The Future of Search and Discovery in Big Data Analytics: Ultrametric Information Spaces

F. Murtagh (1, 2) and P. Contreras (2, 3)
(1) Science Foundation Ireland
(2) Thinking Safe Ltd.
(3) Computer Learning Research Centre
Department of Computer Science
Royal Holloway, University of London
February 17, 2012

Abstract
Consider observation data, comprised of \( n \) observation vectors with values on a set of attributes. This gives us \( n \) points in attribute space. Having data structured as a tree, implied by having our observations embedded in an ultrametric topology, offers great advantage for proximity searching. If we have preprocessed data through such an embedding, then an observation’s nearest neighbor is found in constant computational time, i.e. \( O(1) \) time. A further powerful approach is discussed in this work: the inducing of a hierarchy, and hence a tree, in linear computational time, i.e. \( O(n) \) time for \( n \) observations. It is with such a basis for proximity search and best match that we can address the burgeoning problems of processing very large, and possibly also very high dimensional, data sets.

1 Introduction
Under the heading of “Addressing the big data challenge”, the European 7th Framework Programme sees the issue thus (see INFSO, 2012): “Recent industry reports detail how data volumes are growing at a faster rate than our ability to interpret and exploit them for innovative ICT applications, for decision support, planning, monitoring, control and interaction. This includes unstructured data types such as video, audio, images and free text as well as structured data types such as database records, sensor readings and 3D. While each of these types requires some specific form of processing and analytics, many of the general principles for managing and storing them at extreme scales are common across all of them.” Analytics tool capability is called for, to address these burgeoning issues in the data intensive industries, to support “effective policy making and implementation” of public bodies resulting in “significant annual savings from
Big Data applications”, and also to exploit open, linked data – “foster the reuse of public sector information and strengthen other open data activities linked to commercial exploitation.” The “big data” marketplace is stated to be potentially worth approximately USD 600 billion.

To address the challenges of search and discovery in massive and complex data sets and data flows, it is our contention in this work that we must move to an appropriate topology – to an appropriate framework such that computation is greatly facilitated. Our work is all about empowering those who are involved in data analytics, through clustering and related algorithms, to face these new challenges. Scalability and interactivity are two of the performance issues that follow directly from clustering algorithms, for search, retrieval and discovery, that are of linear computational complexity or better (logarithmic, or constant).

2 Ultrametric Information Spaces

For high dimensional spaces and also for massive data spaces, it has been shown in Murtagh (2004) that one can exploit both symmetry and sparsity to great effect in order to carry out nearest neighbor or best match search and other related operations.

The triangular inequality holds for a metric space: \( d(x, z) \leq d(x, y) + d(y, z) \) for any triplet of points, \( x, y, z \). In addition the properties of symmetry and positive definiteness are respected. The “strong triangular inequality” or ultrametric inequality is: \( d(x, z) \leq \max\{d(x, y), d(y, z)\} \) for any triplet \( x, y, z \). An ultrametric space (Benzécri, 1979; van Rooij, 1978) implies respect for a range of stringent properties. For example, the triangle formed by any triplet is necessarily isosceles, with the two large sides equal; or is equilateral.

2.1 Computational Costs of Operations in an Ultrametric Space

Given that sparse forms of coding are considered for how complex stimuli are represented in the cortex (see Young and Yamane, 1992), the ultrametricity of such spaces becomes important because of this sparseness of coding. Among other implications, this points to the possibility that semantic pattern matching is best accomplished through ultrametric computation.

A convenient data structure for points in an ultrametric space is a dendrogram. We define a dendrogram as a rooted, labeled, ranked, binary tree (Murtagh, 1984a). For \( n \) observations, with such a definition of tree, there are precisely \( n - 1 \) levels. With each level there is an associated rank \( 1, 2, \ldots, n - 1 \), with level 1 corresponding to the singletons, and level \( n - 1 \) corresponding to the root node, and also to the cluster that encompasses all observations. With such a tree, there is an associated distance on the tree, termed the ultrametric distance, which is a mapping (of the Cartesian product of the observation set with itself) into the positive reals.
We will use the terms point and observation interchangeably, when the context allows. That is to say, an observation vector is a point in a space of ambient dimensionality defined by the cardinality of the attribute set, on which the observation takes values.

