Density Tree and Density Ranking in Singular Measures

Yen-Chi Chen

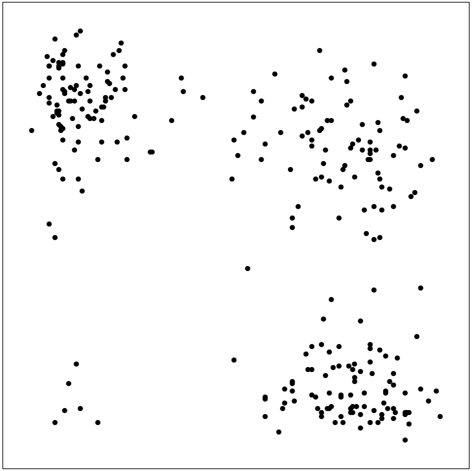
Department of Statistics
University of Washington

Outline

- Density Trees
- Density Ranking
- Density Ranking: Multiple Datasets
- Summary

Density Trees

Clusters and Density Function: an Illustration



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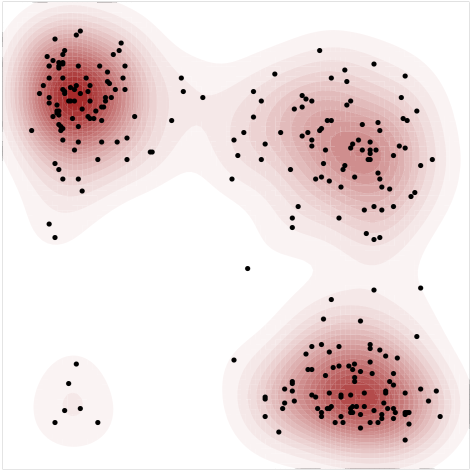

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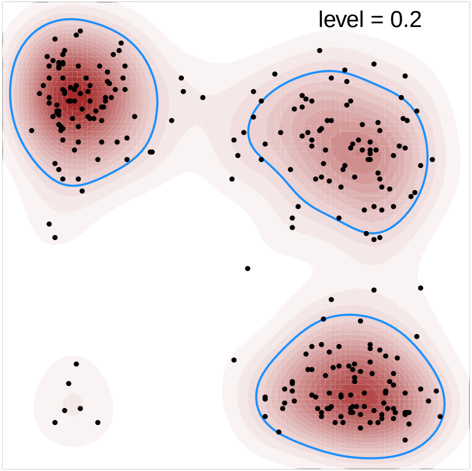

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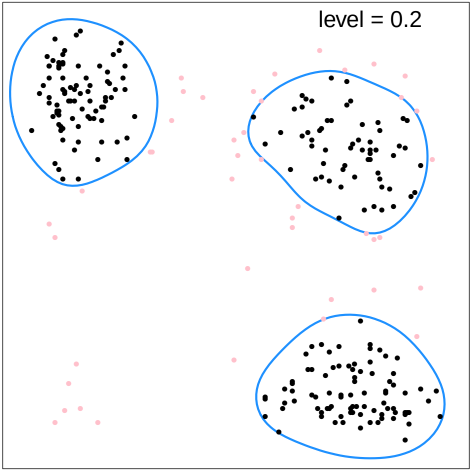

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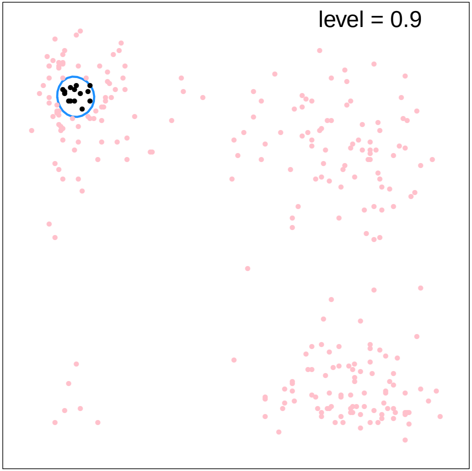
- Thus, the level λ has an effect on the clustering result.
- Varying the level λ may lead to a creation of a new cluster or a merging of existing clusters.

Clusters and Density Function: Different Levels



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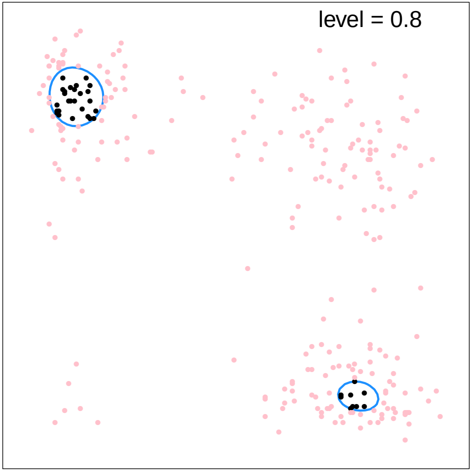

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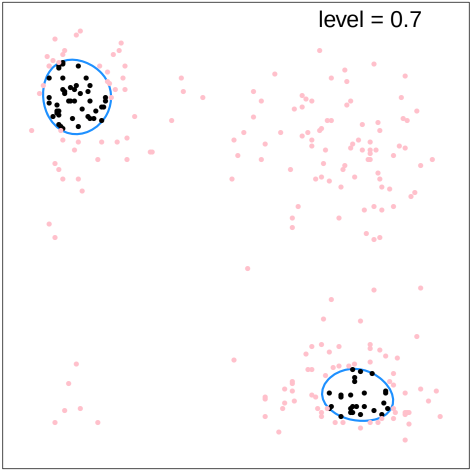

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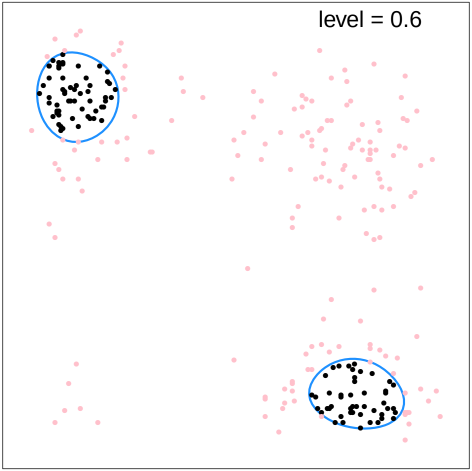

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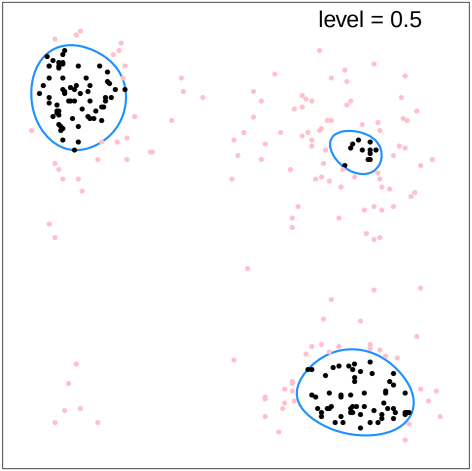

