The Importance of Data Clustering Stability

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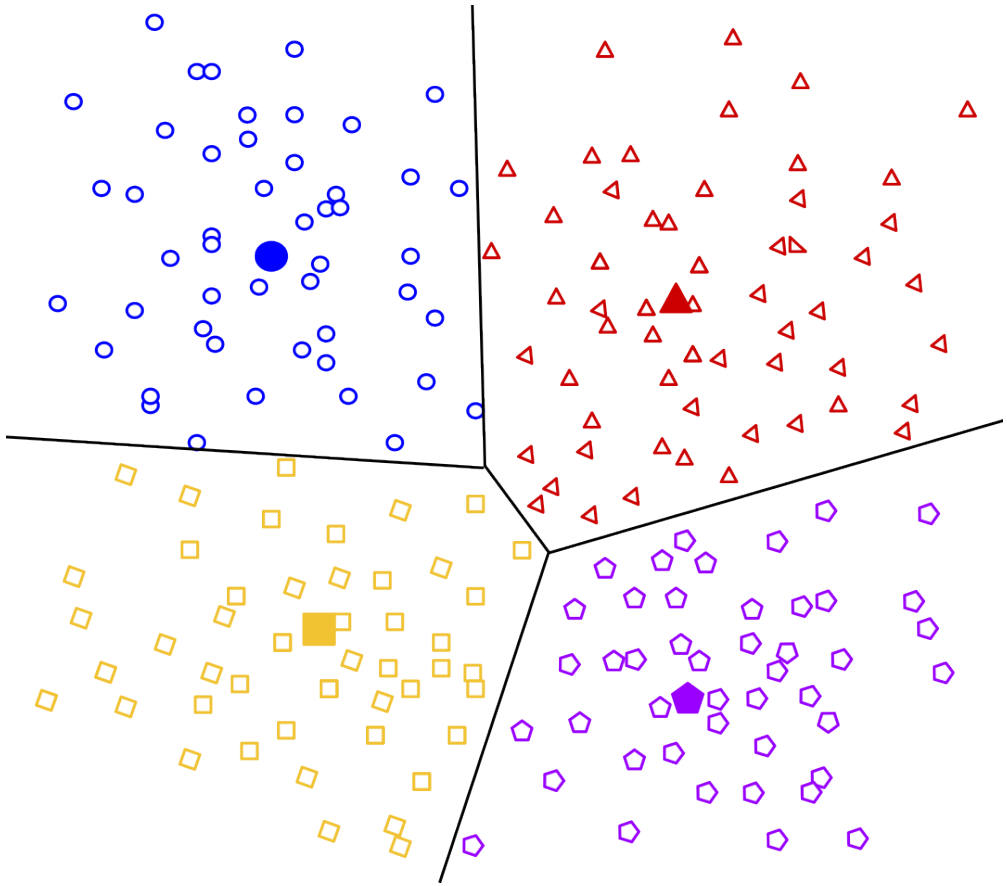
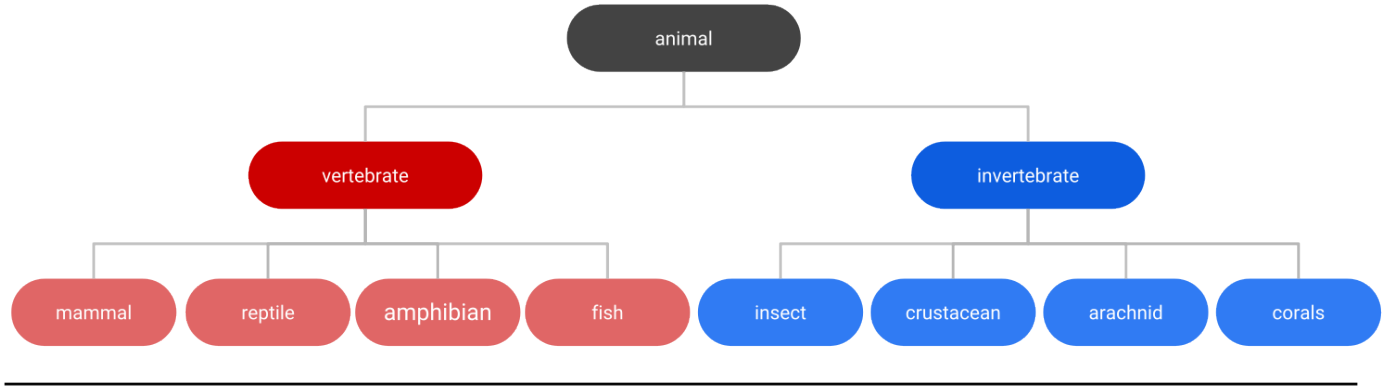
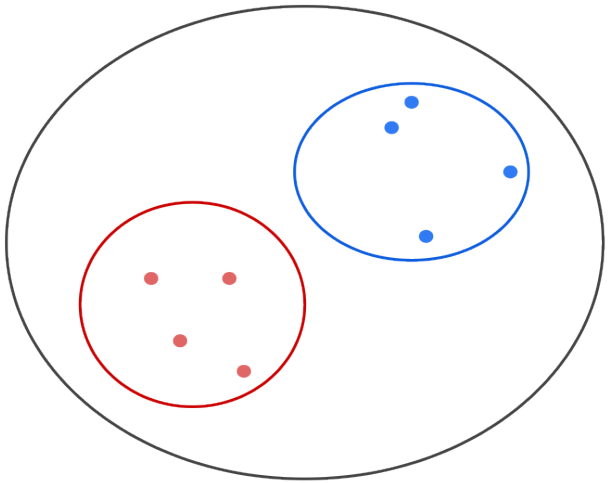
  - Sports Training?
- It can uncover hidden insights and make data more manageable and understandable.