Operations on binary trees are often based on tree traversal between root and terminal. See e.g. van Rijsbergen (1979). Hence computational cost of such operations is dependent on root-to-terminal(s) path length. The total path length of a root-to-terminal traversal varies for each terminal (or point in the corresponding ultrametric space). It is simplest to consider path length in terms of level or tree node rank (and if it is necessary to avail of path length in terms of ultrametric distances, then constant computational time, only, is needed for table lookup). A dendrogram’s root-to-terminal path length can vary from close to \( \log_2 n \) (“close to” because the path length has to be an integer) to \( n - 1 \) (Murtagh, 1984b). Let us call this computational cost of a tree traversal \( O(t) \).

Most operations that we will now consider make use of a dendrogram data structure. Hence the cost of building a dendrogram is important. For the problem in general, see Krivánek and Morávek (1984, 1986) and Day (1996). For \( O(n^2) \) implementations of most commonly used hierarchical clustering algorithms, see Murtagh (1983, 1985). In section 3 we will address the issue of efficiently constructing a hierarchical clustering, and hence mapping observed data into an ultrametric topology. We will discuss a linear time approach for this.

To place a new point (from an ultrametric space) into a dendrogram, we need to find its nearest neighbor. We can do this, in order to write the new terminal into the dendrogram, using a root-to-terminal traversal in the current version of a dendrogram. This leads to our first proposition.

**Proposition 1**: The computational complexity of adding a new terminal to a dendrogram is \( O(t) \), where \( t \) is one traversal from root to terminals in the dendrogram.

**Proposition 2**: The computational complexity of finding the ultrametric distance between two terminal nodes is twice the length of a traversal from root to terminals in the dendrogram. Therefore distance is computed in \( O(t) \) time. Informally: we potentially have to traverse from each terminal to the root in order to find the common, “parent” node.

**Proposition 3**: The traversal length from dendrogram root to dendrogram terminals is best case 1, and worst case \( n - 1 \). When the dendrogram is optimally balanced or structured, the traversal length from root to terminals is \([\log_2 n]\), where \([\cdot]\) is the floor, or integer part, function. Hence \( 1 \geq O(t) \geq n - 1 \), and for a balanced tree \( O(t) = \log_2 n \).

Depending on the agglomerative criterion used, we can approximate the balanced or structured dendrogram – and hence favorable case – quite well in practice (Murtagh, 1984b). The Ward, or minimum variance, agglomerative criterion is shown empirically to be best.
**Proposition 4**: Nearest neighbor search in ultrametric space can be carried out in $O(1)$ or constant time.

This results from the following: the nearest neighbor pair must be in the same tightest cluster that contains them both. There is only one candidate to check for in a dendrogram. Hence nearest neighbor finding results in firstly finding the lowest level cluster containing the given terminal; followed by finding the other terminal in this cluster. Two operations are therefore required.

### 2.2 Implications

In Murtagh (2004a, 2004b) we have shown that high dimensional and sparse codings tend to be ultrametric. This is an interesting result in its own right. However a far more important result is that certain computational operations can be carried out very efficiently indeed in space endowed with an ultrametric.

Chief among these computational operations, we have noted, is that nearest neighbor finding can be carried out in (worst case) constant computational time, relative to the number of observables considered, $n$. Depending on the structure of the ultrametric space (i.e. if we can build a balanced dendrogram data structure), pairwise distance calculation can be carried out in logarithmic computational time.

We have also (Murtagh, 2004a) reviewed approaches to using ultrametric distances in order to expedite best match, or nearest neighbor, or more generally proximity search. The usual constructive approach, viz. build a hierarchic clustering, is simply not computationally feasible in very high dimensional spaces as are typically found in such fields as speech processing, information retrieval, or genomics and proteomics.

Forms of sparse coding are considered to be used in the human or animal cortex. We raise the interesting question as to whether human or animal thinking can be computationally efficient precisely because such computation is carried out in an ultrametric space. For further elaboration on this, see Murtagh (2012a, 2012b).

### 3 Linear Time and Direct Reading Hierarchical Clustering

In areas such as search, matching, retrieval and general data analysis, massive increase in data requires new methods that can cope well with the explosion in volume and dimensionality of the available data. The Baire metric, which is furthermore an ultrametric, has particular advantages when used to induce a hierarchy and in turn to support clustering, matching and other operations. See Murtagh and Contreras (2012), and Contreras and Murtagh (2012).

Arising directly out of the Baire distance is an ultrametric tree, which also can be seen as a tree that hierarchically clusters data. This presents a number of advantages when storing and retrieving data. When the data source is in
numerical form this ultrametric tree can be used as an index structure making matching and search, and thus retrieval, much easier.