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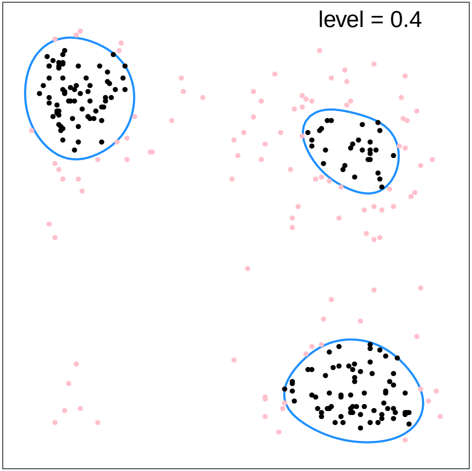

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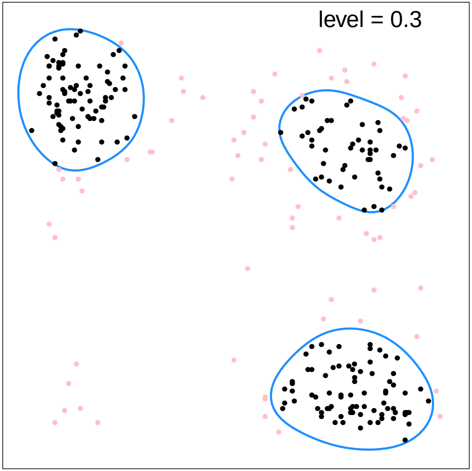

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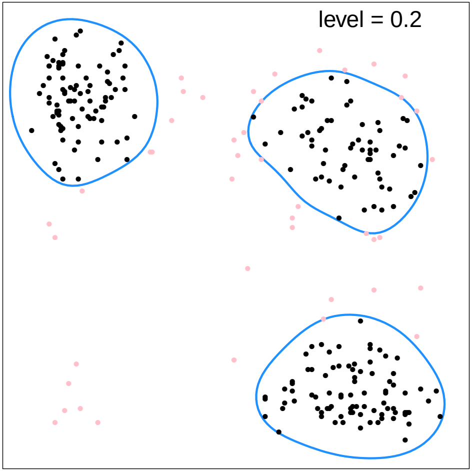

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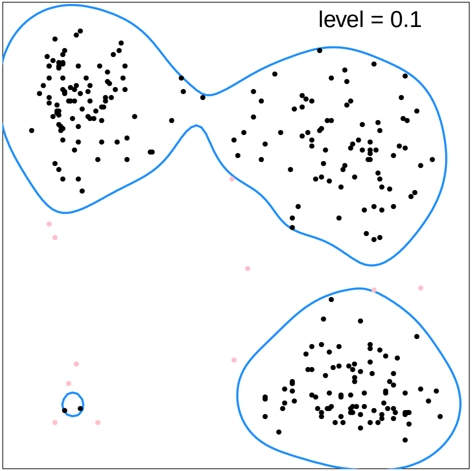

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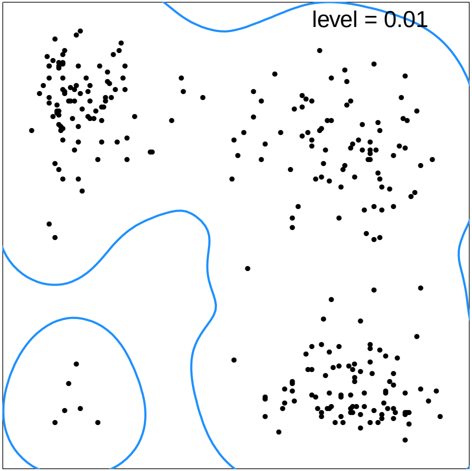

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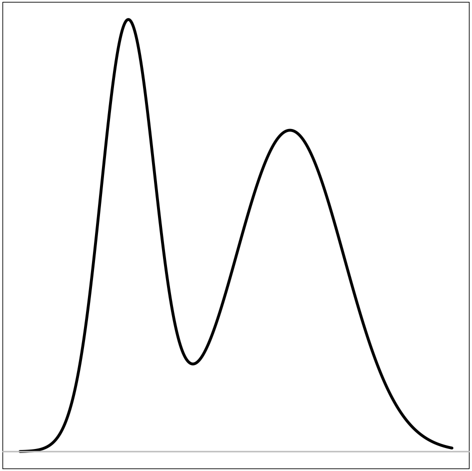
- Cluster tree (Stuetzle 2003) is to summarize such an evolution process by a tree.
- When applied to a density function, a cluster tree is also called a density tree (Klemelä 2004).

Density Tree: an Illustration



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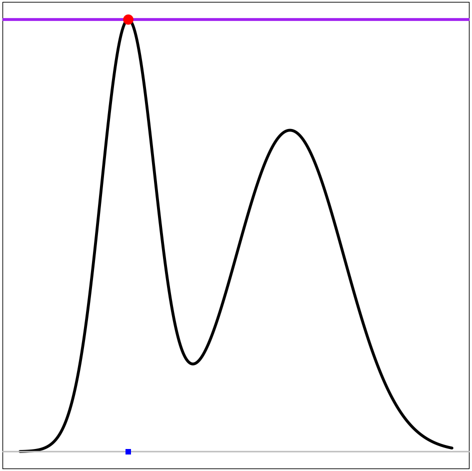

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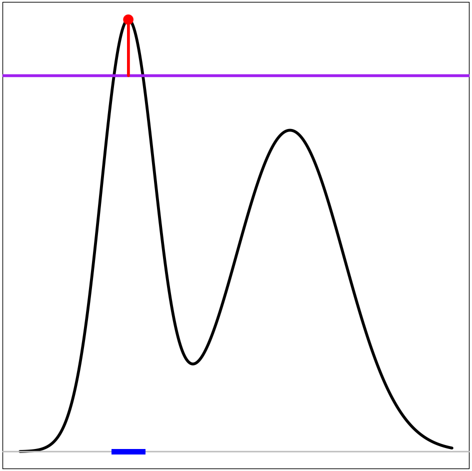

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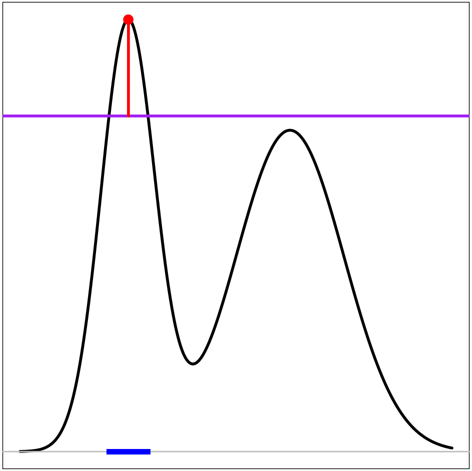

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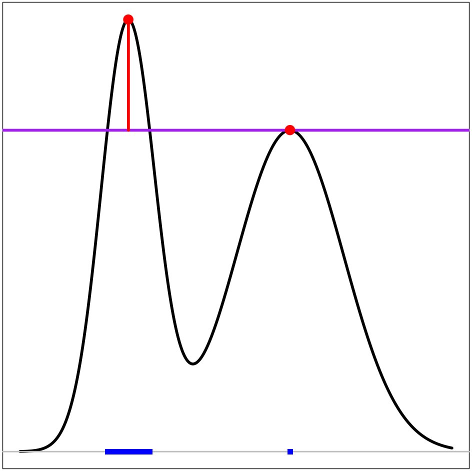