Centroid-Based Clustering

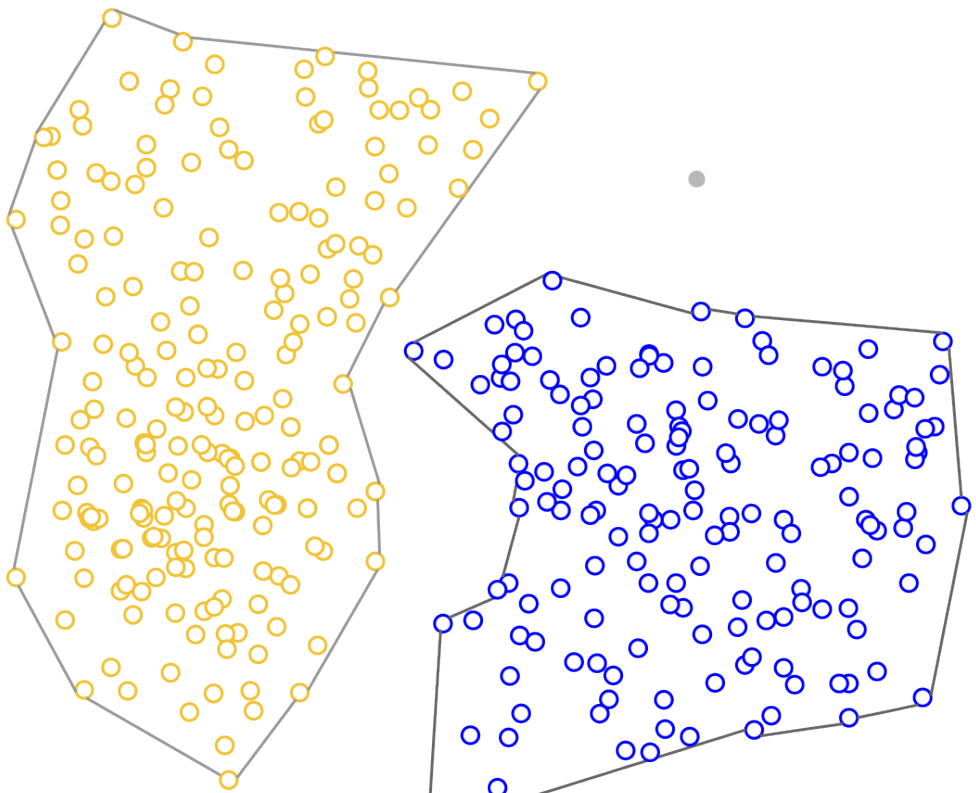


Hierarchical Clustering

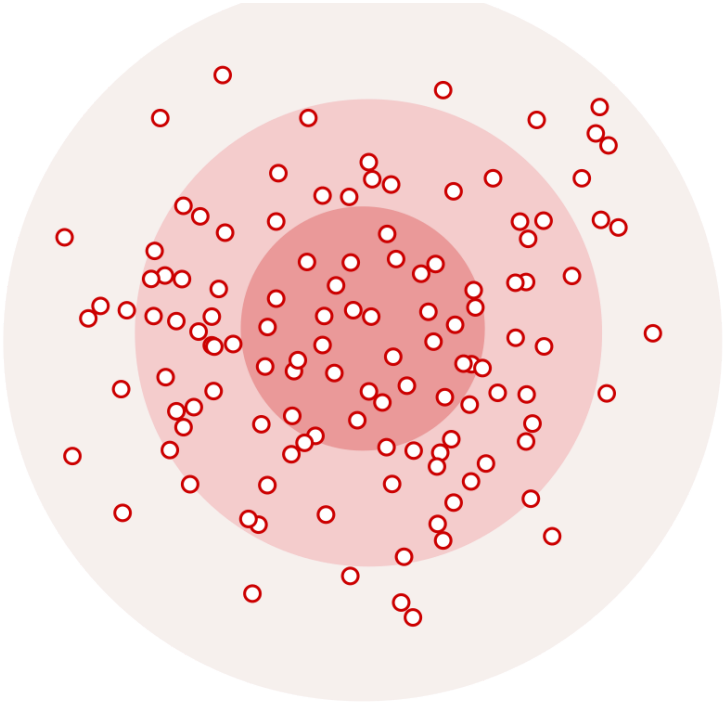


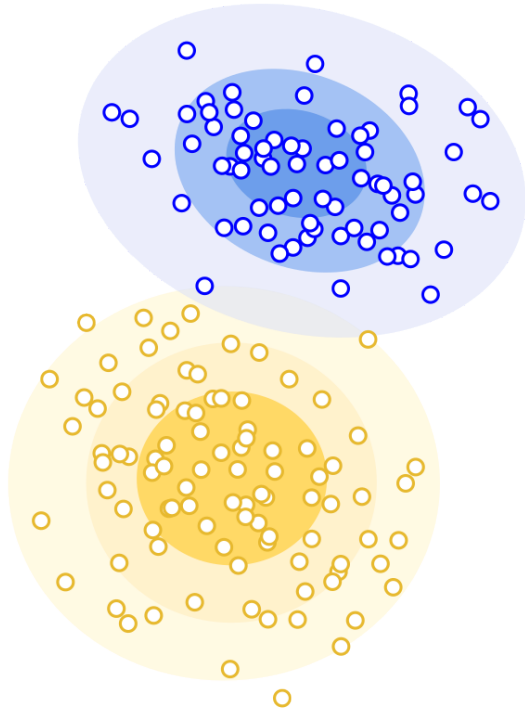


Density-Based Clustering



Distribution-Based Clustering





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  - *Density-Based Spatial Clustering of Applications with Noise*
- Gaussian Mixture Models
  - assumes that the data is generated from a mixture of several Gaussian distributions

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- It uses a "mutual reachability distance", and identifies clusters by iteratively merging or splitting groups of data points.

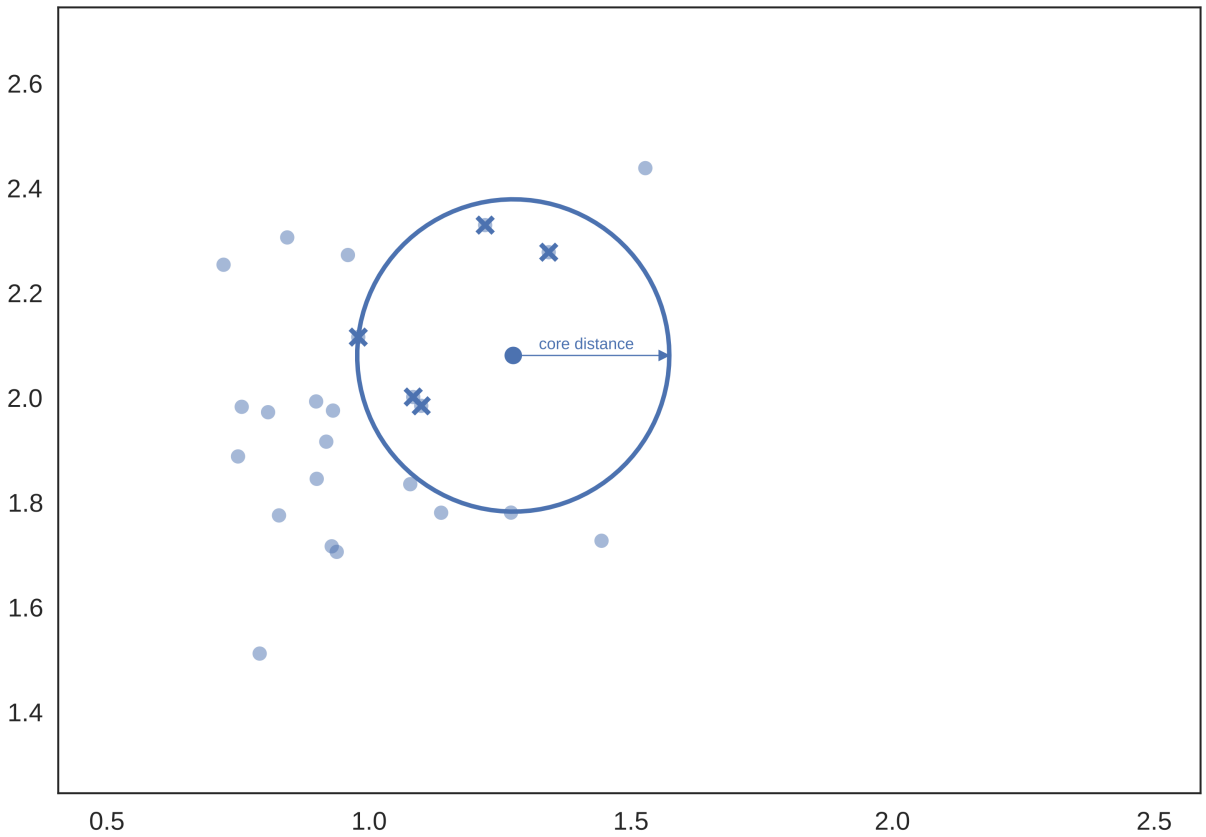
core_k

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.

core_k Illustration



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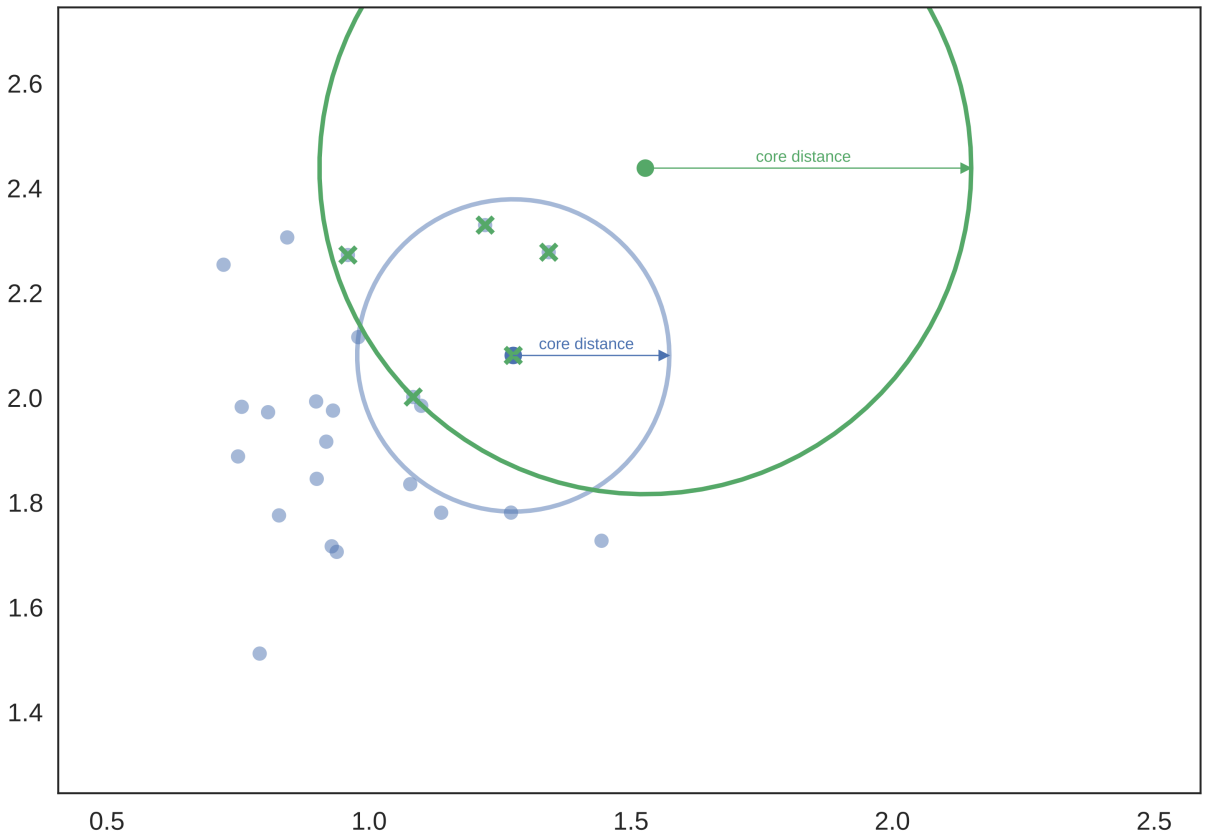

