The Importance of Data Clustering Stability

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figures/letu.png

- HDBSCAN stands for "Hierarchical Density-Based Spatial Clustering of Applications with Noise"
- It was introduced in 2015, by Campello, Moulavi, and Zimek [2], for automatic clustering of n-dimensional data sets.
- It uses a "mutual reachability distance", and identifies clusters by iteratively merging or splitting groups of data points.

Mutual Reachability Distance

Definition

The **mutual reachability distance** of two data points x and y, written $\mathrm{mrd}(x, y)$, with a paramater $k \in \mathbb{Z}^+$, is the maximum of

$$\begin{cases} \text{Distance between } x \text{ and } y \\ \text{Distance to } k\text{-nearest neighbor of } x \\ \text{Distance to } k\text{-nearest neighbor of } y \end{cases}$$

where "distance" refers to the standard ℓ^2 norm of $x - y$, or euclidian distance.

Note: The k-nearest neighbor is the kth closest point *not counting the point itself*. Undefined if there are k or less total data points.

HDBSCAN

figures/from_tutorial/scatterplot.png

figures/from_tutorial/mst.png

figures/from_tutorial/clusters.png

"Unreasonable Stability"

In [1], Dr. Blevins and her advisor Dr. Bridges of Oak Ridge National Labratory showed that distinct minimum spanning trees on the same data set give the same clusters.

figures/stability.png

Goals

1. Verify that it is possible to get different minimum spanning trees over the same data
2. Test whether this can occur in real-world data (and get a rough sense of how often)
3. Classify exactly when we get non-unique minimum spanning trees

Base Case

Example

Different orderings of the simple data set $[[0,0],[0,1],[1,1],[1,0]]$ give different minimum spanning trees

figures/base_case.png

Iris

Example

the Iris data set [6] records information about various types of iris flowers.

figures/iris2d.png

Iris Closeup

figures/iris2d_closeup.png

Note: All graphs (except the first) are a two-dimensional projection of the higher-dimensional data sets, but the python script verifies that there are truly multiple trees in the native dimension.

MNIST Closeup

Example

MNIST is a massive data set of handwritten digits. We plotted the first 50.

figures/mnist2d_closeup.png

core_k

Definition

Given some $k \in \mathbb{Z}^+$, for a data point x, the $\text{core}_k(x)$ is the distance to the k-nearest neighbor of x.

Note that this definition depends on which distance we are using. Usually we will use the ℓ^2 norm.
If the language seems strange, it is inspired by the HDBSCAN algorithm itself.

NECKSc

Definition

Let X, along with some distance definition dist, be a metric space. And, with a paramater $k \in \mathbb{Z}^+$, define

$$\epsilon = \min_{x \in X} \text{core}_k(x) = \text{core}_k(x_0) \text{ for some } x_0 \in X.$$

Then X is a 'not-everywhere core$_k$ sparse (closed)' (**NECKSc**) metric space, if and only if

$$\exists y, z \in \{x \in X : 0 < \text{dist}(x, x_0) \leq \epsilon\} \text{ with } y \neq z \text{ and } \text{dist}(y, z) \leq \epsilon.$$

In other words, a metric space is NECKSc if there are two points in the k-nearest neighbors of x_0 that are also within ϵ of each other.

Original NECKS Definition

Note: This is a tweaked version of a NECKS metric space.

figures/necks_def.png

NECKSc $\implies$ Multiple Minimum Spanning Trees

Theorem

(From [1]) Let (X, dist) *be a NECKS metric space for some* $k \in \mathbb{N}$*. Let* $G(V, E)$ *be the complete graph such that* $V = X$ *and for* $(a, b) \in E$*,* $w(a, b) = \mathrm{mrd}(a, b)$*. Then* G *has multiple minimum spanning trees.*

Dr. Blevins and Dr. Bridges showed this for NECKS spaces, but it also holds for NECKSc spaces. So we need only to show that a data set (along with a definition of distance) is a NECKSc metric space to show that it has multiple minimum spanning trees.

