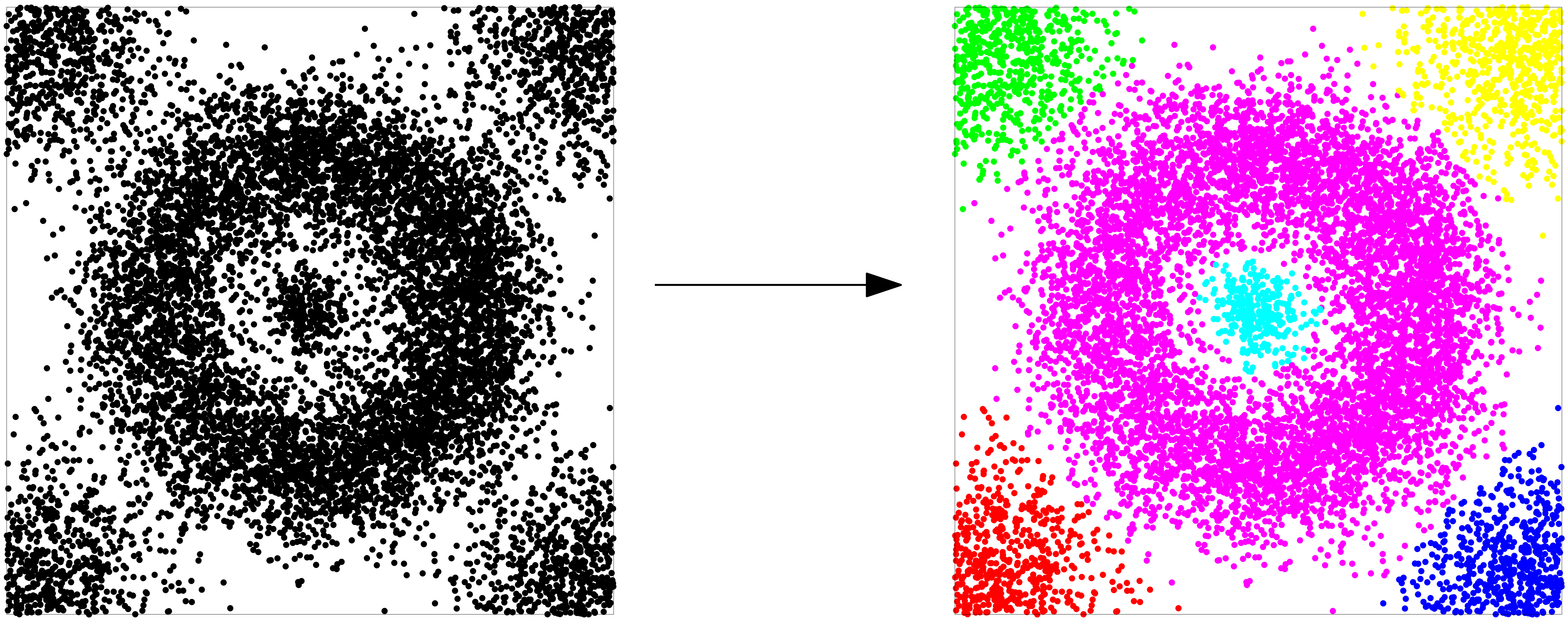
Introduction to persistence theory through an application in clustering

[F. Chazal, L. Guibas, S. Oudot, P. Skraba: Persistence-Based Clustering in Riemannian Manifolds, *Journal of the ACM*, 60(6):1–38, 2013]

Clustering

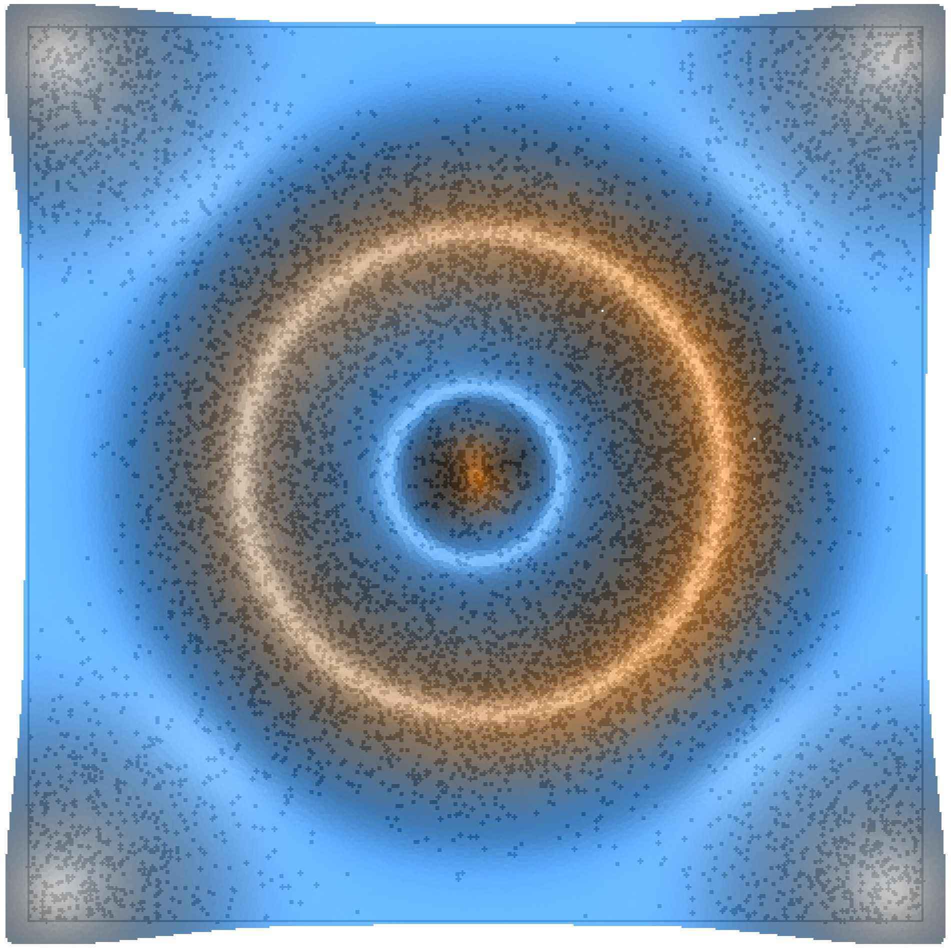
Input: a finite set P of data in some metric space



Task: partition the data set P into *homogeneous* subsets (clusters)

Mode-Seeking Paradigm

- Hyp: data are sampled iid from a probability measure μ with density f (both **unknown**)



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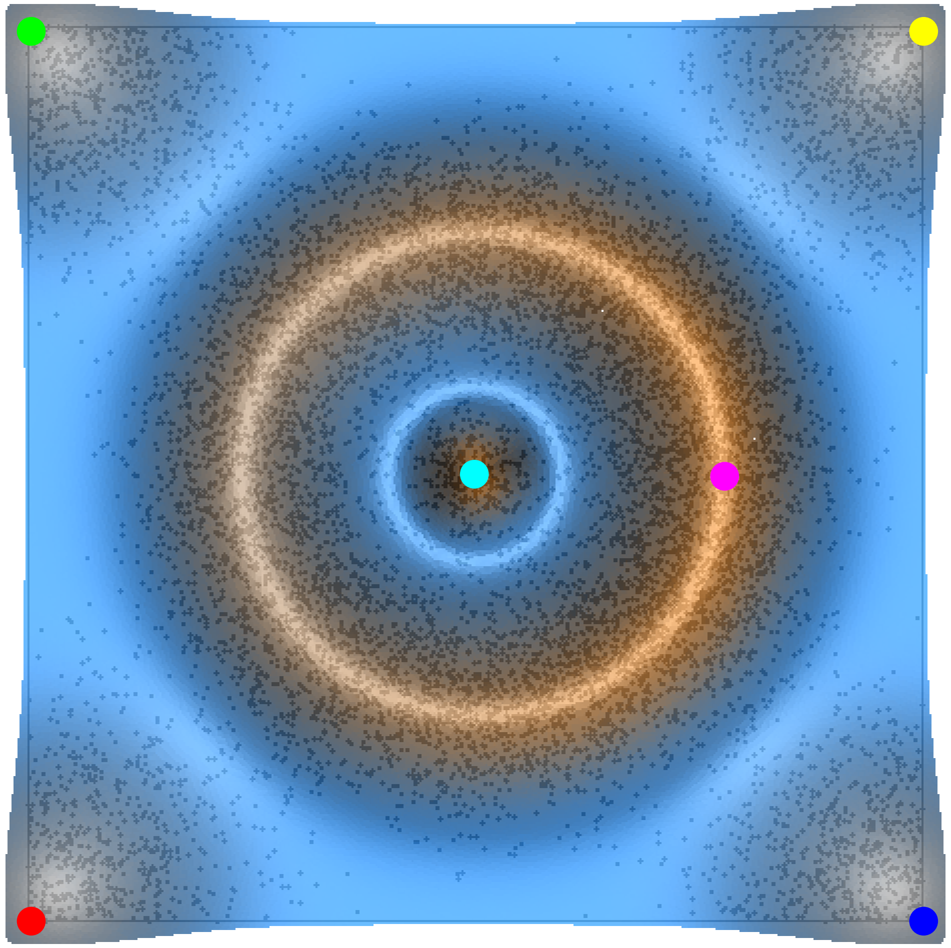
- Hyp: data are sampled iid from a probability measure μ with density f (both **unknown**)

