

Chapter 5

Hierarchical Clustering for Finding Symmetries and Other Patterns in Massive, High Dimensional Datasets

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Abstract. Data analysis and data mining are concerned with unsupervised pattern finding and structure determination in data sets. “Structure” can be understood as symmetry and a range of symmetries are expressed by hierarchy. Such symmetries directly point to invariants, that pinpoint intrinsic properties of the data and of the background empirical domain of interest. We review many aspects of hierarchy here, including ultrametric topology, generalized ultrametric, linkages with lattices and other discrete algebraic structures and with p-adic number representations. By focusing on symmetries in data we have a powerful means of structuring and analyzing massive, high dimensional data stores. We illustrate the powerfulness of hierarchical clustering in case studies in chemistry and finance, and we provide pointers to other published case studies.

Keywords: Data analytics, multivariate data analysis, pattern recognition, information storage and retrieval, clustering, hierarchy, p-adic, ultrametric topology, complexity.

1 Introduction: Hierarchy and Other Symmetries in Data Analysis

Herbert A. Simon, Nobel Laureate in Economics, originator of “bounded rationality” and of “satisficing”, believed in hierarchy at the basis of the human and social sciences, as the following quotation shows: “... my central theme is that complexity frequently takes the form of hierarchy and that hierarchic systems have some common properties independent of their specific content. Hierarchy, I shall argue, is one of the central structural schemes that the architect of complexity uses.” ([74], p. 184.)

Partitioning a set of observations [75, 76, 49] leads to some very simple symmetries. This is one approach to clustering and data mining. But such approaches, often based on optimization, are not of direct interest to us here. Instead we

will pursue the theme pointed to by Simon, namely that the notion of hierarchy is fundamental for interpreting data and the complex reality which the data expresses. Our work is very different too from the marvelous view of the development of mathematical group theory – but viewed in its own right as a complex, evolving system – presented by Foote [19].

Weyl [80] makes the case for the fundamental importance of symmetry in science, engineering, architecture, art and other areas. As a “guiding principle”, “Whenever you have to do with a structure-endowed entity ... try to determine its group of automorphisms, the group of those element-wise transformations which leave all structural relations undisturbed. You can expect to gain a deep insight in the constitution of [the structure-endowed entity] in this way. After that you may start to investigate symmetric configurations of elements, i.e. configurations which are invariant under a certain subgroup of the group of all automorphisms; ...” ([80], p. 144).

1.1 About This Article

In section 2, we describe ultrametric topology as an expression of hierarchy. This provides comprehensive background on the commonly used quadratic computational time (i.e., $O(n^2)$, where n is the number of observations) agglomerative hierarchical clustering algorithms.

In section 3, we look at the generalized ultrametric context. This is closely linked to analysis based on lattices. We use a case study from chemical database matching to illustrate algorithms in this area.

In section 4, p-adic encoding, providing a number theory vantage point on ultrametric topology, gives rise to additional symmetries and ways to capture invariants in data.

Section 5 deals with symmetries that are part and parcel of a tree, representing a partial order on data, or equally a set of subsets of the data, some of which are embedded. An application of such symmetry targets from a dendrogram expressing a hierarchical embedding is provided through the Haar wavelet transform of a dendrogram and wavelet filtering based on the transform.

Section 6 deals with new and recent results relating to the remarkable symmetries of massive, and especially high dimensional data sets. An example is discussed of segmenting a financial forex (foreign exchange) trading signal.

1.2 A Brief Introduction to Hierarchical Clustering

For the reader new to analysis of data a very short introduction is now provided on hierarchical clustering. Along with other families of algorithm, the objective is automatic classification, for the purposes of data mining, or knowledge discovery. Classification, after all, is fundamental in human thinking, and machine-based decision making. But we draw attention to the fact that our objective is *unsupervised*, as opposed to *supervised* classification, also known as discriminant analysis or (in a general way) machine learning. So here we are *not* concerned with generalizing the decision making capability of training data, nor are we concerned

with fitting statistical models to data so that these models can play a role in generalizing and predicting. Instead we are concerned with having “data speak for themselves”. That this unsupervised objective of classifying data (observations, objects, events, phenomena, etc.) is a huge task in our society is unquestionably true. One may think of situations when precedents are very limited, for instance.

Among families of clustering, or unsupervised classification, algorithms, we can distinguish the following: (i) array permuting and other visualization approaches; (ii) partitioning to form (discrete or overlapping) clusters through optimization, including graph-based approaches; and – of interest to us in this article – (iii) embedded clusters interrelated in a tree-based way.

For the last-mentioned family of algorithm, agglomerative building of the hierarchy from consideration of object pairwise distances has been the most common approach adopted. As comprehensive background texts, see [48, 30, 81, 31].

1.3 A Brief Introduction to p-Adic Numbers

The real number system, and a p-adic number system for given prime, p , are potentially equally useful alternatives. p-Adic numbers were introduced by Kurt Hensel in 1898.

Whether we deal with Euclidean or with non-Euclidean geometry, we are (nearly) always dealing with reals. But the reals start with the natural numbers, and from associating observational facts and details with such numbers we begin the process of measurement. From the natural numbers, we proceed to the rationals, allowing fractions to be taken into consideration.

The following view of how we do science or carry out other quantitative study was proposed by Volovich in 1987 [78, 79]. See also the surveys in [15, 22]. We can always use rationals to make measurements. But they will be approximate, in general. It is better therefore to allow for observables being “continuous, i.e. endow them with a topology”. Therefore we need a completion of the field \mathbb{Q} of rationals. To complete the field \mathbb{Q} of rationals, we need Cauchy sequences and this requires a norm on \mathbb{Q} (because the Cauchy sequence must converge, and a norm is the tool used to show this). There is the Archimedean norm such that: for any $x, y \in \mathbb{Q}$, with $|x| < |y|$, then there exists an integer N such that $|Nx| > |y|$. For convenience here, we write: $|x|_\infty$ for this norm. So if this completion is Archimedean, then we have $\mathbb{R} = \mathbb{Q}_\infty$, the reals. That is fine if space is taken as commutative and Euclidean.

What of alternatives? Remarkably all norms are known. Besides the \mathbb{Q}_∞ norm, we have an infinity of norms, $|x|_p$, labeled by primes, p . By Ostrowski’s theorem [65] these are all the possible norms on \mathbb{Q} . So we have an unambiguous labeling, via p , of the infinite set of non-Archimedean completions of \mathbb{Q} to a field endowed with a topology.

In all cases, we obtain locally compact completions, \mathbb{Q}_p , of \mathbb{Q} . They are the fields of p-adic numbers. All these \mathbb{Q}_p are continua. Being locally compact, they have additive and multiplicative Haar measures. As such we can integrate over them, such as for the reals.

1.4 Brief Discussion of p-Adic and m-Adic Numbers

We will use p to denote a prime, and m to denote a non-zero positive integer. A p -adic number is such that any set of p integers which are in distinct residue classes modulo p may be used as p -adic digits. (Cf. remark below, at the end of section 4.1, quoting from [25]. It makes the point that this opens up a range of alternative notation options in practice.) Recall that a ring does not allow division, while a field does. m -Adic numbers form a ring; but p -adic numbers form a field. So a priori, 10-adic numbers form a ring. This provides us with a reason for preferring p -adic over m -adic numbers.

We can consider various p -adic expansions:

1. $\sum_{i=0}^n a_i p^i$, which defines positive integers. For a p -adic number, we require $a_i \in 0, 1, \dots, p-1$. (In practice: just write the integer in binary form.)
2. $\sum_{i=-\infty}^n a_i p^i$ defines rationals.
3. $\sum_{i=k}^{\infty} a_i p^i$ where k is an integer, not necessarily positive, defines the field \mathbb{Q}_p of p -adic numbers.

\mathbb{Q}_p , the field of p -adic numbers, is (as seen in these definitions) the field of p -adic expansions.

The choice of p is a practical issue. Indeed, adelic numbers use all possible values of p (see [6] for extensive use and discussion of the adelic number framework). Consider [14, 37]. DNA (deoxyribonucleic acid) is encoded using four nucleotides: A, adenine; G, guanine; C, cytosine; and T, thymine. In RNA (ribonucleic acid) T is replaced by U, uracil. In [14] a 5-adic encoding is used, since 5 is a prime and thereby offers uniqueness. In [37] a 4-adic encoding is used, and a 2-adic encoding, with the latter based on 2-digit boolean expressions for the four nucleotides (00, 01, 10, 11). A default norm is used, based on a longest common prefix – with p -adic digits from the start or left of the sequence (see section 4.2 below where this longest common prefix norm or distance is used and, before that, section 3.3 where an example is discussed in detail).

2 Ultrametric Topology

In this section we mainly explore symmetries related to: geometric shape; matrix structure; and lattice structures.

2.1 Ultrametric Space for Representing Hierarchy

Consider Figures 1 and 2, illustrating the ultrametric distance and its role in defining a hierarchy. An early, influential paper is Johnson [35] and an important survey is that of Rammal et al. [67]. Discussion of how a hierarchy expresses the semantics of change and distinction can be found in [61].

The ultrametric topology was introduced by Marc Krasner [40], the ultrametric inequality having been formulated by Hausdorff in 1934. Essential motivation for the study of this area is provided by [70] as follows. Real and complex fields

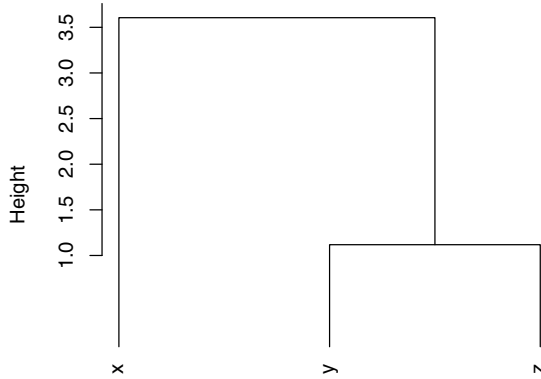


Fig. 1. The strong triangular inequality defines an ultrametric: every triplet of points satisfies the relationship: $d(x, z) \leq \max\{d(x, y), d(y, z)\}$ for distance d . Cf. by reading off the hierarchy, how this is verified for all x, y, z : $d(x, z) = 3.5$; $d(x, y) = 3.5$; $d(y, z) = 1.0$. In addition the symmetry and positive definiteness conditions hold for any pair of points.

