Geometric and Topological Data Analysis

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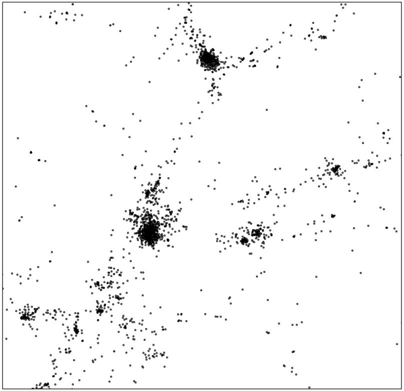
Geometric and Topological Data Analysis: Big Picture



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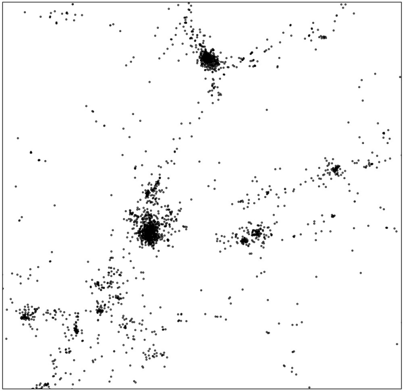
$$X_1, \cdots, X_n \sim p,$$

p is a probability density function.



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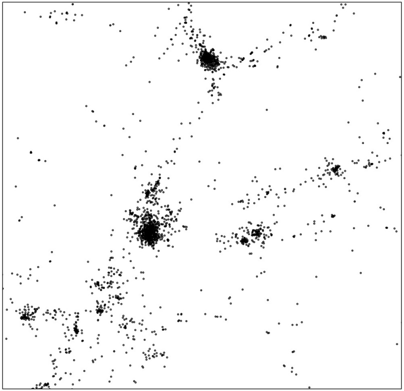

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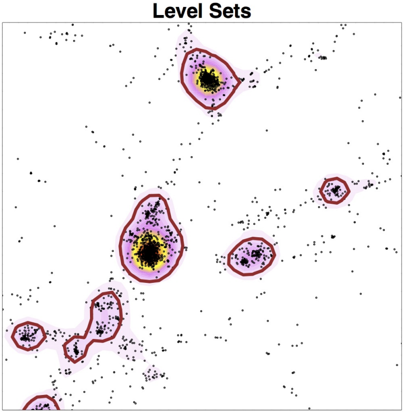

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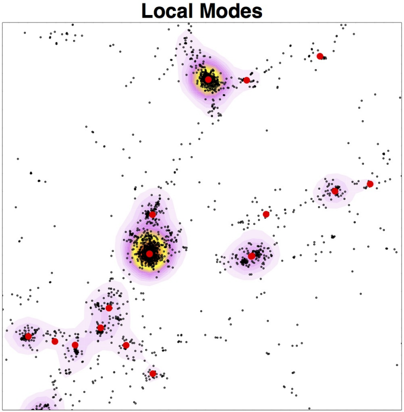

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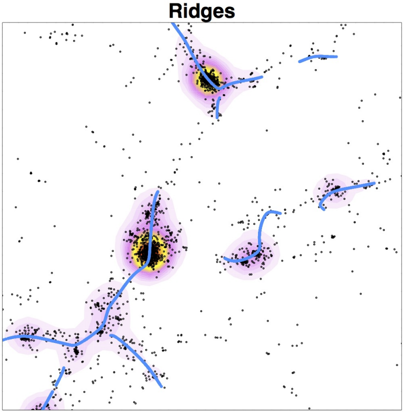

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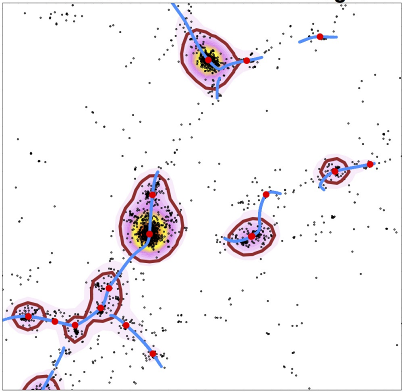

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- But this idea may fail.