- Partition the data according to the **stable manifolds** of the peaks of f



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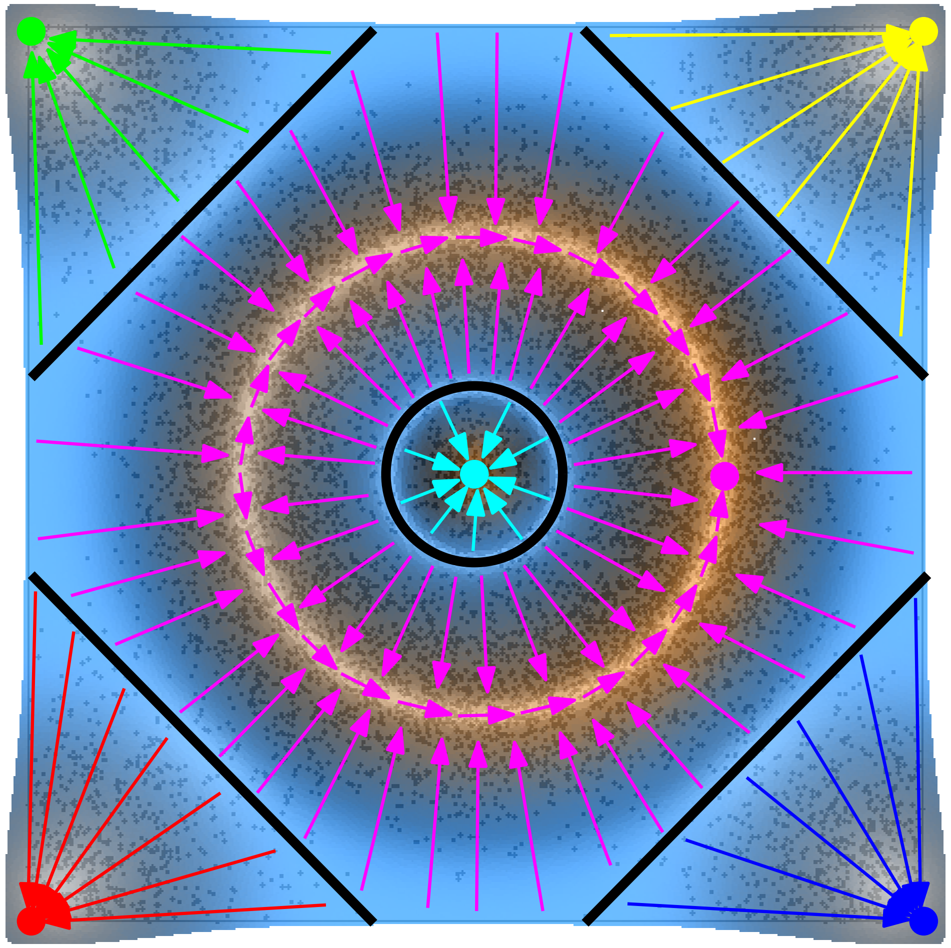

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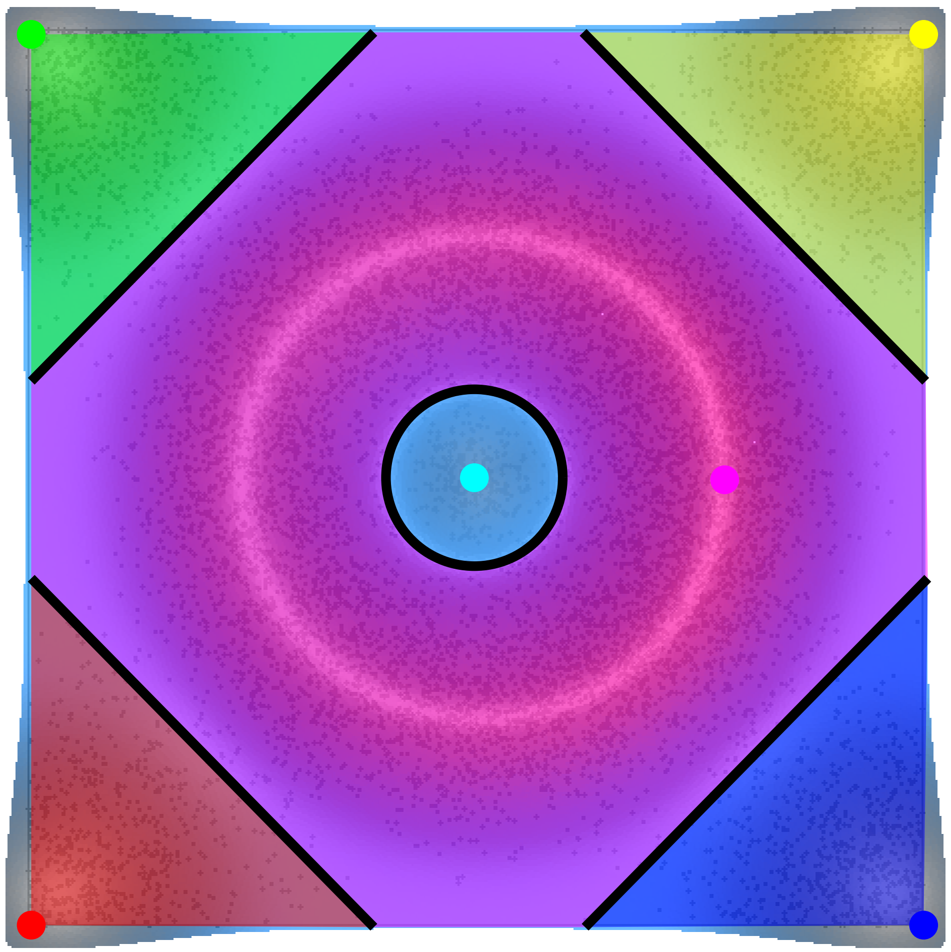
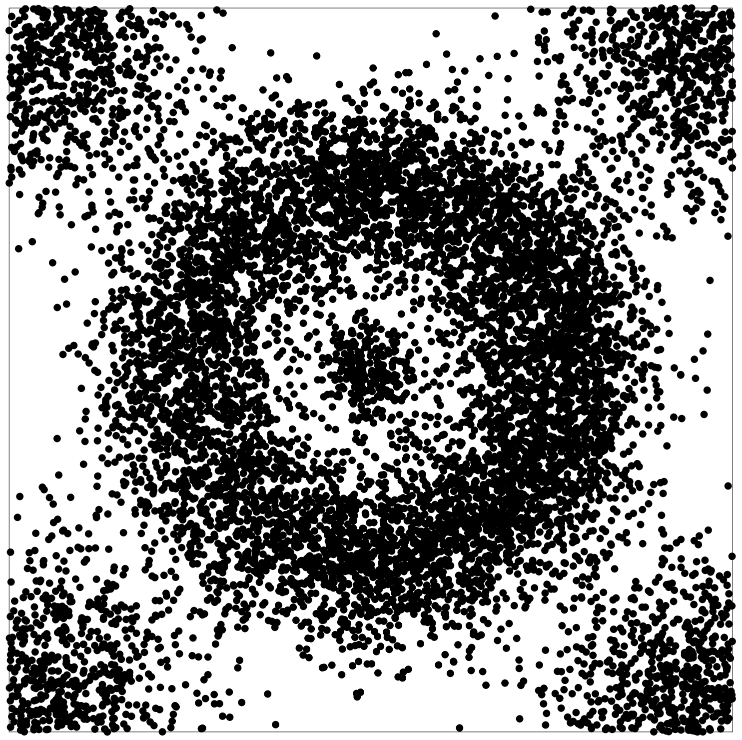


Hill-Climbing Schemes

- **Numerical**, e.g. D. Comaniciu and P. Meer. Mean shift: A robust approach toward feature space analysis. *IEEE Trans. on Pattern Analysis and Machine Intelligence*, 24(5):603–619, May 2002.

- **Combinatorial**, e.g. W. L. Koontz, P. M. Narendra, and K. Fukunaga. A graph-theoretic approach to nonparametric cluster analysis. *IEEE Trans. on Computers*, 24:936–944, September 1976.

[Koontz, Narendra, Fukunaga'76] in a Nutshell



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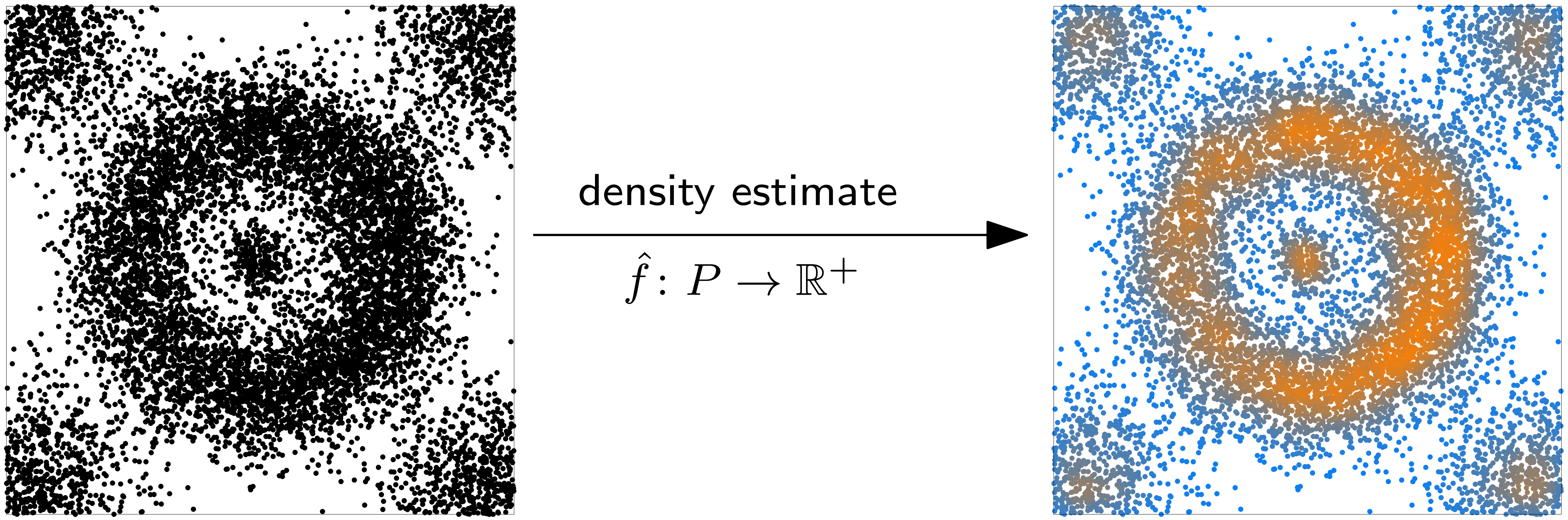