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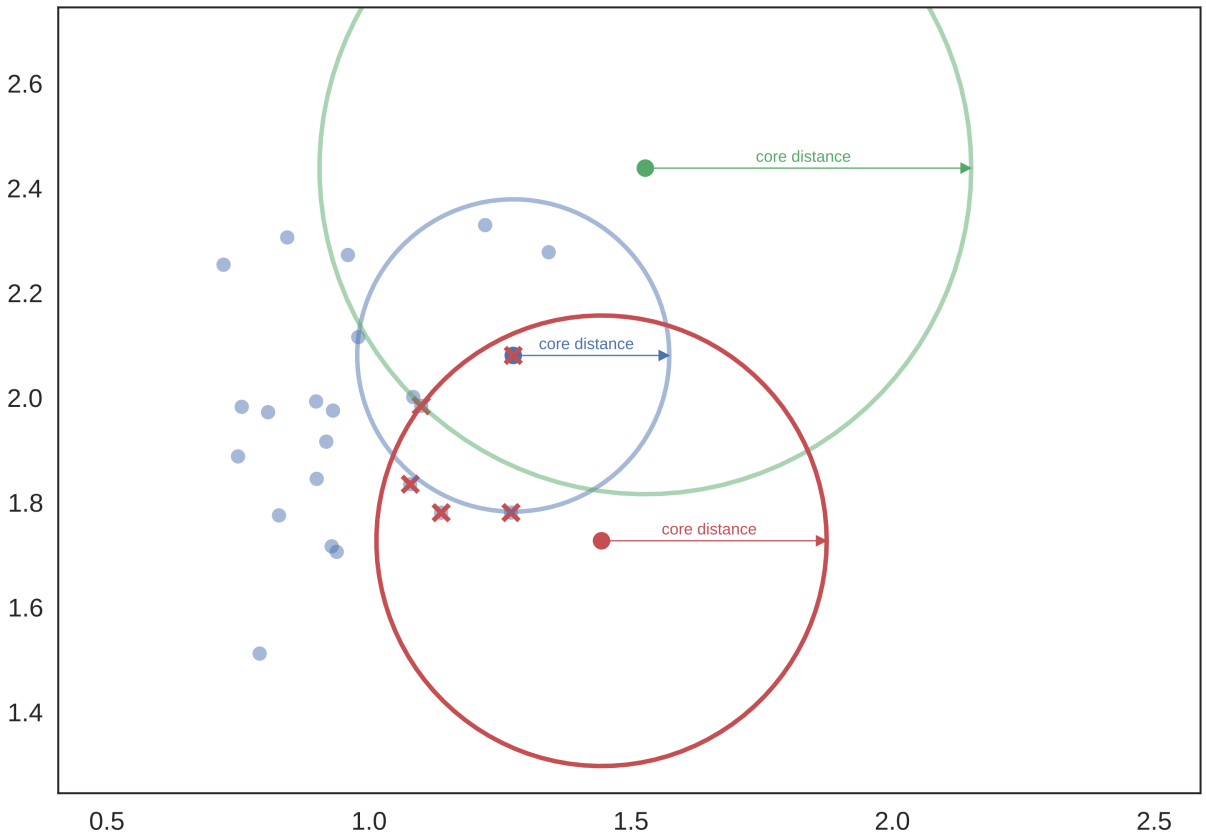


Mutual Reachability Distance

Definition

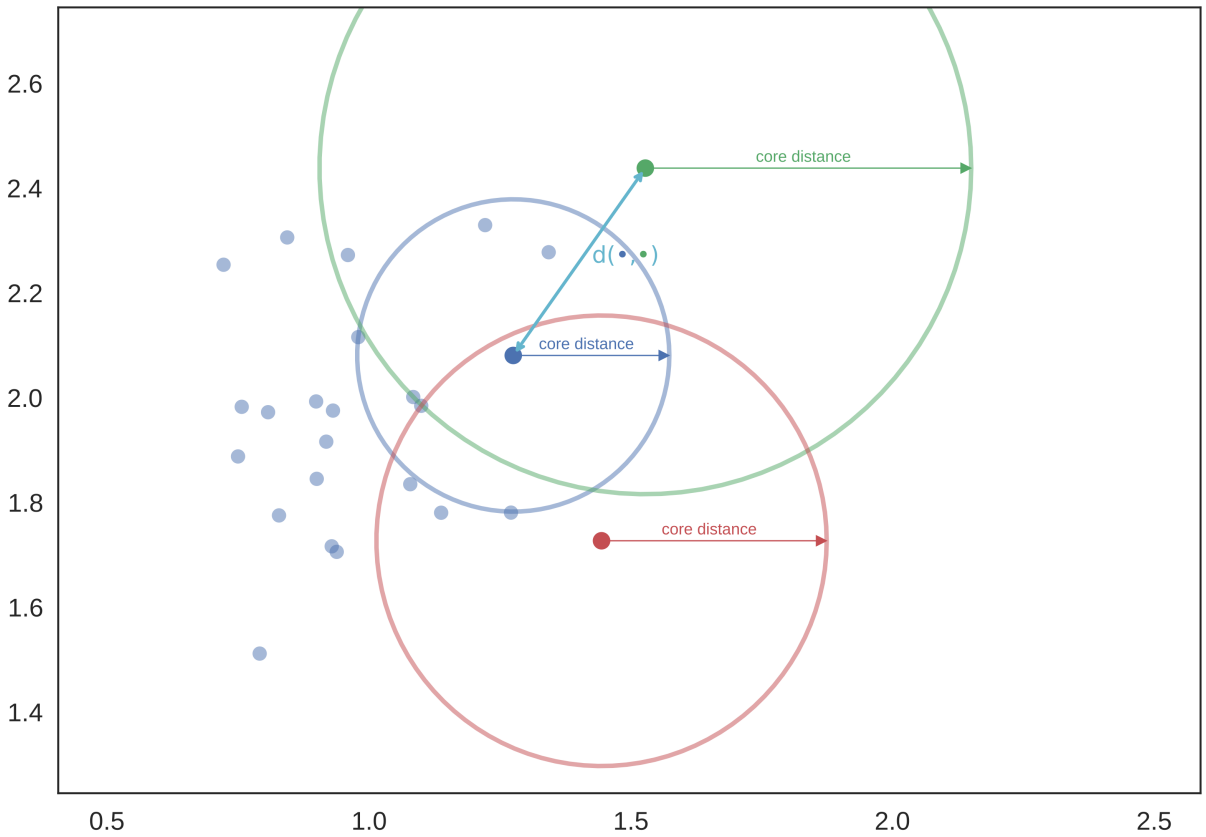
The **mutual reachability distance** of two data points x and y, written $\text{mrd}(x, y)$, with a paramater $k \in \mathbb{Z}^+$ and a metric dist, is

$$\max \begin{cases} \text{dist}(x, y): & \text{Distance between } x \text{ and } y \\ \text{core}_k(x): & \text{Distance to } k\text{-nearest neighbor of } x \\ \text{core}_k(y): & \text{Distance to } k\text{-nearest neighbor of } y \end{cases}$$

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

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.

core_k Illustration



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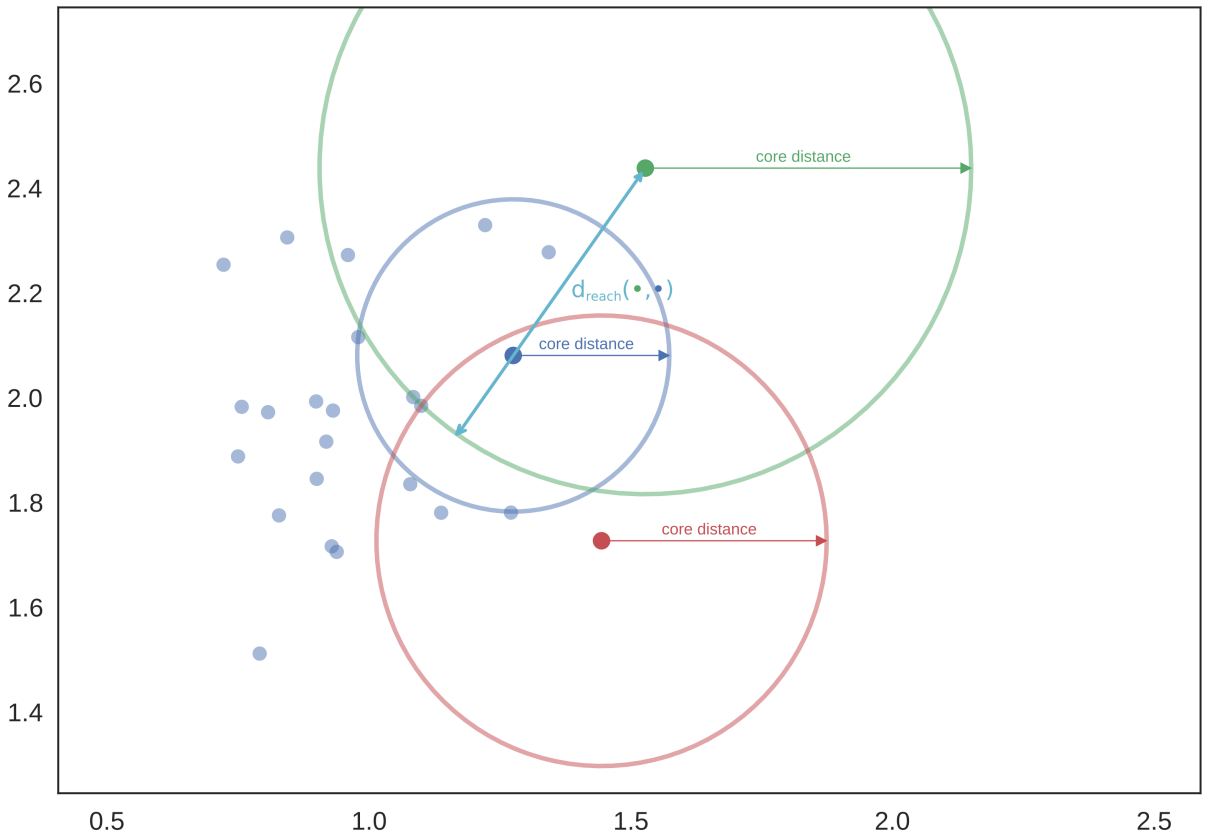