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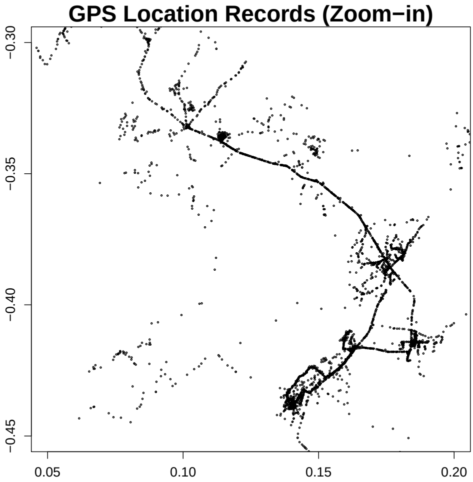

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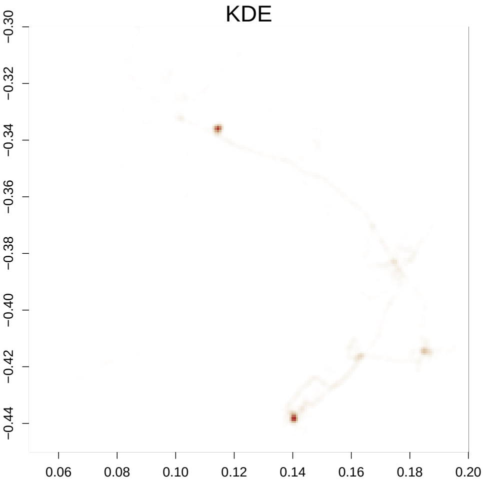

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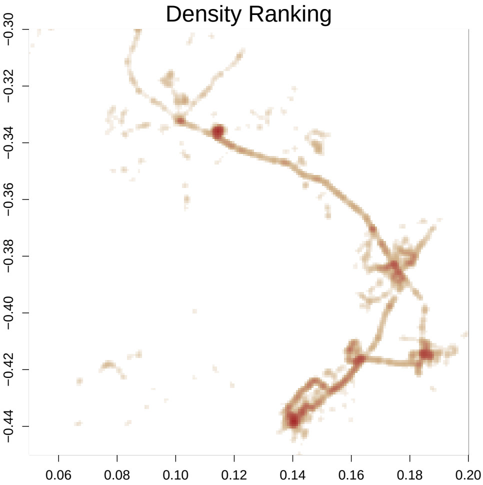

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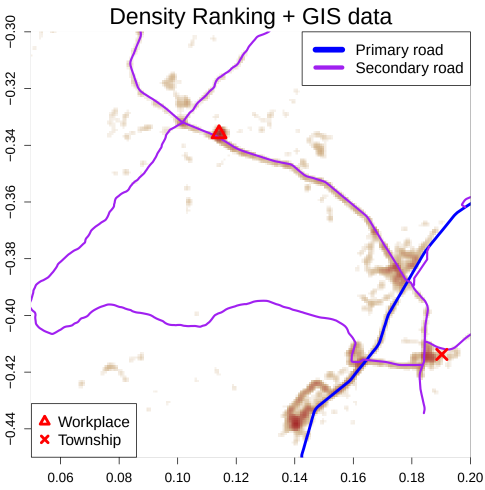

Density Ranking: Introduction

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- The KDE cannot detect intricate structures inside the GPS data.
- But the density ranking works!
- This comes from the fact that the underlying probability density function (PDF) does not exist!
- Namely, our probability distribution function is a singular measure.

