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# DeBaCl: A Python Package for Interactive DEnsity-BAsed CLustering

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#### Abstract

The level set tree approach of Hartigan (1975) provides a probabilistically based and highly interpretable encoding of the clustering behavior of a dataset. By representing the hierarchy of data modes as a dendrogram of the level sets of a density estimator, this approach offers many advantages for exploratory analysis and clustering, especially for complex and high-dimensional data. Several R packages exist for level set tree estimation, but their practical usefulness is limited by computational inefficiency, absence of interactive graphical capabilities and, from a theoretical perspective, reliance on asymptotic approximations. To make it easier for practitioners to capture the advantages of level set trees, we have written the Python package **DeBaCl** for DEnsity-BAsed CLustering. In this article we illustrate how **DeBaCl**'s level set tree estimates can be used for difficult clustering tasks and interactive graphical data analysis. The package is intended to promote the practical use of level set trees through improvements in computational efficiency and a high degree of user customization. In addition, the flexible algorithms implemented in **DeBaCl** enjoy finite sample accuracy, as demonstrated in recent literature on density clustering. Finally, we show the level set tree framework can be easily extended to deal with functional data.

*Keywords*: density-based clustering, level set tree, Python, interactive graphics, functional data analysis.

# 1. Introduction

Clustering is one of the most fundamental tasks in statistics and machine learning, and numerous algorithms are available to practitioners. Some of the most popular methods, such as K-means (MacQueen 1967; Lloyd 1982) and spectral clustering (Shi and Malik 2000), rely

on the key operational assumption that there is one optimal partition of the data into K well-separated groups, where K is assumed to be known *a priori*. While effective in some cases, this flat or scale-free notion of clustering is inadequate when the data are very noisy or corrupted, or exhibit complex multimodal behavior and spatial heterogeneity, or simply when the value of K is unknown. In these cases, hierarchical clustering affords a more realistic and flexible framework in which the data are assumed to have multi-scale clustering features that can be captured by a hierarchy of nested subsets of the data. The expression of these subsets and their order of inclusions—typically depicted as a dendrogram—provide a great deal of information that goes beyond the original clustering task. In particular, it frees the practitioner from the requirement of knowing in advance the "right" number of clusters, provides a useful global summary of the entire dataset, and allows the practitioner to identify and focus on interesting sub-clusters at different levels of spatial resolution.

There are, of course, myriad algorithms just for hierarchical clustering. However, in most cases their usage is advocated on the basis of heuristic arguments or computational ease, rather than well-founded theoretical guarantees. The high-density hierarchical clustering paradigm put forth by Hartigan (1975) is an exception. It is based on the simple but powerful definition of clusters as the maximal connected components of the super-level sets of the probability density specifying the data-generating distribution. This formalization has numerous advantages: (1) it provides a probabilistic notion of clustering that conforms to the intuition that clusters are the regions with largest probability to volume ratio; (2) it establishes a direct link between the clustering task and the fundamental problem of nonparametric density estimation; (3) it allows for a clear definition of clustering performance and consistency (Hartigan 1981) that is amenable to rigorous theoretical analysis and (4) as we show below, the dendrogram it produces is highly interpretable, offers a compact yet informative representation of a distribution, and can be interactively queried to extract and visualize subsets of data at desired resolutions. Though the notion of high-density clustering has been studied for quite some time (Polonik 1995), recent theoretical advances have further demonstrated the flexibility and power of density clustering. See, for example, Rinaldo, Singh, Nugent, and Wasserman (2012); Rinaldo and Wasserman (2010); Kpotufe and Luxburg (2011); Chaudhuri and Dasgupta (2010); Steinwart (2011); Sriperumbudur and Steinwart (2012); Lei, Robins, and Wasserman (2013); Balakrishnan, Narayanan, Rinaldo, Singh, and Wasserman (2013) and the refences therein.

This paper introduces the Python package **DeBaCl** for efficient and statistically-principled DEnsity-BAsed CLustering. **DeBaCl** is not the first implementation of level set tree estimation and clustering; the R packages **denpro** (Klemelä 2004), **gslclust** (Stuetzle and Nugent 2010), and **pdfCluster** (Azzalini and Menardi 2012) also contain various level set tree estimators. However, they tend to be too inefficient for most practical uses and rely on methods lacking rigorous theoretical justification. The popular nonparametric density-based clustering algorithm DBSCAN (Ester, Kriegel, and Xu 1996) is implemented in the R package **fpc** (Hennig 2013) and the Python library **scikit-learn** (Pedregosa, Varoquaux, Gramfort, Michel, Thirion, Grisel, Blondel, Prettenhofer, Weiss, Dubourg, Vanderplas, Passos, Cournapeau, Brucher, Perrot, and Duchesnay 2011), but this method does not provide an estimate of the level set tree.

**DeBaCl** handles much larger datasets than existing software, improves computational speed,

and extends the utility of level set trees in three important ways: (1) it provides several novel visualization tools to improve the readability and interpetability of density cluster trees; (2) it offers a high degree of user customization; and (3) it implements several recent methodological advances. In particular, it enables construction of level set trees for arbitrary functions over a dataset, building on the idea that level set trees can be used even with data that lack a bona fide probability density function. **DeBaCl** also includes the first practical implementation of the recent, theoretically well-supported algorithm from Chaudhuri and Dasgupta (2010).

#### 2. Level set trees

Suppose we have a collection of points  $\mathbb{X}_n = \{x_1, \ldots, x_n\}$  in  $\mathbb{R}^d$ , which we model as i.i.d. draws from an unknown probability distribution with probability density function f (with respect to Lebesgue measure). Our goal is to identify and extract clusters of  $\mathbb{X}_n$  without any *a priori* knowledge about f or the number of clusters. Following the statistically-principled approach of Hartigan (1975), clusters can be identified as modes of f. For any threshold value  $\lambda \geq 0$ , the  $\lambda$ -upper level set of f is

$$L_{\lambda}(f) = \{ x \in \mathbb{R}^d : f(x) \ge \lambda \}.$$
(1)

The connected components of  $L_{\lambda}(f)$  are called the  $\lambda$ -clusters of f and high-density clusters are  $\lambda$ -clusters for any value of  $\lambda$ . It is easy to see that  $\lambda$ -clusters associated with larger values of  $\lambda$  are regions where the ratio of probability content to volume is higher. Also note that for a fixed value of  $\lambda$ , the corresponding set of clusters will typically not give a partition of  $\{x : f(x) \ge 0\}$ .