Sufficient k value

Theorem

For $k \geq 6$, any two dimensional data set, with the ℓ^2 norm as distance, is a NECKSc space, and thus has multiple minimum spanning trees.

Proof Sketch

Increasing k cannot decrease ϵ, so proving the theorem for $k = 6$ is sufficient to show it's truth for all $k \geq 6$.

- Assume BWOC there exists some two-dimensional data set X that is not a NECKSc metric space for $k = 6$ (with standard euclidian distance).
- Order the six closest points to x_0 in terms of their angle relative to x_0.
- By the definition of $\mathrm{core}_6(x_0)$, these are all within ϵ of x_0.
- No pair of these points is within ϵ of each other, becuase X is not a NECKSc space.

Proof Sketch (continued)

- This means that blue lines are strictly greater than ϵ, and red/green lines are less than or equal to ϵ.
- The angles formed around x_0 sum to more than 2π.

`figures/2d_proof_fig.png`

The Kissing Number

Definition

Given an n-dimensional sphere S with radius r, the n-**dimensional kissing number** $\text{kiss}(n)$ is the maximum number of spheres of radius r that can be tangent to S without the interiors of any two spheres overlapping*.

*Two spheres' interiors overlap if their intersection is neither the empty set nor a single point.

Background on the Kissing Number

Already hard in three dimensions: Newton disagreed with David Gregory about kiss(3). "Extra" space in 3D unlike in 2D.

figures/1dkn.png

figures/kissing_picture.jpg

Kissing Numbers (from [3])

figures/kissing_nums_list.png

$k > \text{kiss}(n) \implies \text{NECKSc}$

Theorem

Let X be n-dimensional data set, and let dist *be euclidian distance. Then* (X, dist) *is a NECKSc space if*

1. $k > \text{kiss}(n)$ *and*
2. $|X| > k$*

*This second point is formally necessary but practically meaningless: $|X| \leq k$ would mean the data is all in one cluster.

Proof Sketch

Let X be an n-dimensional data set, and let (X, dist) **not** be a NECKSc space. We show that this implies $k \leq \text{kiss}(n)$.

- Consider the k closest points to x_0, call this set A.
- Notice that $|A| = k$.
- Let each $p \in A$ correspond to a new p', on $\overrightarrow{x_0 p}$, with $\text{dist}(x_0, p') = \epsilon \geq \text{dist}(x_0, p)$. (Call this set of new points A').
- $|A'| = |A| = k$.
- For all $p, q \in A$ with $p \neq q$, $\text{dist}(p, q) > \epsilon$, becuase X is not a NECKSc space.
- Because new points travel outward along diverging lines, we also know $\text{dist}(p', q') > \epsilon$ for all $p', q' \in A'$ with $p' \neq q'$.

Proof Sketch (continued)

- We place a hypersphere of radius $\frac{\epsilon}{2}$ centered at each $p' \in A'$, as well as one centered at x_0.
- These hyperspheres are all tangent to the hypersphere centered at x_0, because for each $p' \in A'$, $\text{dist}(p', x_0) = \epsilon$.
- But no hypersphere is tangent to any other, because $\text{dist}(p', q') > \epsilon$ for all $p', q' \in A'$ with $p' \neq q'$.
- These all have radius $\frac{\epsilon}{2}$, so $\text{kiss}(n) \geq k$ by definition.

Proof Illustration

figures/kiss_proof_a.png

figures/kiss_proof_b.png

figures/kiss_proof_c.png

Conclusion

- We have verified that it is possible to get different minimum spanning trees from HDBSCAN over the same data set.
- We have tested that this can occur in real-world data, and have empirically shown that this is often.
- We have shown conditions that gurantee a metric space is NECKSc, which implies non-unique minimum spanning trees.

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