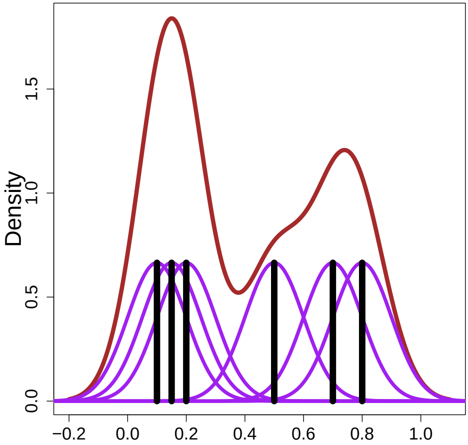
Definition of Density Ranking - 1

- Given random variables $X_1, \cdots, X_n \in \mathbb{R}^d$, the KDE is

$$\widehat{p}(x) = \frac{1}{nh^d} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right),$$

  where $K(\cdot)$ is called the kernel function such as a Gaussian and $h > 0$ is called the smoothing bandwidth that controls the amount of smoothing.
- The KDE smoothes out the observations into small bumps and sum over all of them to obtain a PDF.

Definition of Density Ranking - 2



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- The formal definition of density ranking is

$$\begin{aligned}\widehat{\alpha}(x) &= \frac{1}{n}\sum_{i=1}^{n} I\left(\widehat{p}(x) \geq \widehat{p}(X_i)\right)\\ &= \text{ratio of observations' density below the density of point } x.\end{aligned}$$

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- Namely, $\widehat{\alpha}(x) = 0.3$ implies that the (estimated) density of point x is above the (estimated) density of 30% of all observations.

Property of Density Ranking

- For an observation $X_{\max}$ with $\widehat{\alpha}(X_{\max}) = 1$, then it means

$$\widehat{p}(X_{\max}) = \max\left\{\widehat{p}(X_1), \cdots, \widehat{p}(X_n)\right\}.$$

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- If an observation X_ℓ satisfies $\widehat{\alpha}(X_\ell) = 0.25$, this means that the ranking of density at X_ℓ is the 25%.
- Moreover, for any pairs of points x_1, x_2,

$$\begin{aligned}
\widehat{p}(x_1) > \widehat{p}(x_2) &\Longrightarrow \widehat{\alpha}(x_1) > \widehat{\alpha}(x_2)\\
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- Under regularity conditions,

$$\int \left|\widehat{\alpha}(x) - \alpha(x)\right|^2 dP(x) \xrightarrow{P} 0, \quad \sup_x \left|\widehat{\alpha}(x) - \alpha(x)\right| \xrightarrow{P} 0.$$

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$$\mathcal{H}_s(x) = \lim_{r\to 0} \frac{P(B(x,r))}{C_s r^s}.$$

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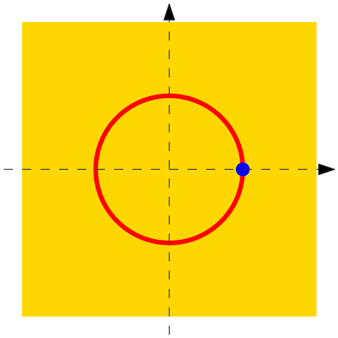
- For a point x, we then define

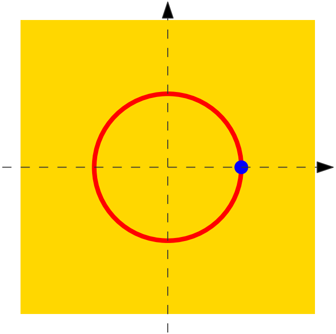
$$\tau(x) = \max\{s \le d : \mathcal{H}_s(x) < \infty\}, \quad \rho(x) = \mathcal{H}_{\tau(x)}(x).$$

Geometric Density: Example - 1

- Assume the distribution function P is a mixture of a $2D$ uniform distribution within $[-1, 1]^2$, a $1D$ uniform distribution over the ring $\{(x, y) : x^2 + y^2 = 0.5^2\}$, and a point mass at $(0.5, 0)$, then the support can be partitioned as follows:



Geometric Density: Example - 2



- Orange region: $\tau(x) = 2$.
- Red region: $\tau(x) = 1$.
- Blue region: $\tau(x) = 0$.

Geometric Density and Ranking

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- Namely, we first compare the dimension of the two points, the lower dimensional structure wins. If they are on regions of the same dimension, we then compare the density of that dimension.