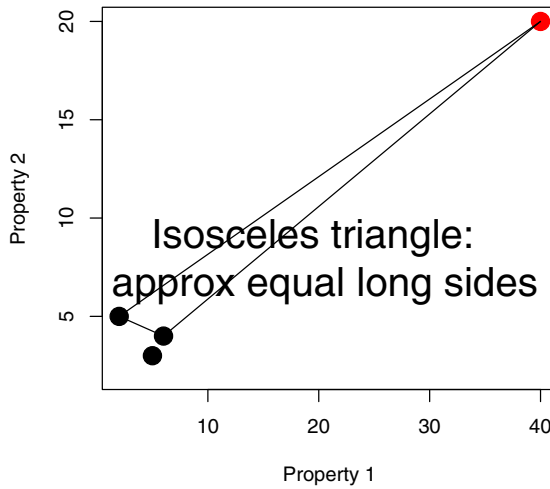


Fig. 2. How metric data can approximate an ultrametric, or can be made to approximate an ultrametric in the case of a stepwise, agglomerative algorithm. A “query” is on the far right. While we can easily determine the closest target (among the three objects represented by the dots on the left), is the closest really that much different from the alternatives? This question motivates an ultrametric view of the metric relationships shown.

gave rise to the idea of studying any field K with a complete valuation $|\cdot|$ comparable to the absolute value function. Such fields satisfy the “strong triangle inequality” $|x + y| \leq \max(|x|, |y|)$. Given a valued field, defining a totally ordered Abelian (i.e. commutative) group, an ultrametric space is induced through $|x - y| = d(x, y)$. Various terms are used interchangeably for analysis in and over such fields such as p-adic, ultrametric, non-Archimedean, and isosceles. The natural geometric ordering of metric valuations is on the real line, whereas in the ultrametric case the natural ordering is a hierarchical tree.

2.2 Some Geometrical Properties of Ultrametric Spaces

We see from the following, based on [41] (chapter 0, part IV), that an ultrametric space is quite different from a metric one. In an ultrametric space everything “lives” on a tree.

In an ultrametric space, all triangles are either isosceles with small base, or equilateral. We have here very clear symmetries of shape in an ultrametric topology. These symmetry “patterns” can be used to fingerprint data sets and time series: see [55, 57] for many examples of this.

Some further properties that are studied in [41] are: (i) Every point of a circle in an ultrametric space is a center of the circle. (ii) In an ultrametric topology, every ball is both open and closed (termed clopen). (iii) An ultrametric space is 0-dimensional (see [7, 69]). It is clear that an ultrametric topology is very different from our intuitive, or Euclidean, notions. The most important point to keep in mind is that in an ultrametric space everything “lives” in a hierarchy expressed by a tree.

2.3 Ultrametric Matrices and Their Properties

For an $n \times n$ matrix of positive reals, symmetric with respect to the principal diagonal, to be a matrix of distances associated with an ultrametric distance on X , a sufficient and necessary condition is that a permutation of rows and columns satisfies the following form of the matrix:

1. Above the diagonal term, equal to 0, the elements of the same row are non-decreasing.
2. For every index k , if

$$d(k, k + 1) = d(k, k + 2) = \cdots = d(k, k + \ell + 1)$$

then

$$d(k + 1, j) \leq d(k, j) \text{ for } k + 1 < j \leq k + \ell + 1$$

and

$$d(k + 1, j) = d(k, j) \text{ for } j > k + \ell + 1$$

Under these circumstances, $\ell \geq 0$ is the length of the section beginning, beyond the principal diagonal, the interval of columns of equal terms in row k .

Table 1. Input data: 8 iris flowers characterized by sepal and petal widths and lengths. From Fisher’s iris data [17].

| | Sepal.Length | Sepal.Width | Petal.Length | Petal.Width |
|-------|--------------|-------------|--------------|-------------|
| iris1 | 5.1 | 3.5 | 1.4 | 0.2 |
| iris2 | 4.9 | 3.0 | 1.4 | 0.2 |
| iris3 | 4.7 | 3.2 | 1.3 | 0.2 |
| iris4 | 4.6 | 3.1 | 1.5 | 0.2 |
| iris5 | 5.0 | 3.6 | 1.4 | 0.2 |
| iris6 | 5.4 | 3.9 | 1.7 | 0.4 |
| iris7 | 4.6 | 3.4 | 1.4 | 0.3 |

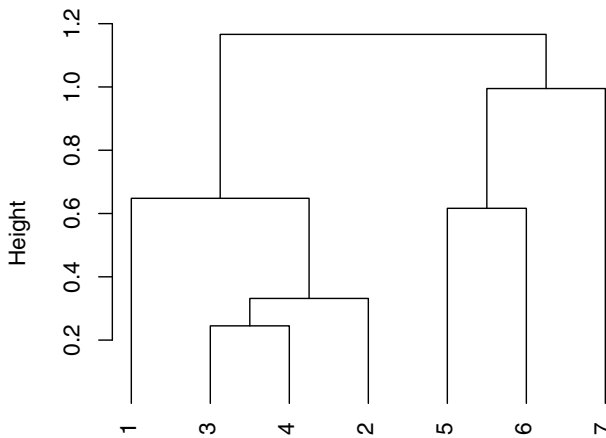


Fig. 3. Hierarchical clustering of 7 iris flowers using data from Table 1. No data normalization was used. The agglomerative clustering criterion was the minimum variance or Ward one.

To illustrate the ultrametric matrix format, consider the small data set shown in Table 1. A dendrogram produced from this is in Figure 3. The ultrametric matrix that can be read off this dendrogram is shown in Table 2. Finally a visualization of this matrix, illustrating the ultrametric matrix properties discussed above, is in Figure 4.

2.4 Clustering through Matrix Row and Column Permutation

Figure 4 shows how an ultrametric distance allows a certain structure to be visible (quite possibly, in practice, subject to an appropriate row and column permuting), in a matrix defined from the set of all distances. For set X , then, this matrix expresses the distance mapping of the Cartesian product, $d : X \times X \longrightarrow \mathbb{R}^+$. \mathbb{R}^+ denotes the non-negative reals. A priori the rows and columns of the

Table 2. Ultrametric matrix derived from the dendrogram in Figure 3

| | iris1 | iris2 | iris3 | iris4 | iris5 | iris6 | iris7 |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| iris1 | 0 | 0.6480741 | 0.6480741 | 0.6480741 | 1.1661904 | 1.1661904 | 1.1661904 |
| iris2 | 0.6480741 | 0 | 0.3316625 | 0.3316625 | 1.1661904 | 1.1661904 | 1.1661904 |
| iris3 | 0.6480741 | 0.3316625 | 0 | 0.2449490 | 1.1661904 | 1.1661904 | 1.1661904 |
| iris4 | 0.6480741 | 0.3316625 | 0.2449490 | 0 | 1.1661904 | 1.1661904 | 1.1661904 |
| iris5 | 1.1661904 | 1.1661904 | 1.1661904 | 1.1661904 | 0 | 0.6164414 | 0.9949874 |
| iris6 | 1.1661904 | 1.1661904 | 1.1661904 | 1.1661904 | 0.6164414 | 0 | 0.9949874 |
| iris7 | 1.1661904 | 1.1661904 | 1.1661904 | 1.1661904 | 0.9949874 | 0.9949874 | 0 |

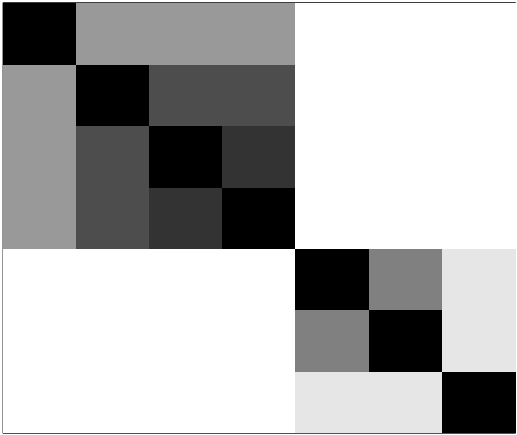


Fig. 4. A visualization of the ultrametric matrix of Table 2, where bright or white = highest value, and black = lowest value

function of the Cartesian product set X with itself could be in any order. The ultrametric matrix properties establish what is possible when the distance is an ultrametric one. Because the matrix (a 2-way data object) involves one *mode* (due to set X being crossed with itself; as opposed to the 2-mode case where an observation set is crossed by an attribute set) it is clear that both rows and columns can be permuted to yield the *same* order on X . A property of the form of the matrix is that small values are at or near the principal diagonal.

A generalization opens up for this sort of clustering by visualization scheme. Firstly, we can directly apply row and column permuting to 2-mode data, i.e. to the rows and columns of a matrix crossing indices I by attributes J , $a : I \times J \longrightarrow \mathbb{R}$. A matrix of values, $a(i, j)$, is furnished by the function a acting on the sets I and J . Here, each such term is real-valued. We can also generalize the principle of permuting such that small values are on or near the principal diagonal to instead allow similar values to be near one another, and thereby to facilitate visualization. An optimized way to do this was pursued in [45, 44]. Comprehensive surveys of clustering algorithms in this area, including objective functions,

visualization schemes, optimization approaches, presence of constraints, and applications, can be found in [46, 43]. See too [12, 53].

For all these approaches, underpinning them are row and column permutations, that can be expressed in terms of the permutation group, S_n , on n elements.

2.5 Other Miscellaneous Symmetries

As examples of various other local symmetries worthy of consideration in data sets consider subsets of data comprising clusters, and reciprocal nearest neighbor pairs.

Given an observation set, X , we define dissimilarities as the mapping $d : X \times X \longrightarrow \mathbb{R}^+$. A dissimilarity is a positive, definite, symmetric measure (i.e., $d(x, y) \geq 0$; $d(x, y) = 0$ if $x = y$; $d(x, y) = d(y, x)$). If in addition the triangular inequality is satisfied (i.e., $d(x, y) \leq d(x, z) + d(z, y)$, $\forall x, y, z \in X$) then the dissimilarity is a distance.

If X is endowed with a metric, then this metric is mapped onto an ultrametric. In practice, there is no need for X to be endowed with a metric. Instead a dissimilarity is satisfactory.

A hierarchy, H , is defined as a binary, rooted, node-ranked tree, also termed a dendrogram [3, 35, 41, 53]. A hierarchy defines a set of embedded subsets of a given set of objects X , indexed by the set I . That is to say, object i in the object set X is denoted x_i , and $i \in I$. These subsets are *totally ordered* by an index function ν , which is a stronger condition than the *partial order* required by the subset relation. The index function ν is represented by the ordinate in Figure 3 (the “height” or “level”). A bijection exists between a hierarchy and an ultrametric space.

Often in this article we will refer interchangeably to the object set, X , and the associated set of indices, I .

