivalent, and which are not. During
training, the algorithm is given metadata for the nodes in the graph, and is told to report “equivalent” pieces of equipment to be close together, and “non-equivalent” equipment to be far apart, on a scale from 0 to 1. These predictions, thus, make up a dissimilarity measure.

In Figure 7 we provide a visual presentation of the results from clustering the DAG. We show how the clustering proceeds both when using $\mathcal{H}_{\text{opt}, \varepsilon}^{\mathcal{CL}}$ and $\mathcal{H}_{\text{opt}}^{\mathcal{CL}}$, that is, with and without order preserving clustering. The left column shows the order preserving clustering, and the right column contains output from optimised clustering without the order relation. Since the number of merges for $\mathcal{H}_{\text{opt}, \varepsilon}^{\mathcal{CL}}$ is less than for $\mathcal{H}_{\text{opt}}^{\mathcal{CL}}$, the rows in the figure present selected steps in the clustering processes. The clusters are identified by colors, and components in the partial dendrograms with corresponding color represent the dendrograms over the clusters. As can be seen, when clustering without taking the order relation into account, the clustering process has a tendency to agglomerate parents and children. This only reflects the fact that the metadata exhibits high similarity between those elements. When the order relation is taken into account, no such clusters are formed. The bottom left hand side plot shows the terminal state of the order preserving clustering; no further agglomeration is possible beyond this state. For the right hand side, the process continues two more steps, merging the last three clusters into one.

The ultrametric produced by the order preserving hierarchical clustering is presented in Table 2 and the difference between the ultrametric and the original dissimilarity measure is shown in Table 3. The bold face values in Table 3 correspond to pairs of elements that are comparable, and can therefore never be merged. A bold face of minimal value means that the original dissimilarity measure correctly identified this (assigning a large dissimilarity), whereas a bold positive value indicates the opposite. The most significant values of the latter kind are colored red.

|   | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     | 10    | 11    | 12    | 13     |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|
| 1 | 0.9600| 0.9933| 0.9933| 0.1224| 0.7206| 0.7586| 0.5214| 0.9993| 0.1506| 0.6881| 0.7878| 0.1105 |
| 2 | 0.9993| 0.9900| 0.5449| 0.4970| 0.9600| 0.9993| 0.6450| 0.9600| 0.1149| 0.5600|       |       |
| 3 | 0.5449| 0.9993| 0.9993| 0.9993| 0.9993| 0.9982| 0.4340| 0.9993| 0.9993| 0.9993|       |       |
| 4 | 0.9993| 0.9993| 0.9993| 0.9993| 0.9993| 0.9993| 0.9993| 0.9993| 0.9993|       |       |       |
| 5 | 0.0997| 0.9600| 0.2210| 0.9549| 0.1760| 0.1105| 0.9600| 0.1355|       |       |       |       |
| 6 | 0.8666| 0.5826| 0.9993| 0.5639| 0.7123| 0.5449| 0.7180|       |       |       |       |       |
| 7 |       | 0.9600| 0.9993| 0.5529| 0.8697| 0.1149| 0.5600|       |       |       |       |       |
| 8 |       | 0.9993| 0.4864| 0.4308| 0.6132| 0.2567|       |       |       |       |       |       |
| 9 |       | 0.9993| 0.9993| 0.9993| 0.9549|       |       |       |       |       |       |       |
| 10|       |       | 0.1105| 0.4862| 0.2136|       |       |       |       |       |       |       |
| 11|       |       |       | 0.9600| 0.0778|       |       |       |       |       |       |       |
| 12|       |       |       |       | 0.9600|       |       |       |       |       |       |       |

Table 1: Input dissimilarity measure.

|   | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     | 10    | 11    | 12    | 13     |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|
| 1 | 0.6451| 0.6451| 0.6451| 0.1224| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451 |
| 2 | 0.6451| 0.6451| 0.6451| 0.6450| 0.4970| 0.6451| 0.6451| 0.6450| 0.6450| 0.4970| 0.6451|       |
| 3 | 0.5449| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.4340| 0.6451| 0.6451| 0.6451|       |
| 4 | 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451|       |       |
| 5 | 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451|       |       |
| 6 | 0.6450| 0.6451| 0.6451| 0.5639| 0.6451| 0.6450| 0.6451|       |       |       |       |       |
| 7 | 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451|       |       |       |       |       |
| 8 |       | 0.6451| 0.6451| 0.6451| 0.6451| 0.6451| 0.6451|       |       |       |       |       |
| 9 |       |       | 0.6451| 0.6451| 0.6451| 0.6451| 0.6451|       |       |       |       |       |
| 10|       |       |       | 0.6451| 0.6450| 0.6451|       |       |       |       |       |       |
| 11|       |       |       |       | 0.6451| 0.6451|       |       |       |       |       |       |
| 12|       |       |       |       |       | 0.6451|       |       |       |       |       |       |

Table 2: Ultrametric produced by order preserving clustering. For the clustering, we used $\varepsilon = 0.0001$ to be able to distinguish the completed links in the table.
Figure 7: $\mathcal{H}_{\text{opt},\varepsilon}^{<CC}$ vs. $\mathcal{H}_{\text{opt}}^{CC}$ applied to ordered data, using the dissimilarity in Table 1.
Currently assumed that the problem is NP-hard.