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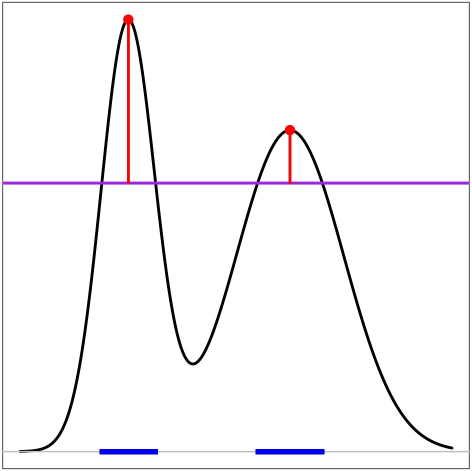

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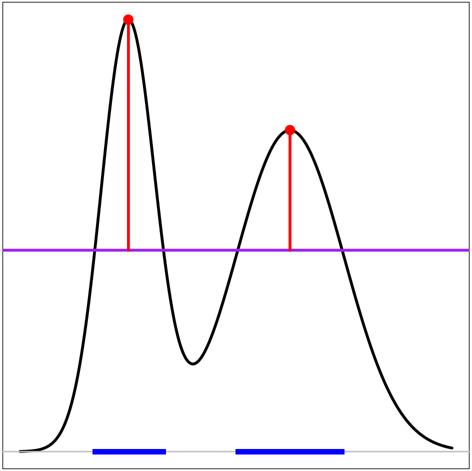

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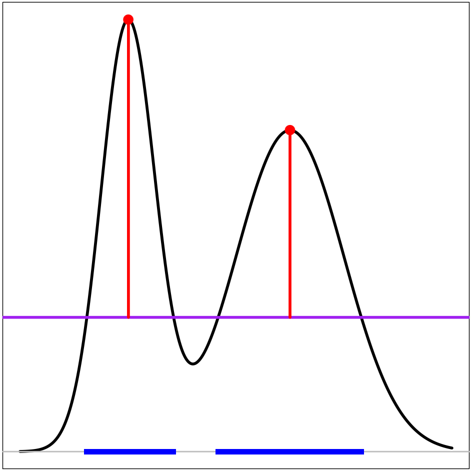

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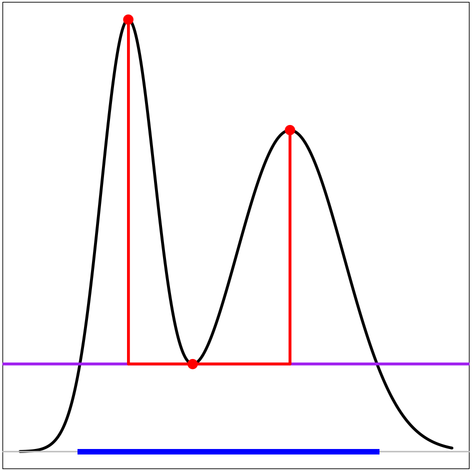

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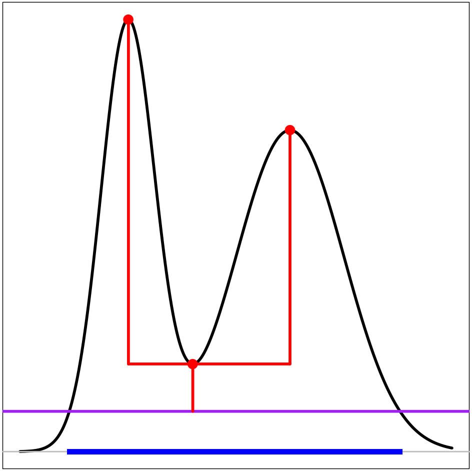

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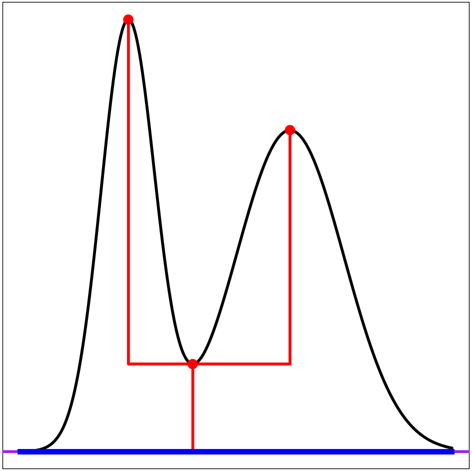

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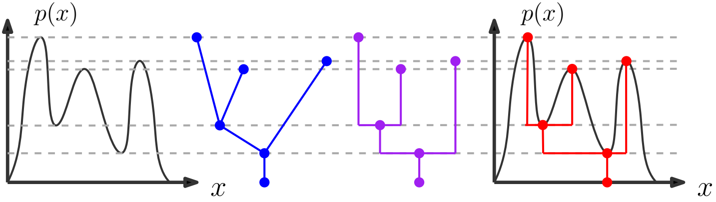

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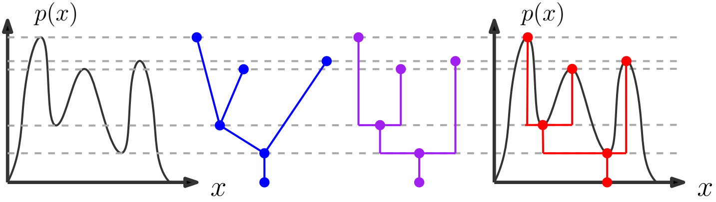

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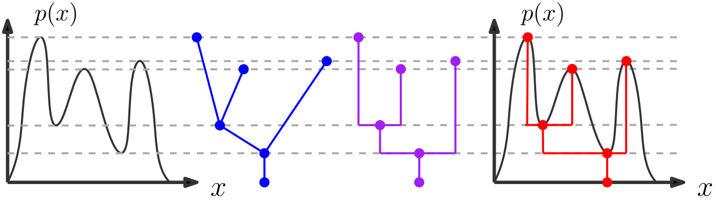

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- The merging of connected components is often associated with local minima or saddle points.

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- We define a collection $T_p = \bigcup_{\lambda \geq 0} \{C_{\lambda,1}, \cdots, C_{\lambda,J(\lambda)}\}$. Namely, T_p is the collection of all connected components from every level.
- Then the elements of T_p admits a tree structure – this tree structure is the density tree.

Estimating a Density Tree - 1

- In statistics, we often do not know the true density function p.
- Instead, we observe a random sample $X_1, \cdots, X_n \in \mathbb{R}^d$ that are IID from p.
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- Here we use the kernel density estimator (KDE):

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

  where $K(\cdot)$ is the kernel function that is often a smooth function like a Gaussian, and $h > 0$ is the smoothing bandwidth that controls the amount of smoothing.

Estimating a Density Tree - 2

- To measure the estimation error, a simple metric is

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- Under smoothness conditions and $n \to \infty, h \to 0$,

$$P_n \geq 1 - e^{-nh^{d+4} \cdot C_p},$$

for some constant C_p depending on the density function p.