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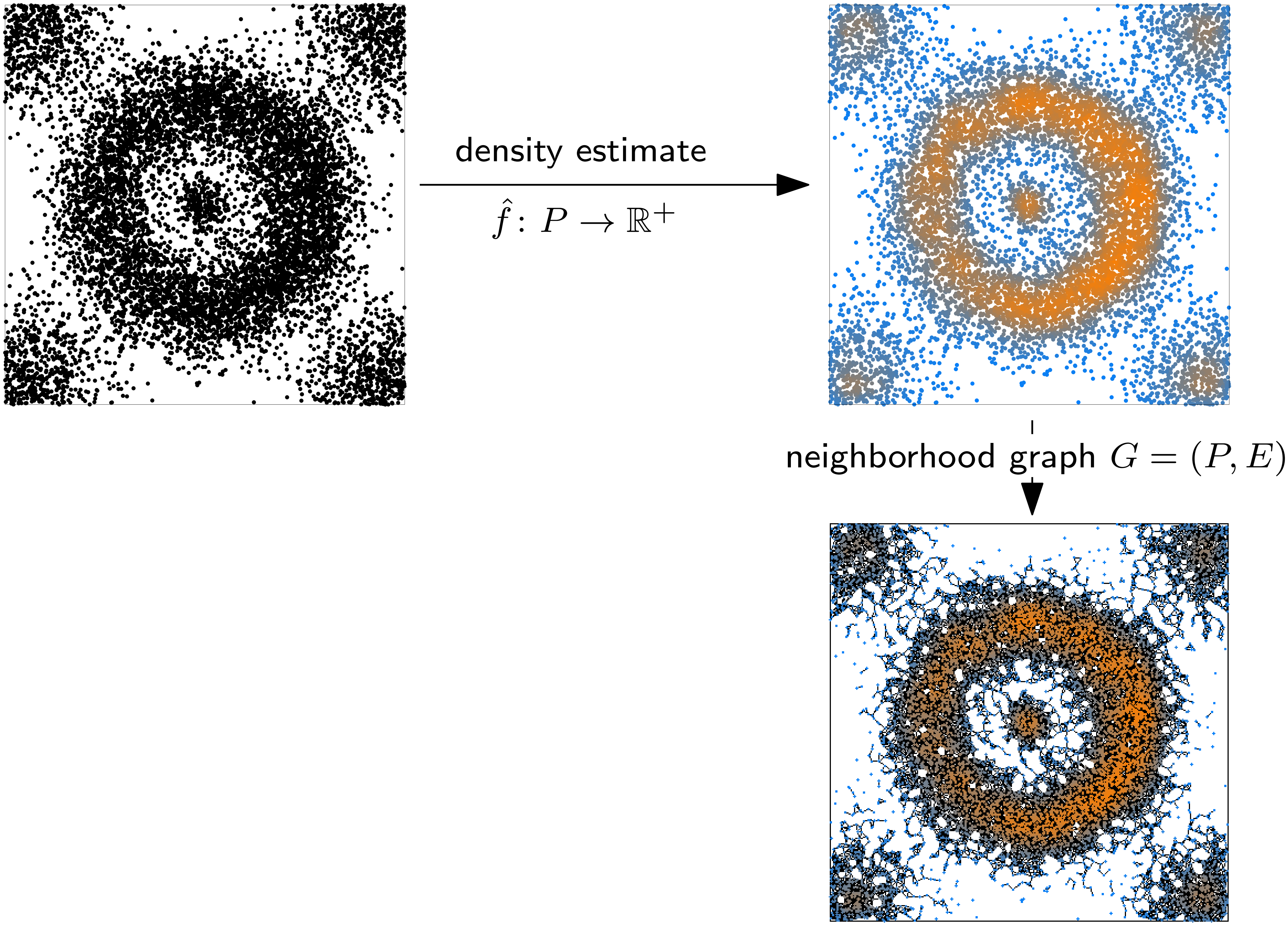

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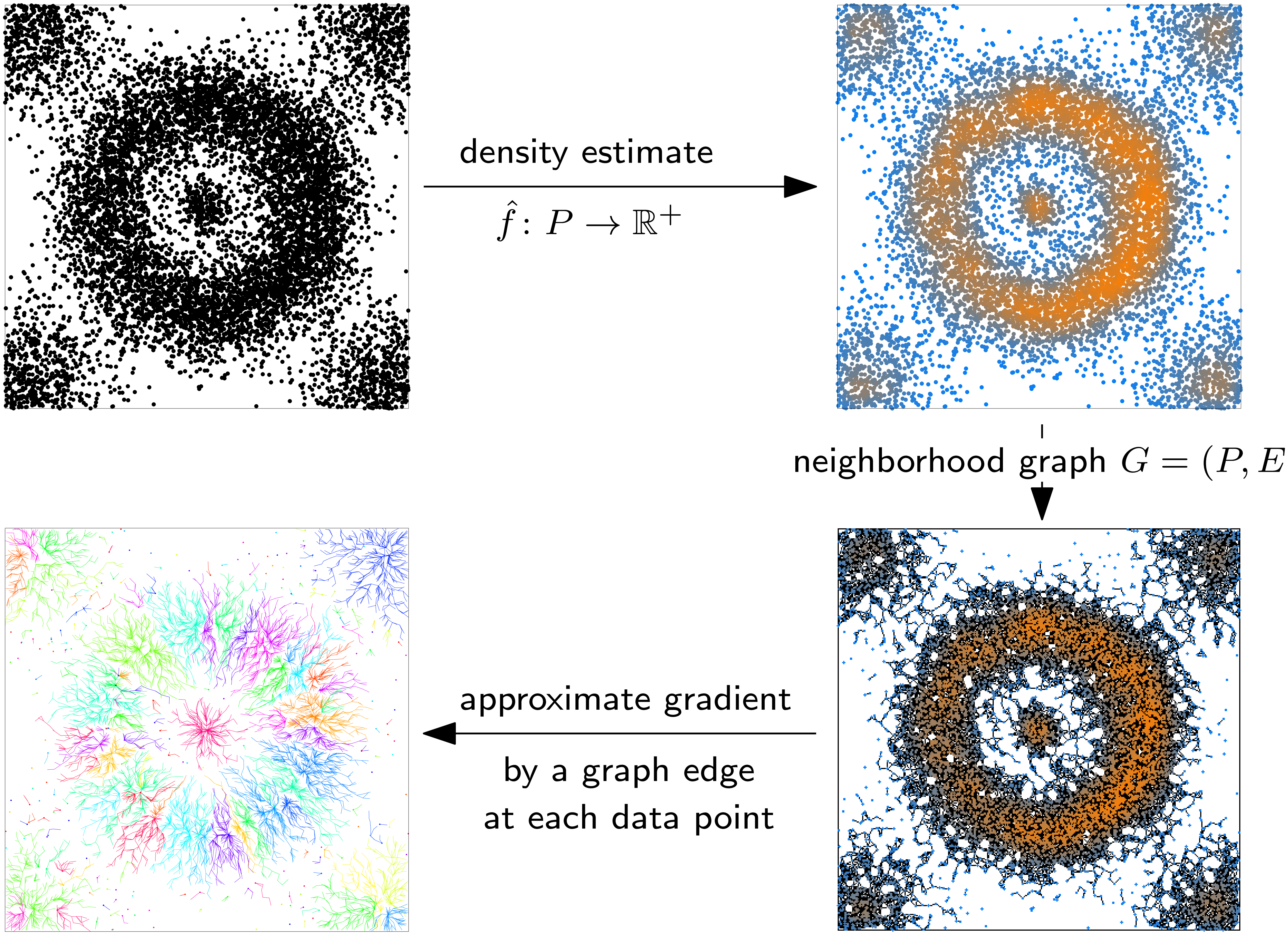


Pseudo-code:

Input: neighborhood graph G with n vertices, n-dimensional vector $\hat{f}$ (density estimator)

Sort the vertex indices $\{1, 2, \cdots, n\}$ so that $\hat{f}(1) \geq \hat{f}(2) \geq \cdots \geq \hat{f}(n)$;
Initialize a union-find data structure (disjoint-set forest) $\mathcal{U}$ and two vectors g, r of size n;