The clusters can be associated with hash keys, that is to say, the cluster members can be mapped onto “bins” or “buckets”.

Another vantage point in this work is precision of measurement. Data measurement precision can be either used as given or modified in order to enhance the inherent ultrametric and hence hierarchical properties of the data.

Rather than mapping pairwise relationships onto the reals, as distance does, we can alternatively map onto subsets of the power set of, say, attributes of our observation set. This is expressed by the generalized ultrametric, which maps pairwise relationships into a partially ordered set (see Murtagh, 2011). It is also current practice as formal concept analysis where the range of the mapping is a lattice.

Relative to other algorithms the Baire-based hierarchical clustering method is fast. It is a direct reading algorithm involving one scan of the input data set, and is of linear computational complexity.

Many vantage points are possible, all in the Baire metric framework. The following vantage points are discussed in Murtagh and Contreras (2012).

- Metric that is simultaneously an ultrametric.
- Hierarchy induced through m-adic encoding (m positive integer, e.g. 10).
- p-Adic (p prime) or m-adic clustering.
- Hashing of data into bins.
- Data precision of measurement implies how hierarchical the data is.
- Generalized ultrametric.
- Lattice-based formal concept analysis.
- Linear computational time hierarchical clustering.

3.1 Ultrametric Baire Space and Distance

A Baire space 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. What is of interest to us is this longest common prefix metric, which we call the Baire distance (Bradley, 2009; Mirkin and Fishburn, 1979; Murtagh et al., 2008).

We begin with the longest common prefixes at issue being digits of precision of univariate or scalar values. For example, let us consider two such decimal values, $x$ and $y$, with both measured to some maximum precision. We take as maximum precision the length of the value with the fewer decimal digits. With no loss of generality we take $x$ and $y$ to be bounded by 0 and 1. Thus we consider ordered sets $x_k$ and $y_k$ for $k \in K$. So $k = 1$ is the first decimal place of
precision; \( k = 2 \) is the second decimal place; \( \ldots \); \( k = |K| \) is the \( |K| \)th decimal place. The cardinality of the set \( K \) is the precision with which a number, \( x \) or \( y \), is measured.

Consider as examples \( x_3 = 0.478 \); and \( y_3 = 0.472 \). Start from the first decimal position. For \( k = 1 \), we find \( x_1 = y_1 = 4 \). For \( k = 2 \), \( x_2 = y_2 = 7 \). But for \( k = 3 \), \( x_3 \neq y_3 \).

We now introduce the following distance (case of vectors \( x \) and \( y \), with 1 attribute, hence unidimensional):

\[
d_B(x_K, y_K) = \begin{cases} 
1 & \text{if } x_1 \neq y_1 \\
\inf \mathcal{B}^{-\nu} & \text{if } x_1 = y_1, \ 1 \leq \nu \leq |K|
\end{cases}
\]  

(1)

We call this \( d_B \) value Baire distance, which is a 1-bounded ultrametric (Bradley, 2009; Murtagh, 2007) distance, \( 0 < d_B \leq 1 \). When dealing with binary (boolean) data \( B = 2 \). When working with real numbers the base is best defined to be \( B = 10 \). With \( B = 10 \), for instance, it can be seen that the Baire distance is embedded in a 10-way tree which leads to a convenient data structure to support search and other operations when we have decimal data. As a consequence data can be organized, stored and accessed very efficiently and effectively in such a tree.

For \( B \) prime, this distance has been studied by Benoist-Pineau et al. (2001) and by Bradley (2009, 2010), with many further (topological and number theoretic, leading to algorithmic and computational) insights arising from the \( p \)-adic (where \( p \) is prime) framework. See also Anashin and Khrennikov (2009).

For use of random projections to allow for analysis of multidimensional data in the scope of the Baire distance, see Contreras and Murtagh (2012) and also Murtagh and Contreras (2012). In these works, a range of very large data sets are considered, for clustering and for proximity search, in domains that include astronomy (photometric and astrometric redshifts), and chemoinformatics.

### 3.2 Linear Time, or \( O(N) \) Computational Complexity, Hierarchical Clustering

A point of departure for our work has been the computational objective of bypassing computationally demanding hierarchical clustering methods (typically quadratic time, or \( O(n^2) \) for \( n \) input observation vectors), but also having a framework that is of great practical importance in terms of the application domains.