Constructing Density Ranking using Geometric Density

- Using the ordering $\succ_{\tau,\rho}$, we then define the population density ranking as

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- Using the ordering $\succ_{\tau,\rho}$, we then define the population density ranking as
$$\alpha(x) = P(x \succeq_{\tau,\rho} X_1)$$
- When the PDF exists, the ordering $\succ_{\tau,\rho}$ equals to $\succ_{d,p}$ so
$$\alpha(x) = P(x \succeq_{d,p} X_1) = P(p(x) \geq p(X_1)),$$
which recovers our original definition.

Convergence under Singular Measure

- When P is a singular distribution and satisfies certain regularity conditions,

$$\int \left|\widehat{\alpha}(x) - \alpha(x)\right|^2 dP(x) \xrightarrow{P} 0$$

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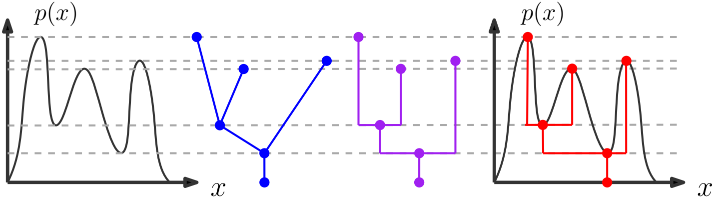
  but no guarantee for the convergence of $\sup_x \left|\widehat{\alpha}(x) - \alpha(x)\right|$.
- Example of non-convergence of supreme norm: points very close to a lower dimensional structure will not converge.

Density Ranking and Cluster Tree - 1

- Cluster tree is a technique to summarize a function using a tree.
- When the PDF exists, the cluster tree of a PDF and the cluster tree of the corresponding density ranking has the same tree topology.



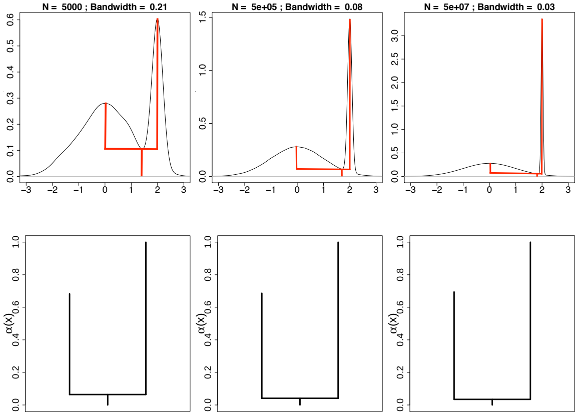
- The idea of building a cluster tree of a function f relies on matching the connecting components of level sets $\{x : f(x) \geq \lambda\}$ when we vary the level λ.

Density Ranking and Cluster Tree - 2

- Using the level sets of $\widehat{\alpha}(x)$ or $\alpha(x)$, we can define the cluster tree of the density ranking and the population density ranking.
- When the distribution function is singular and satisfies certain regularity conditions, the cluster tree of $\widehat{\alpha}(x)$ converges to the cluster tree of $\alpha(x)$.

Density Ranking and Cluster Tree: Example

Here the population distribution function is a mixture of a $1D$ standard normal distribution and a point mass at 2. We consider three sample sizes: $n = 5 \times 10^3, 5 \times 10^5, 5 \times 10^7$.