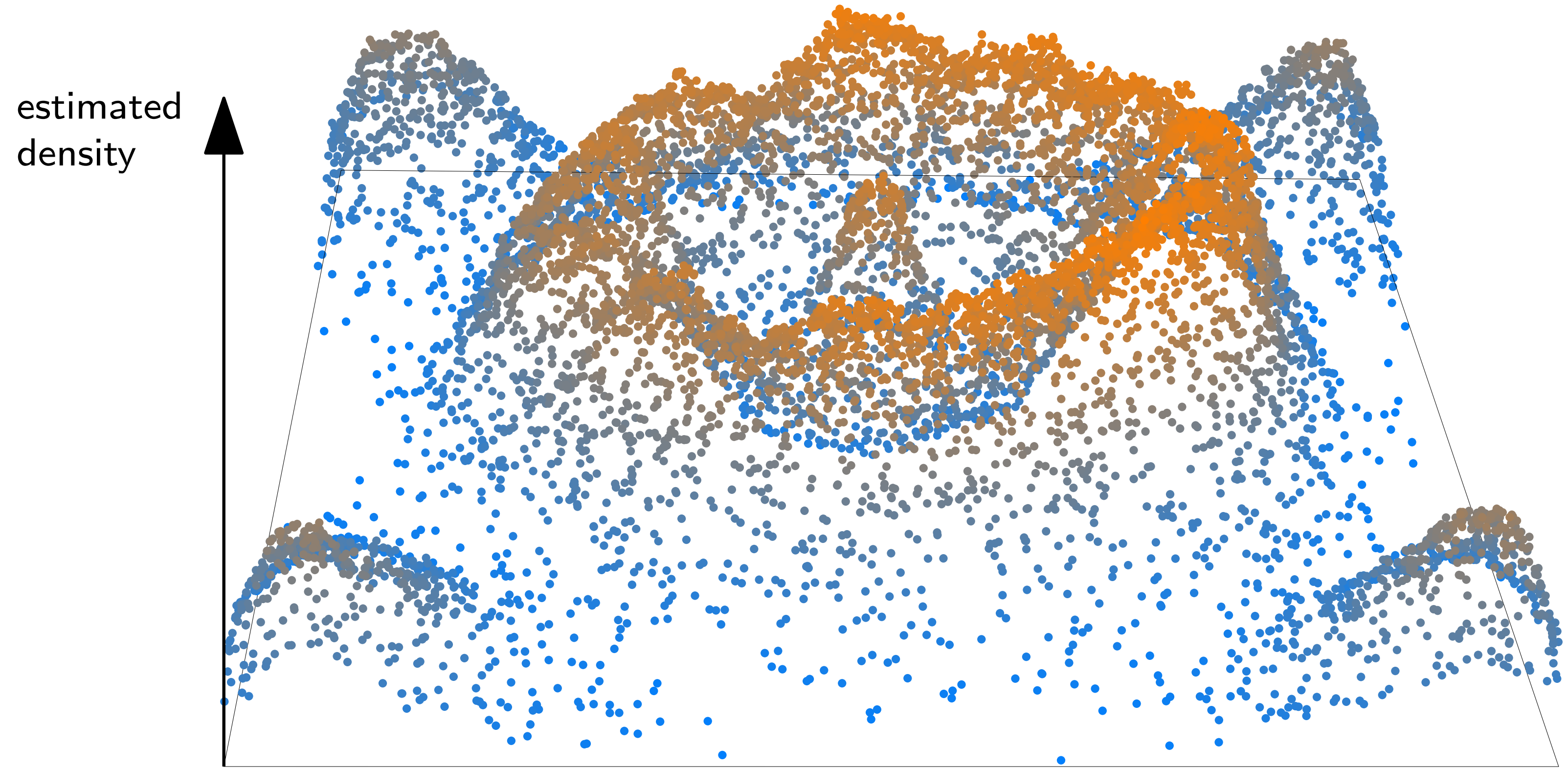
for $i = 1$ to n **do**
  Let $\mathcal{N}$ be the set of neighbors of i in G that have indices lower than i;
  if $\mathcal{N} = \emptyset$ *// vertex i is a peak of $\hat{f}$ within G*
    Create a new entry e in $\mathcal{U}$ and attach vertex i to it;
    $r(e) \leftarrow i$ *// $r(e)$ stores the root vertex associated with the entry e*
  else *// vertex i is not a peak of $\hat{f}$ within G*
    $g(i) \leftarrow \mathrm{argmax}_{j \in \mathcal{N}} \hat{f}(j)$ *// $g(i)$ stores the approximate gradient at vertex i*
    $e_i \leftarrow \mathcal{U}.\mathtt{find}(g(i))$;
    Attach vertex i to the entry e_i;

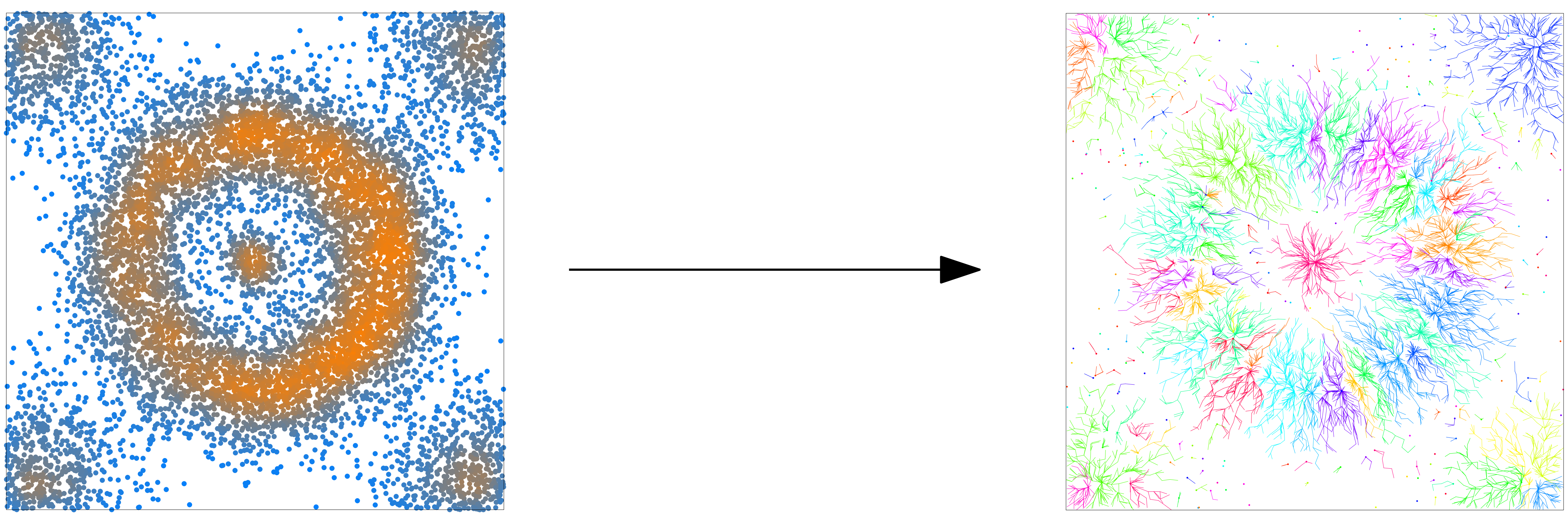
graph-based
hill-climbing
(1976)