The level set tree is simply the set of all high-density clusters. This collection is a tree because it has the following property: for any two high-density clusters A and B, either A is a subset of B, B is a subset of A, or they are disjoint. This property allows us to visualize the level set tree with a dendrogram that shows all high-density clusters simultaneously and can be queried quickly and directly to obtain specific cluster assignments. Branching points of the dendrogram correspond to density levels where two or more modes of the pdf, i.e. new clusters, emerge. Each vertical line segment in the dendrogram represents the high-density clusters within a single pdf mode; these clusters are all subsets of the cluster at the level where the mode emerges. Line segments that do not branch are considered high-density modes, which we call the leaves of the tree. For simplicity, we tend to refer to the dendrogram as the level set tree itself.

Because f is unknown, the level set tree must be estimated from the data. Ideally we would use the high-density clusters of a suitable density estimate  $\hat{f}$  to do this; for a well-behaved fand a large sample size,  $\hat{f}$  is close to f with high probability so the level set tree for  $\hat{f}$  would be a good estimate for the level set tree of f (Chaudhuri and Dasgupta 2010). Unfortunately, this approach is not computationally feasible even for low-dimensional data because finding the upper level sets of  $\hat{f}$  requires evaluating the function on a dense mesh and identifying  $\lambda$ -clusters requires a combinatorial search over all possible paths connecting any two points in the mesh.

Many methods have been proposed to overcome these computational obstacles. The first

category includes techniques that remain faithful to the idea that clusters are regions of the sample space. Members of this family include histogram-based partitions (Klemelä 2004), binary tree partitions (Klemelä 2005) (implemented in the R package **denpro**) and Delaunay triangulation partitions (Azzalini and Torelli 2007) (implemented in R package **pdfCluster**). These techniques tend to work well for low-dimension data, but suffer from the curse of dimensionality because partitioning the sample space requires an exponentially increasing number of cells or algorithmic complexity (Azzalini and Torelli 2007).

In contrast, another family of estimators produces high-density clusters of data points rather than sample space regions; this is the approach taken by our package. Conceptually, these methods estimate the level set tree of f by intersecting the level sets of f with the sample points  $X_n$  and then evaluating the connectivity of each set by graph theoretic means. This typically consists of three high-level steps: estimation of the probability density  $\hat{f}(x)$  from the data; construction of a graph G that describes the similarity between each pair of data points; and a search for connected components in a series of subgraphs of G induced by removing nodes and/or edges of insufficient weight, relative to various density levels.

The variations within the latter category are found in the definition of G, the set of density levels over which to iterate, and the way in which G is restricted to a subgraph for a given density level  $\lambda$ . Edge iteration methods assign a weight to the edges of G based on the proximity of the incident vertices in feature space (Chaudhuri and Dasgupta 2010) or the value of  $\hat{f}(x)$  at the incident vertices (Wong and Lane 1983) or on a line segment connecting them (Stuetzle and Nugent 2010). For these procedures, the relevant density levels are the edge weights of G. Frequently, iteration over these levels is done by initializing G with an empty edge set and adding successively more heavily weighted edges, in the manner of traditional single linkage clustering. In this family, the Chaudhuri and Dasgupta algorithm (which is a generalization of Wishart (1969)) is particularly interesting because the authors prove finite sample rates for convergence to the true level set tree (Chaudhuri and Dasgupta 2010). To the best of our knowledge, however, only Stuetzle and Nugent (2010) has a publicly available implementation, in the R package **gslclust**.

Point iteration methods construct G so the vertex for observation  $x_i$  is weighted according to  $\widehat{f}(x_i)$ , but the edges are unweighted. In the simplest form, there is an edge between the vertices for observations  $x_i$  and  $x_j$  if the distance between  $x_i$  and  $x_j$  is smaller than some threshold value, or if  $x_i$  and  $x_j$  are among each other's k-closest neighbors (Kpotufe and Luxburg 2011; Maier, Hein, and von Luxburg 2009). A more complicated version places an edge  $(x_i, x_j)$  in G if the amount of probability mass that would be needed to fill the valleys along a line segment between  $x_i$  and  $x_j$  is smaller than a user-specified threshold (Menardi and Azzalini 2013). The latter method is available in the R package **pdfCluster**.

## 3. Implementation

The default level set tree algorithm in **DeBaCl** is described in Algorithm 1, based on the method proposed by Kpotufe and Luxburg (2011) and Maier *et al.* (2009). For a sample with

*n* observations in  $\mathbb{R}^d$ , the k-nearest neighbor (kNN) density estimate is:

$$\widehat{f}(x_j) = \frac{k}{n \cdot v_d \cdot r_k^d(x_j)} \tag{2}$$

where  $v_d$  is the volume of the Euclidean unit ball in  $\mathbb{R}^d$  and  $r_k(x_j)$  is the Euclidean distance from point  $x_j$  to its k'th closest neighbor. The process of computing subgraphs and finding connected components of those subgraphs is implemented with the **igraph** package (Csardi and Nepusz 2006). Our package also depends on the **NumPy** and **SciPy** packages for basic computation (Jones, Oliphant, and Peterson 2001) and the **Matplotlib** package for plotting (Hunter 2007). We use this algorithm because it is straightforward and fast; although it does require

Algorithm 1: Baseline DeBaCl level set tree estimation procedure

Input:  $\{x_1, \ldots, x_n\}, k, \gamma$ Output:  $\widehat{\mathcal{T}}$ , a hierarchy of subsets of  $\{x_1, \ldots, x_n\}$   $G \leftarrow k$ -nearest neighbor similarity graph on  $\{x_1, \ldots, x_n\}$ ;  $\widehat{f}(\cdot) \leftarrow k$ -nearest neighbor density estimate based on  $\{x_1, \ldots, x_n\}$ ; for  $j \leftarrow 1$  to n do  $\lambda_j \leftarrow \widehat{f}(x_j)$ ;  $L_{\lambda_j} \leftarrow \{x_i : \widehat{f}(x_i) \ge \lambda_j\}$ ;  $G_j \leftarrow$  subgraph of G induced by  $L_j$ ; Find the connected components of  $G_{\lambda_j}$ ;  $\widehat{\mathcal{T}} \leftarrow$  dendrogram of connected components of graphs  $G_1, \ldots, G_n$ , ordered by inclusions;  $\widehat{\mathcal{T}} \leftarrow$  remove components of size smaller than  $\gamma$ ; return  $\widehat{\mathcal{T}}$ 

computation of all  $\binom{n}{2}$  pairwise distances, the procedure can be substantially shortened by estimating connected components on a sparse grid of density levels. The implementation of this algorithm is novel in its own right (to the best of our knowledge), and **DeBaCl** includes several other new visualization and methodological tools.