We have shown that the family of partial dendrograms over a set embed into the family of classical dendrograms. The difference being that partial dendrograms have several connected components. We have showed that the clustering is idempotent and permutation invariant.

We have established order preserving hierarchical agglomerative clustering for strictly partially ordered sets. The clustering uses classical linkage functions such as single-, average-, and complete linkage. We have showed that the clustering is idempotent and permutation invariant.

The output of hierarchical clustering of strict posets results in partial dendrograms, sub-trees of classical dendrograms. The difference being that partial dendrograms have several connected components. We have shown that the family of partial dendrograms over a set embed into the family of dendrograms over the set.

When applying the theory to non-ordered sets, we see that we have a new theory for hierarchical agglomerative clustering that is very close to the classical theory. But, differently from classical hierarchical clustering, our theory is permutation invariant. We have shown that for single linkage, our theory coincide with classical hierarchical clustering, while for complete linkage, the clustering problem becomes NP-hard. However, the computational complexity is directly linked to the number of tied connections, and in the absence of tied connections, the theories coincide again.

7 Summing up

We have established order preserving hierarchical agglomerative clustering for strictly partially ordered sets. The clustering uses classical linkage functions such as single-, average-, and complete linkage. We have showed that the clustering is idempotent and permutation invariant.

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7.1 Discussion and future work

Several practical issues and open questions remain:

7.1.1 Performance

We do provide a Python based implementation of the theory described in this paper Bakkelund, 2020; the code that was used for the demonstration in Section 6. However, the algorithm running time is not adequate for industrial applications, and more research is required in order to establish more efficient algorithms.

7.1.2 Complexity

Since $\mathcal{HC}^{<\mathcal{CL}}_{\text{opt},\varepsilon}(X, \emptyset, d) = \mathcal{HC}^{\mathcal{CL}}_{\text{opt}}(X, d)$, it follows that $\mathcal{HC}^{<\mathcal{CL}}_{\text{opt},\varepsilon}$ is NP-hard in the general case.

For single- and average linkage, we have no corresponding results. However, the problem of solving $\mathcal{HC}^{\mathcal{CL}}_{\text{opt},\varepsilon}(X, <, d)$ generally shares commonality with several known NP-hard problems, such as Optimal Linear Arrangement and Acyclic Partition Garey and Johnson, 1977, so it is currently assumed that the problem is NP-hard.

|   | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
|---|---|---|---|---|---|---|---|---|----|----|----|----|
| 1 | -0.3149 | -0.3542 | -0.3542 | 0.0000 | -0.0755 | -0.1057 | 0.1237 | -0.3542 | 0.4945 | 0.5570 | -0.1427 | 0.5346 |
| 2 | -0.3542 | -0.3542 | -0.3149 | 0.0000 | -0.3149 | -0.3542 | 0.0000 | -0.3149 | 0.3821 | -0.3149 | 0.3149 |
| 3 | 0.0000 | -0.3542 | -0.3542 | -0.3542 | -0.3531 | 0.0000 | -0.3542 | -0.3542 | -0.3542 | -0.3542 | -0.3542 |
| 4 | -0.3542 | -0.3542 | -0.3542 | -0.3542 | -0.3531 | 0.0537 | -0.3542 | -0.3542 | -0.3542 | -0.3542 | -0.3542 |
| 5 | 0.0254 | -0.3149 | 0.4241 | -0.3098 | 0.4091 | 0.5346 | -0.3149 | 0.5096 |
| 6 | -0.3149 | -0.3542 | 0.0625 | -0.3542 | 0.0000 | -0.0672 | 0.1001 | -0.0649 |
| 7 | -0.3542 | -0.3542 | 0.0921 | -0.2246 | 0.0000 | -0.3149 |
| 8 | -0.3531 | 0.1587 | 0.2143 | 0.0319 | 0.3884 |
| 9 | -0.3542 | -0.3542 | -0.3542 | -0.3542 | -0.3098 |
| 10 | 0.1588 | 0.5346 | 0.1588 | 0.4315 |
| 11 | -0.3149 | 0.0000 |
| 12 | 0.0000 |

Table 3: Difference between the ultrametric and the original dissimilarity measure. The red numbers indicate comparisons where the original dissimilarity measure identified the elements as being similar, and therefore likely to be merged early in the process, while the order preserving clustering identified them as being comparable, and therefore never to be merged.
7.1.3 Order versus dissimilarity

The order relation has a significant effect on the output from the clustering process: If the dissimilarity measure starts out by associating “wrong” elements, the induced order may exclude future merges of elements correctly belonging together. Also, if the order relation erroneously identifies elements as comparable, this may prevent elements that belong together from being merged, regardless of the quality of the dissimilarity measure.

Together, these observations call for a need to “loosen up” the stringent nature of the order relation, or to allow to balance the merge-affinity of the dissimilarity measure against the prohibitions of the order relation.

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