Output: the collection of entries e in $\mathcal{U}$

Why things go ill

Noisy estimator



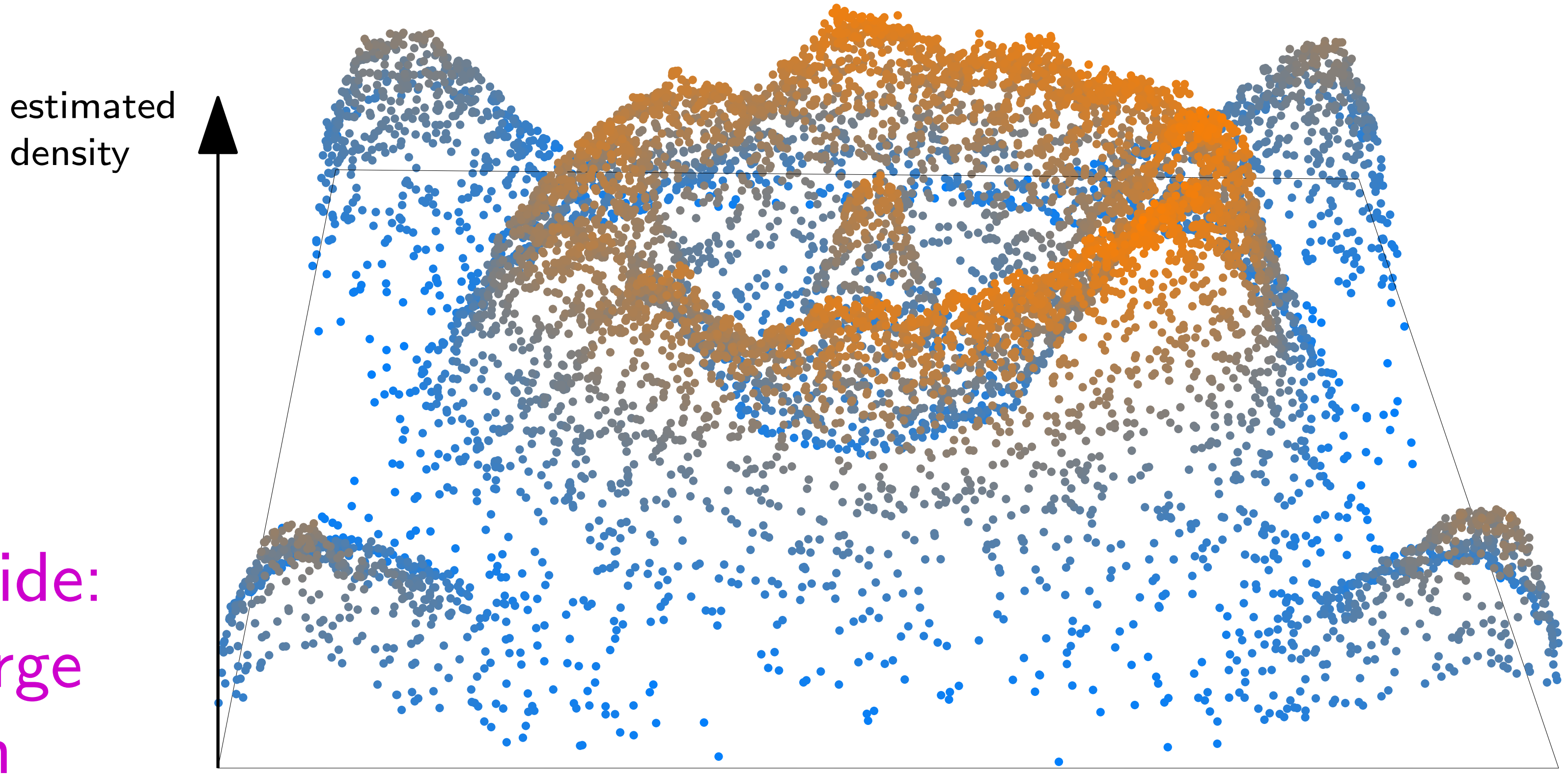


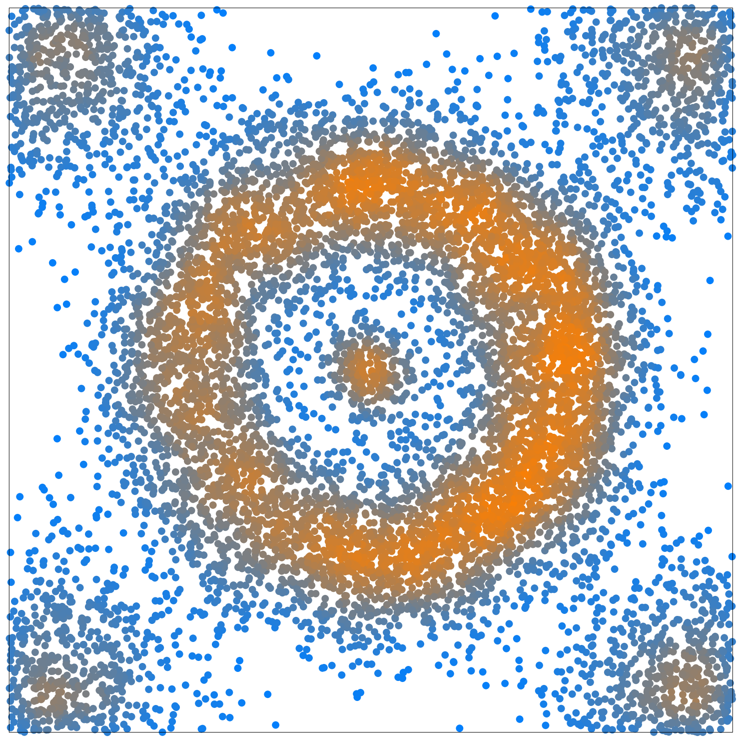
Why things go ill

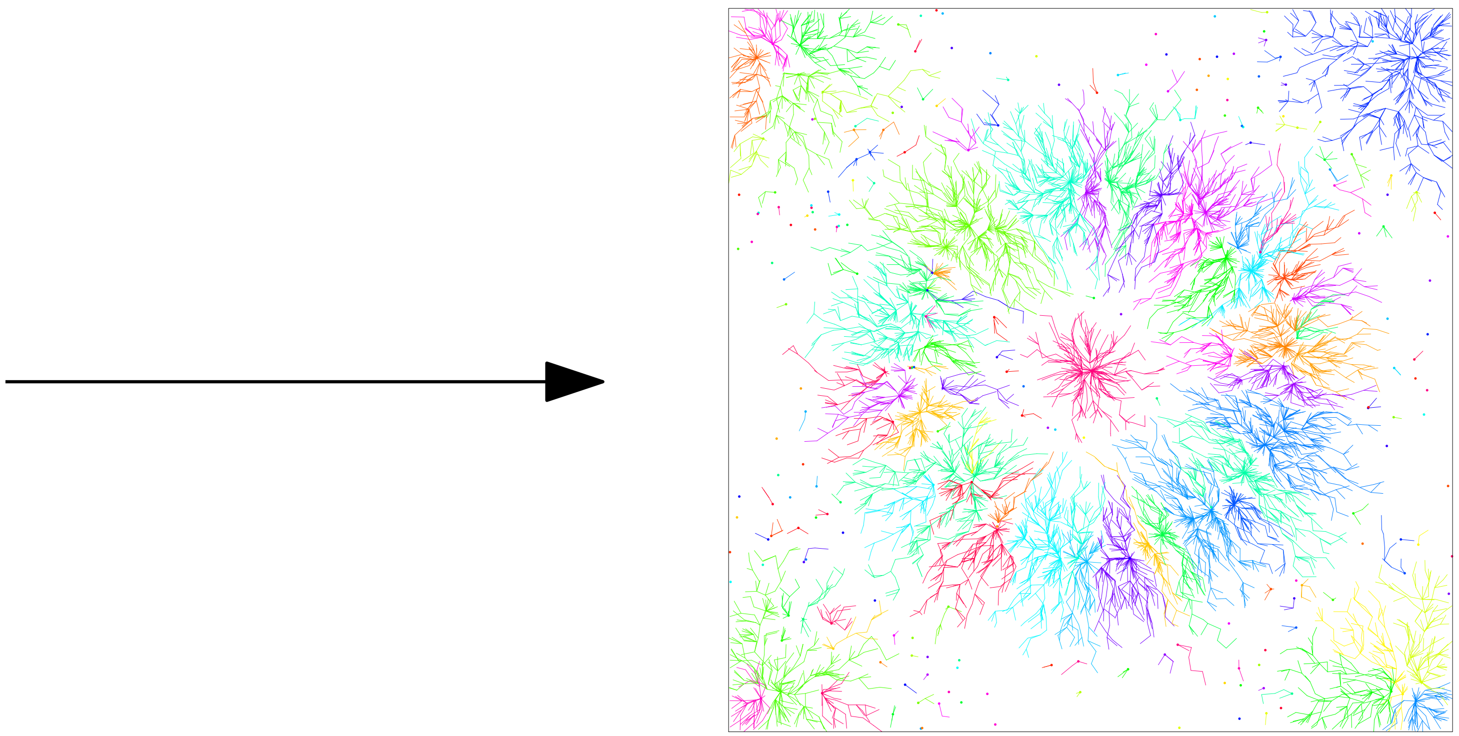
Noisy estimator

Solution:

- merge clusters in post-processing step
- use persistence as a guide:
  - which clusters to merge
  - where to merge them

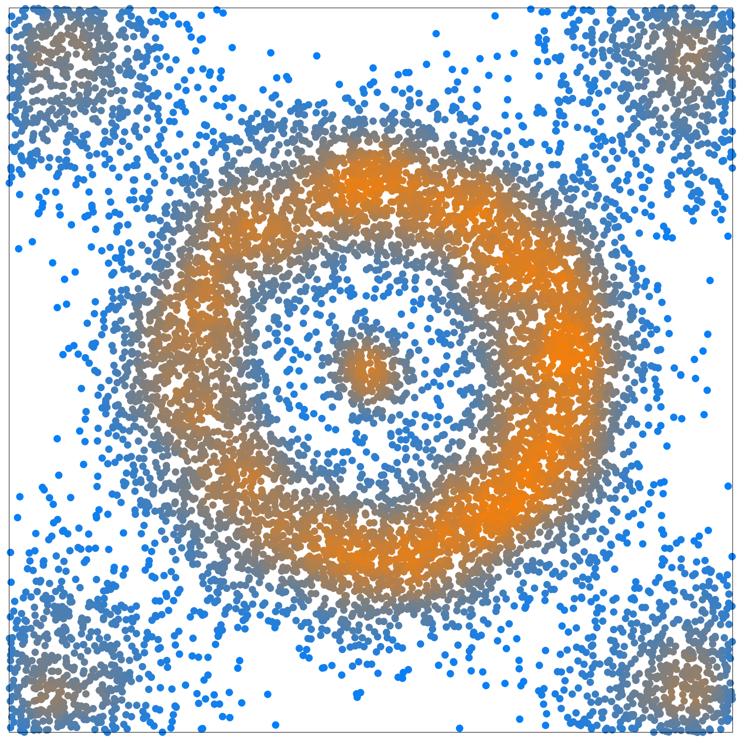




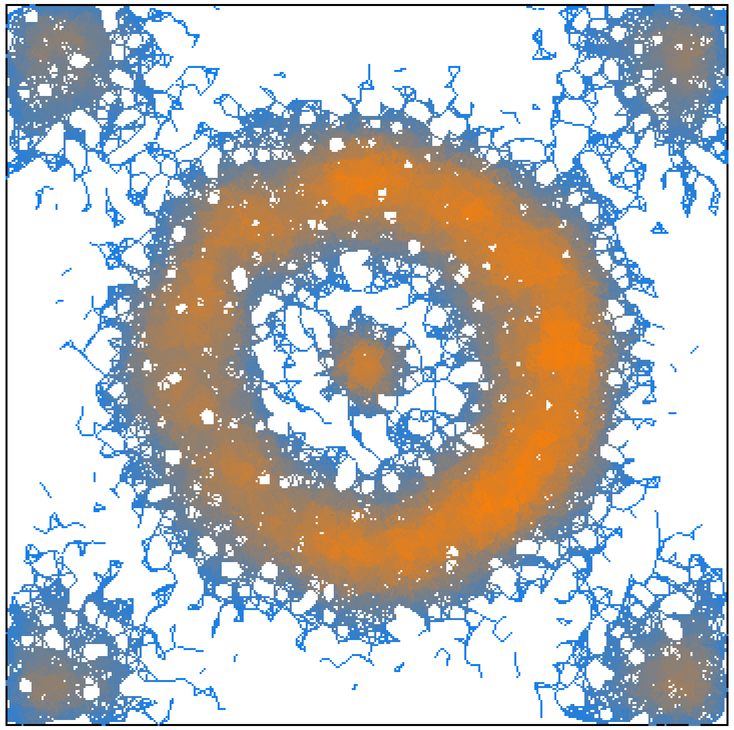


Persistence of the estimated density in the graph

- Extend $\hat{f}\colon P \to \mathbb{R}$ to a map $G \to \mathbb{R}$ by $\hat{f}((u,v)) := \min\left\{\hat{f}(u),\ \hat{f}(v)\right\}$