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- Note: density tree can also be recovered by a kNN approach; see Chaudhuri and Dasgupta (2010) and Chaudhuri et al. (2014) for more details.

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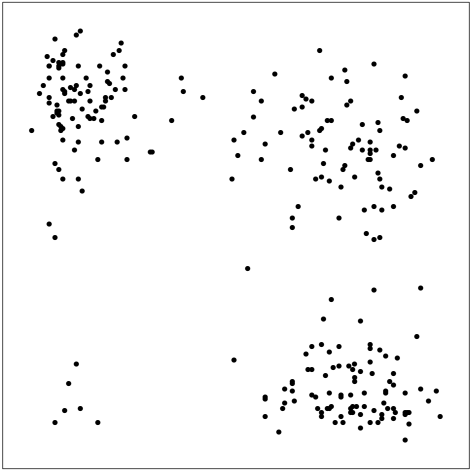

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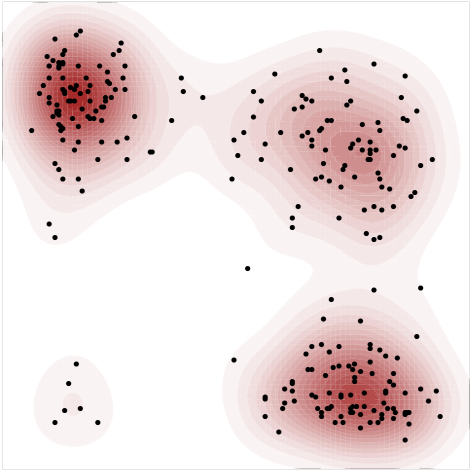

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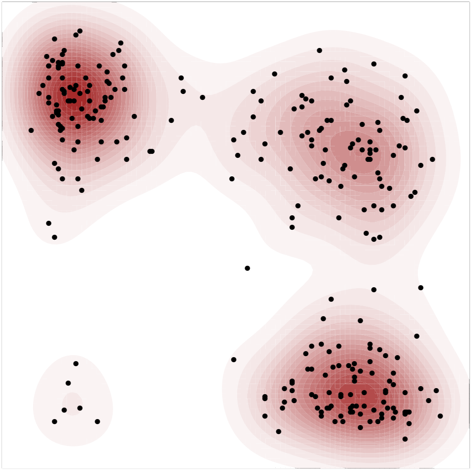

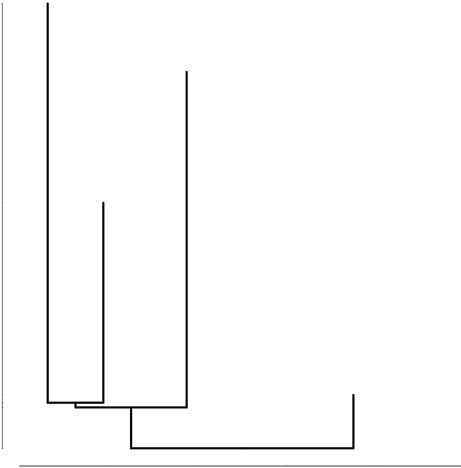

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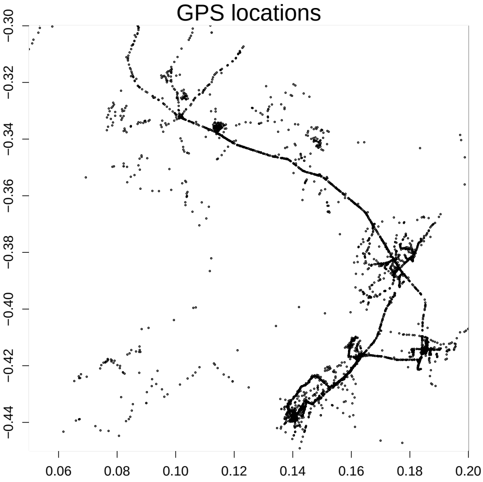
- When using a density level sets to define clusters, the density tree contains the information about the evolution and stability of clusters.
- Moreover, density trees can always be displayed in 2D plane. So they are good tools for visualizing multivariate functions.

Density Ranking

Failure of Density Trees and KDE

- Although density trees and KDE are good approaches, sometimes they may fail.
- In particular, when the PDF does not exist, we cannot use the usual definition for density trees and the KDE to analyze our data.

Failure of Density Trees and KDE: an Example



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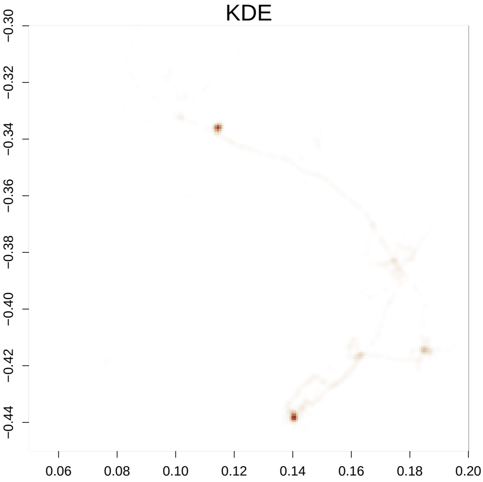

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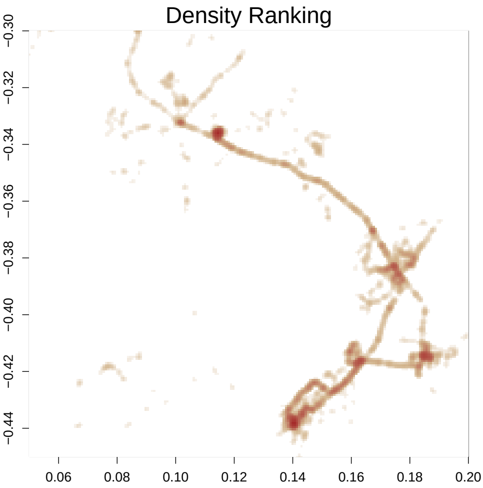

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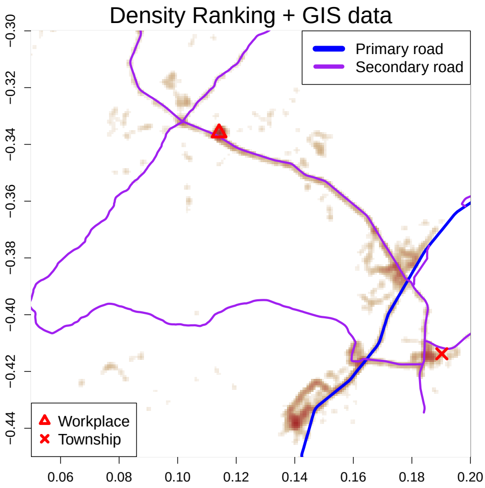

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- However, density ranking still works!