Usually a constructive approach is used to induce H on a set I . The most efficient algorithms are based on nearest neighbor chains, which by definition end in a pair of agglomerable reciprocal nearest neighbors. Further information can be found in [50, 51, 53, 54].

3 Generalized Ultrametric

In this subsection, we consider an ultrametric defined on the power set or join semilattice. Comprehensive background on ordered sets and lattices can be found in [10]. A review of generalized distances and ultrametrics can be found in [72].

3.1 Link with Formal Concept Analysis

Typically hierarchical clustering is based on a distance (which can be relaxed often to a dissimilarity, not respecting the triangular inequality, and *mutatis mutandis* to a similarity), defined on all pairs of the object set: $d : X \times X \rightarrow \mathbb{R}^+$.

I.e., a distance is a positive real value. Usually we require that a distance cannot be 0-valued unless the objects are identical. That is the traditional approach.

A different form of ultrametrization is achieved from a dissimilarity defined on the power set of attributes characterizing the observations (objects, individuals, etc.) X . Here we have: $d : X \times X \longrightarrow 2^J$, where J indexes the attribute (variables, characteristics, properties, etc.) set.

This gives rise to a different notion of distance, that maps pairs of objects onto elements of a join semilattice. The latter can represent all subsets of the attribute set, J . That is to say, it can represent the power set, commonly denoted 2^J , of J .

As an example, consider, say, $n = 5$ objects characterized by 3 boolean (presence/absence) attributes, shown in Figure 5 (top). Define dissimilarity between a pair of objects in this table as a *set* of 3 components, corresponding to the 3 attributes, such that if both components are 0, we have 1; if either component is 1 and the other 0, we have 1; and if both components are 1 we get 0. This is the simple matching coefficient [33]. We could use, e.g., Euclidean distance for each of the values sought; but we prefer to treat 0 values in both components as signaling a 1 contribution. We get then $d(a, b) = 1, 1, 0$ which we will call **d1**, **d2**. Then, $d(a, c) = 0, 1, 0$ which we will call **d2**. Etc. With the latter we create lattice nodes as shown in the middle part of Figure 5.

In Formal Concept Analysis [10, 24], it is the lattice itself which is of primary interest. In [33] there is discussion of, and a range of examples on, the close relationship between the traditional hierarchical cluster analysis based on $d : I \times I \rightarrow \mathbb{R}^+$, and hierarchical cluster analysis “based on abstract posets” (a poset is a partially ordered set), based on $d : I \times I \rightarrow 2^J$. The latter, leading to clustering based on dissimilarities, was developed initially in [32].

3.2 Applications of Generalized Ultrametrics

As noted in the previous subsection, the usual ultrametric is an ultrametric distance, i.e. for a set I , $d : I \times I \longrightarrow \mathbb{R}^+$. The generalized ultrametric is also consistent with this definition, where the range is a subset of the power set: $d : I \times I \longrightarrow \Gamma$, where Γ is a partially ordered set. In other words, the *generalized* ultrametric distance is a set. Some areas of application of generalized ultrametrics will now be discussed.

In the theory of reasoning, a monotonic operator is rigorous application of a succession of conditionals (sometimes called consequence relations). However negation or multiple valued logic (i.e. encompassing intermediate truth and falsehood) require support for non-monotonic reasoning.

Thus [28]: “Once one introduces negation ... then certain of the important operators are not monotonic (and therefore not continuous), and in consequence the Knaster-Tarski theorem [i.e. for fixed points; see [10]] is no longer applicable to them. Various ways have been proposed to overcome this problem. One such [approach is to use] syntactic conditions on programs ... Another is to consider different operators ... The third main solution is to introduce techniques

| | v_1 | v_2 | v_3 |
|---|-------|-------|-------|
| a | 1 | 0 | 1 |
| b | 0 | 1 | 1 |
| c | 1 | 0 | 1 |
| e | 1 | 0 | 0 |
| f | 0 | 0 | 1 |

| Potential lattice vertices | Lattice vertices found | Level |
|----------------------------|--|-------|
| d1,d2,d3 | d1,d2,d3 | 3 |
| d1,d2 d2,d3 d1,d3 | $ \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \\ \diagup \quad \diagdown \\ \diagdown \quad \diagup \\ \diagup \quad \diagdown \end{array} $ | 2 |
| d1 d2 d3 | d2 | 1 |

The set d1,d2,d3 corresponds to: $d(b, e)$ and $d(e, f)$
The subset d1,d2 corresponds to: $d(a, b), d(a, f), d(b, c), d(b, f),$ and $d(c, f)$
The subset d2,d3 corresponds to: $d(a, e)$ and $d(c, e)$
The subset d2 corresponds to: $d(a, c)$

Clusters defined by all pairwise linkage at level ≤ 2 :
 a, b, c, f
 a, c, e

Clusters defined by all pairwise linkage at level ≤ 3 :
 a, b, c, e, f

Fig. 5. Top: example data set consisting of 5 objects, characterized by 3 boolean attributes. Then: lattice corresponding to this data and its interpretation.

from topology and analysis to augment arguments based on order ... [the latter include:] methods based on metrics ... on quasi-metrics ... and finally ... on ultrametric spaces.”

The convergence to fixed points that are based on a generalized ultrametric system is precisely the study of spherically complete systems and expansive automorphisms discussed in section 4.3 below. As expansive automorphisms we see here again an example of symmetry at work.

3.3 Example of Application: Chemical Database Matching

In the 1990s, the Ward minimum variance hierarchical clustering method became the method of choice in the chemoinformatics community due to its hierarchical nature and the quality of the clusters produced. Unfortunately the method

reached its limits once the pharmaceutical companies tried processing datasets of more than 500,000 compounds due to: the $O(n^2)$ processing requirements of the reciprocal nearest neighbor algorithm; the requirement to hold all chemical structure “fingerprints” in memory to enable random access; and the requirement that parallel implementation use a shared-memory architecture. Let us look at an alternative hierarchical clustering algorithm that bypasses these computational difficulties.

A direct application of generalized ultrametrics to data mining is the following. The potentially huge advantage of the generalized ultrametric is that it allows a hierarchy to be read directly off the $I \times J$ input data, and bypasses the $O(n^2)$ consideration of all pairwise distances in agglomerative hierarchical clustering. In [62] we study application to chemoinformatics. Proximity and best match finding is an essential operation in this field. Typically we have one million chemicals upwards, characterized by an approximate 1000-valued attribute encoding.

Consider first our need to normalize the data. We divide each boolean (presence/absence) value by its corresponding column sum.

We can consider the hierarchical cluster analysis from abstract posets as based on $d : I \times I \rightarrow \mathbb{R}^{|J|}$. In [33], the median of the $|J|$ distance values is used, as input to a traditional hierarchical clustering, with alternative schemes discussed. See also [32] for an early elaboration of this approach.

Let us now proceed to take a particular approach to this, which has very convincing computational benefits.

3.3.1 Ultrametrization through Baire Space Embedding: Notation

A Baire space [42] consists of countably infinite sequences with a metric defined in terms of the longest common prefix: the longer the common prefix, the closer a pair of sequences. The Baire metric, and simultaneously ultrametric, will be defined in definition 1 in the next subsection. What is of interest to us here is this longest common prefix metric, which additionally is an ultrametric. The longest common prefixes at issue here are those of precision of any value (i.e., x_{ij} , for chemical compound i , and chemical structure code j). Consider two such values, x_{ij} and y_{ij} , which, when the context easily allows it, we will call x and y . Each are of some precision, and we take the integer $|K|$ to be the maximum precision. We pad a value with 0s if necessary, so that all values are of the same precision. Finally, we will assume for convenience that each value $\in [0, 1)$ and this can be arranged by normalization.

3.3.2 The Case of One Attribute

Thus we consider ordered sets x_k and y_k for $k \in K$. In line with our notation, we can write x_K and y_K for these numbers, with the set K now ordered. (So, $k = 1$ is the first decimal place of precision; $k = 2$ is the second decimal place; \dots ; $k = |K|$ is the $|K|$ th decimal place.) The cardinality of the set K is the precision with which a number, x_K , is measured. Without loss of generality, through normalization, we will take all $x_K, y_K \leq 1$. We will also consider decimal

numbers, only, in this article (hence $x_k \in \{0, 1, 2, \dots, 9\}$ for all numbers x , and for all digits k), again with no loss of generality to non-decimal number representations.

Consider as examples $x_K = 0.478$; and $y_K = 0.472$. In these cases, $|K| = 3$. For $k = 1$, we find $x_k = y_k = 4$. For $k = 2$, $x_k = y_k$. But for $k = 3$, $x_k \neq y_k$.

We now introduce the following distance:

$$d_B(x_K, y_K) = \begin{cases} 1 & \text{if } x_1 \neq y_1 \\ \inf 2^{-n} & x_n = y_n \quad 1 \leq n \leq |K| \end{cases} \quad (1)$$

So for $x_K = 0.478$ and $y_K = 0.472$ we have $d_B(x_K, y_K) = 2^{-2} = 0.25$.

The Baire distance is used in denotational semantics where one considers x_K and y_K as words (of equal length, in the finite case), and then this distance is defined from a common n -length prefix, or left substring, in the two words. For a set of words, a prefix tree can be built to expedite word matching, and the Baire distance derived from this tree.

We have $1 \geq d_B(x_K, y_K) \geq 2^{-|K|}$. Identical x_K and y_K have Baire distance equal to $2^{-|K|}$. The Baire distance is a 1-bounded ultrametric.

The Baire ultrametric defines a hierarchy, which can be expressed as a multi-way tree, on a set of numbers, x_{IK} . So the number x_{iK} , indexed by i , $i \in I$, is of precision $|K|$. It is actually simple to determine this hierarchy. The partition at level $k = 1$ has clusters defined as all those numbers indexed by i that share the same 1st digit. The partition at level $k = 2$ has clusters defined as all those numbers indexed by i that share the same 2nd digit; and so on, until we reach $k = |K|$. A strictly finer, or identical, partition is to be found at each successive level (since once a pair of numbers becomes dissimilar, $d_B > 0$, this non-zero distance cannot be reversed). Identical numbers at level $k = 1$ have distance $\leq 2^{-1} = 0.5$. Identical numbers at level $k = 2$ have distance $\leq 2^{-2} = 0.25$. Identical numbers at level $k = 3$ have distance $\leq 2^{-3} = 0.125$; and so on, to level $k = |K|$, when distance $= 2^{-|K|}$.