$\hat{f}$



$\hat{f}$ extended to G

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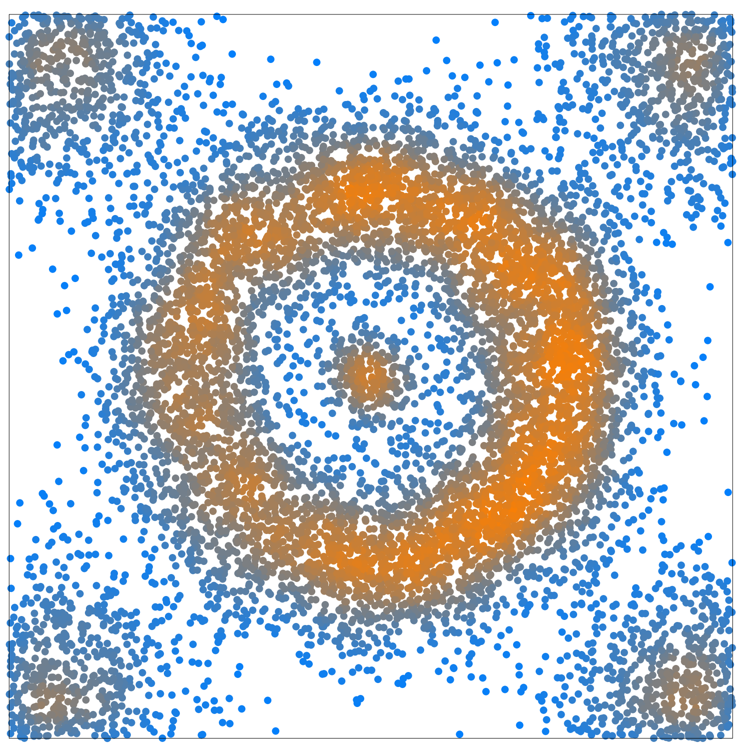
- $D(\hat{f})$ encodes the lifespans of the peaks of $\hat{f}$ as independent components in G



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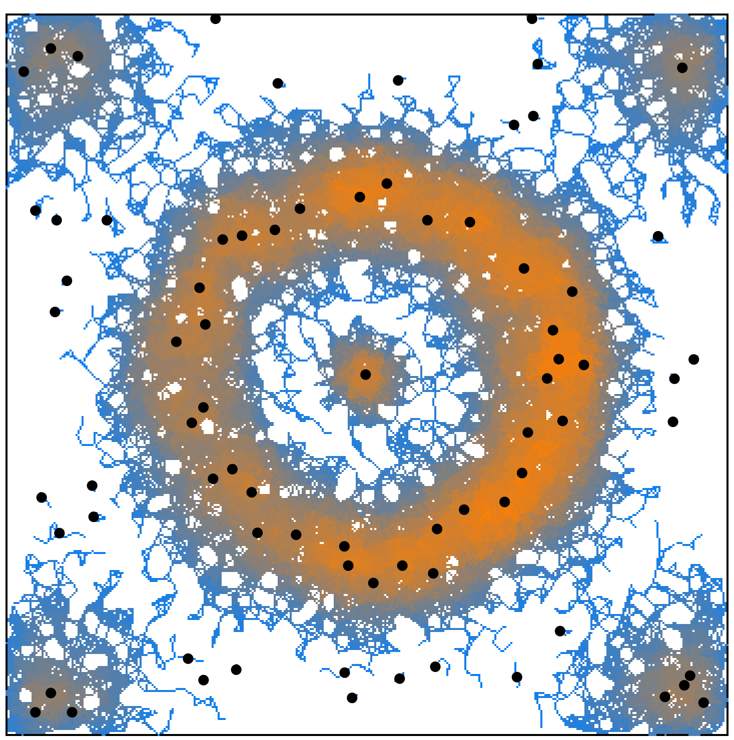

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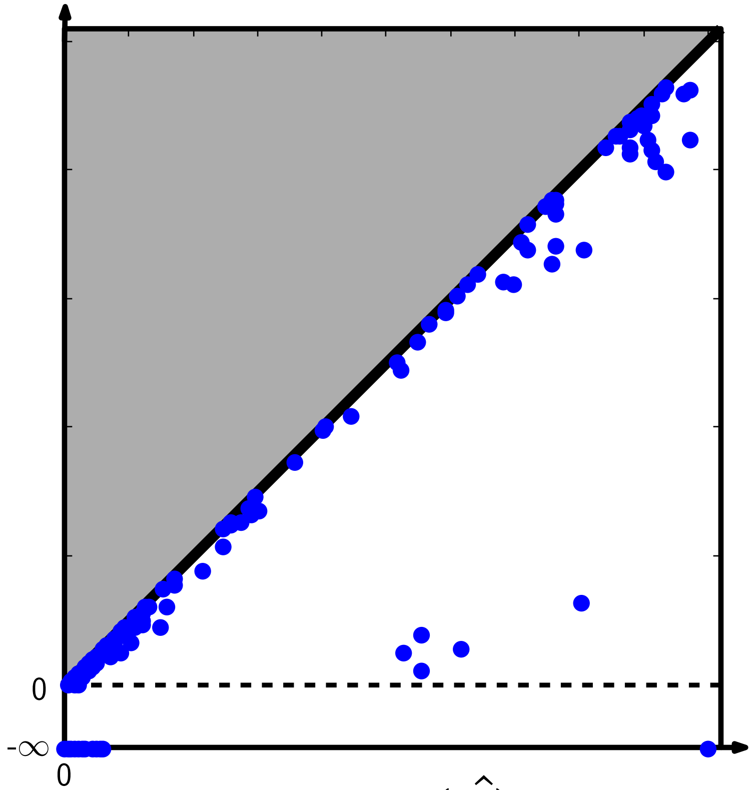

$D(\hat{f})$

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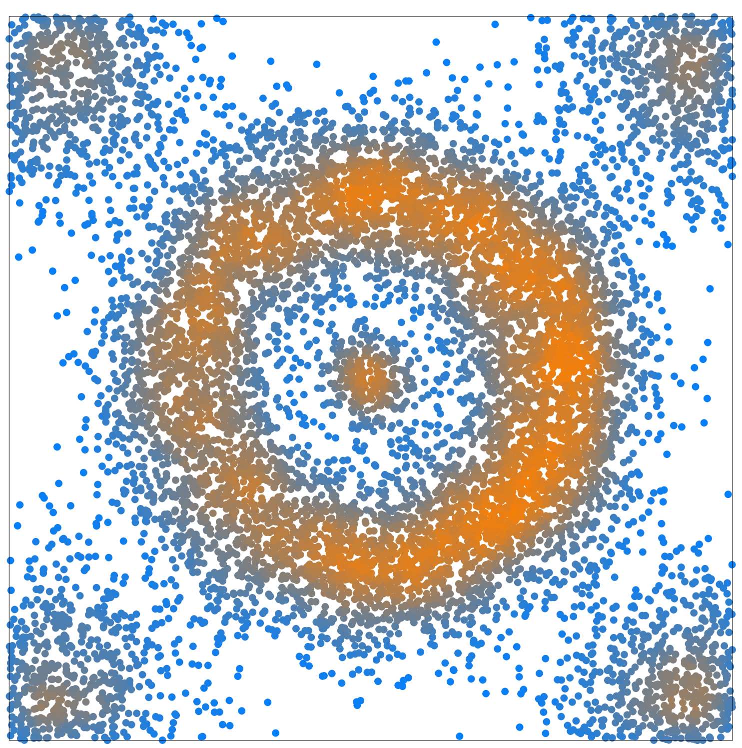
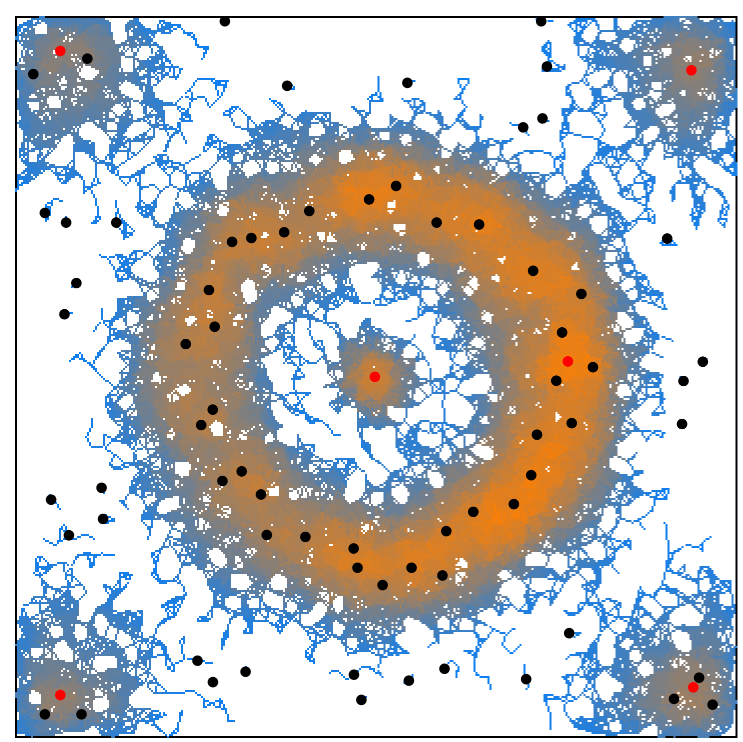
- $D(\hat{f})$ encodes the lifespans of the peaks of $\hat{f}$ as independent components in G
- from $D(\hat{f})$, the user can infer a persistence threshold τ