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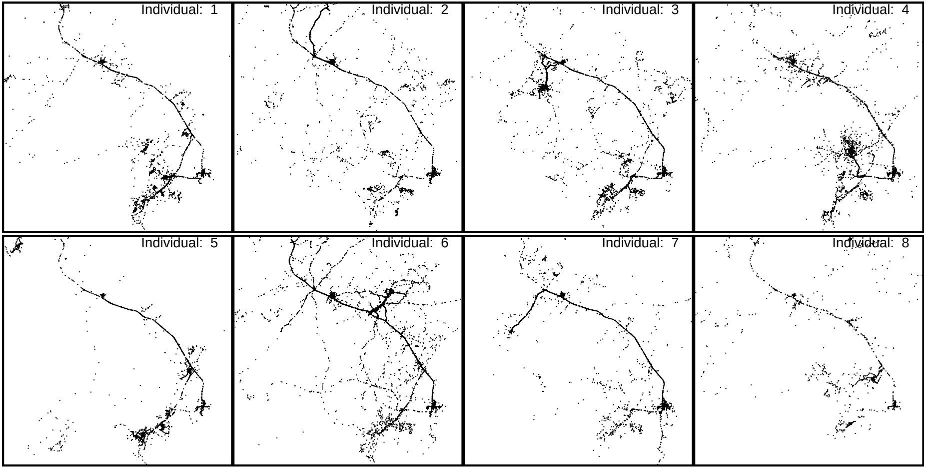
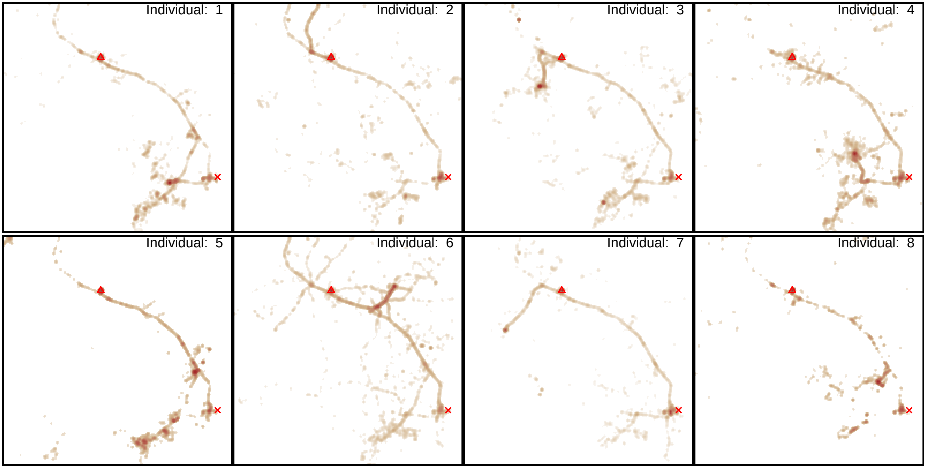


Application of Density Ranking: GPS dataset - 2



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- For a density ranking $\widehat{\alpha}$, let

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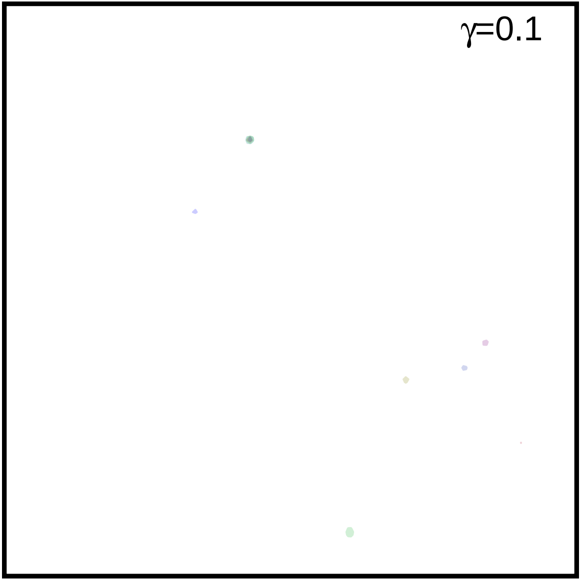
  be the (upper) level set.
- We can compare the density ranking of each individual by overlapping their level sets at each level.