#### 3.1. Visualization tools

Our level set tree plots increase the amount of information contained in a tree visualization and greatly improve interpretability relative to existing software. Suppose a sample of 2,000 observations in  $\mathbb{R}^2$  from a mixture of three Gaussian distributions (Figure 1a). The traditional level set tree is illustrated in Figure 1b and the **DeBaCl** version in Figure 1c. A plot based only on the mathematical definition of a level set tree conveys the structure of the mode hierarchy and indicates the density levels where each tree node begins and ends, but does not indicate how many points are in each branch or visually associate the branches with a particular subset of data. In the proposed software package, level set trees are plotted to emphasize the empirical mass in each branch (i.e. the fraction of data in the associated cluster): tree branches are sorted from left-to-right by decreasing empirical mass, branch widths are proportional to empirical mass, and the white space around the branches is proportional to empirical mass. For matching tree nodes to the data, branches can be colored to correspond to high-density data clusters (Figures 1c and 1d). Clicking on a tree branch produces a banner that indicates the start and end levels of the associated high-density cluster as well as its empirical mass (Figure 5a).

The level set tree plot is an excellent tool for interactive exploratory data analysis because it acts as a handle for identifying and plotting spatially coherent, high-density subsets of data. The full power of this feature can be seen clearly with the more complex data of Section 4.



Figure 1: Level set tree plots and cluster labeling for a simple simulation. A level set tree is constructed from a sample of 2,000 observations drawn from a mix of three Gaussians in  $\mathbb{R}^2$ . a) The kNN density estimator evaluated on the data. b) A plot of the tree based only on the mathematical definition of level set trees. c) The new level set tree plot, from **DeBaCl**. Tree branches emphasize empirical mass through ordering, spacing, and line width, and they are colored to match the cluster labels in d. A second vertical axis is added that indicates that fraction of background mass at each critical density level. d) Cluster labels from the *all-mode* labeling technique, where each leaf of the level set tree is designated as a cluster.

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#### 3.2. Alternate scales

By construction, the nodes of a level set tree are indexed by density levels  $\lambda$ , which determine the scale of the vertical axis in a plot of the tree. While this does encode the parent-child relationships in the tree, interpretability of the  $\lambda$  scale is limited by the fact that it depends on the height of the density estimate  $\hat{f}$ . It is not clear, for example, whether  $\lambda = 1$  would be a low- or a high-density threshold; this depends on the particular distribution.

To remove the scale dependence we can instead index level set tree nodes based on the probability content of upper level sets. Specifically, let  $\alpha$  be a number between 0 and 1 and define

$$\lambda_{\alpha} = \sup\left\{\lambda \colon \int_{x \in L_{\lambda}(f)} f(x) dx \ge \alpha\right\}$$
(3)

to be the value of  $\lambda$  for which the upper level set of f has probability content no smaller than  $\alpha$  (Rinaldo *et al.* 2012). The map  $\alpha \mapsto \lambda_{\alpha}$  gives a monotonically decreasing one-to-one correspondence between values of  $\alpha$  in [0, 1] and values of  $\lambda$  in  $[0, \max_x f(x)]$ . In particular,  $\lambda_1 = 0$  and  $\lambda_0 = \max_x f(x)$ . For an empirical level set tree, set  $\lambda_{\alpha}$  to the  $\alpha$ -quantile of  $\{\hat{f}(x_i)\}_{i=1}^n$ . Expressing the height of the tree in terms of  $\alpha$  instead of  $\lambda$  does not change the topology (i.e. number and ordering of the branches) of the tree; the re-indexed tree is a deformation of the original tree in which some of its nodes are stretched out and others are compressed.

 $\alpha$ -indexing is more interpretable and useful for several reasons. The  $\alpha$  level of the tree indexes clusters corresponding to the  $1 - \alpha$  fraction of "most clusterable" data points; in particular, larger  $\alpha$  values yield more compact and well-separated clusters, while smaller values can be used for de-noising and outlier removal. Because  $\alpha$  is always between 0 and 1, scaling by probability content also enables comparisons of level set trees arising from data sets drawn from different pdfs, possibly in spaces of different dimensions. Finally, the  $\alpha$ -index is more effective than  $\lambda$ -indexing in representing regions of large probability content but low density and is less affected by small fluctuations in density estimates.

A common (incorrect) intuition when looking at an  $\alpha$ -indexed level set tree plot is to interpret the height of the branches as the size of the corresponding cluster, as measured by its empirical mass. However, with  $\alpha$ -indexing the height of any branch depends on its empirical mass as well as the empirical mass of all other branches that coexist with it. In order to obtain trees that do conform to this intuition, we introduce the  $\kappa$ -indexed level set tree.

Recall from Section 2 that clusters are defined as maximal connected components of the sets  $L_{\lambda}(f)$  (see equation 1) as  $\lambda$  varies from 0 to  $\max_x f(x)$ , and that the level set tree is the dendrogram representing the hierarchy of all clusters. Assume the tree is binary and with tooted. Let  $\{1, 2, \ldots, K\}$  be an enumeration of the nodes of the level set tree and let  $\mathcal{C} = \{C_0, \ldots, C_K\}$  be the corresponding clusters. We can always choose the enumeration in a way that is consistent with the hierarchy of inclusions of the elements of  $\mathcal{C}$ ; that is,  $C_0$  is the support of f (which we assume for simplicity to be a connected set) and if  $C_i \subset C_j$ , then i > j. For a node i > 0, we denote with parent<sub>i</sub> the unique node j such that  $C_j$  is the smallest element of  $\mathcal{C}$  such that  $C_j \supset C_i$ . Similarly, kid<sub>i</sub> is the pair of nodes (j, j') such that  $C_j$  and

 $C_{j'}$  are the maximal subsets of  $C_i$ . Finally, for i > 0, sib<sub>i</sub> is the node j such there exists a k for which kid<sub>k</sub> = (i, j). For a cluster  $C_i \in C$ , we set

$$M_i = \int_{C_i} f(x) dx, \tag{4}$$

which we refer to as the mass of  $C_i$ .