3.3.3 Analysis: Baire Ultrametrization from Numerical Precision

In this section we use (i) a random projection of vectors into a 1-dimensional space (so each chemical structure is mapped onto a scalar value, by design ≥ 0 and ≤ 1) followed by (ii) implicit use of a prefix tree constructed on the digits of the set of scalar values. First we will look at this procedure. Then we will return to discuss its properties.

We seek all i, i' such that:

1. for all $j \in J$,
2. $x_{ijK} = x_{i'jK}$
3. to fixed precision K

Recall that K is an ordered set. We impose a user specified upper limit on precision, $|K|$.

Table 3. Results for the three different data sets, each consisting of 7500 chemicals, are shown in immediate succession. The number of significant decimal digits is 4 (more precise, and hence more different clusters found), 3, 2, and 1 (lowest precision in terms of significant digits).

| Sig. dig. c | No. clusters |
|---------------|--------------|
| 4 | 6591 |
| 4 | 6507 |
| 4 | 5735 |
| 3 | 6481 |
| 3 | 6402 |
| 3 | 5360 |
| 2 | 2519 |
| 2 | 2576 |
| 2 | 2135 |
| 1 | 138 |
| 1 | 148 |
| 1 | 167 |

Now rather than $|J|$ separate tests for equality (point 1 above), a *sufficient condition* is that $\sum_j w_j x_{ijK} = \sum_j w_j x_{i'jK}$ for a set of weights w_j . What helps in making this sufficient condition for equality work well in practice is that many of the x_{iJK} values are 0: cf. the approximate 8% matrix occupancy rate that holds here. We experimented with such possibilities as $w_j = j$ (i.e., $\{1, 2, \dots, |J|\}$ and $w_j = |J| + 1 - j$ (i.e., $\{|J|, |J| - 1, \dots, 3, 2, 1\}$). A first principal component would allow for the definition of the least squares optimal linear fit of the projections. The best choice of w_j values we found for uniformly distributed values in $(0, 1)$: for each j , $w_j \sim U(0, 1)$.

Table 3 shows, in immediate succession, results for three data sets. The normalizing column sums were calculated and applied independently to each of the three data sets. Insofar as x_J is directly proportional, whether calculated on 7500 chemical structures or 1.2 million, leads to a constant of proportionality, only, between the two cases. As noted, a random projection was used. Finally, identical projected values were read off, to determine clusters.

3.3.4 Discussion: Random Projection and Hashing

Random projection is the finding of a low dimensional embedding of a point set – dimension equals 1, or a line or axis, in this work – such that the distortion

of any pair of points is bounded by a function of the lower dimensionality [77]. There is a burgeoning literature in this area, e.g. [16]. While random projection *per se* will not guarantee a bijection of best match in original and in lower dimensional spaces, our use of projection here is effectively a hashing method ([47] uses MD5 for nearest neighbor search), in order to deliberately find hash collisions – thereby providing a *sufficient* condition for the mapped vectors to be identical.

Collision of identically valued vectors is guaranteed, but what of collision of non-identically valued vectors, which we want to avoid?

To prove such a result may require an assumption of what distribution our original data follow. A general class is referred to as a stable distribution [29]: this is a distribution such that a limited number of weighted sums of the variables is also itself of the same distribution. Examples include both Gaussian and long-tailed or power law distributions.

Interestingly, however, very high dimensional (or equivalently, very low sample size or low n) data sets, by virtue of high relative dimensionality alone, have points mostly lying at the vertices of a regular simplex or polygon [55, 27]. This intriguing aspect is one reason, perhaps, why we have found random projection to work well. Another reason is the following: if we work on normalized data, then the values on any two attributes j will be small. Hence x_j and x'_j are small. Now if the random weight for this attribute is w_j , then the random projections are, respectively, $\sum_j w_j x_j$ and $\sum_j w_j x'_j$. But these terms are dominated by the random weights. We can expect near equal x_j and x'_j terms, for all j , to be mapped onto fairly close resultant scalar values.

Further work is required to confirm these hypotheses, viz., that high dimensional data may be highly “regular” or “structured” in such a way; and that, as a consequence, hashing is particularly well-behaved in the sense of non-identical vectors being nearly always collision-free. There is further discussion in [8].

We remark that a prefix tree, or trie, is well-known in the searching and sorting literature [26], and is used to expedite the finding of longest common prefixes. At level one, nodes are associated with the first digit. At level two, nodes are associated with the second digit, and so on through deeper levels of the tree.

3.3.5 Simple Clustering Hierarchy from the Baire Space Embedding

The Baire ultrametrization induces a (fairly flat) multiway tree on the given data set.

Consider a partition yielded by identity (over all the attribute set) at a given precision level. Then for precision levels k_1, k_2, k_3, \dots we have, at each, a partition, such that all member clusters are ordered by reverse embedding (or set inclusion): $q_{(1)} \supseteq q_{(2)} \supseteq q_{(3)} \supseteq \dots$. Call each such sequence of embeddings a chain. The entire data set is covered by a set of such chains. This sequence of partitions is ordered by set inclusion.

The computational time complexity is as follows. Let the number of chemicals be denoted $n = |I|$; the number of attributes is $|J|$; and the total number of digits precision is $|K|$. Consider a particular number of digits precision, k_0 , where $1 \leq k_0 \leq |K|$. Then the random projection takes $n \cdot k_0 \cdot |J|$ operations. A sort follows, requiring $O(n \log n)$ operations. Then clusters are read off with $O(n)$ operations. Overall, the computational effort is bounded by $c_1 \cdot |I| \cdot |J| \cdot |K| + c_2 \cdot |I| \cdot \log |I| + c_3 |I|$ (where c_1, c_2, c_3 are constants), which is equal to $O(|I| \log |I|)$ or $O(n \log n)$.

Further evaluation and a number of further case studies are covered in [8].

4 Hierarchy in a p-Adic Number System

A dendrogram is widely used in hierarchical, agglomerative clustering, and is induced from observed data. In this article, one of our important goals is to show how it lays bare many diverse symmetries in the observed phenomenon represented by the data. By expressing a dendrogram in p-adic terms, we open up a wide range of possibilities for seeing symmetries and attendant invariants.

4.1 p-Adic Encoding of a Dendrogram

We will introduce now the one-to-one mapping of clusters (including singletons) in a dendrogram H into a set of p-adically expressed integers (a fortiori, rationals, or \mathbb{Q}_p). The field of p-adic numbers is the most important example of ultrametric spaces. Addition and multiplication of p-adic integers, \mathbb{Z}_p (cf. expression in subsection 1.4), are well-defined. Inverses exist and no zero-divisors exist.

A terminal-to-root traversal in a dendrogram or binary rooted tree is defined as follows. We use the path $x \subset q \subset q' \subset q'' \subset \dots q_{n-1}$, where x is a given object specifying a given terminal, and q, q', q'', \dots are the embedded classes along this path, specifying nodes in the dendrogram. The root node is specified by the class q_{n-1} comprising all objects.

A terminal-to-root traversal is the shortest path between the given terminal node and the root node, assuming we preclude repeated traversal (backtrack) of the same path between any two nodes.

By means of terminal-to-root traversals, we define the following p-adic encoding of terminal nodes, and hence objects, in Figure 6.

$$\begin{aligned}
 x_1 : & +1 \cdot p^1 + 1 \cdot p^2 + 1 \cdot p^5 + 1 \cdot p^7 \\
 x_2 : & -1 \cdot p^1 + 1 \cdot p^2 + 1 \cdot p^5 + 1 \cdot p^7 \\
 x_3 : & \quad -1 \cdot p^2 + 1 \cdot p^5 + 1 \cdot p^7 \\
 x_4 : & +1 \cdot p^3 + 1 \cdot p^4 - 1 \cdot p^5 + 1 \cdot p^7 \\
 x_5 : & -1 \cdot p^3 + 1 \cdot p^4 - 1 \cdot p^5 + 1 \cdot p^7 \\
 x_6 : & \quad -1 \cdot p^4 - 1 \cdot p^5 + 1 \cdot p^7 \\
 x_7 : & \quad \quad +1 \cdot p^6 - 1 \cdot p^7 \\
 x_8 : & \quad \quad -1 \cdot p^6 - 1 \cdot p^7
 \end{aligned} \tag{2}$$

If we choose $p = 2$ the resulting decimal equivalents could be the same: cf. contributions based on $+1 \cdot p^1$ and $-1 \cdot p^1 + 1 \cdot p^2$. Given that the coefficients of the p^j terms ($1 \leq j \leq 7$) are in the set $\{-1, 0, +1\}$ (implying for x_1 the additional terms: $+0 \cdot p^3 + 0 \cdot p^4 + 0 \cdot p^6$), the coding based on $p = 3$ is required to avoid ambiguity among decimal equivalents.

A few general remarks on this encoding follow. For the labeled ranked binary trees that we are considering (for discussion of combinatorial properties based on labeled, ranked and binary trees, see [52]), we require the labels $+1$ and -1 for the two branches at any node. Of course we could interchange these labels, and have these $+1$ and -1 labels reversed at any node. By doing so we will have different p-adic codes for the objects, x_i .

The following properties hold: (i) *Unique encoding*: the decimal codes for each x_i (lexicographically ordered) are unique for $p \geq 3$; and (ii) *Reversibility*: the dendrogram can be uniquely reconstructed from any such set of unique codes.

The p-adic encoding defined for any object set can be expressed as follows for any object x associated with a terminal node:

$$x = \sum_{j=1}^{n-1} c_j p^j \text{ where } c_j \in \{-1, 0, +1\} \quad (3)$$

In greater detail we have:

$$x_i = \sum_{j=1}^{n-1} c_{ij} p^j \text{ where } c_{ij} \in \{-1, 0, +1\} \quad (4)$$

Here j is the level or rank (root: $n - 1$; terminal: 1), and i is an object index.

In our example we have used: $c_j = +1$ for a left branch (in the sense of Figure 6), $= -1$ for a right branch, and $= 0$ when the node is not on the path from that particular terminal to the root.

A matrix form of this encoding is as follows, where $\{\cdot\}^t$ denotes the transpose of the vector.

Let \mathbf{x} be the column vector $\{x_1 \ x_2 \ \dots \ x_n\}^t$.

Let \mathbf{p} be the column vector $\{p^1 \ p^2 \ \dots \ p^{n-1}\}^t$.