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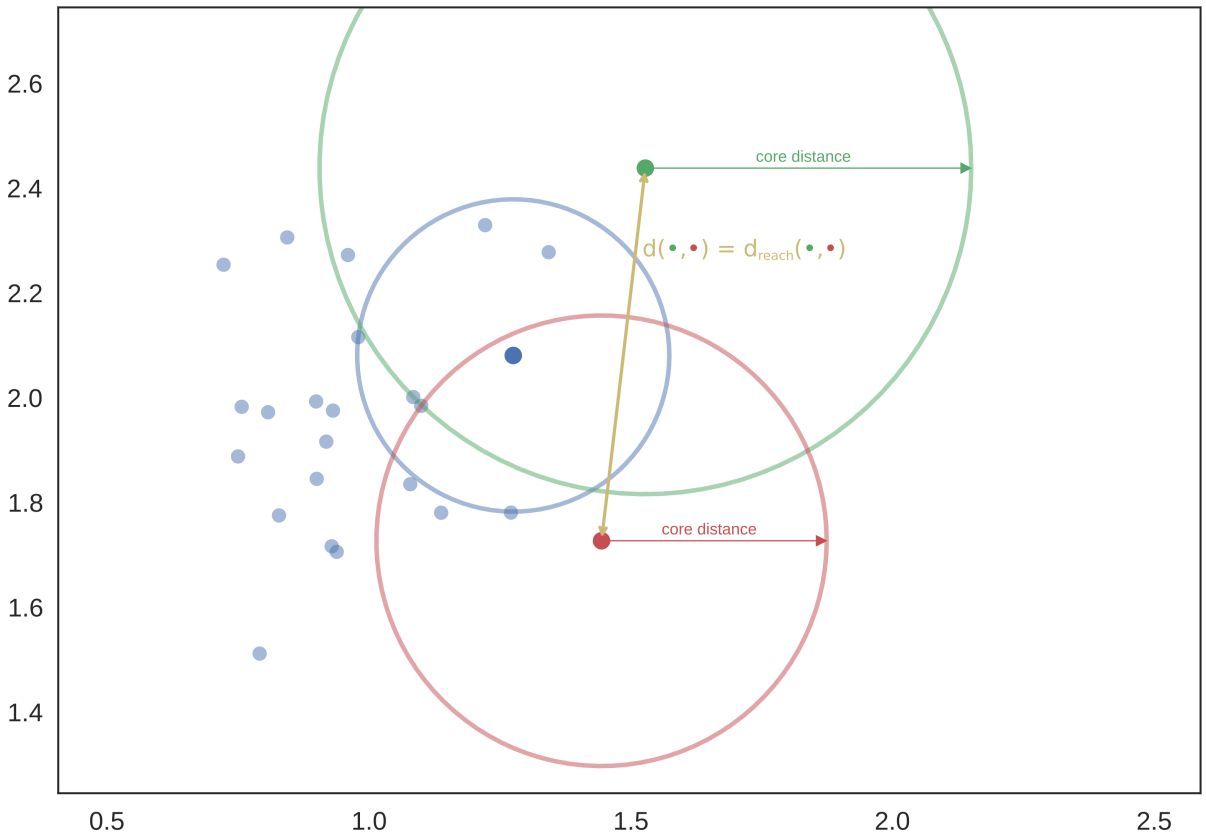
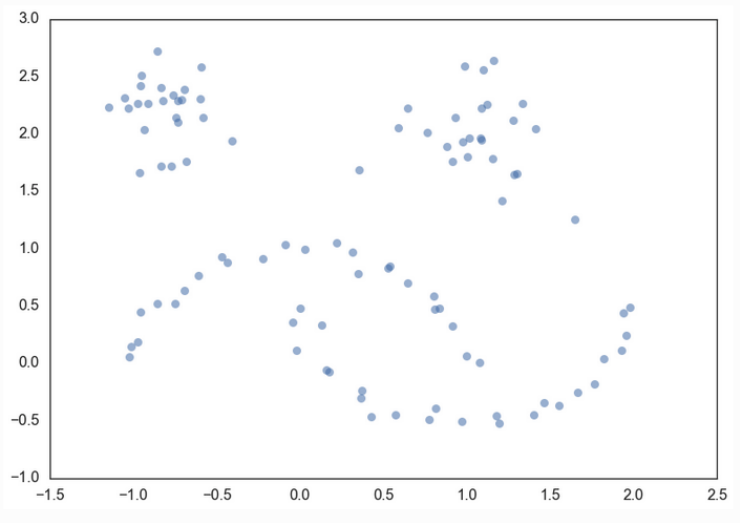


HDBSCAN



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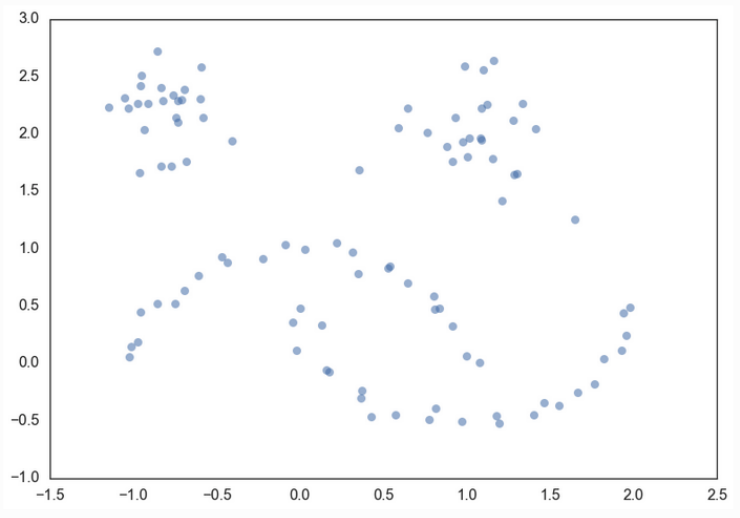
3.0
2.5
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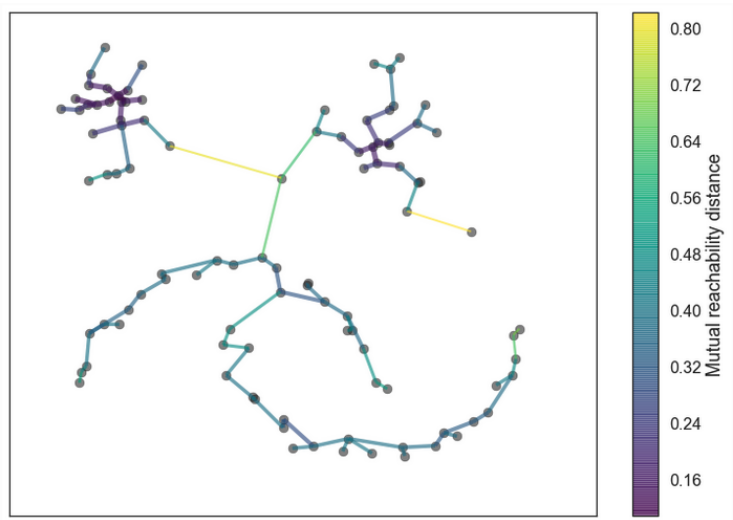
0.80
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0.48
0.40
0.32
0.24
0.16
Mutual reachability distance