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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

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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 data points X_i, X_j,

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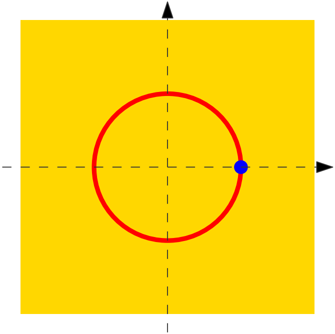
- For a point x, we then define

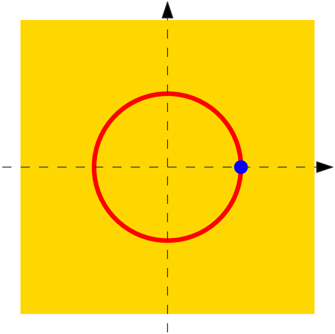
$$\tau(x) = \max\{s \le d : \mathscr{H}_s(x) < \infty\}, \quad \rho(x) = \mathscr{H}_{\tau(x)}(x).$$

Hausdorff 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 Hausdorff: Example - 2



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

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- For two points x_1, x_2, we define an ordering such that $x_1 \succ_{\tau,\rho} x_2$ if

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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 Hausdorff Density

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

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- 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.

Ranking Tree: a Generalization of Density Tree

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- We call this tree the ranking tree.
- Formally, the ranking tree is the set

$$T_\alpha = \bigcup_\lambda \{A_{\lambda,1}, \cdots, A_{\lambda,J(\lambda)}\}$$

where

$$A_{\lambda,1}, \cdots, A_{\lambda,J(\lambda)}$$

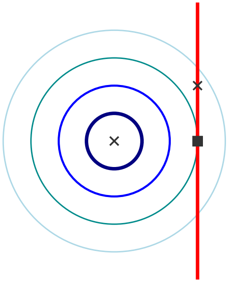
are the connected components of the λ-level set of $\alpha(x)$.

Dimensional Critical Points - 1

- In singular measure, there is a new type of critical points. We call them the *dimensional critical points*.
- These critical points contribute to the change of topology of level sets as the usual critical points but they cannot be defined by setting gradient to be 0.

Dimensional Critical Points - 2

- The box in the following figure is a dimensional critical point.
- Note: this is a mixture of 2D distribution and a 1D distribution on the black line (maximum value occurs at the cross).



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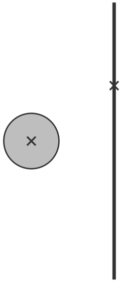

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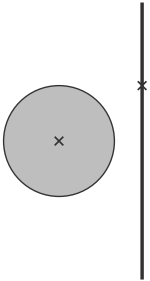

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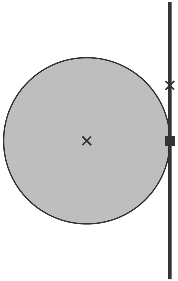

Convergence under Singular Measure: Density Ranking - 1

- 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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- However, the speed of diverging depends on $\tau(x)$. The smaller $\tau(x)$, the faster (actually the diverging rate is $O(h^{\tau(x)-d})$).
- So eventually, we can separate different dimensional structures.

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- Example of non-convergence of supreme norm: consider a sequence of points on a higher dimensional space but moving toward a lower dimensional space within distance $\frac{h}{2}$.

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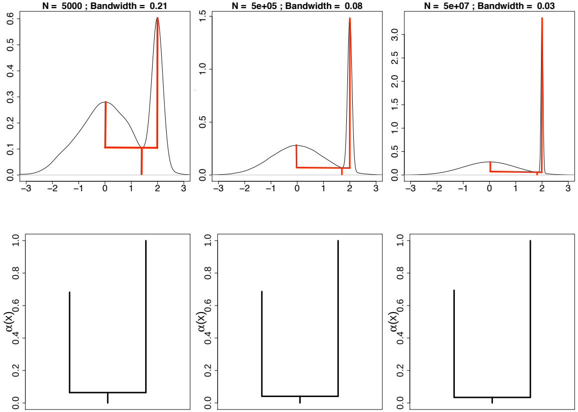
- In addition, the height of each branch of the tree will also converge.

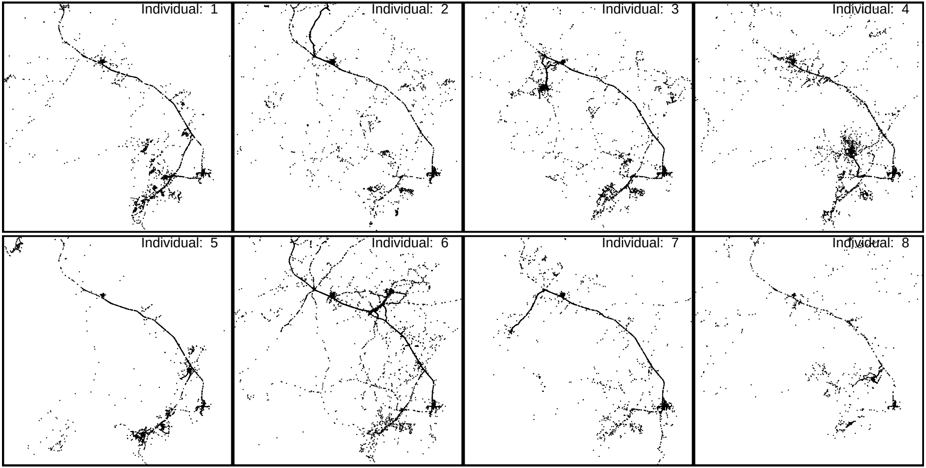
Density Ranking and Cluster Tree: Example

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: $n = 5 \times 10^3, 5 \times 10^5, 5 \times 10^7$.



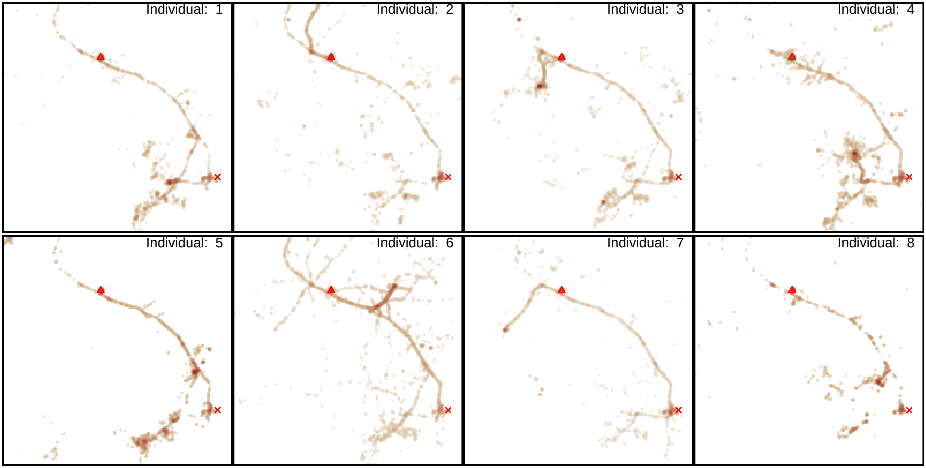
Density Ranking: Multiple Datasets

Application of Density Ranking: GPS dataset - 1



Joint work with Adrian Dobra and Zhihang Dong.

Application of Density Ranking: GPS dataset - 2



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Summarizing Multiple Density Ranking: Level Plots - 1

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- We can compare the density ranking of each individual by overlapping their level sets at different levels.