Define a characteristic matrix C of the branching codes, $+1$ and -1 , and an absent or non-existent branching given by 0, as a set of values c_{ij} where $i \in I$, the indices of the object set; and $j \in \{1, 2, \dots, n - 1\}$, the indices of the dendrogram levels or nodes ordered increasingly. For Figure 6 we therefore have:

$$C = \{c_{ij}\} = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 0 & 1 \\ -1 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & -1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 & -1 & 0 & 1 \\ 0 & 0 & 0 & -1 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 \end{pmatrix} \quad (5)$$

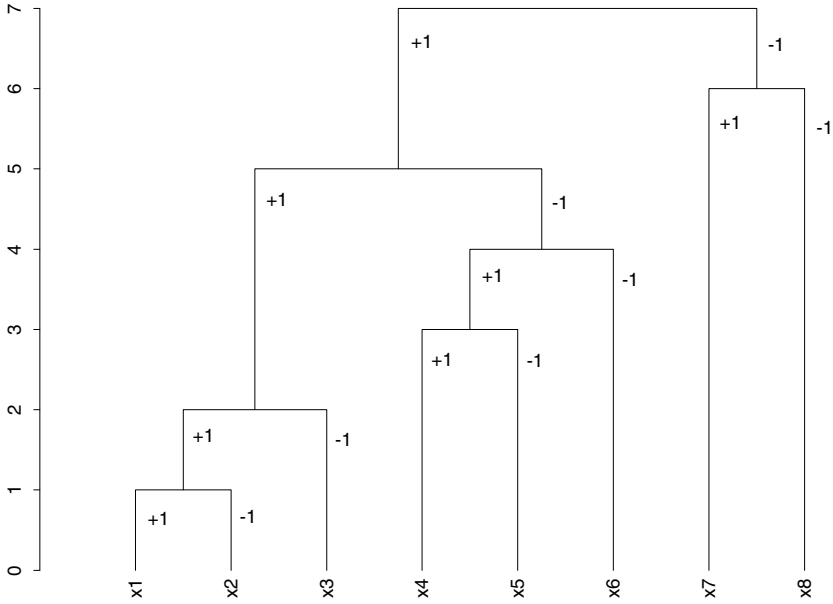


Fig. 6. Labeled, ranked dendrogram on 8 terminal nodes, x_1, x_2, \dots, x_8 . Branches are labeled +1 and -1. Clusters are: $q_1 = \{x_1, x_2\}$, $q_2 = \{x_1, x_2, x_3\}$, $q_3 = \{x_4, x_5\}$, $q_4 = \{x_4, x_5, x_6\}$, $q_5 = \{x_1, x_2, x_3, x_4, x_5, x_6\}$, $q_6 = \{x_7, x_8\}$, $q_7 = \{x_1, x_2, \dots, x_7, x_8\}$.

For given level j , $\forall i$, the absolute values $|c_{ij}|$ give the membership function either by node, j , which is therefore read off columnwise; or by object index, i , which is therefore read off rowwise.

The matrix form of the p-adic encoding used in equations (3) or (4) is:

$$\mathbf{x} = C\mathbf{p} \quad (6)$$

Here, \mathbf{x} is the decimal encoding, C is the matrix with dendrogram branching codes (cf. example shown in expression (5)), and \mathbf{p} is the vector of powers of a fixed integer (usually, more restrictively, fixed prime) p .

The tree encoding exemplified in Figure 6, and defined with coefficients in equations (3) or (4), (5) or (6), with labels +1 and -1 was required (as opposed to the choice of 0 and 1, which might have been our first thought) to fully cater for the ranked nodes (i.e. the total order, as opposed to a partial order, on the nodes).

We can consider the objects that we are dealing with to have equivalent integer values. To show that, all we must do is work out decimal equivalents of the p-adic expressions used above for x_1, x_2, \dots . As noted in [25], we have equivalence between: a p-adic number; a p-adic expansion; and an element of \mathbb{Z}_p (the p-adic integers). The coefficients used to specify a p-adic number, [25] notes (p. 69), “must be taken in a set of representatives of the class modulo p . The numbers

between 0 and $p - 1$ are only the most obvious choice for these representatives. There are situations, however, where other choices are expedient.”

We note that the matrix C is used in [9]. A somewhat trivial view of how “hierarchical trees can be perfectly scaled in one dimension” (the title and theme of [9]) is that p-adic numbering is feasible, and hence a one dimensional representation of terminal nodes is easily arranged through expressing each p-adic number with a real number equivalent.

4.2 p-Adic Distance on a Dendrogram

We will now induce a metric topology on the p-adically encoded dendrogram, H . It leads to various symmetries relative to identical norms, for instance, or identical tree distances.

We use the following longest common subsequence, starting at the root: we look for the term p^r in the p-adic codes of the two objects, where r is the lowest level such that the values of the coefficients of p^r are equal.

Let us look at the set of p-adic codes for x_1, x_2, \dots above (Figure 6 and relations 3), to give some examples of this.

For x_1 and x_2 , we find the term we are looking for to be p^1 , and so $r = 1$.

For x_1 and x_5 , we find the term we are looking for to be p^5 , and so $r = 5$.

For x_5 and x_8 , we find the term we are looking for to be p^7 , and so $r = 7$.

Having found the value r , the distance is defined as p^{-r} [3, 25].

This longest common prefix metric is also known as the Baire distance, and has been discussed in section 3.3. In topology the Baire metric is defined on infinite strings [42]. It is more than just a distance: it is an ultrametric bounded from above by 1, and its *infimum* is 0 which is relevant for very long sequences, or in the limit for infinite-length sequences. The use of this Baire metric is pursued in [62] based on random projections [77], and providing computational benefits over the classical $O(n^2)$ hierarchical clustering based on all pairwise distances.

The longest common prefix metric leads directly to a *p-adic hierarchical classification* (cf. [5]). This is a special case of the “fast” hierarchical clustering discussed in section 3.2.

Compared to the longest common prefix metric, there are other related forms of metric, and simultaneously ultrametric. In [23], the metric is defined via the integer part of a real number. In [3], for integers x, y we have: $d(x, y) = 2^{-\text{order}_p(x-y)}$ where p is prime, and $\text{order}_p(i)$ is the exponent (non-negative integer) of p in the prime decomposition of an integer. Furthermore let $S(x)$ be a series: $S(x) = \sum_{i \in \mathbb{N}} a_i x^i$. (\mathbb{N} are the natural numbers.) The order of $S(i)$ is the rank of its first non-zero term: $\text{order}(S) = \inf\{i : i \in \mathbb{N}; a_i \neq 0\}$. (The series that is all zero is of order infinity.) Then the ultrametric similarity between series is: $d(S, S') = 2^{-\text{order}(S-S')}$.

4.3 Scale-Related Symmetry

Scale-related symmetry is very important in practice. In this subsection we introduce an operator that provides this symmetry. We also term it a dilation operator, because of its role in the wavelet transform on trees (see section 5.3 below, and [58] for discussion and examples). This operator is p -adic multiplication by $1/p$.

Consider the set of objects $\{x_i | i \in I\}$ with its p -adic coding considered above. Take $p = 2$. (Non-uniqueness of corresponding decimal codes is not of concern to us now, and taking this value for p is without any loss of generality.) Multiplication of $x_1 = +1 \cdot 2^1 + 1 \cdot 2^2 + 1 \cdot 2^5 + 1 \cdot 2^7$ by $1/p = 1/2$ gives: $+1 \cdot 2^1 + 1 \cdot 2^4 + 1 \cdot 2^6$. Each level has decreased by one, and the lowest level has been lost. Subject to the lowest level of the tree being lost, the form of the tree remains the same. By carrying out the multiplication-by- $1/p$ operation on all objects, it is seen that the effect is to rise in the hierarchy by one level.

Let us call product with $1/p$ the operator A . The effect of losing the bottom level of the dendrogram means that either (i) each cluster (possibly singleton) remains the same; or (ii) two clusters are merged. Therefore the application of A to all q implies a subset relationship between the set of clusters $\{q\}$ and the result of applying A , $\{Aq\}$.

Repeated application of the operator A gives Aq, A^2q, A^3q, \dots . Starting with any singleton, $i \in I$, this gives a path from the terminal to the root node in the tree. Each such path ends with the null element, which we define to be the p -adic encoding corresponding to the root node of the tree. Therefore the intersection of the paths equals the null element.

Benedetto and Benedetto [1, 2] discuss A as an expansive automorphism of I , i.e. form-preserving, and locally expansive. Some implications [1] of the expansive automorphism follow. For any q , let us take q, Aq, A^2q, \dots as a sequence of open subgroups of I , with $q \subset Aq \subset A^2q \subset \dots$, and $I = \bigcup \{q, Aq, A^2q, \dots\}$. This is termed an inductive sequence of I , and I itself is the inductive limit ([68], p. 131).

Each path defined by application of the expansive automorphism defines a spherically complete system [70, 23, 69], which is a formalization of well-defined subset embeddedness. Such a methodological framework finds application in multi-valued and non-monotonic reasoning, as noted in section 3.2.

5 Tree Symmetries through the Wreath Product Group

In this section the wreath product group, used up to now in the literature as a framework for tree structuring of image or other signal data, is here used on a 2-way tree or dendrogram data structure. An example of wreath product invariance is provided by the wavelet transform *of* such a tree.

5.1 Wreath Product Group Corresponding to a Hierarchical Clustering

A dendrogram like that shown in Figure 6 is invariant as a representation or structuring of a data set relative to rotation (alternatively, here: permutation) of left and right child nodes. These rotation (or permutation) symmetries are defined by the wreath product group (see [20, 21, 18] for an introduction and applications in signal and image processing), and can be used with any m -ary tree, although we will treat the binary or 2-way case here.

For the group actions, with respect to which we will seek invariance, we consider independent cyclic shifts of the subnodes of a given node (hence, at each level). Equivalently these actions are adjacency preserving permutations of subnodes of a given node (i.e., for given q , with $q = q' \cup q''$, the permutations of $\{q', q''\}$). We have therefore cyclic group actions at each node, where the cyclic group is of order 2.

The symmetries of H are given by structured permutations of the terminals. The terminals will be denoted here by $\text{Term } H$. The full group of symmetries is summarized by the following generative algorithm:

1. For level $l = n - 1$ down to 1 do:
2. Selected node, $\nu \leftarrow$ node at level l .
3. And permute subnodes of ν .

Subnode ν is the root of subtree H_ν . We denote H_{n-1} simply by H . For a subnode ν' undergoing a relocation action in step 3, the internal structure of subtree $H_{\nu'}$ is not altered.

The algorithm described defines the automorphism group which is a wreath product of the symmetric group. Denote the permutation at level ν by P_ν . Then the automorphism group is given by:

$$G = P_{n-1} \text{ wr } P_{n-2} \text{ wr } \dots \text{ wr } P_2 \text{ wr } P_1$$

where wr denotes the wreath product.