Level Plots: Example



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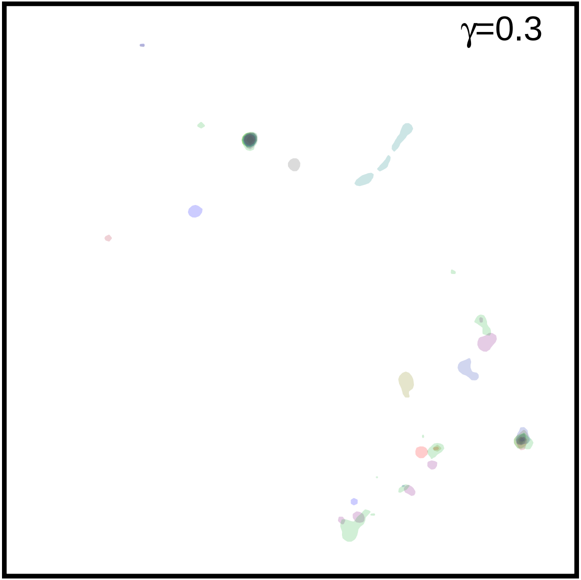

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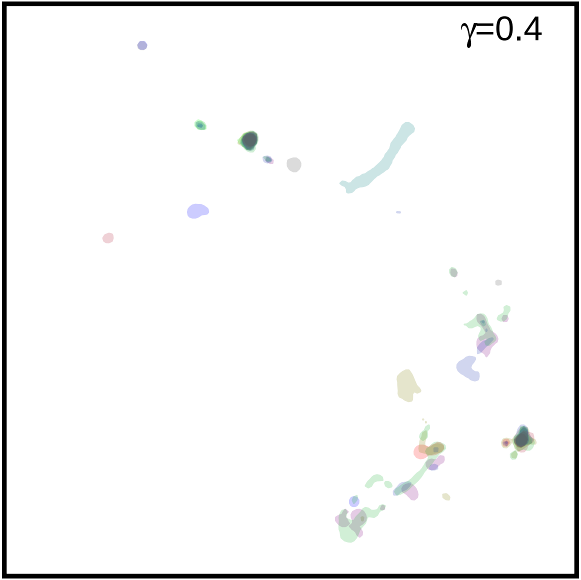

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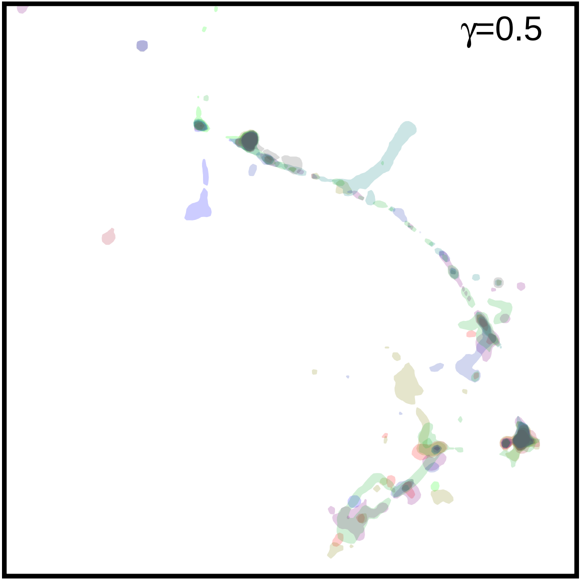

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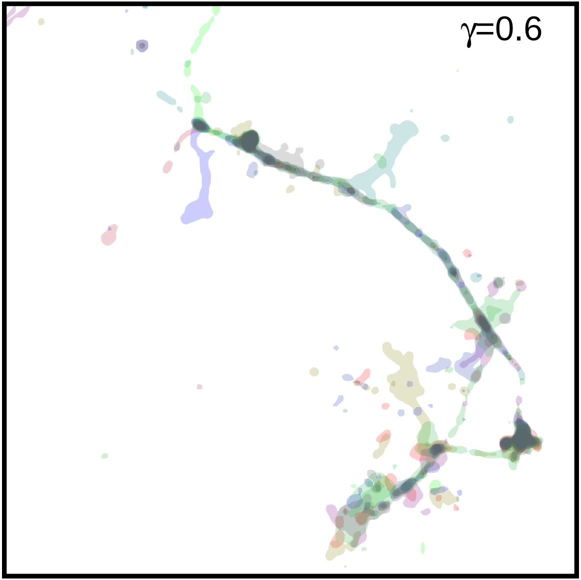