The true  $\kappa$ -tree can be defined recursively by associating with each node *i* two numbers  $\kappa'_i$  and  $\kappa''_i$  such that  $\kappa'_i - \kappa''_i$  is the *salient mass* of node *i*. For leaf nodes, the salient mass is the mass of the cluster, and for non-leaves it is the mass of the cluster boundary region.  $\kappa'$  and  $\kappa''$  are defined differently for each node type.

1. Internal nodes, including the root node.

$$\kappa_0' = M_0 = 1,$$
  

$$\kappa_i' = \kappa_{\text{parent}_i}''$$
  

$$\kappa_i'' = \sum_{j \in \text{kid}_i} M_j + \sum_{k \in \text{sib}_i} M_k$$

2. Leaf nodes.

$$\kappa_i' = \kappa_{\text{parent}_i}''$$
$$\kappa_i'' = \kappa_i' - M_i$$

To estimate the  $\kappa$ -tree, we use  $\hat{f}$  instead of f and let  $m_i$  be the fraction of data contained in the cluster for the tree node i at birth. Again, define the estimated tree recursively:

$$\begin{aligned} \widehat{\kappa}'_0 &= 1, \\ \widehat{\kappa}'_i &= \widehat{\kappa}''_{\text{parent}_i}, \\ \widehat{\kappa}''_i &= \widehat{\kappa}'_i - m_i + \sum_{j \in \text{kid}_i} m_j. \end{aligned}$$

In practice we subtract the above quantities from 1 to get an increasing scale that matches the  $\lambda$  and  $\kappa$  scales.

Note that switching between the  $\lambda$  to  $\alpha$  index does not change the overall shape of the tree, but switching to the  $\kappa$  index *does*. In particular, the tallest leaf of the  $\kappa$  tree corresponds to the cluster with largest empirical mass. In both the  $\lambda$  and  $\alpha$  trees, on the other hand, leaves correspond to clusters composed of points with high density values. The difference can be substantial. Figure 3 illustrates the differences between the three types of indexing for the "crater" example in Figure 2. This example consists of a central Gaussian with high density and low mass surrounded by a ring with high mass but uniformly low density. The  $\lambda$ -scale tree (Figure 3a) correctly indicates the heights of the modes of  $\hat{f}$ , but tends to produce the incorrect intuition that the ring (blue node and blue points in Figure 2b) is small. The  $\alpha$ -scale plot (Figure 3b) ameliorates this problem by indexing node heights to the quantiles of  $\hat{f}$ . The blue node appears at  $\alpha = 0.35$ , when 65% of the data remains in the upper level set, and vanishes at  $\alpha = 0.74$ , when only 26% of the data remains in the upper level set. It is tempting to say that this means the blue node contains 0.74 - 0.35 = 0.39 of the mass but this is incorrect because some of the difference in mass is due to the red node. This interpretation is precisely the design of the  $\kappa$ -tree, however, where we can say that the blue node contains 0.72 - 0.35 = 0.37 of the data.



Figure 2: The crater simulation. 2,000 points are sampled from a mixture of a central Gaussian and an outer ring (Gaussian direction with uniform noise). Roughly 70% of the points are in the outer ring. a) The kNN density estimator evaluated on the data. b) Cluster labels from the *all-mode* labeling technique, where each leaf of the level set tree is designated as a cluster. Gray points are unlabeled low-density background observations.



Figure 3: Level set tree scales for the crater simulation. a) The  $\lambda$  scale is dominant, corresponding directly to density level values. There is a one-to-one correspondence with  $\alpha$  values shown on the right y-axis. Note the blue branch, corresponding to the outer ring in the crater simulation, appears to be very small in this plot, despite the fact that the true group contains about 70% of data b) The  $\alpha$  scale is dominant, corresponding to the fraction of data excluded from the upper level set at each  $\lambda$  value. The blue cluster is more exaggerated but the topology of the tree remains unchanged. c) The  $\kappa$  scale. The blue cluster now appears larger than the red, facilitating the intuitive connection between branch height and cluster mass.

#### 3.3. Cluster retrieval options

Many clustering algorithms are designed to only output a partition of the data, whose elements are then taken to be the clusters. As we argued in the introduction, such a paradigm is often inadequate for data exhibiting complex and multi-scale clustering features. In contrast, hierarchical clustering in general and level set tree clustering in particular give a more complete and informative description of the clusters in a dataset. However, many applications require that each data point be assigned to a single cluster label. Much of the work on level set trees ignores this phase of a clustering application or assumes that labels will be assigned according to the connected components at a chosen  $\lambda$  (density) or  $\alpha$  (mass) level, which **DeBaCl** accomodates through the *upper set clustering* option. Rather than choosing a single density level, a practitioner might prefer to specify the number of clusters K (as with Kmeans). One way (of many) that this can be done is to find the first K-1 splits in the level set tree and identify each of the children from these splits as a cluster, known in **DeBaCl** as the first-K clustering technique. A third, preferred, option avoids the choice of  $\lambda$ ,  $\alpha$ , or K altogether and treats each leaf of the level set tree as a separate cluster (Azzalini and Torelli 2007). We call this the *all-mode clustering* method. Use of these labeling options is illustrated in Section 4.

Note that each of these methods assigns only a fraction of points to clusters (the *foreground* points), while leaving low-density observations (*background* points) unlabeled. Assigning the background points to clusters can be done with any classification algorithm, and **DeBaCl** includes a handful of simple options, including a k-nearest neighbor classifer, for the task.