5.2 Wreath Product Invariance

Call $\text{Term } H_\nu$ the terminals that descend from the node at level ν . So these are the terminals of the subtree H_ν with its root node at level ν . We can alternatively call $\text{Term } H_\nu$ the cluster associated with level ν .

We will now look at shift invariance under the group action. This amounts to the requirement for a constant function defined on $\text{Term } H_\nu, \forall \nu$. A convenient way to do this is to define such a function on the set $\text{Term } H_\nu$ via the root node alone, ν . By definition then we have a constant function on the set $\text{Term } H_\nu$.

Let us call V_ν a space of functions that are constant on $\text{Term } H_\nu$. That is to say, the functions are constant in clusters that are defined by the subset of n objects. Possibilities for V_ν that were considered in [58] are:

1. Basis vector with $|\text{Term } H_{n-1}|$ components, with 0 values except for value 1 for component i .
2. Set (of cardinality $n = |\text{Term } H_{n-1}|$) of m -dimensional observation vectors.

Consider the resolution scheme arising from moving from Term $H_{\nu'}$, Term $H_{\nu''}$ to Term H_{ν} . From the hierarchical clustering point of view it is clear what this represents, simply, an agglomeration of two clusters called Term $H_{\nu'}$ and Term $H_{\nu''}$, replacing them with a new cluster, Term H_{ν} .

Let the spaces of functions that are constant on subsets corresponding to the two cluster agglomerands be denoted $V_{\nu'}$ and $V_{\nu''}$. These two clusters are disjoint initially, which motivates us taking the two spaces as a couple: $(V_{\nu'}, V_{\nu''})$.

5.3 Example of Wreath Product Invariance: Haar Wavelet Transform of a Dendrogram

Let us exemplify a case that satisfies all that has been defined in the context of the wreath product invariance that we are targeting. It is the algorithm discussed in depth in [58]. Take the constant function from $V_{\nu'}$ to be $f_{\nu'}$. Take the constant function from $V_{\nu''}$ to be $f_{\nu''}$. Then define the constant function, the *scaling function*, in V_{ν} to be $(f_{\nu'} + f_{\nu''})/2$. Next define the zero mean function, $(w_{\nu'} + w_{\nu''})/2 = 0$, the *wavelet function*, as follows:

$$w_{\nu'} = (f_{\nu'} + f_{\nu''})/2 - f_{\nu'}$$

in the support interval of $V_{\nu'}$, i.e. Term $H_{\nu'}$, and

$$w_{\nu''} = (f_{\nu'} + f_{\nu''})/2 - f_{\nu''}$$

in the support interval of $V_{\nu''}$, i.e. Term $H_{\nu''}$.

Since $w_{\nu'} = -w_{\nu''}$ we have the zero mean requirement.

We now illustrate the Haar wavelet transform of a dendrogram with a case study.

The discrete wavelet transform is a decomposition of data into spatial and frequency components. In terms of a dendrogram these components are with respect to, respectively, within and between clusters of successive partitions. We show how this works taking the data of Table 4.

Table 4. First 8 observations of Fisher's iris data. L and W refer to length and width.

| | Sepal.L | Sepal.W | Petal.L | Petal.W |
|---|---------|---------|---------|---------|
| 1 | 5.1 | 3.5 | 1.4 | 0.2 |
| 2 | 4.9 | 3.0 | 1.4 | 0.2 |
| 3 | 4.7 | 3.2 | 1.3 | 0.2 |
| 4 | 4.6 | 3.1 | 1.5 | 0.2 |
| 5 | 5.0 | 3.6 | 1.4 | 0.2 |
| 6 | 5.4 | 3.9 | 1.7 | 0.4 |
| 7 | 4.6 | 3.4 | 1.4 | 0.3 |
| 8 | 5.0 | 3.4 | 1.5 | 0.2 |

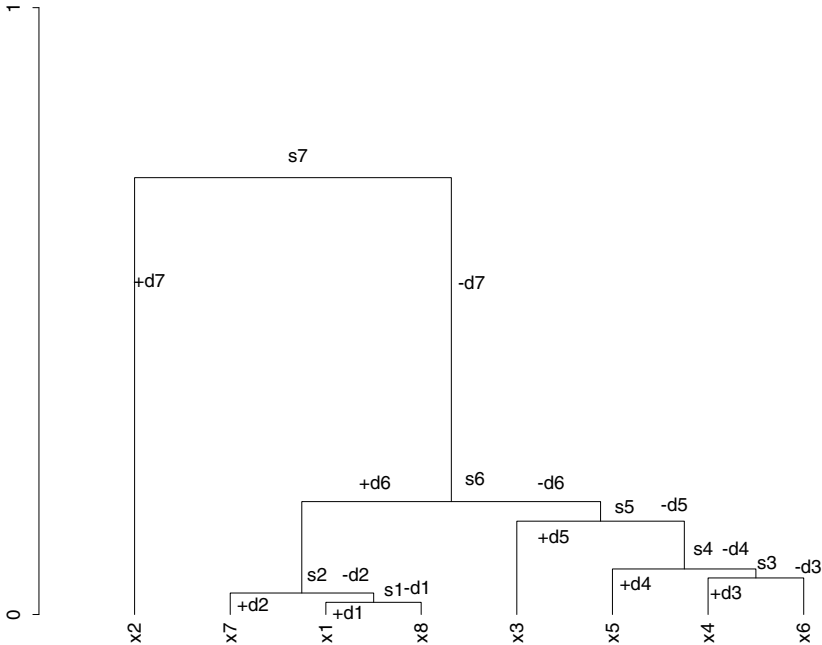


Fig. 7. Dendrogram on 8 terminal nodes constructed from first 8 values of Fisher iris data. (Median agglomerative method used in this case.) Detail or wavelet coefficients are denoted by d , and data smooths are denoted by s . The observation vectors are denoted by x and are associated with the terminal nodes. Each *signal smooth*, s , is a vector. The (positive or negative) *detail signals*, d , are also vectors. All these vectors are of the same dimensionality.

Table 5. The hierarchical Haar wavelet transform resulting from use of the first 8 observations of Fisher’s iris data shown in Table 4. Wavelet coefficient levels are denoted d1 through d7, and the continuum or smooth component is denoted s7.

| | s7 | d7 | d6 | d5 | d4 | d3 | d2 | d1 |
|---------|----------|----------|----------|---------|--------|-------|--------|-------|
| Sepal.L | 5.146875 | 0.253125 | 0.13125 | 0.1375 | -0.025 | 0.05 | -0.025 | 0.05 |
| Sepal.W | 3.603125 | 0.296875 | 0.16875 | -0.1375 | 0.125 | 0.05 | -0.075 | -0.05 |
| Petal.L | 1.562500 | 0.137500 | 0.02500 | 0.0000 | 0.000 | -0.10 | 0.050 | 0.00 |
| Petal.W | 0.306250 | 0.093750 | -0.01250 | -0.0250 | 0.050 | 0.00 | 0.000 | 0.00 |

The hierarchy built on the 8 observations of Table 4 is shown in Figure 7. Here we denote irises 1 through 8 as, respectively: $x_1, x_3, x_4, x_6, x_8, x_2, x_5, x_7$.

Something more is shown in Figure 7, namely the detail signals (denoted $\pm d$) and overall smooth (denoted s), which are determined in carrying out the wavelet transform, the so-called forward transform.

The inverse transform is then determined from Figure 7 in the following way. Consider the observation vector x_2 . Then this vector is reconstructed exactly by reading the tree from the root: $s_7 + d_7 = x_2$. Similarly a path from root to terminal is used to reconstruct any other observation. If x_2 is a vector of dimensionality m , then so also are s_7 and d_7 , as well as all other detail signals.

This procedure is the same as the Haar wavelet transform, only applied to the dendrogram and using the input data.

This wavelet transform for the data in Table 4, based on the “key” or intermediary hierarchy of Figure 7, is shown in Table 5.

Wavelet regression entails setting small and hence unimportant detail coefficients to 0 before applying the inverse wavelet transform. More discussion can be found in [58].

Early work on p-adic and ultrametric wavelets can be found in Kozyrev [38, 39]. While we have treated the case of the wavelet transform on a particular graph, a tree, recent applications of wavelets to general graphs are in [34] and, by representing the graph as a matrix, in [63].

6 Remarkable Symmetries in Very High Dimensional Spaces

In the work of [66, 67] it was shown how as ambient dimensionality increased distances became more and more ultrametric. That is to say, a hierarchical embedding becomes more and more immediate and direct as dimensionality increases. A better way of quantifying this phenomenon was developed in [55]. What this means is that there is inherent hierarchical structure in high dimensional data spaces.

It was shown experimentally in [66, 67, 55] how points in high dimensional spaces become increasingly equidistant with increase in dimensionality. Both [27] and [13] study Gaussian clouds in very high dimensions. The latter finds that “not only are the points [of a Gaussian cloud in very high dimensional space] on the convex hull, but all reasonable-sized subsets span faces of the convex hull. This is wildly different than the behavior that would be expected by traditional low-dimensional thinking”.

That very simple structures come about in very high dimensions is not as trivial as it might appear at first sight. Firstly, even very simple structures (hence with many symmetries) can be used to support fast and perhaps even constant time worst case proximity search [55]. Secondly, as shown in the machine learning framework by [27], there are important implications ensuing from the simple high dimensional structures. Thirdly, [59] shows that very high dimensional clustered data contain symmetries that in fact can be exploited to “read off” the clusters in a computationally efficient way. Fourthly, following [11], what we might want to look for in contexts of considerable symmetry are the “impurities” or small irregularities that detract from the overall dominant picture.

See Table 6 exemplifying the change of topological properties as ambient dimensionality increases. It behoves us to exploit the symmetries that arise when we have to process very high dimensional data.