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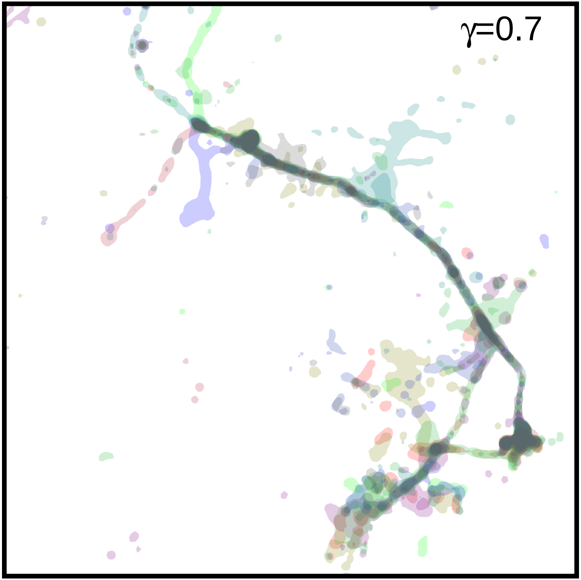

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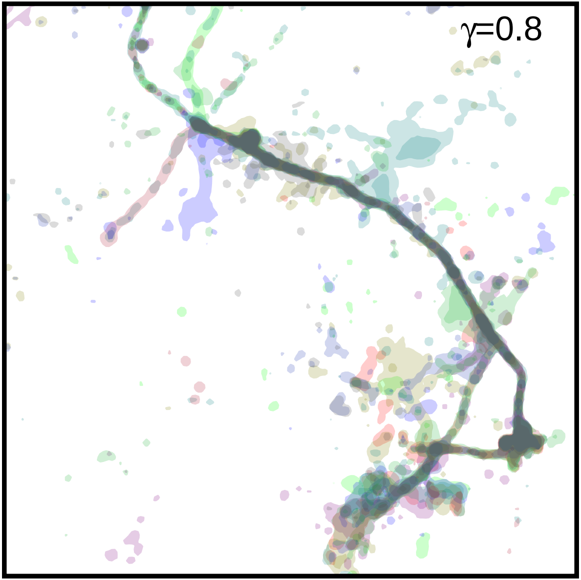

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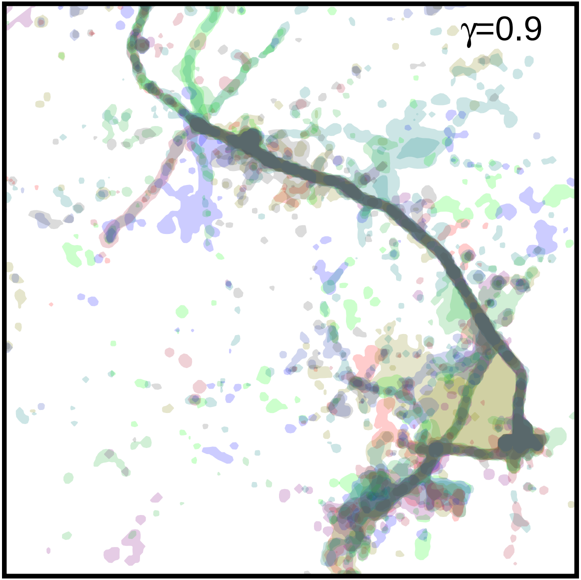