#### 3.4. Chaudhuri and Dasgupta algorithm

Chaudhuri and Dasgupta (2010) introduce an algorithm for estimating a level set tree that is particularly notable because the authors prove finite-sample convergence rates (where consistency is in the sense of Hartigan (1981)). The algorithm is a generalization of single linkage, reproduced here for convenience in Algorithm 2. To translate this program into a practical

Algorithm 2: Chaudhuri and Dasgupta (2010) level set tree estimation procedure.

**Input**:  $\{x_1, ..., x_n\}, k, \alpha$ 

**Output**:  $\widehat{\mathcal{T}}$ , a hierarchy of subsets of  $\{x_1, \ldots, x_n\}$ 

 $r_k(x_i) \leftarrow \text{distance to the } k$ 'th neighbor of  $x_i$ ;

for  $r \leftarrow 0$  to  $\infty$  do

 $G_r \leftarrow \text{graph with vertices } \{x_i : r_k(x_i) \le r\} \text{ and edges } \{(x_i, x_j) : ||x_i - x_j|| \le \alpha r\};$ 

Find the connected components of  $G_{\lambda_r}$ ;

 $\widehat{\mathcal{T}} \leftarrow$  dendrogram of connected components of graphs  $G_r$ , ordered by inclusions; return  $\widehat{\mathcal{T}}$ 

implementation, we must find a finite set of values for r such that the graph  $G_r$  can only change at these values. When  $\alpha = 1$ , the only values of r where the graph can change are the edge lengths in the graph  $e_{ij} = ||x_i - x_j||$  for all *i* and *j*. Let *r* take on each value of  $e_{ij}$  in descending order; in each iteration remove vertices and edges with larger k-neighbor radius

When  $\alpha \neq 1$ , the situation is trickier. First, note that including r values where the graph *does* not change is not a problem, since the original formulation of the method includes all values of  $r \in \mathbb{R}^{+0}$ . Clearly, the vertex set can still change at any edge length  $e_{ij}$ . The edge set can only change at values where  $r = e_{ij}/\alpha$  for some i, j. Suppose  $e_{u,v}$  and  $e_{r,s}$  are consecutive values in a descending ordered list of edge lengths. Let  $r = e/\alpha$ , where  $e_{u,v} < e < e_{r,s}$ . Then the edge set  $E = \{(x_i, x_j) : ||x_i - x_j|| \leq \alpha r = e\}$  does not change as r decreases until  $r = e_{u,v}/\alpha$ , where the threshold of  $\alpha r$  now excludes edge  $(x_u, x_v)$ . Thus, by letting r iterate over the values in  $\bigcup_{i,j} \{e_{ij}, \frac{e_{ij}}{\alpha}\}$ , we capture all possible changes in  $G_r$ .

In practice, starting with a complete graph and removing one edge at a time is extremely slow because this requires  $2*\binom{n}{2}$  connected component searches. The **DeBaCl** implementation includes an option to initialize the algorithm at the k-nearest neighbor graph instead, which is a substantially faster approximation to the Chaudhuri-Dasgupta method. This shortcut is still dramatically slower than **DeBaCl**'s geometric tree algorithm, which is one reason why we prefer the latter. Future development efforts will focus on improvements in the speed of both procedures.

#### 3.5. Pseudo-densities for functional data

and edge length, respectively.

The level set tree estimation procedure in Algorithm 1 can be extended to work with data sampled from non-Euclidean spaces that do not admit a well-defined pdf. The lack of a density function would seem to be an insurmountable problem for a method defined on the levels of a pdf. In this case, however, level set trees can be built on the levels of a pseudodensity estimate that measures the similarity of observations and the overall connectivity of the sample space. Pseudo-densities cannot be used to compute probabilities as in Euclidean spaces, but are proportional to the statistical expectations of estimates of the form  $\hat{f}$ , which remain well-defined random quantities (Ferraty and Vieu 2006).

Random functions, for example, may have well-defined probability distributions that cannot be represented by pdfs (Billingsley 2012). To build level set trees for this type of data, **DeBaCl** accepts very general functions for  $\hat{f}$ , including pseudo-densities, although the user must compute the pairwise distances. The package includes a utility function for evaluating a k-nearest neighbor pseudo-density estimator on the data based on the pairwise distances. Specifically, equation 2 is modified by expunging the term  $v^d$  and setting d arbitrarily to 1. An application is shown in Section 4.

#### 3.6. User customization

One advantage of **DeBaCl** over existing cluster tree software is that **DeBaCl** is intended to be easily modified by the user. As described above, two major algorithm types are offered, as well as the ability to use pseudo-densities for functional data. In addition, the package allows a high degree of customization in the type of similarity graph, *data ordering function* (density, pseudo-density, or arbitrary function), pruning function, cluster labeling scheme, and background point classifier. In effect, the only fixed aspect of **DeBaCl** is that clusters are defined for every level to be connected components of a geometric graph.

# 4. Usage

#### 4.1. Basic Example

In this section we walk through the density-based clustering analysis of 10,000 fiber tracks mapped in a human brain with diffusion-weighted imaging. For this analysis we use only the subcortical endpoint of each fiber track, which is in  $\mathbb{R}^3$ . Despite this straightforward context of finite, low-dimensional data, the clustering problem is somewhat challenging because the data are known to have complicated striatal patterns. For this paper we add the **DeBaCl** package to the Python path at run time, but this can be done in a more persistent manner for repeated use. The **NumPy** library is also needed for this example, and we assume the dataset is located in the working directory. We use our preferred algorithm, the geometric level set tree, which is located in the **geom\_tree** module.

```
## Import DeBaCl package
import sys
sys.path.append('/home/brian/Projects/debacl/DeBaCl/')
from debacl import geom_tree as gtree
from debacl import utils as utl
## Import other Python libraries
import numpy as np
## Load the data
X = np.loadtxt('0187_endpoints.csv', delimiter=',')
n, p = X.shape
```

The next step is to define parameters for construction and pruning of the level set tree, as well as general plot aesthetics. For this example we set the density and connectivity smoothness parameter k to 0.01n and the pruning parameter  $\gamma$  is set to 0.05n. Tree branches with fewer points than this will be merged into larger sibling branches. For the sake of speed, we use a small subsample in this example.

```
## Downsample
n_samp = 5000
ix = np.random.choice(range(n), size=n_samp, replace=False)
X = X[ix, :]
n, p = X.shape
## Set level set tree parameters
```

```
p_k = 0.01
p_gamma = 0.05
k = int(p_k * n)
gamma = int(p_gamma * n)
## Set plotting parameters
utl.setPlotParams(axes_labelsize=28, xtick_labelsize=20, ytick_labelsize=20,
figsize=(8,8))
```