Agglomerative hierarchical clustering algorithms are based on pairwise distances (or dissimilarities) implying computational time that is \( O(n^2) \) where \( n \) is the number of observations. The implementation required to achieve this is, for most agglomerative criteria, the nearest neighbor chain, together with the reciprocal nearest neighbors, algorithm (furnishing inversion-free hierarchies whenever Bruynooghe’s reducibility property, see Murtagh (1985), is satisfied by the cluster criterion).

This quadratic time requirement is a worst case performance result. It is most often the average time also since the pairwise agglomerative algorithm

\[6\]
is applied directly to the data without any preprocessing speed-ups (such as preprocessing that facilitates fast nearest neighbor finding). An example of a linear average time algorithm for (worst case quadratic computational time) agglomerative hierarchical clustering is in Murtagh (1983).

With the Baire-based hierarchical clustering algorithm, we have an algorithm for linear time worst case hierarchical clustering. It can be characterized as a divisive rather than an agglomerative algorithm.

### 3.3 Grid-Based Clustering Algorithms

The Baire-based hierarchical clustering algorithm has characteristics that are related to grid-based clustering algorithms, and density-based clustering algorithms, which – often – were developed in order to handle very large data sets.

The main idea here is to use a grid like structure to split the information space, separating the dense grid regions from the less dense ones to form groups. In general, a typical approach within this category will consist of the following steps (Grabusts and Borisov, 2002):

1. Creating a grid structure, i.e. partitioning the data space into a finite number of non-overlapping cells.
2. Calculating the cell density for each cell.
3. Sorting of the cells according to their densities.
4. Identifying cluster centers.
5. Traversal of neighbor cells.

Additional background on grid-based clustering can be found in the following works: Chang and Jin (2002), Gan et al. (2007), Park and Lee (2004), and Xu and Wunsch (2008).

Cluster bins, derived from an m-adic tree, provide us with a grid-based framework or data structuring. We can read off the cluster bin members from an m-adic tree. An m-adic tree requires one scan through the data, and therefore this data structure is constructed in linear computational time.

In such a preprocessing context, clustering with the Baire distance can be seen as a “crude” method for getting clusters. After this we can use more traditional techniques to refine the clusters in terms of their membership. Alternatively (and we have quite extensively compared Baire clustering with, e.g. k-means, where it compares very well, see Murtagh et al., 2008, and Contreras and Murtagh, 2012) clustering with the Baire distance can be seen as fully on a par with any optimization algorithm for clustering. As optimization, and just as one example from the many examples reviewed in this article, the Baire approach optimizes an m-adic fit of the data simply by reading the m-adic structure directly from the data.
4 Conclusions

Baire distance is an ultrametric, so we can think of reading off observations as a tree.

Through data precision of measurement, alone, we can enhance inherent ultrametricity, or inherent hierarchical properties in the data.

Clusters in such a Baire-based hierarchy are simple “bins” and assignments are determined through a very simple hashing. (E.g. $0.3475 \rightarrow$ bin 3, and $0.34 \rightarrow$ bin 34, and $0.347 \rightarrow$ bin 347, and $0.3475 \rightarrow$ bin 3475.)

As we have observed, certain search-related computational operations can be carried out very efficiently indeed in space endowed with an ultrametric. Chief among these computational operations is that nearest neighbor finding can be carried out in (worst case) constant computational time. Depending on the structure of the ultrametric space (i.e. if we can build a balanced dendrogram data structure), pairwise distance calculation can be carried out in logarithmic computational time.

In conclusion we have here a comprehensive approach, founded on ultrametric topology rather than more traditional metric geometry, in order to address the burgeoning problems presented by “big data” analytics, i.e. massive data sets in potentially very high dimensional spaces.

References

1. V. Anashin and A. Khrennikov, Applied Algebraic Dynamics, De Gruyter, 2009.

2. J. Benois-Pineau, A.Yu. Khrennikov and N.V. Kotovich, “Segmentation of images in p-adic and Euclidean metrics”, Dokl. Math., 64, 450–455, 2001.

3. J.P. Benzécri, La Taxinomie, Dunod, 2nd edition, 1979.

4. P.E. Bradley, “On p-adic classification”, p-Adic Numbers, Ultrametric Analysis, and Applications, 1:271–285, 2009.

5. P.E. Bradley, “Mumford dendrograms”, Journal of Classification, 53:393–404, 2010.

6. Jae-Woo Chang and Du-Seok Jin, “A new cell-based clustering method for large, high-dimensional data in data mining applications”, in SAC ’02: Proceedings of the 2002 ACM symposium on Applied computing, pages 503–507, 2002.