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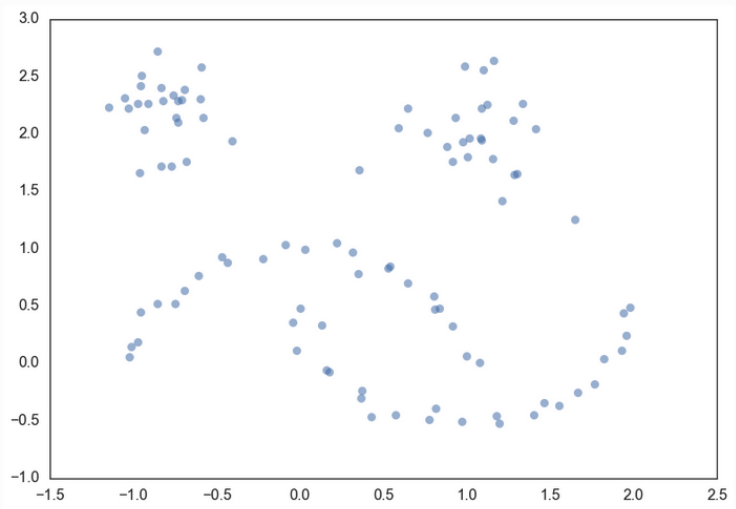
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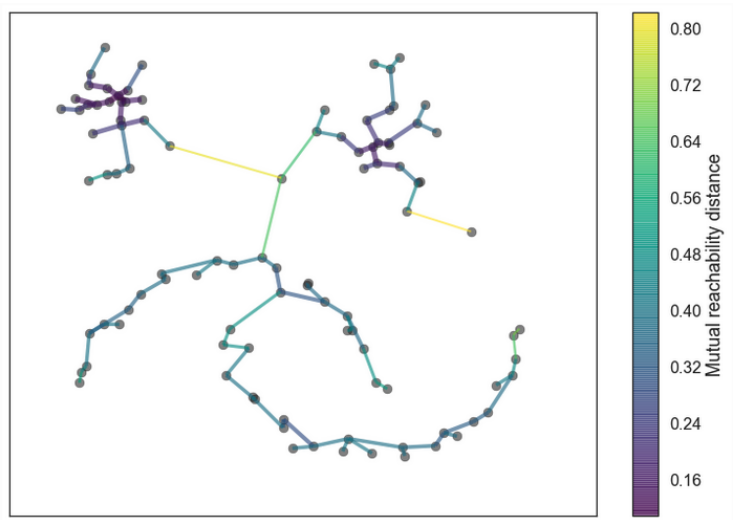
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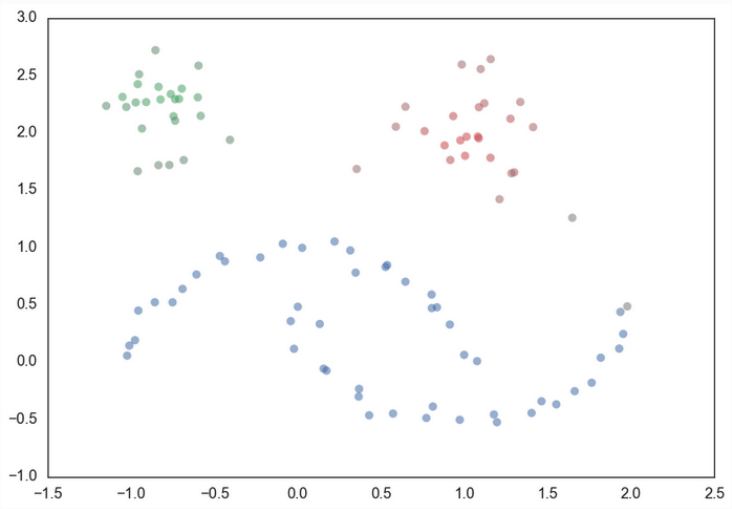
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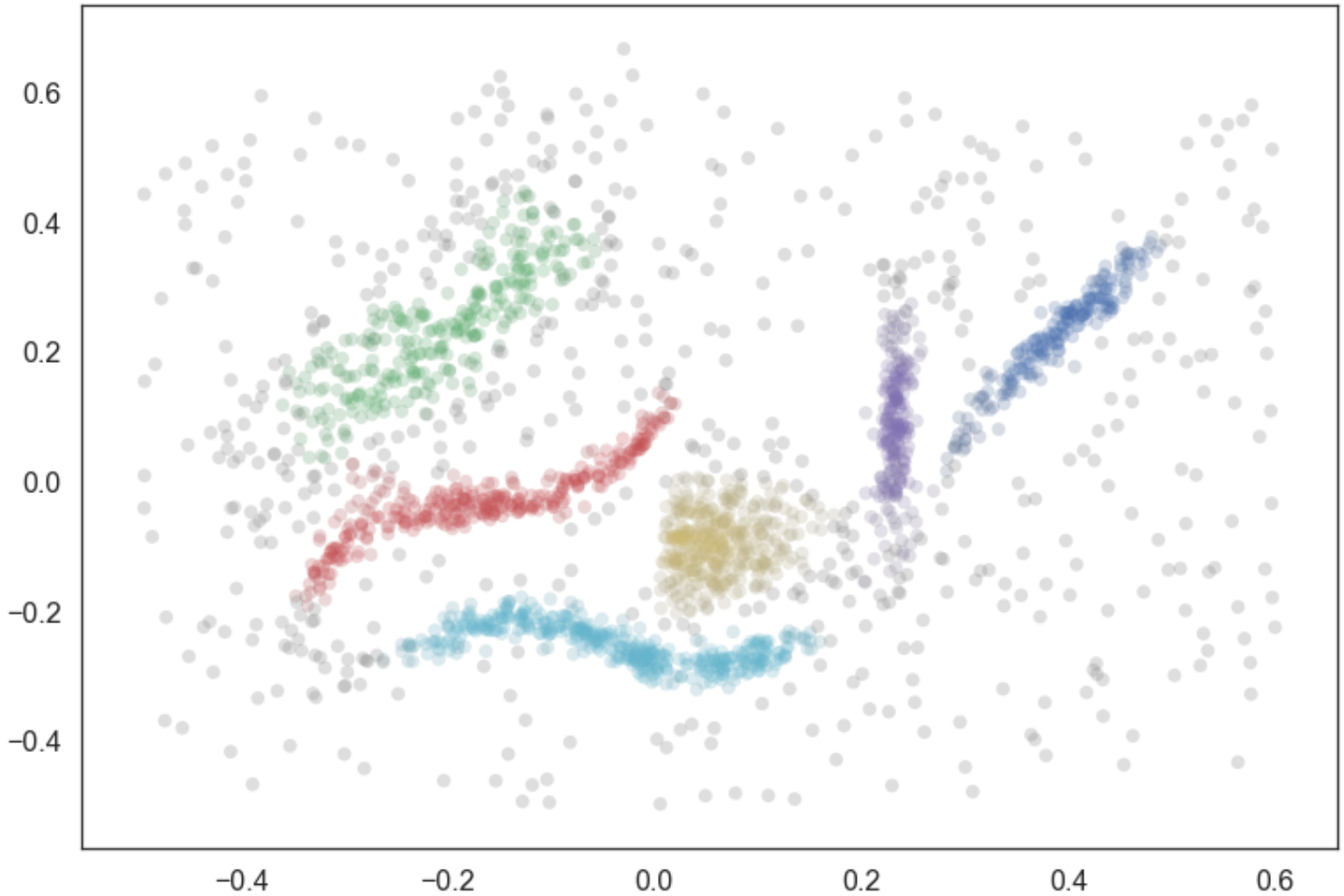
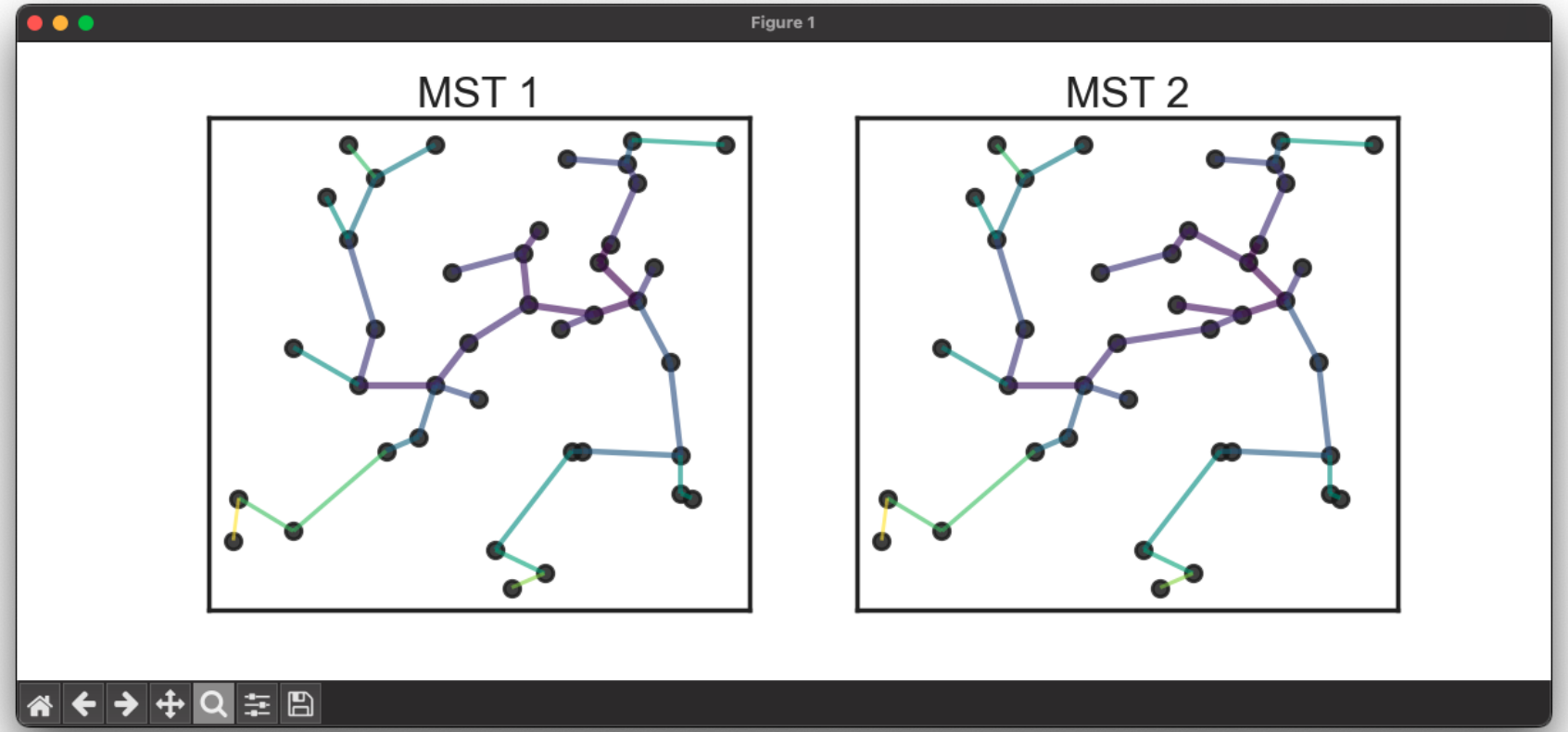
Example HDBSCAN Run