For straightforward cases like this one, we use a single convenience function to do density estimation, similarity graph definition, level set tree construction, and pruning. In the following example, each of these steps will be done separately. Note the **print** function is overloaded to show a summary of the tree.

```
## Build the level set tree with the all-in-one function
tree = gtree.geomTree(X, k, gamma, n_grid=None, verbose=False)
print tree
```

	alpha1	alpha2	children	lambda1	lambda2	parent	size
key							
0	0.0000	0.0040	[1, 2]	0.000000	0.00003	None	5000
1	0.0040	0.0716	[11, 12]	0.00003	0.000133	0	2030
2	0.0040	0.1278	[21, 22]	0.00003	0.000425	0	2950
11	0.0716	0.3768	[27, 28]	0.000133	0.004339	1	1437
12	0.0716	0.3124	[]	0.000133	0.002979	1	301
21	0.1278	0.9812	[]	0.000425	0.045276	2	837
22	0.1278	0.3882	[29, 30]	0.000425	0.004584	2	1410
27	0.3768	0.4244	[31, 32]	0.004339	0.005586	11	863
28	0.3768	1.0000	[]	0.004339	0.071075	11	406
29	0.3882	0.9292	[]	0.004584	0.032849	22	262
30	0.3882	0.9786	[]	0.004584	0.043969	22	668
31	0.4244	0.9896	[]	0.005586	0.048706	27	428
32	0.4244	0.9992	[]	0.005586	0.064437	27	395

The next step is to assign cluster labels to a set of foreground data points with the function GeomTree.getClusterLabels. The desired labeling method is specified with the method argument. When the correct number of clusters K is known, the first-k option retrieves the first K disjoint clusters that appear when  $\lambda$  is increased from 0. Alternately, the upper-set option cuts the tree at a single level, which is useful if the goal is to include or exclude a certain fraction of the data from the upper level set. Here we use this function with  $\alpha$  set to 0.05, which removes the 5% of the observations with the lowest estimated density (i.e. outliers) and clusters the remainder. Finally, the all-mode option returns a foreground cluster for each leaf of the level set tree, which avoids the need to specify either K,  $\lambda$ , or  $\alpha$ .

Additional arguments for each method are specified by keyword argument; the getClusterLabels method parses them intelligently. For all of the labeling methods the

function returns two objects. The first is an  $m \times 2$  matrix, where m is the number of points in the foreground set. The first column is the index of an observation in the full data matrix, and the second column is the cluster label. The second object is a list of the tree nodes that are foreground clusters. This is useful for coloring level set tree nodes to match observations plotted in feature space.

The GeomTree.plot method draws the level set tree dendrogram, with the vertical scale controlled by the form parameter. See Section 3.2 for more detail. The three plot forms are shown in Figure 4, foreground clusters are derived from *first-k* clustering with K set to 3. the plotForeground function from the DeBaCl utils module is used to match the node colors in the dendrogram to the clusters in feature space. Note that the plot function returns a tuple with several objects, but only the first is useful for most applications.

```
## Plot the level set tree with three different vertical scales, colored by the
first-K clustering
fig = tree.plot(form='lambda', width='mass', color_nodes=nodes_k)[0]
fig.savefig('../figures/endpt_tree_lambda.png')
fig = tree.plot(form='alpha', width='mass', color_nodes=nodes_k)[0]
fig = tree.plot(form='kappa', width='mass', color_nodes=nodes_k)[0]
fig.savefig('../figures/endpt_tree_alpha.png')
## Plot the foreground points from the first-K labeling
fig, ax = utl.plotForeground(X, uc_k, fg_alpha=0.6, bg_alpha=0.4, edge_alpha=0.3, s
=22)
ax.elev = 14; ax.azim=160 # adjust the camera angle
fig.savefig('../figures/endpt_firstK_fg.png', bbox_inches='tight')
```

A level set tree plot is also useful as a scaffold for interactive exploration of spatially coherent subsets of data, either by selecting individual nodes of the tree or by retreiving high-density clusters at a selected density or mass level. These tools are particularly useful for exploring clustering features at multiple data resolutions. In Figure 5, for example, there are two dominant clusters, but each one has highly salient clustering behavior at higher resolutions. The interactive tools allow for exploration of the parent-child relationships between these clusters.

```
tool1 = gtree.ComponentGUI(tree, X, form='alpha', output=['scatter'], size=18, width=
    'mass')
tool1.show()
```



Figure 4: First-k clustering results with different vertical scales and the clusters in feature space.



Figure 5: The level set tree can be used as a scaffold for interactive exploration of data subsets or upper level set clusters.

# tool2 = gtree.ClusterGUI(tree, X, form='alpha', width='mass', size=18) tool2.show()

The final step of our standard data analysis is to assign background points to a foreground cluster. **DeBaCl**'s **utils** module includes several very simple classifiers for this task, although more sophisticated methods have been proposed (Azzalini and Torelli 2007). For this example we assign background points with a k-nearest neighbor classifier. The observations are plotted a final time, with a full data partition (Figure 6).

```
## Assign background points with a simple kNN classifier
segment = utl.assignBackgroundPoints(X, uc_k, method='knn', k=k)
```



Figure 6: Endpoint data, with background points assigned to the *first-K* foreground clusters with a k-nearest neighbor classifier.

```
## Plot all observations, colored by cluster
fig, ax = utl.plotForeground(X, segment, fg_alpha=0.6, bg_alpha=0.4, edge_alpha
=0.3, s=22)
ax.elev = 14; ax.azim=160
fig.savefig('../figures/endpt_firstK_segment.png', bbox_inches='tight')
```