$\hat{f}$



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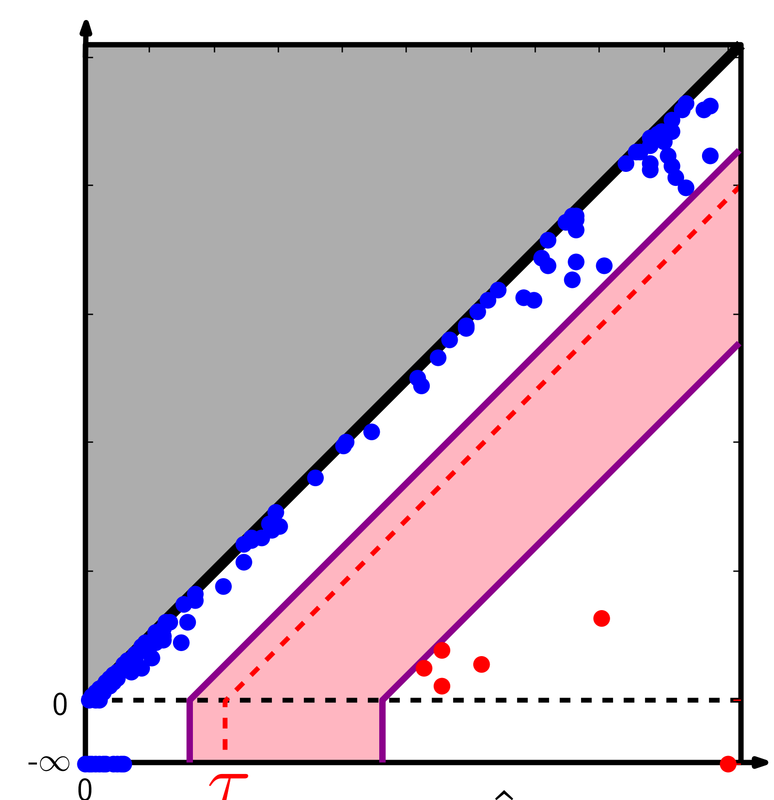
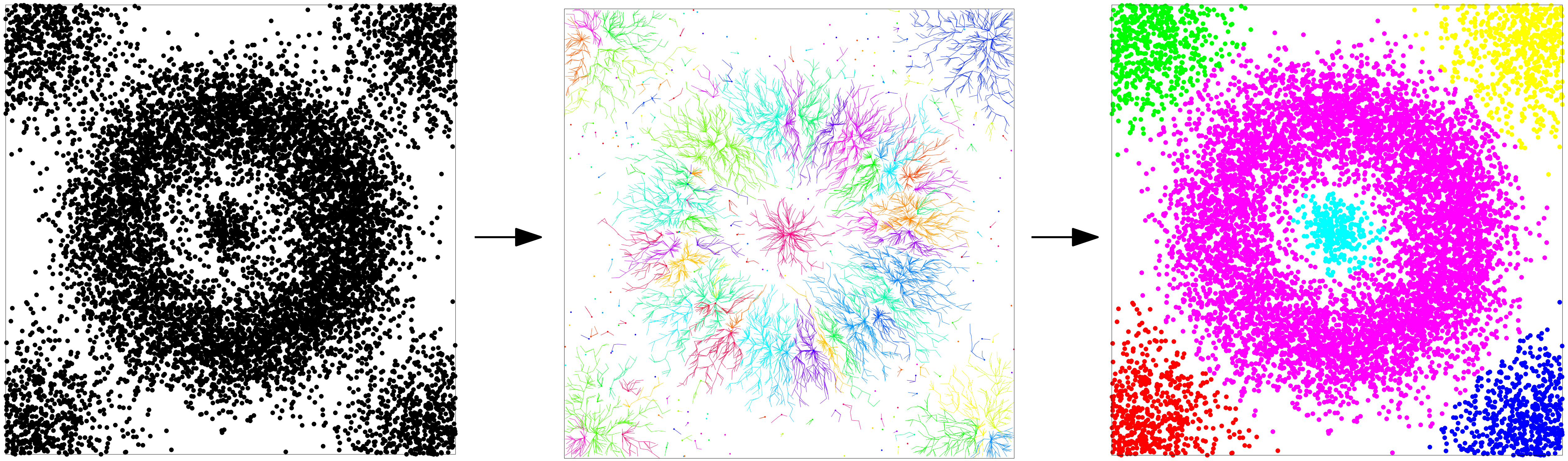


$D(\hat{f})$

Persistence of the estimated density in the graph

- Extend $\hat{f}\colon P \to \mathbb{R}$ to a map $G \to \mathbb{R}$ by $\hat{f}((u,v)) := \min\left\{\hat{f}(u),\ \hat{f}(v)\right\}$
- $D(\hat{f})$ encodes the lifespans of the peaks of $\hat{f}$ as independent components in G
- from $D(\hat{f})$, the user can infer a persistence threshold τ
- inductively merge clusters of peaks of prominence $\leq \tau$ into their parent's cluster



Pseudo-code:

Input: simple graph G with n vertices, n-dimensional vector $\hat{f}$, real parameter $\tau \geq 0$.

Sort the vertex indices $\{1, 2, \cdots, n\}$ so that $\hat{f}(1) \geq \hat{f}(2) \geq \cdots \geq \hat{f}(n)$;
Initialize a union-find data structure $\mathcal{U}$ and two vectors g, r of size n;

for $i = 1$ to n **do**
    Let $\mathcal{N}$ be the set of neighbors of i in G that have indices lower than i;
    if $\mathcal{N} = \emptyset$ *// vertex i is a peak of $\hat{f}$ within G*
        Create a new entry e in $\mathcal{U}$ and attach vertex i to it;
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        $g(i) \leftarrow \mathrm{argmax}_{j \in \mathcal{N}} \hat{f}(j)$ *// $g(i)$ stores the approximate gradient at vertex i*
        $e_i \leftarrow \mathcal{U}.\mathtt{find}(g(i))$;
        Attach vertex i to the entry e_i;

graph-based hill-climbing (1976)

        for $j \in \mathcal{N}$ **do**
            $e \leftarrow \mathcal{U}.\mathtt{find}(j)$;
            if $e \neq e_i$ and $\min\{\hat{f}(r(e)),\ \hat{f}(r(e_i))\} < \hat{f}(i) + \tau$
                $\mathcal{U}.\mathtt{union}(e,\ e_i)$;
                $r(e \cup e_i) \leftarrow \mathrm{argmax}_{\{r(e),\ r(e_i)\}} \hat{f}$;
                $e_i \leftarrow e \cup e_i$;

cluster merges with persistence (2013)

Output: the collection of entries e of $\mathcal{U}$ such that $\hat{f}(r(e)) \geq \tau$.

Complexity of the Algorithm

Given a neighborhood graph with n vertices (with density estimates) and m edges:

1. the algorithm sorts the vertices by decreasing density estimates,

2. the algorithm makes a single pass through the vertex set, creating the spanning forest and merging clusters on the fly using a union-find data structure.

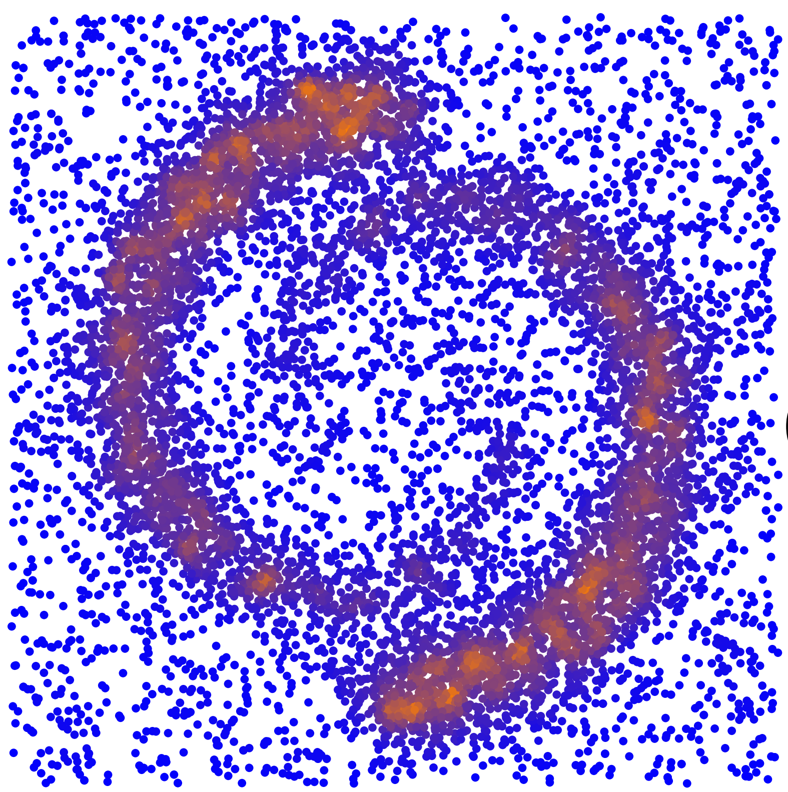
$\rightarrow$ Running time: $O(n \log n + (n+m)\alpha(n))$