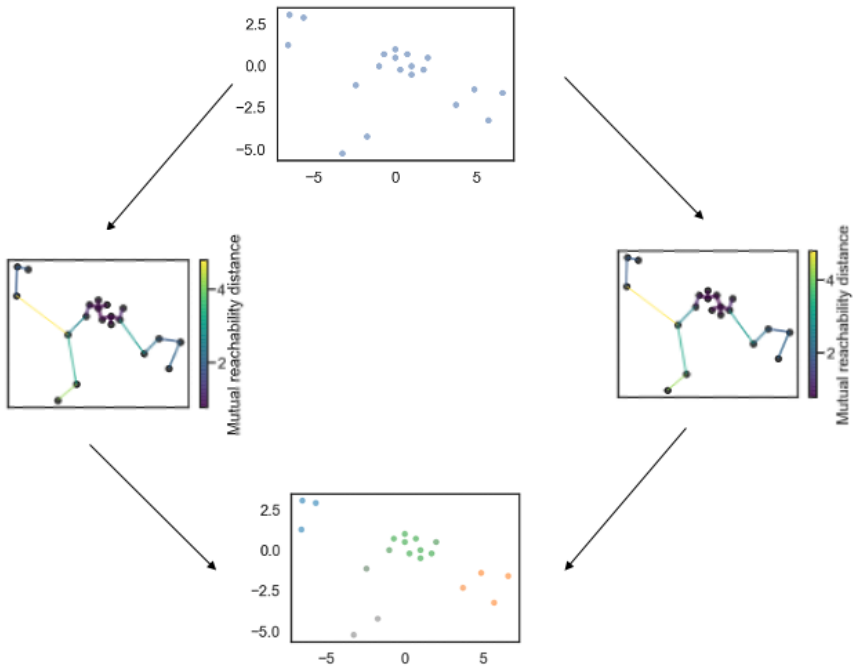


Forty Random Points



"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.



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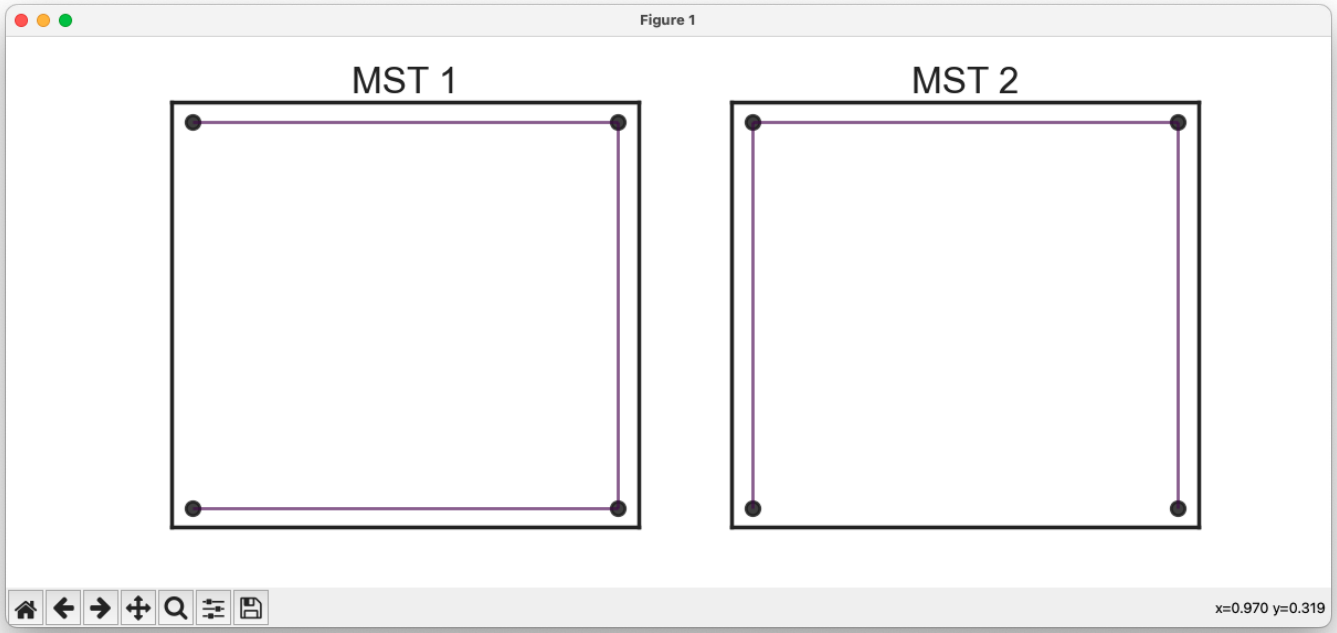
3. Describe sufficient conditions for non-unique minimum spanning trees

Base Case

Example

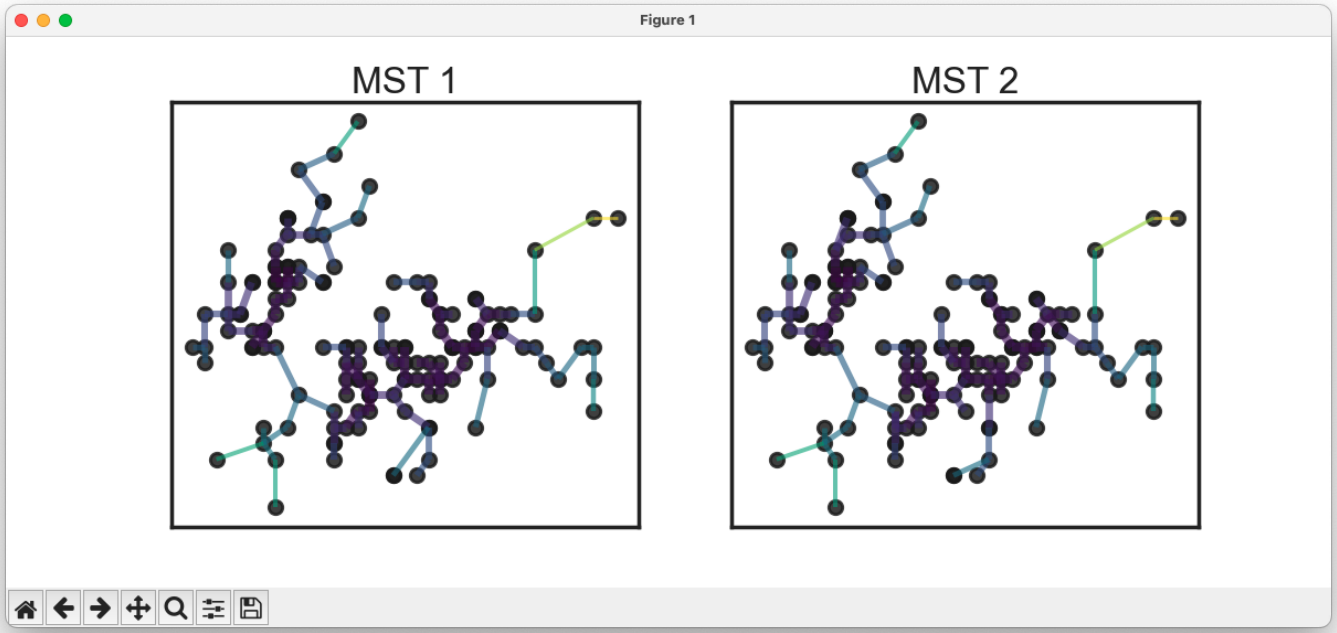
Different orderings of the simple data set $[[0, 0], [0, 1], [1, 1], [1, 0]]$ give different minimum spanning trees