To customize the level set tree estimator, each phase can be done manually. Here we use methods in **DeBaCl**'s **utils** module to build a k-nearest neighbor similarity graph W, a k-nearest neighbor density estimate **fhat**, a grid of density levels **levels**, and the background observation sets at each density level (**bg\_sets**). The **constructTree** method of the **geom\_tree** module puts the pieces together to make the tree and the **prune** function removes tree leaf nodes that are small and likely due to random noise.

```
## Similarity graph and density estimate
W, k_radius = utl.knnGraph(X, k, self_edge=False)
fhat = utl.knnDensity(k_radius, n, p, k)
## Tree construction and pruning
bg_sets, levels = utl.constructDensityGrid(fhat, mode='mass', n_grid=None)
tree = gtree.constructTree(W, levels, bg_sets, mode='density', verbose=False)
tree.prune(method='size-merge', gamma=gamma)
print tree
```

	alpha1	alpha2	children	lambda1	lambda2	parent	size
key							
0	0.0000	0.0040	[1, 2]	0.000000	0.00003	None	5000
1	0.0040	0.0716	[11, 12]	0.00003	0.000133	0	2030
2	0.0040	0.1278	[21, 22]	0.00003	0.000425	0	2950
11	0.0716	0.3768	[27, 28]	0.000133	0.004339	1	1437
12	0.0716	0.3124	[]	0.000133	0.002979	1	301
21	0.1278	0.9812	[]	0.000425	0.045276	2	837
22	0.1278	0.3882	[29, 30]	0.000425	0.004584	2	1410
27	0.3768	0.4244	[31, 32]	0.004339	0.005586	11	863
28	0.3768	1.0000	[]	0.004339	0.071075	11	406
29	0.3882	0.9292	[]	0.004584	0.032849	22	262
30	0.3882	0.9786	[]	0.004584	0.043969	22	668
31	0.4244	0.9896	[]	0.005586	0.048706	27	428
32	0.4244	0.9992	[]	0.005586	0.064437	27	395

In the definition of density levels and background sets, the constructDensityGrid allows the user to specify the n\_grid parameter to speed up the algorithm by computing the upper level set and connectivity for only a subset of density levels. The mode parameter determines whether the grid of density levels is based on evenly-sized blocks of observations (mode='mass') or density levels (mode='levels'); we generally prefer the 'mass' mode for our own analyses.

The mode parameter of the tree construction function is usually set to be 'density', which treats the underlying function **fhat** as a density or pseudo-density function, with a floor value of 0. This algorithm can be applied to arbitrary functions that do not have a floor value, in which case the mode should be set to 'general'.

### 4.2. Extension: The Chaudhuri-Dasgupta Tree

Usage of the Chaudhuri-Dasgupta algorithm is similar to the standalone geomTree function. First load the **DeBaCl** module **cd\_tree** (labeled here for brevity as **cdt**) and the utility functions in **utils**, as well as the data.

```
## Import DeBaCl package
import sys
sys.path.append('/home/brian/Projects/debacl/DeBaCl/')
from debacl import cd_tree as cdt
from debacl import utils as utl
## Import other Python libraries
import numpy as np
## Load the data
X = np.loadtxt('0187_endpoints.csv', delimiter=',')
```

n, p = X.shape

Because the straightforward implementation of the Chaudhuri-Dasgupta algorithm is extremely slow, we use a random subset of only 200 observations (out of the total of 10,000). The smoothing parameter is set to be 2.5% of n, or 5. The pruning parameter is 5% of n, or 10. The pruning parameter is slightly less important for the Chaudhuri-Dasgupta algorithm.

```
## Downsample
n_samp = 200
ix = np.random.choice(range(n), size=n_samp, replace=False)
X = X[ix, :]
n, p = X.shape
## Set level set tree parameters
p_k = 0.025
p_gamma = 0.05
k = int(p_k * n)
gamma = int(p_gamma * n)
## Set plotting parameters
utl.setPlotParams(axes_labelsize=28, xtick_labelsize=20, ytick_labelsize=20,
figsize=(8,8))
```

The straightforward implementation of the Chaudhuri-Dasgupta algorithm starts with a complete graph and removes one edge a time, which is extremely slow. The **start** parameter of the **cdTree** function allows for shortcuts. These are approximations to the method, but are necessary to make the algorithm practical. Currently, the only implemented shortcut is to start with a k-nearest neighbor graph.

```
## Construct the level set tree estimate
tree = cdt.cdTree(X, k, alpha=1.4, start='knn', verbose=False)
tree.prune(method='size-merge', gamma=gamma)
```

As with the geometric tree, we can print a summary of the tree, plot the tree, retrieve foreground cluster labels, and plot the foreground clusters. This is illustrated below for the 'all-mode' labeling method.

```
## Print/make output
print tree
fig = tree.plot()
fig.savefig('../figures/cd_tree.png')
uc, nodes = tree.getClusterLabels(method='all-mode')
fig, ax = utl.plotForeground(X, uc, fg_alpha=0.6, bg_alpha=0.4, edge_alpha=0.3, s
        =60)
ax.elev = 14; ax.azim=160
```



Figure 7: The Chaudhuri-Dasgupta tree for the fiber track endpoint data, downsampled from 10,000 to 200 observations to make computation feasible. Foreground clusters based on all-mode clustering are shown on the right.

fig	<pre>fig.savefig('/figures/cd_allmode.png')</pre>							
	child	dren	parent	r1	r2	size		
key								
0	[3	, 4]	None	8.134347	4.374358	200		
3	[15,	16]	0	4.374358	2.220897	109		
4	[23,	24]	0	4.374358	1.104121	75		
15		[]	3	2.220897	0.441661	32		
16		[]	3	2.220897	0.343408	55		
23		[]	4	1.104121	0.445529	28		
24		[]	4	1.104121	0.729226	24		

#### 4.3. Extension: Functional Data

Nothing in the process of estimating a level set tree requires  $\hat{f}$  to be a bona fide probability density function, and the **DeBaCl** package allows us to use this fact to use level set trees for much more complicated datasets. To illustrate we use the phoneme dataset from Ferraty and Vieu (2006), which contains 2000 total observations of five short speech patterns. Each observation is recorded on a regular grid of 150 frequencies, but we treat this as an approximation of a continuous function on an interval of  $\mathbb{R}^1$ . Because the observations are random curves they do not have bona fide density functions, but we can still construct a sample level set tree by estimating a pseudo-density function that measures the proximity of each curve to its neighbors.