Summarizing Multiple Density Ranking: Level Plots - 2

- Note that we use $1-\gamma$ as the level in the set $\widehat{A}_{\gamma}$.
- This is because such a set has a natural interpretation in activity space.
- Activity space: the spatial regions where an individual undertakes his/her daily life.

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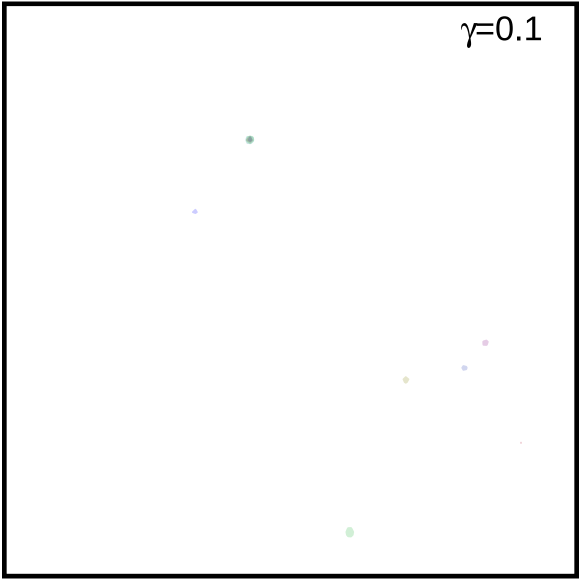
- We can interpret $\widehat{A}_\gamma$ as the (top) $\gamma \cdot 100\%$ activity space because they are regions containing at least $\gamma \cdot 100\%$ GPS records.
- Namely, $\widehat{A}_{\gamma=0.3}$ is the (top) 30% activity space.

Level Plots: Example



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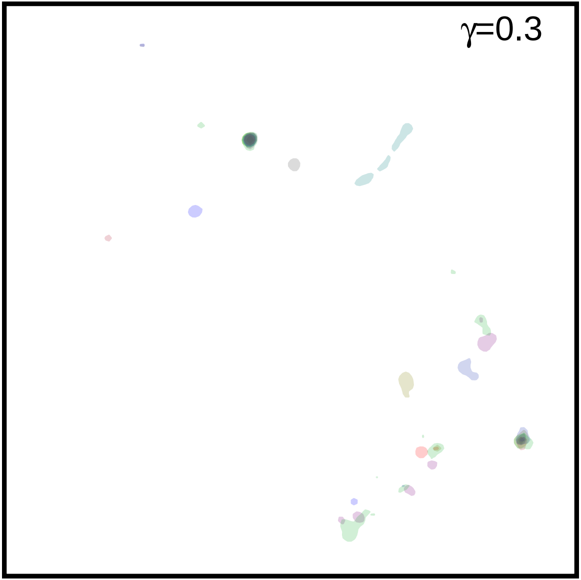

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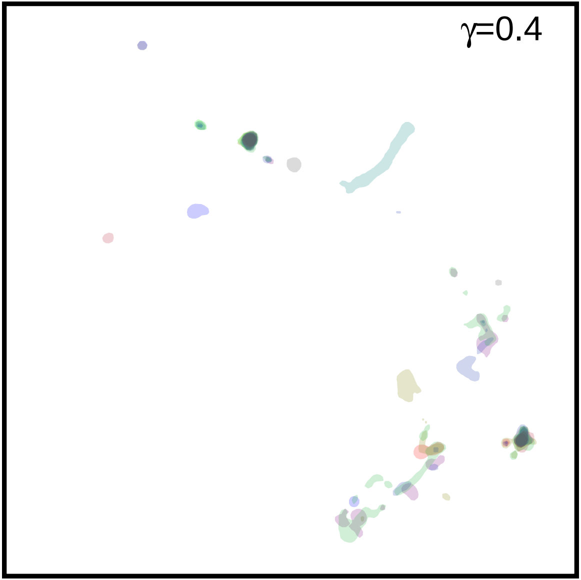

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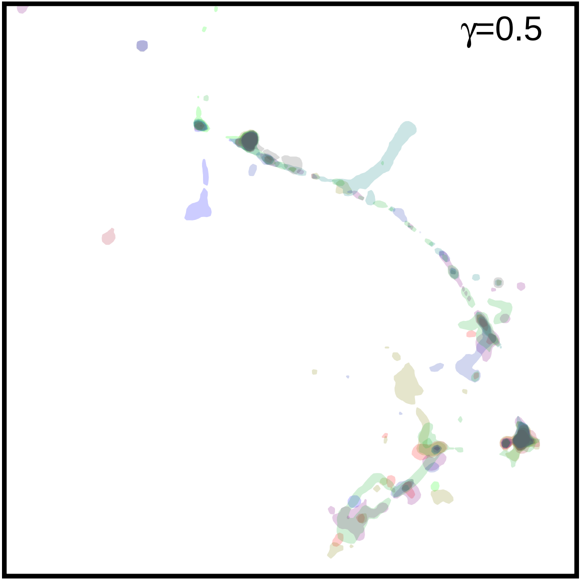

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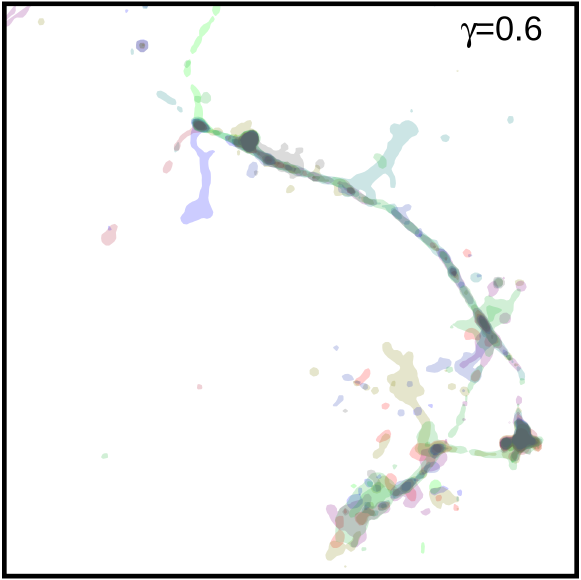

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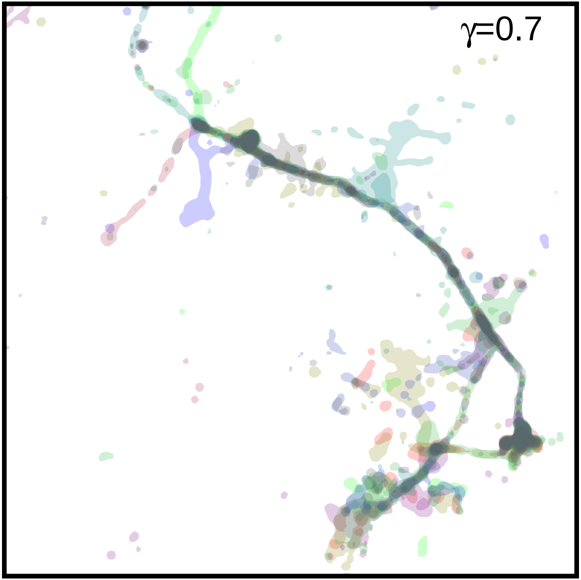