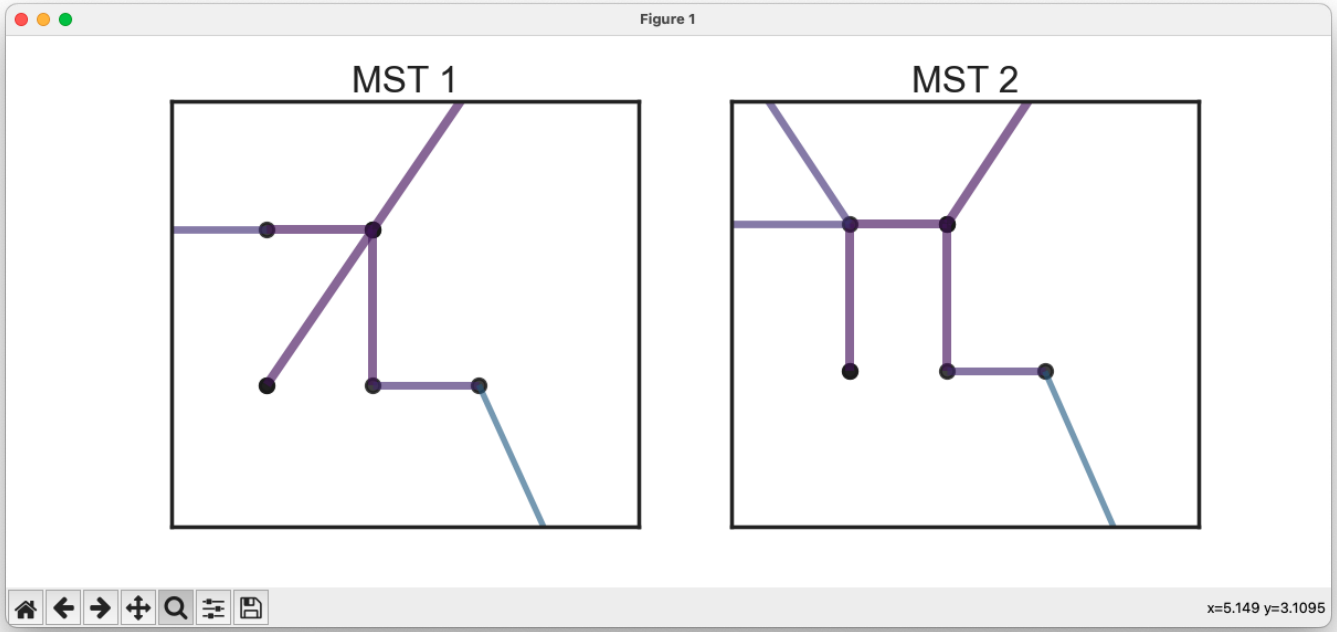
Iris

Example

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



Iris Closeup

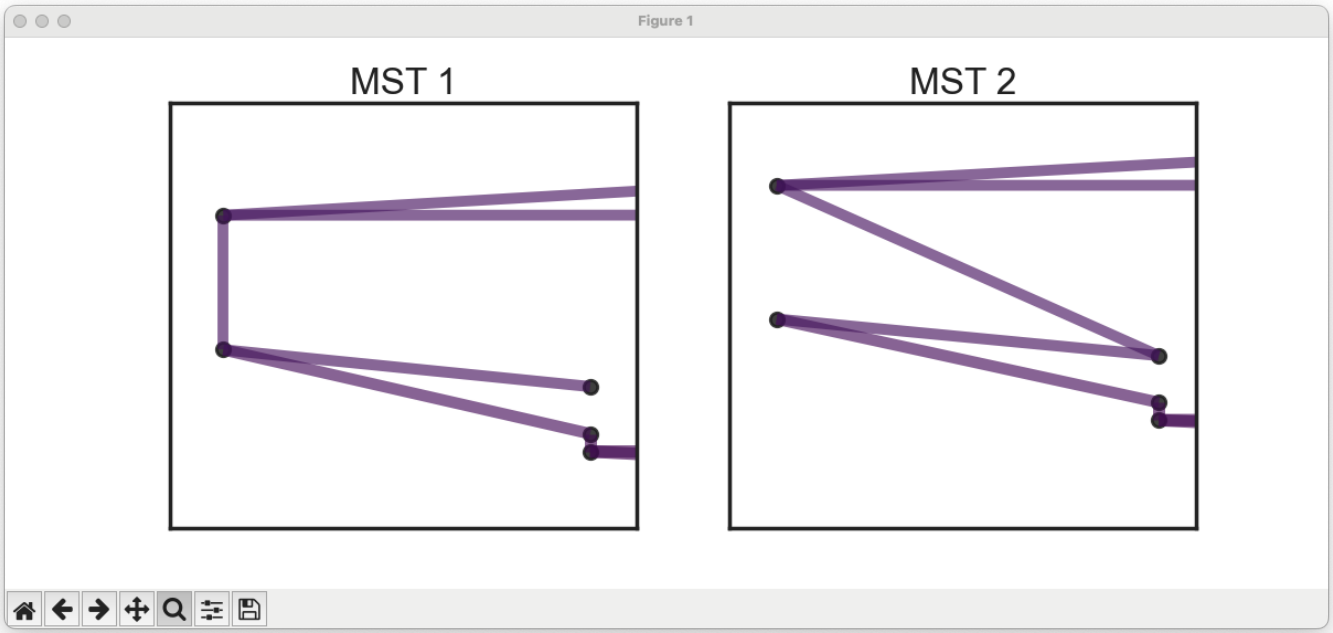


Note: All graphs (except the first) are a two-dimensional projection of the higher-dimensional data sets, but the python script verifies that there are truly multiple trees in the native dimension.

MNIST Closeup

Example

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



NECkSc

Definition

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

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

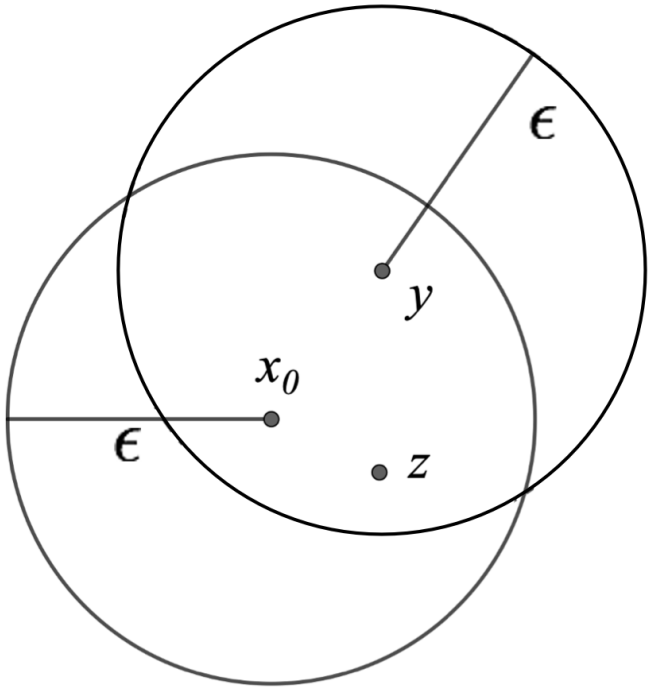
Then X is a 'not-everywhere core$_k$ sparse (closed)' (**NECkSc**) metric space, if and only if

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

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.



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 $(a, b) \in E$, $w(a, b) = \text{mrd}(a, b)$. 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 $k \geq 6$.

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- Order the six closest points to x_0 in terms of their angle relative to x_0.
- By the definition of $\text{core}_6(x_0) = \epsilon$, 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.

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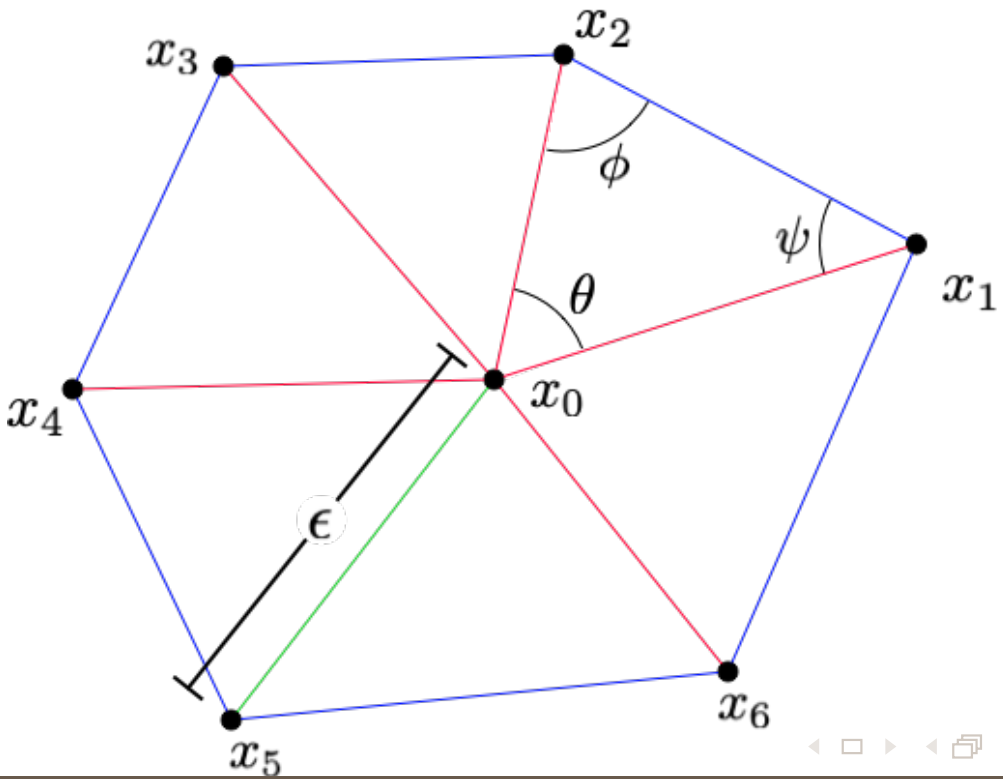