7. P. Contreras and F. Murtagh, “A very fast, linear time p-adic and hierarchical clustering algorithm using the Baire metric”, Journal of Classification, forthcoming, 2012.
8. W.H.E. Day, “Complexity theory: An introduction for practitioners of classification”, in P. Arabie, L.J. Hubert and G. De Soete, Eds., Clustering and Classification, Singapore: World Scientific, 199–233, 1996.

9. Guojun Gan, Chaoqun Ma, and Jianhong Wu, Data Clustering Theory, Algorithms, and Applications, Society for Industrial and Applied Mathematics. SIAM, 2007.

10. P. Grabusts and A. Borisov, “Using grid-clustering methods in data classification”, In PARELEC 02: Proceedings of the International Conference on Parallel Computing in Electrical Engineering, p. 425, Washington, DC, USA, 2002. IEEE Computer Society.

11. INFSO – Directorate General Information Society, European Commission, FP7 ICT Work Programme 2013 Orientations, Overview, Version 10/01/2012, white paper INFSO-C2/10/01/2012.

12. M. Krivánek and J. Morávek, “NP-hard problems in hierarchical-tree clustering”, Acta Informatica, 23, 311–323, 1986.

13. M. Krivánek and J. Morávek, “On NP-hardness in hierarchical clustering”, in T. Havránek, Z. Sidák and M. Novák, ed., Compstat 1984: Proceedings in Computational Statistics, 189–194, Vienna: Physica-Verlag, 1984.

14. B. Mirkin and P. Fishburn, Group Choice, V.H. Winston, 1979.

15. F. Murtagh, “Expected time complexity results for hierarchic clustering algorithms that use cluster centers”, Information Processing Letters, 16:237–241, 1983.

16. F. Murtagh, Multidimensional Clustering Algorithms, Physica-Verlag, 1985.

17. F. Murtagh, “Counting dendrograms: a survey”, Discrete Applied Mathematics, 7, 191–199, 1984a.

18. F. Murtagh, “Structures of hierarchic clusterings: Implications for information retrieval and for multivariate data analysis”, Information Processing and Management, 20, 611–617, 1984b.

19. F. Murtagh, “On ultrametricity, data coding, and computation”, Journal of Classification, 21, 167–184, 2004a.

20. F. Murtagh, “Thinking ultrametrically”, in D. Banks, L. House, F.R. McMorris, P. Arabie and W. Gaul, Eds., Classification, Clustering, and Data Mining Applications, Springer, 3–14, 2004b.

21. F. Murtagh, G. Downs, and P. Contreras, “Hierarchical clustering of massive, high dimensional datasets by exploiting ultrametric embedding”, SIAM Journal on Scientific Computing, 30(2):707-730, February 2008.
22. F. Murtagh, “Ultrametric and generalized ultrametric in logic and in data analysis”, in T.S. Clary, Ed., *Horizons in Computer Science, Volume 2*, pp. 251-267, Nova Science Publishers, 2011.

23. F. Murtagh and P. Contreras, “Fast, linear time, m-adic hierarchical clustering for search and retrieval using the Baire metric, with linkages to generalized ultrametrics, hashing, formal concept analysis, and precision of data measurement”, *p-Adic Numbers, Ultrametric Analysis, and Applications*, 4, 45–56, 2012.

24. F. Murtagh, “Ultrametric model of mind, I: Review”, [http://arxiv.org/abs/1201.2711](http://arxiv.org/abs/1201.2711) 2012a.

25. F. Murtagh, “Ultrametric model of mind, II: Application to text content analysis”, [http://arxiv.org/abs/1201.2719](http://arxiv.org/abs/1201.2719) 2012b.

26. Nam Hun Park and Won Suk Lee, “Statistical grid-based clustering over data streams”, *SIGMOD Record*, 33(1):32–37, 2004.

27. C.J. van Rijsbergen, *Information Retrieval*, Butterworths, 1979.

28. A.C.M. van Rooij, *Non-Archimedean Functional Analysis*. Marcel Dekker, 1978.

29. M.P. Young and S. Yamane, “Sparse population coding of faces in the inferotemporal cortex”, *Science*, 256, 1327–1331, 1992.

30. Rui Xu and D.C. Wunsch, *Clustering*, IEEE Computer Society Press, 2008.