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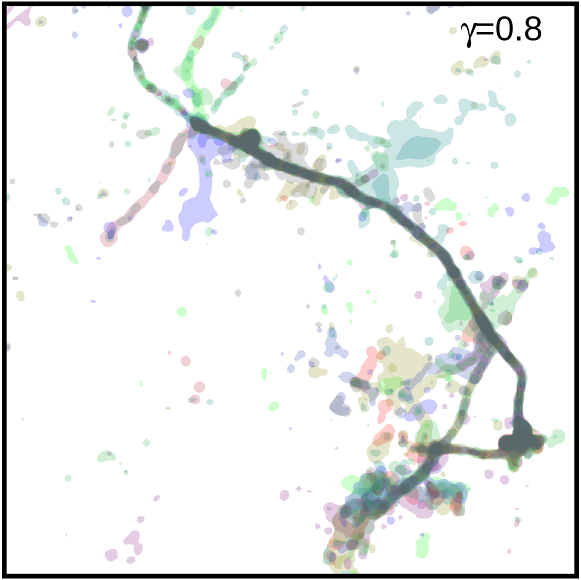

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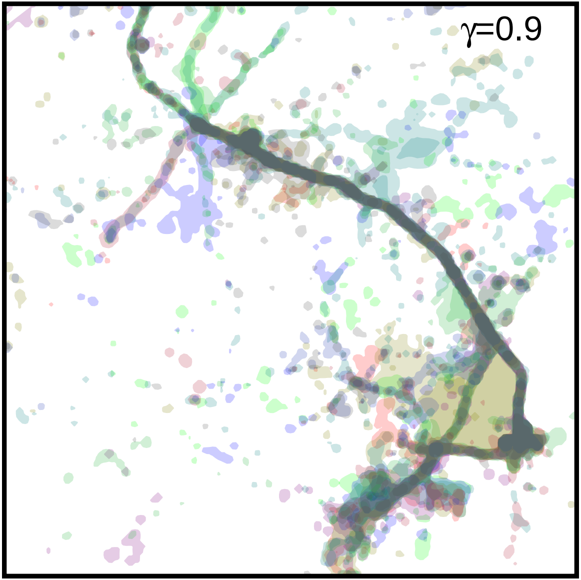

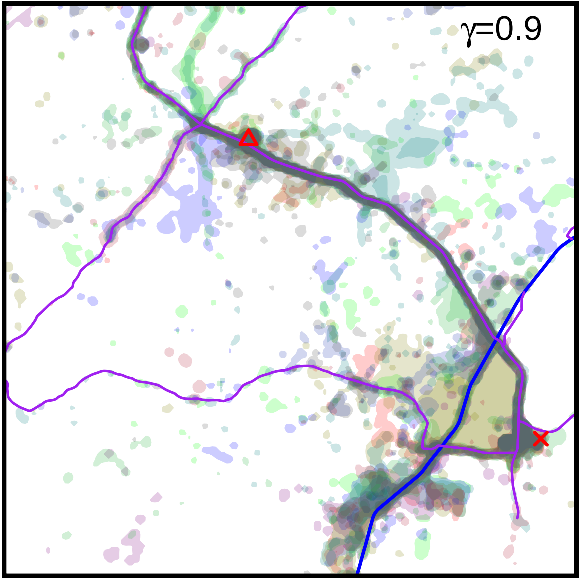
γ=0.9

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- Here we introduce a few curves to summarize geometric and topological features of density ranking.

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

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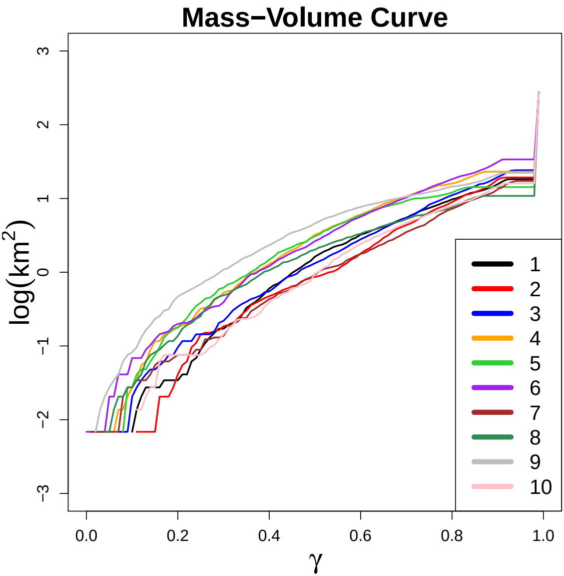

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- Note that the number of connected component is called the 0th order Betti number (0th order topological structure); one can generalize this idea to higher order topological structures.

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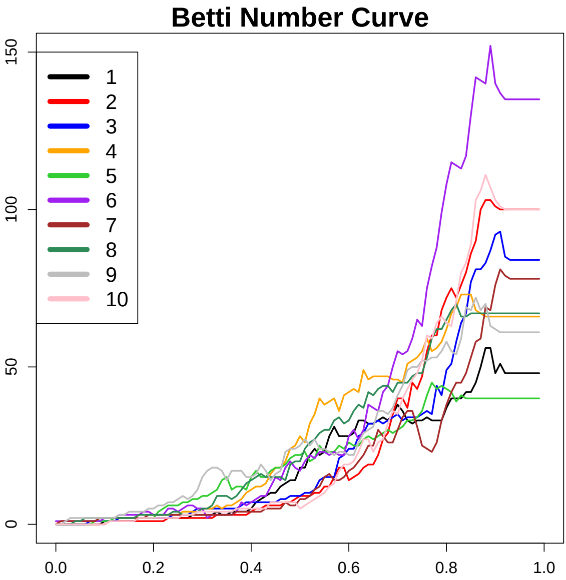

Applying to African Animal Datasets

- We apply our methods to a GPS data about African animals.
- This data is from the Movebank Data Repository[1] and was analyzed in Abrahms et al. (2017).
- Here we compare 4 different types of animals: elephants, jackals, vultures, and zebras.
- In this data, we have 8 elephants, 15 jackals, 10 vultures, and 9 zebras.
- Each animal has a set of GPS records.