To start we load the **DeBaCl** modules and the data, which have been pre-smoothed for this example with cubic splines. The true class of each observation is in the last column of the

raw data object. The curves for each phoneme are shown in Figure 8.

```
## Import DeBaCl package
import sys
sys.path.append('/home/brian/Projects/debacl/DeBaCl/')
from debacl import geom_tree as gtree
from debacl import utils as utl
## Import other Python libraries
import numpy as np
import scipy.spatial.distance as spdist
import matplotlib.pyplot as plt
## Set plotting parameters
utl.setPlotParams(axes_labelsize=28, xtick_labelsize=20, ytick_labelsize=20,
   figsize=(8,8))
## Load data
speech = np.loadtxt('smooth_phoneme.csv', delimiter=',')
phoneme = speech[:, -1].astype(np.int)
speech = speech[:, :-1]
n, p = speech.shape
## Plot the curves, separated by true phoneme
fig, ax = plt.subplots(3, 2, sharex=True, sharey=True)
ax = ax.flatten()
ax[-2].set_xlabel('frequencies')
ax[-1].set_xlabel('frequencies')
for g in np.unique(phoneme):
       ix = np.where(phoneme == g)[0]
       for j in ix:
              ax[g].plot(speech[j, :], c='black', alpha=0.15)
fig.savefig('../figures/phoneme_data.png')
```

For functional data we need to define a distance function, precluding the use of the convenience method GeomTree.geomTree or even the utility function utils.knnGraph. First the bandwith and tree pruning parameters are set to be 0.01n. In the second step all pairwise distances are computed in order to find the k-nearest neighbors for each observation. For simplicity we use Euclidean distance between a pair of curves (which happens to work well in this example), but this is not generally optimal. Next, the adjacency matrix for a k-nearest neighbor graph is constructed, which is no different than the finite-dimensional case. Finally the pseudo-density estimator is built by using the finite-dimensional k-nearest neighbor density estimator with the dimension set (incorrectly) to 1. This function does not integrate to 1, but the function induces an ordering on the observations (from smallest to largest k-neighbor radius) that is invariant to the dimension. This ordering is all that is needed for the final step of building



Figure 8: Smoothed waveforms for spoken phonemes, separated by true phoneme.

the level set tree.

```
## Bandwidth and pruning parameters
p_k = 0.01
p_gamma = 0.01
k = int(p_k * n)
gamma = int(p_gamma * n)
## Find all pairwise distances and the indices of each point's k-nearest neighbors
D = spdist.squareform(spdist.pdist(speech, metric='euclidean'))
rank = np.argsort(D, axis=1)
ix_nbr = rank[:, 0:k]
ix_row = np.tile(np.arange(n), (k, 1)).T
## Construct the similarity graph adjacency matrix
W = np.zeros(D.shape, dtype=np.bool)
W[ix_row, ix_nbr] = True
W = np.logical_or(W, W.T)
np.fill_diagonal(W, False)
## Compute a pseudo-density estimate and evaluate at each observation
k_nbr = ix_nbr[:, -1]
r_k = D[np.arange(n), k_nbr]
fhat = utl.knnDensity(r_k, n, p=1, k=k)
```

```
## Build the level set tree
 bg_sets, levels = utl.constructDensityGrid(fhat, mode='mass', n_grid=None)
 tree = gtree.constructTree(W, levels, bg_sets, mode='density', verbose=False)
 tree.prune(method='size-merge', gamma=gamma)
 print tree
     alpha1 alpha2 children lambda1 lambda2 parent size
key
    0.0000 0.2660
                    [1, 2] 0.000000 0.000261 None 2000
0
1
    0.2660 0.3435 [3, 4] 0.000261 0.000275
                                                 0 1125
  0.2660 1.0000 [] 0.000261 0.000938
                                                   0 343
2
3 0.3435 0.4905 [5, 6] 0.000275 0.000307
                                                   1 565
40.34350.7705[]0.0002750.000426141350.49050.9920[]0.0003070.000808339160.49050.7110[]0.0003070.000382385
```

Once the level set tree is constructed we can plot it and retrieve cluster labels as with finitedimensional data. In this case we choose the all-mode cluster labeling which produces four clusters. The utility function utils.plotForeground is currently designed to work only with two- or three-dimensional data, so plotting the foreground clusters must be done manually for functional data. The clusters from this procedure match the true groups quite well, at least in a qualitative sense.

```
## Retrieve cluster labels
uc, nodes = tree.getClusterLabels(method='all-mode')
## Level set tree plot
fig = tree.plot(form='alpha', width='mass', color_nodes=nodes)[0]
fig.savefig('../figures/phoneme_tree.png')
## Plot the curves, colored by foreground cluster
palette = utl.Palette()
fig, ax = plt.subplots()
ax.set_xlabel("frequency index")
for c in np.unique(uc[:,1]):
    ix = np.where(uc[:,1] == c)[0]
    ix_clust = uc[ix, 0]
    for i in ix_clust:
        ax.plot(speech[i,:], c=np.append(palette.colorset[c], 0.25))
```

fig.savefig('../figures/phoneme\_allMode.png')

# 5. Conclusion



Figure 9: All-mode foreground clusters for the smoothed phoneme data.

The Python package **DeBaCl** for hierarchical density-based clustering provides a highly usable implementation of level set tree estimation and clustering. It improves on existing software through computational efficiency and a high-degree of modularity and customization. Namely, **DeBaCl**:

- offers the first known implementation of the theoretically well-supported Chaudhuri-Dasgupta level set tree algorithm;
- allows for very general data ordering functions, which are typically probability density estimates but could also be pseudo-density estimates for infinite-dimensional functional data or even arbitrary functions;
- accepts any similarity graph, density estimator, pruning function, cluster labeling scheme, and background point assignment classifier;
- includes the all-mode cluster labeling scheme, which does not require an *a priori* choice of the number of clusters;
- incorporates the  $\lambda$ ,  $\alpha$ , and  $\kappa$  vertical scales for plotting level set trees, as well as other plotting tweaks to make level set tree plots more interpretable and usable;
- and finally, includes interactive GUI tools for selecting coherent data subsets or high-density clusters based on the level set tree.

The **DeBaCl** package and user manual is available at https://github.com/CoAxLab/DeBaCl. The project remains under active development; the focus for the next version will be on improvements in computational efficiency, particularly for the Chaudhuri-Dasgupta algorithm.

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