Table 6. Typical results, based on 300 sampled triangles from triplets of points. For uniform, the data are generated on $[0, 1]^m$; hypercube vertices are in $\{0, 1\}^m$, and for Gaussian on each dimension, the data are of mean 0, and variance 1. Dimen. is the ambient dimensionality. Isosc. is the number of isosceles triangles with small base, as a proportion of all triangles sampled. Equil. is the number of equilateral triangles as a proportion of triangles sampled. UM is the proportion of ultrametricity-respecting triangles (= 1 for all ultrametric).

| No. points | Dimen. | Isosc. | Equil. | UM |
|------------|--------|--------|--------|------|
| Uniform | | | | |
| 100 | 20 | 0.10 | 0.03 | 0.13 |
| 100 | 200 | 0.16 | 0.20 | 0.36 |
| 100 | 2000 | 0.01 | 0.83 | 0.84 |
| 100 | 20000 | 0 | 0.94 | 0.94 |
| Hypercube | | | | |
| 100 | 20 | 0.14 | 0.02 | 0.16 |
| 100 | 200 | 0.16 | 0.21 | 0.36 |
| 100 | 2000 | 0.01 | 0.86 | 0.87 |
| 100 | 20000 | 0 | 0.96 | 0.96 |
| Gaussian | | | | |
| 100 | 20 | 0.12 | 0.01 | 0.13 |
| 100 | 200 | 0.23 | 0.14 | 0.36 |
| 100 | 2000 | 0.04 | 0.77 | 0.80 |
| 100 | 20000 | 0 | 0.98 | 0.98 |

6.1 Application to Very High Frequency Data Analysis: Segmenting a Financial Signal

We use financial futures, circa March 2007, denominated in euros from the DAX exchange. Our data stream is at the millisecond rate, and comprises about 382,860 records. Each record includes: 5 bid and 5 asking prices, together with bid and asking sizes in all cases, and action. We extracted one symbol (commodity) with 95,011 single bid values, on which we now report results. See Figure 8.

Embeddings were defined as follows.

- Windows of 100 successive values, starting at time steps: 1, 1000, 2000, 3000, 4000, ..., 94000.
- Windows of 1000 successive values, starting at time steps: 1, 1000, 2000, 3000, 4000, ..., 94000.
- Windows of 10000 successive values, starting at time steps: 1, 1000, 2000, 3000, 4000, ..., 85000.

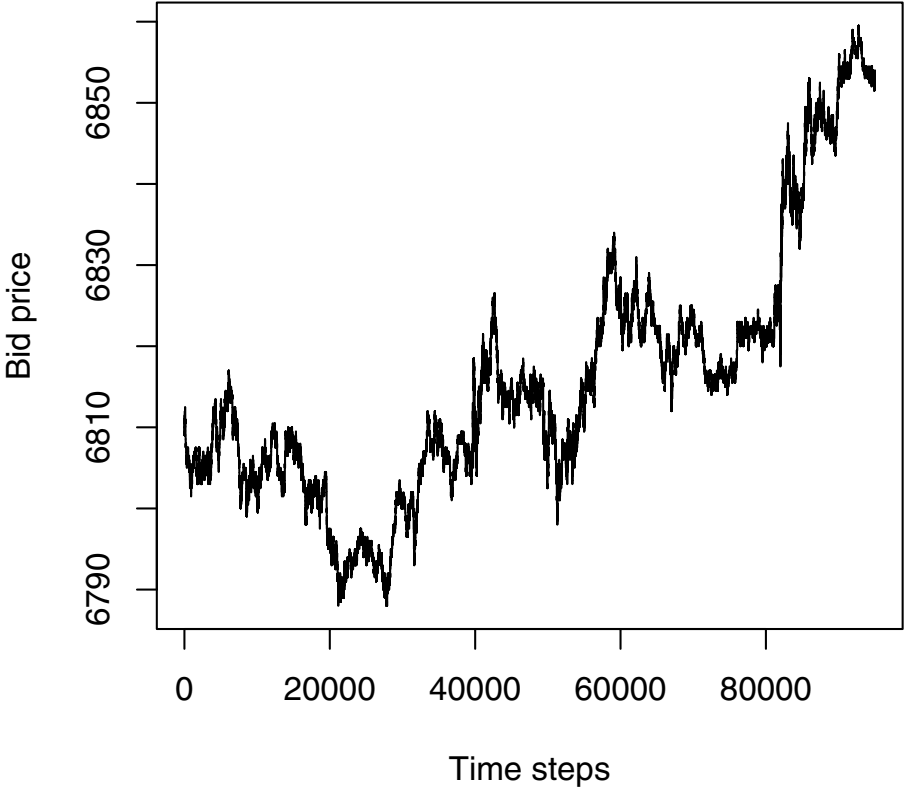


Fig. 8. The signal used: a commodity future, with millisecond time sampling

The histograms of distances between these windows, or embeddings, in respectively spaces of dimension 100, 1000 and 10000, are shown in Figure 9.

Note how the 10000-length window case results in points that are strongly overlapping. In fact, we can say that 90% of the values in each window are overlapping with the next window. Notwithstanding this major overlapping in regard to clusters involved in the pairwise distances, if we can still find clusters in the data then we have a very versatile way of tackling the clustering objective. Because of the greater cluster concentration that we expect (cf. Table 6) from a greater embedding dimension, we use the 86 points in 10000-dimensional space, notwithstanding the fact that these points are from overlapping clusters.

We make the following supposition based on Figure 8: the clusters will consist of successive values, and hence will be justifiably termed segments.

From the distances histogram in Figure 9, bottom, we will carry out Gaussian mixture modeling followed by use of the Bayesian information criterion (BIC, [71]) as an approximate Bayes factor, to determine the best number of clusters (effectively, histogram peaks).

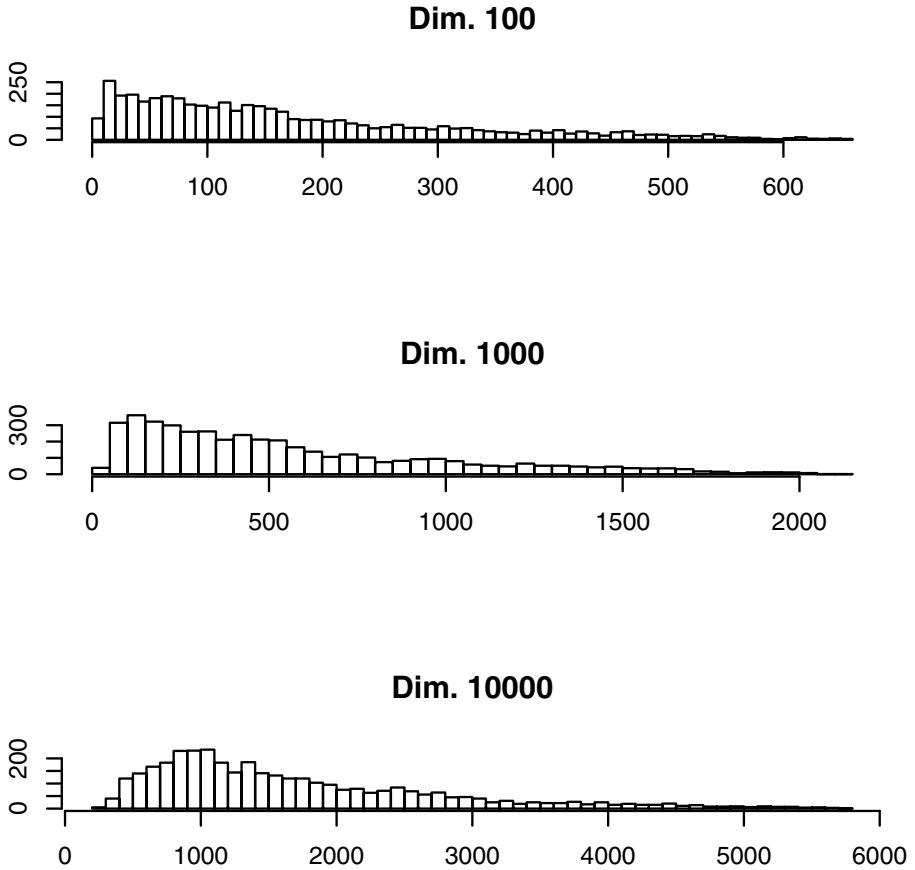


Fig. 9. Histograms of pairwise distances between embeddings in dimensionalities 100, 1000, 10000. Respectively the numbers of embeddings are: 95, 95 and 86.

We fit a Gaussian mixture model to the data shown in the bottom histogram of Figure 9. To derive the appropriate number of histogram peaks we fit Gaussians and use the Bayesian information criterion (BIC) as an approximate Bayes factor for model selection [36, 64]. Figure 10 shows the succession of outcomes, and indicates as best a 5-Gaussian fit. For this result, we find the means of the Gaussians to be as follows: 517, 885, 1374, 2273 and 3908. The corresponding standard deviations are: 84, 133, 212, 410 and 663. The respective cardinalities of the 5 histogram peaks are: 358, 1010, 1026, 911 and 350. Note that this relates so far only to the histogram of pairwise distances. We now want to determine the corresponding clusters in the input data.

While we have the segmentation of the distance histogram, we need the segmentation of the original financial signal. If we had 2 clusters in the original financial signal, then we could expect up to 3 peaks in the distances histogram

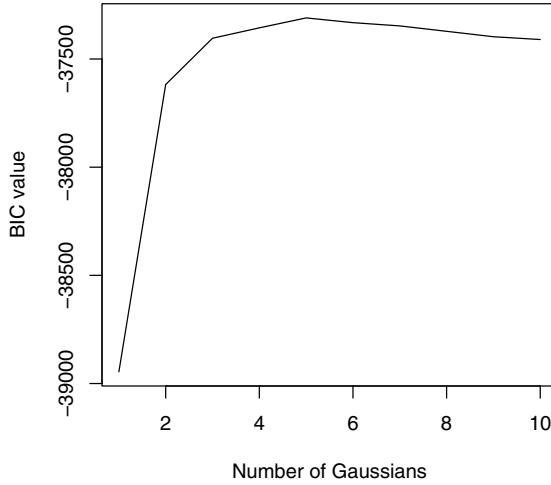


Fig. 10. BIC (Bayesian information criterion) values for the succession of results. The 5-cluster solution has the highest value for BIC and is therefore the best Gaussian mixture fit.

(viz., 2 intra-cluster peaks, and 1 inter-cluster peak). If we had 3 clusters in the original financial signal, then we could expect up to 6 peaks in the distances histogram (viz., 3 intra-cluster peaks, and 3 inter-cluster peaks). This information is consistent with asserting that the evidence from Figure 10 points to two of these histogram peaks being approximately co-located (alternatively: the distances are approximately the same). We conclude that 3 clusters in the original financial signal is the most consistent number of clusters. We will now determine these.

One possibility is to use principal coordinates analysis (Torgerson’s, Gower’s metric multidimensional scaling) of the pairwise distances. In fact, a 2-dimensional mapping furnishes a very similar pairwise distance histogram to that seen using the full, 10000, dimensionality. The first axis in Figure 11 accounts for 88.4% of the variance, and the second for 5.8%. Note therefore how the scales of the planar representation in Figure 11 point to it being very linear.