[1] https://www.datarepository.movebank.org/

Level Plots: Animal Example




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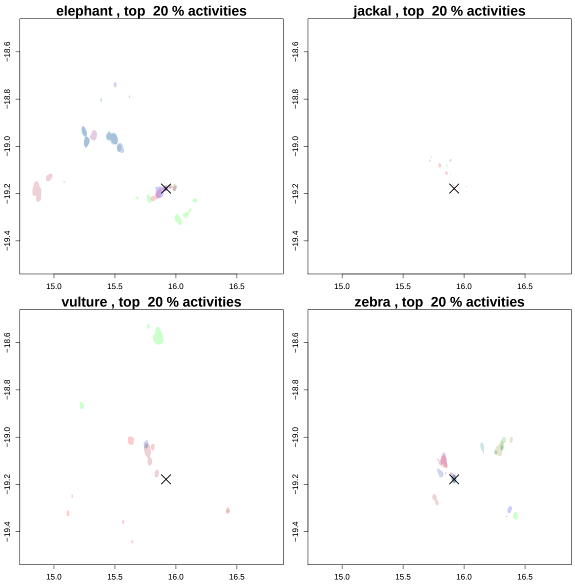

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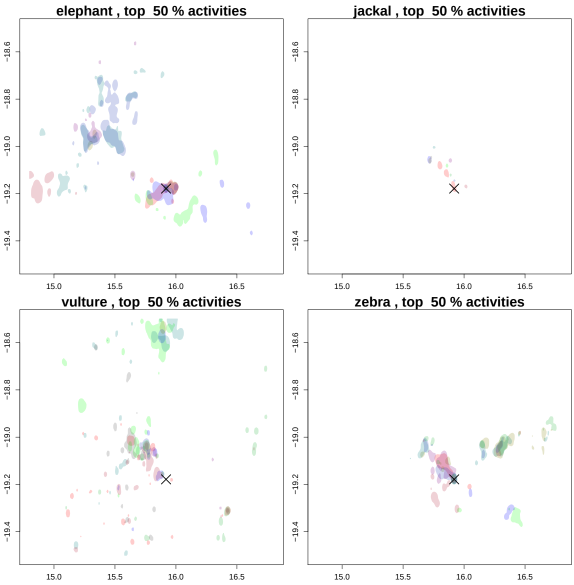

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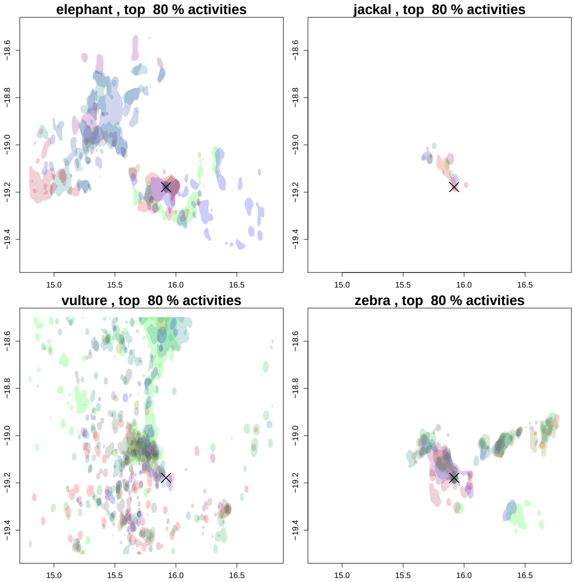

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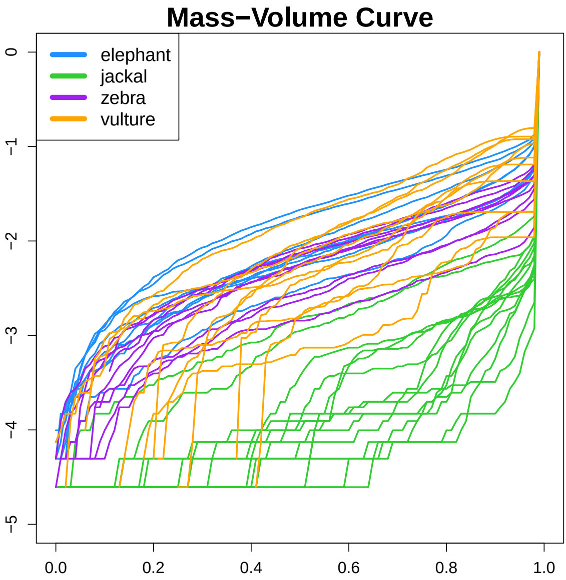

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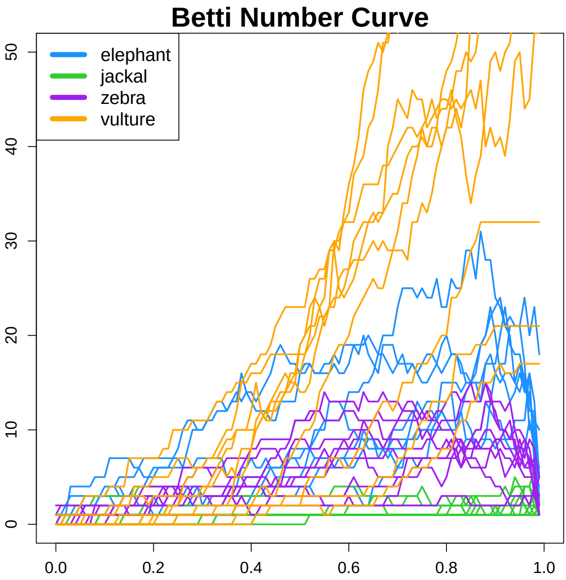

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- Also, density trees provide useful visualization of the underlying density function.
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- Density ranking defines a ranking tree that act as a density tree.

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- Density trees inform how density clusters are related to each other.
- Also, density trees provide useful visualization of the underlying density function.
- However, in complex datasets such as GPS data, we cannot use density tree because the density function does not exist.
- But we can use density ranking to analyze data.
- Density ranking defines a ranking tree that act as a density tree.
- When multiple GPS datasets are available, we can summarize them by functional summaries of density ranking.

Thank You!

An R script for density ranking:

https://github.com/yenchic/density_ranking

More details can be found in

http://faculty.washington.edu/yenchic/

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Assumptions for Regular Distributions

(R1) The density function p has a compact support $\mathbb{K}$.

(R2) The density function is a Morse function and is in $\mathbf{BC}^3$.

(K1) The kernel function K is in $\mathbf{BC}^2$ and integrable.

(K2) K satisfies the VC-type class condition.

Kernel Conditions

(K2) Let

$$\mathscr{K}_r = \left\{ y \mapsto K^{(\alpha)}\left(\frac{x-y}{h}\right) : x \in \mathbb{R}^d, |\alpha| = r \right\},$$

where $K^{(\alpha)}$ is the α-th derivative and let $\mathscr{K}_l^* = \bigcup_{r=0}^{l} \mathscr{K}_r$. We assume that $\mathscr{K}_2^*$ is a VC-type class. i.e. there exists constants A, v and a constant envelope b_0 such that

$$\sup_Q N(\mathscr{K}_2^*, \mathscr{L}^2(Q), b_0\epsilon) \leq \left(\frac{A}{\epsilon}\right)^v, \tag{1}$$

where $N(T, d_T, \epsilon)$ is the ϵ-covering number for an semi-metric set T with metric d_T and $\mathscr{L}^2(Q)$ is the L_2 norm with respect to the probability measure Q.

Assumptions for Singular Distributions

(S1) The support can be partitioned into

$$K = K_0 \bigcup K_1 \bigcup \cdots \bigcup K_d,$$

where $K_\ell = \{x \in \mathbb{K} : \tau(x) = \ell\}$.

(S2) There exist $\rho_{\min}, \rho_{\max}$ such that $0 < \rho_{\min} \leq \rho(x) \leq \rho_{\max} < \infty$ for every $x \in \mathbb{K}$.

(S3) Restricted to each $\mathbb{K}_\ell$ where $\ell > 0$, $\rho(x)$ is a Morse function.

(K1') The kernel function K is in $\mathbf{BC}^2$, integrable, and supported in $[-1, 1]$.

(K2) K satisfies the VC-type class condition.