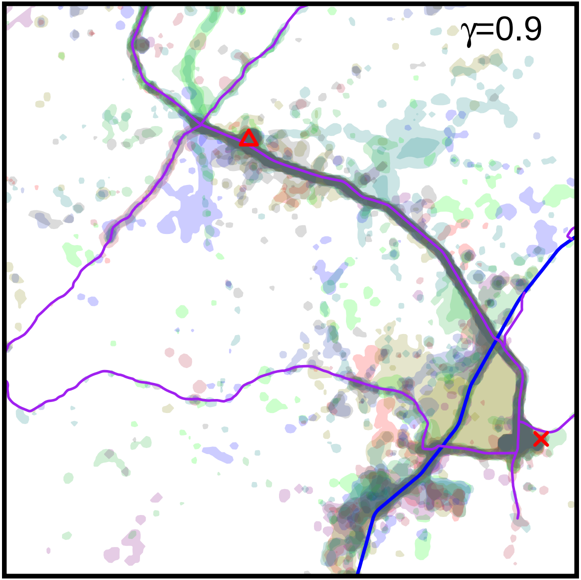
γ=0.9

Summary Curves of Density Ranking

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  - When we have more individuals, this approach might not work (too many contours).
  - We often need to choose a level γ to show the plot but which level to be chosen is unclear.
- Here we introduce a few curves to summarize geometric and topological features of density ranking.

Mass-Volume Curve

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- In practice, we often plot γ versus $\log \mathsf{Vol}(\widehat{\alpha})_\gamma$.

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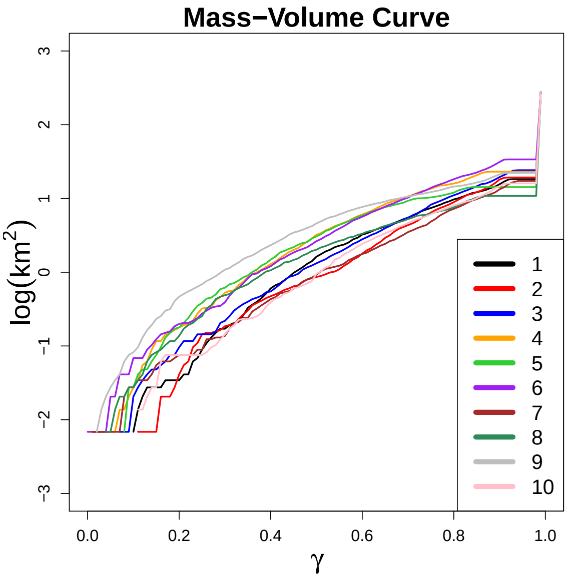

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where for a set A

$$\mathsf{Betti}_0(A) = \text{ number of connected components inside } A.$$

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- It counts the number of connected components of $\widehat{A}_\gamma$ at various level γ.
- Formally, the Betti number curve is

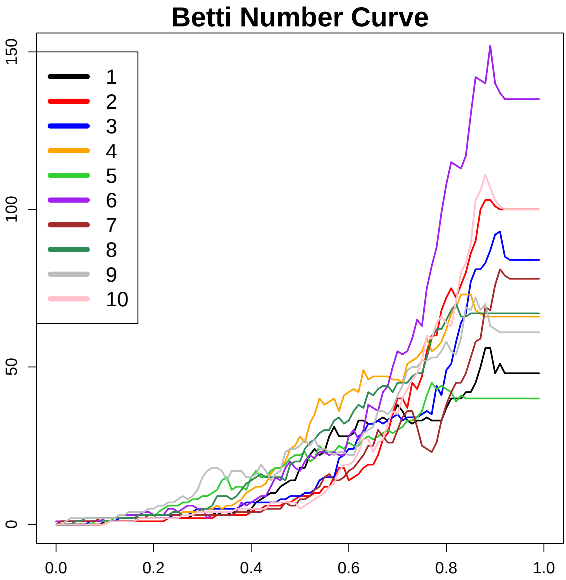
$$\left(\gamma, \mathsf{Betti}_0(\widehat{A}_\gamma)\right) : \gamma \in [0,1],$$

where for a set A

$$\mathsf{Betti}_0(A) = \text{ number of connected components inside } A.$$

- Note that the number of connected component is called the 0th order Betti number (0th order topological structure); one can generalize this idea to higher order topological structures.

Betti Number Curve: Example



Density Ranking: Open Questions

- Convergence of density ranking level sets.
- Convergence of summary curves under singular/non-singular measure.
- Other summary curves.
- Convergence of higher order topological structures.
- Connection to stratified space.