Benzécri ([4], chapter 7, section 3.1) discusses the Guttman effect, or Guttman scale, where factors that are not mutually correlated, are nonetheless functionally related. When there is a “fundamentally unidimensional underlying phenomenon” (there are multiple such cases here) factors are functions of Legendre polynomials. We can view Figure 11 as consisting of multiple horseshoe shapes. A simple explanation for such shapes is in terms of the constraints imposed by lots of equal distances when the data vectors are ordered linearly (see [56], pp. 46-47).

Another view of how embedded (hence clustered) data are capable of being well mapped into a unidimensional curve is Critchley and Heiser [9]. Critchley and Heiser show one approach to mapping an ultrametric into a linearly or

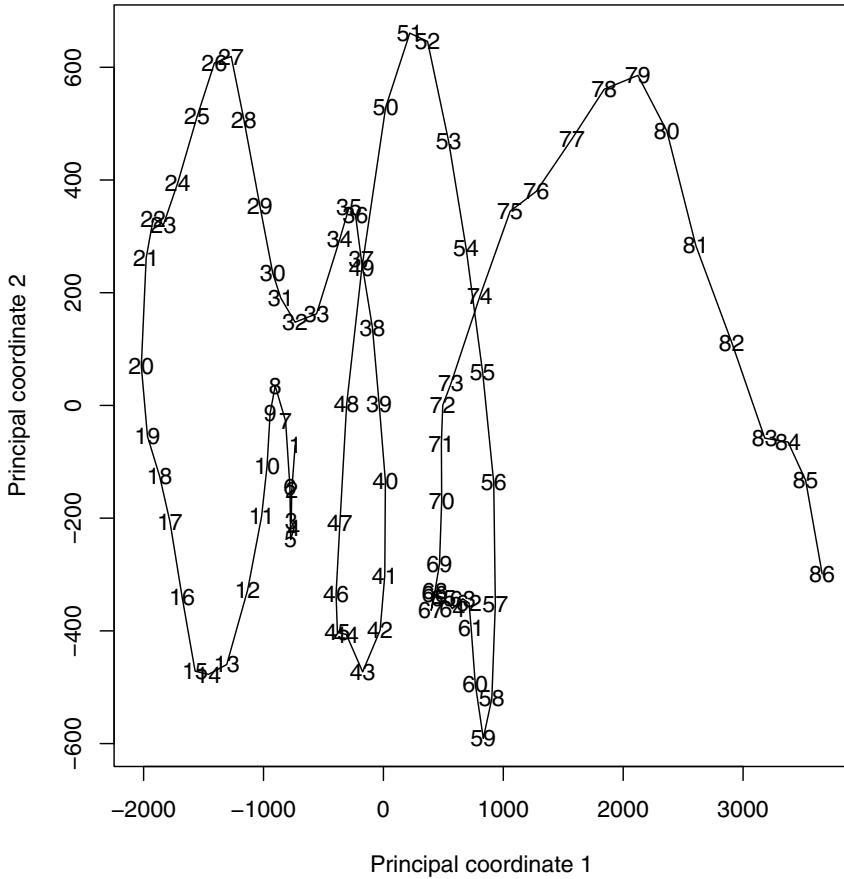


Fig. 11. An interesting representation – a type of “return map” – found using a principal coordinates analysis of the 86 successive 10000-dimensional points. Again a demonstration that very high dimensional structures can be of very simple structure. The planar projection seen here represents most of the information content of the data: the first axis accounts for 88.4% of the variance, while the second accounts for 5.8%.

totally ordered metric. We have asserted and then established how hierarchy in some form is relevant for high dimensional data spaces; and then we find a very linear projection in Figure 11. As a consequence we note that the Critchley and Heiser result is especially relevant for high dimensional data analysis.

Knowing that 3 clusters in the original signal are wanted, we could use Figure 11. There are various ways to do so.

We will use an adjacency-constrained agglomerative hierarchical clustering algorithm to find the clusters: see Figure 12. The contiguity-constrained complete link criterion is our only choice here if we are to be sure that no inversions can come about in the hierarchy, as explained in [53]. As input, we use the coordinates

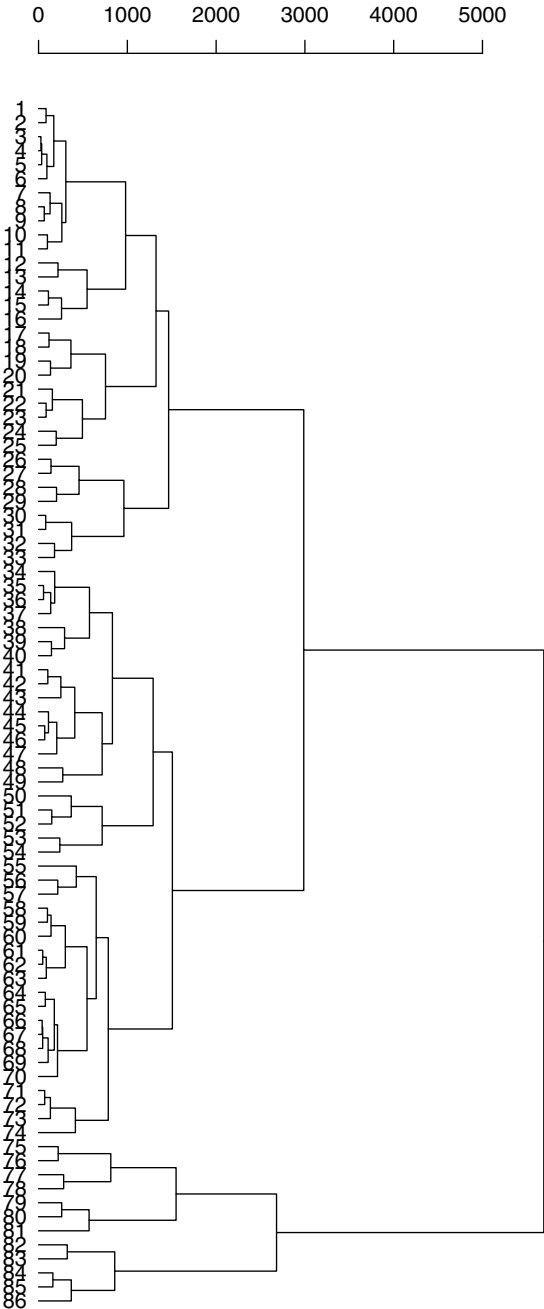


Fig. 12. Hierarchical clustering of the 86 points. Sequence is respected. The agglomerative criterion is the contiguity-constrained complete link method. See [53] for details including proof that there can be no inversion in this dendrogram.

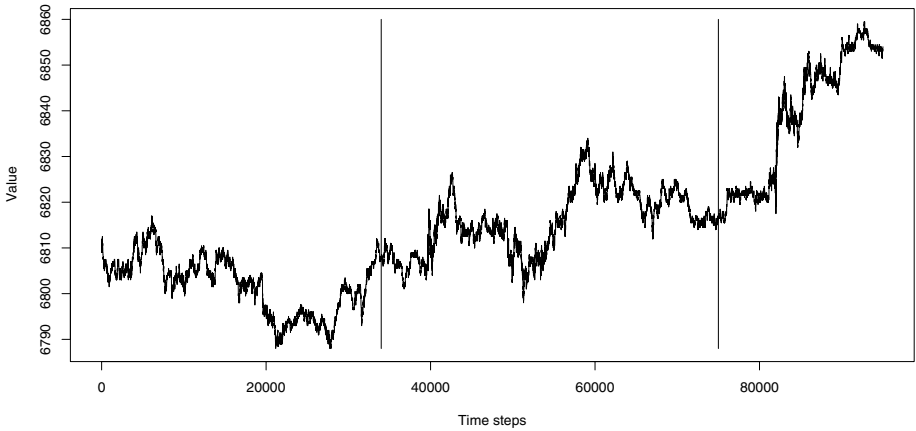


Fig. 13. Boundaries found for 3 segments

in Figure 11. The 2-dimensional Figure 11 representation relates to over 94% of the variance. The most complete basis was of dimensionality 85. We checked the results of the 85-dimensionality embedding which, as noted below, gave very similar results.

Reading off the 3-cluster memberships from Figure 12 gives for the signal actually used (with a very initial segment and a very final segment deleted): cluster 1 corresponds to signal values 1000 to 33999 (points 1 to 33 in Figure 12); cluster 2 corresponds to signal values 34000 to 74999 (points 34 to 74 in Figure 12); and cluster 3 corresponds to signal values 75000 to 86999 (points 75 to 86 in Figure 12). This allows us to segment the original time series: see Figure 13. (The clustering of the 85-dimensional embedding differs minimally. Segments are: points 1 to 32; 33 to 73; and 74 to 86.)

To summarize what has been done:

1. the segmentation is initially guided by the peak-finding in the histogram of distances
2. with high dimensionality we expect simple structure in a low dimensional mapping provided by principal coordinates analysis
3. either the original high dimensional data or the principal coordinates analysis embedding are used as input to a sequence-constrained clustering method in order to determine the clusters
4. which can then be displayed on the original data.

In this case, the clusters are defined using a complete link criterion, implying that these three clusters are determined by minimizing their maximum internal pairwise distance. This provides a strong measure of signal volatility as an explanation for the clusters, in addition to their average value.

7 Conclusions

Among themes not covered in this article are data stream clustering. To provide background and motivation, in [60], we discuss permutation representations of a data stream. Since hierarchies can also be represented as permutations, there is a ready way to associate data streams with hierarchies. In fact, early computational work on hierarchical clustering used permutation representation to great effect (cf. [73]). To analyze data streams in this way, in [57] we develop an approach to ultrametric embedding of time-varying signals, including biomedical, meteorological, financial and other. This work has been pursued in physics by Khrennikov.

Let us now wrap up on the exciting perspectives opened up by our work on the theme of symmetry-finding through hierarchy in very large data collections.

“My thesis has been that one path to the construction of a nontrivial theory of complex systems is by way of a theory of hierarchy.” Thus Simon ([74], p. 216). We have noted symmetry in many guises in the representations used, in the transformations applied, and in the transformed outputs. These symmetries are non-trivial too, in a way that would not be the case were we simply to look at classes of a partition and claim that cluster members were mutually similar in some way. We have seen how the p -adic or ultrametric framework provides significant focus and commonality of viewpoint.

Furthermore we have highlighted the computational scaling properties of our algorithms. They are fully capable of addressing the data and information deluge that we face, and providing us with the best interpretative and decision-making tools. The full elaboration of this last point is to be sought in each and every application domain, and face to face with old and new problems.

In seeking (in a general way) and in determining (in a focused way) structure and regularity in massive data stores, we see that, in line with the insights and achievements of Klein, Weyl and Wigner, in data mining and data analysis we seek and determine symmetries in the data that express observed and measured reality.

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