The Kissing Number

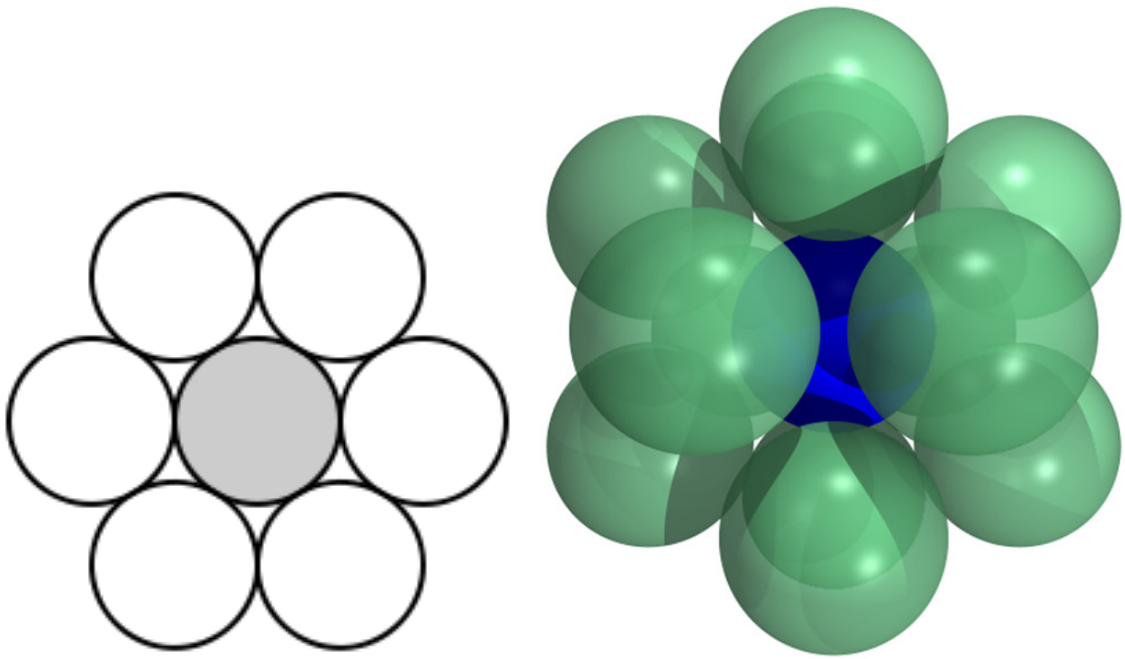
Definition

Given an n-dimensional sphere S with radius r, the n-**dimensional kissing number** 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.



Kissing Numbers (from [3])

Dimension	Lower bound	Upper bound	Ratio	References
1	2		1	
2	6		1	
3	12		1	[18]
4	24		1	[17, 14]
5	40	44	1.100	[7, 13]
6	72	78	1.084	[7, 13]
7	126	134	1.064	[7, 13]
8	240		1	[7, 11, 16]
9	306	363	1.187	[10, 12]
10	510	553	1.085	[5, 12]
11	592	868	1.467	[5, 8]
12	840	1355	1.614	[10, 8]

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

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 $k \leq \text{kiss}(n)$.

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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.

Proof Sketch

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

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- $|A'| = |A| = k$.
- For all $p, q \in A$ with $p \neq q$, $\text{dist}(p, q) > \epsilon$, becuase (X, dist) 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.

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- We place a hypersphere of radius $\frac{\epsilon}{2}$ centered at each $p' \in A'$, as well as one centered at x_0.
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- But no hypersphere is tangent to any other, because $\text{dist}(p', q') > \epsilon$ for all $p', q' \in A'$ with $p' \neq q'$.

Proof Sketch (continued)

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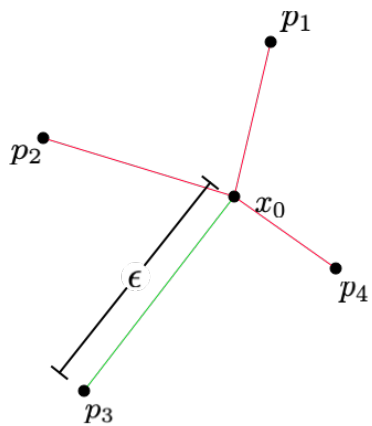
- These hyperspheres are all tangent to the hypersphere centered at x_0, because for each $p' \in A'$, $\text{dist}(p', x_0) = \epsilon$.
- But no hypersphere is tangent to any other, because $\text{dist}(p', q') > \epsilon$ for all $p', q' \in A'$ with $p' \neq q'$.
- These all have radius $\frac{\epsilon}{2}$,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

Proof Illustration in Two Dimensions



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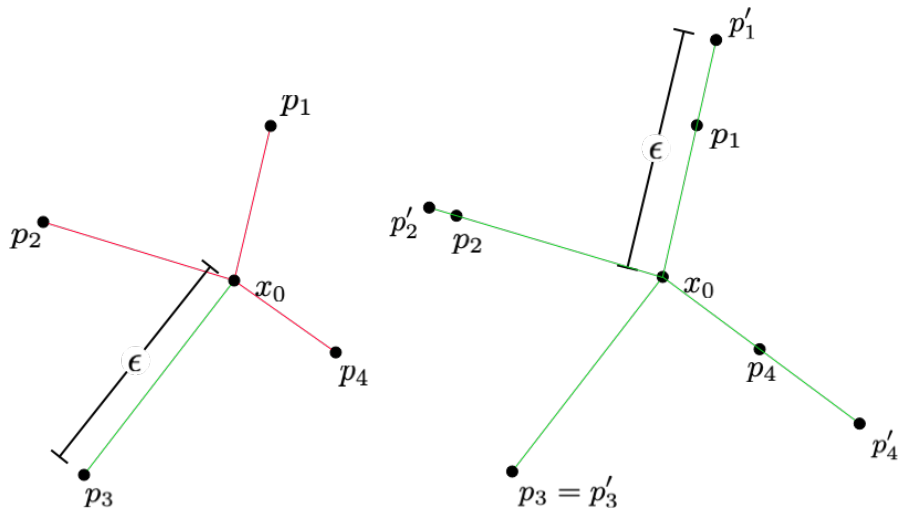

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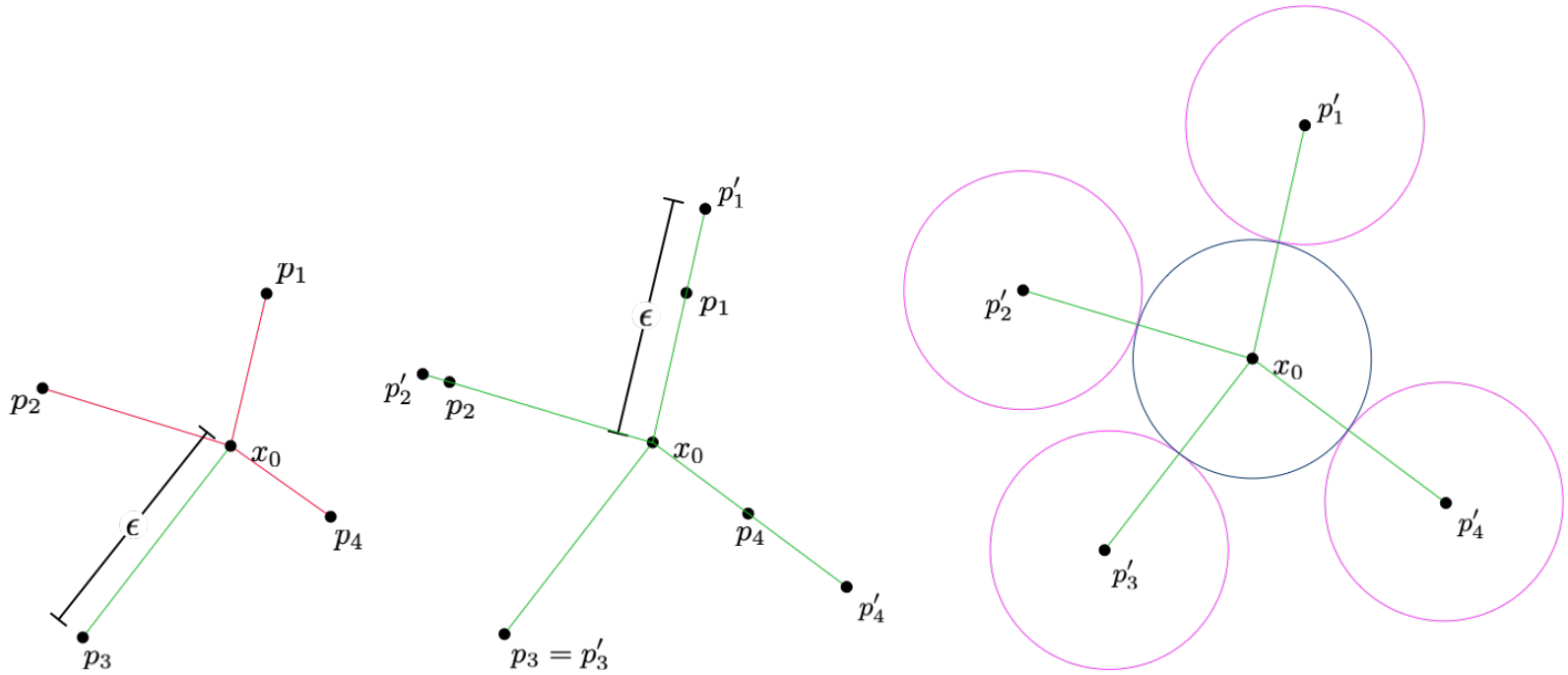

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- We have tested that this can occur in real-world data, and have empirically shown that this is often the case.
- We have shown conditions that gurantee a metric space is NECkSc, which imply non-unique minimum spanning trees.

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