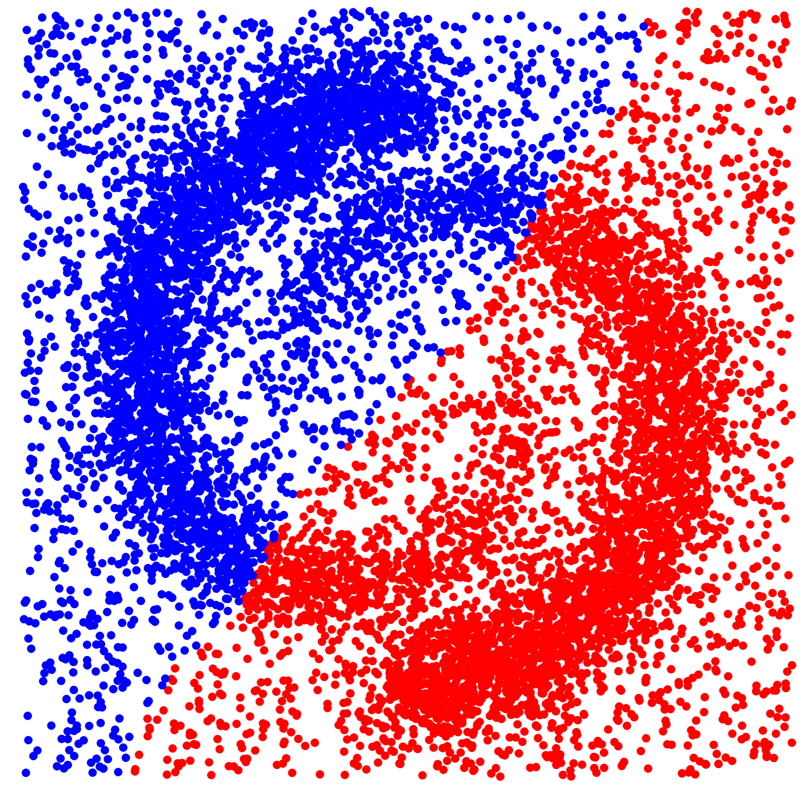
$\rightarrow$ Space complexity: $O(n+m)$

$\rightarrow$ Main memory usage: $O(n)$

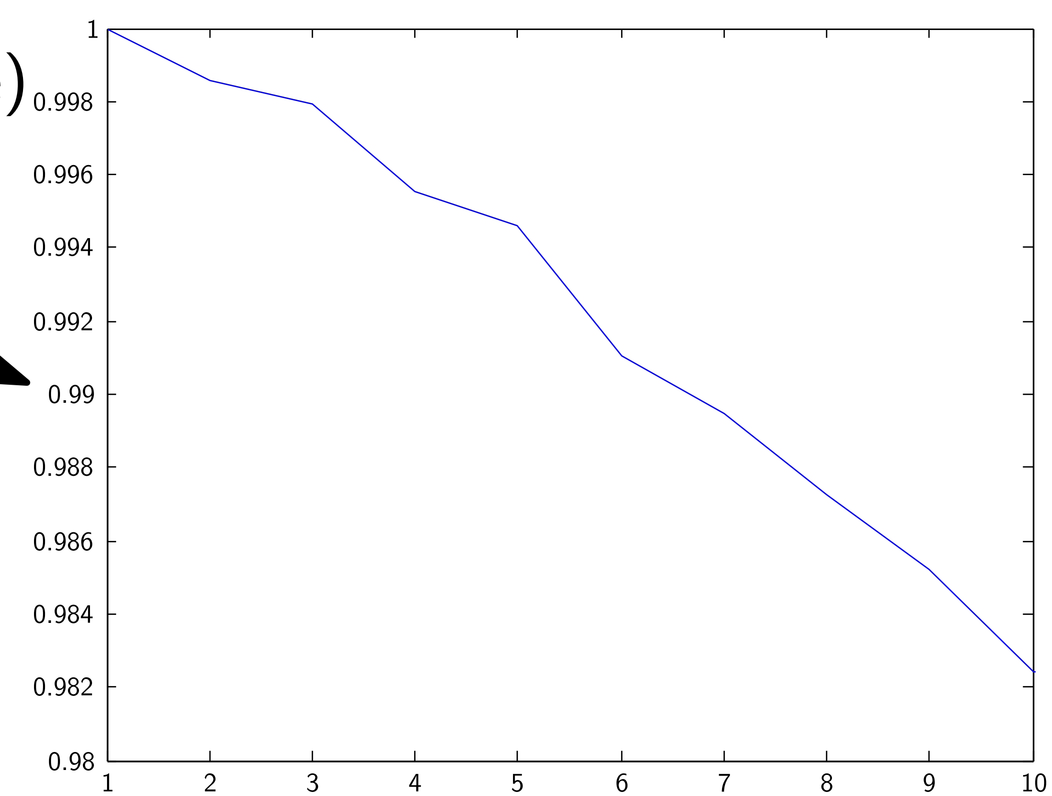
Experimental Results

Synthetic Data





Spectral clustering
(k-means in eigenspace)



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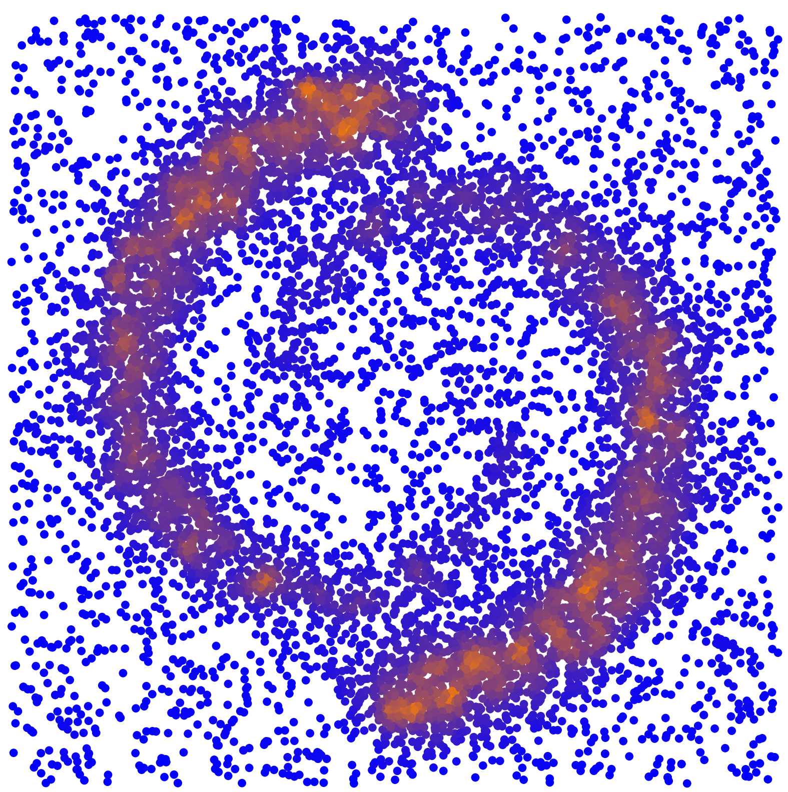
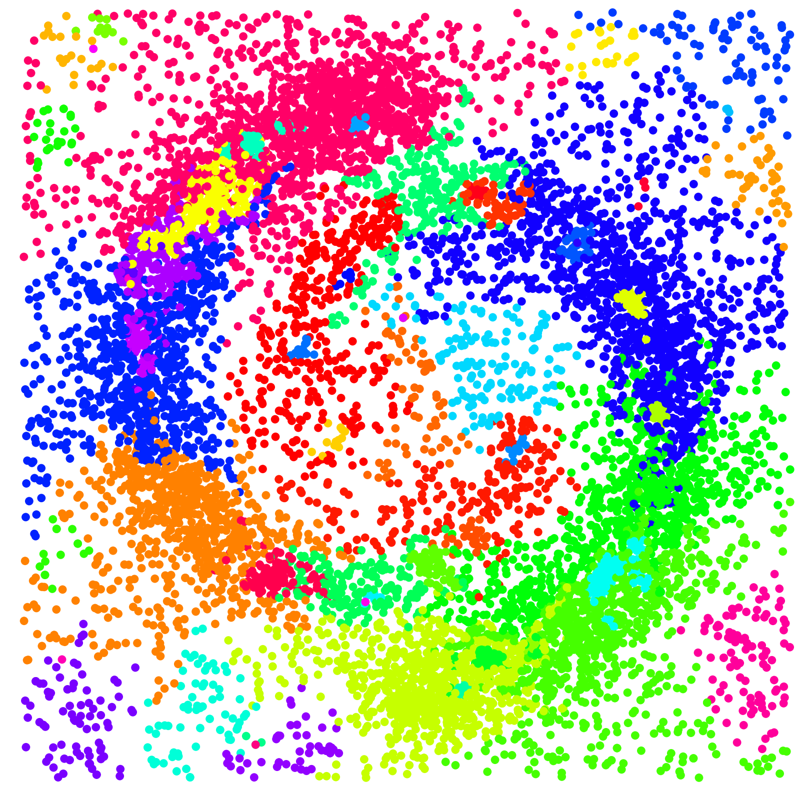
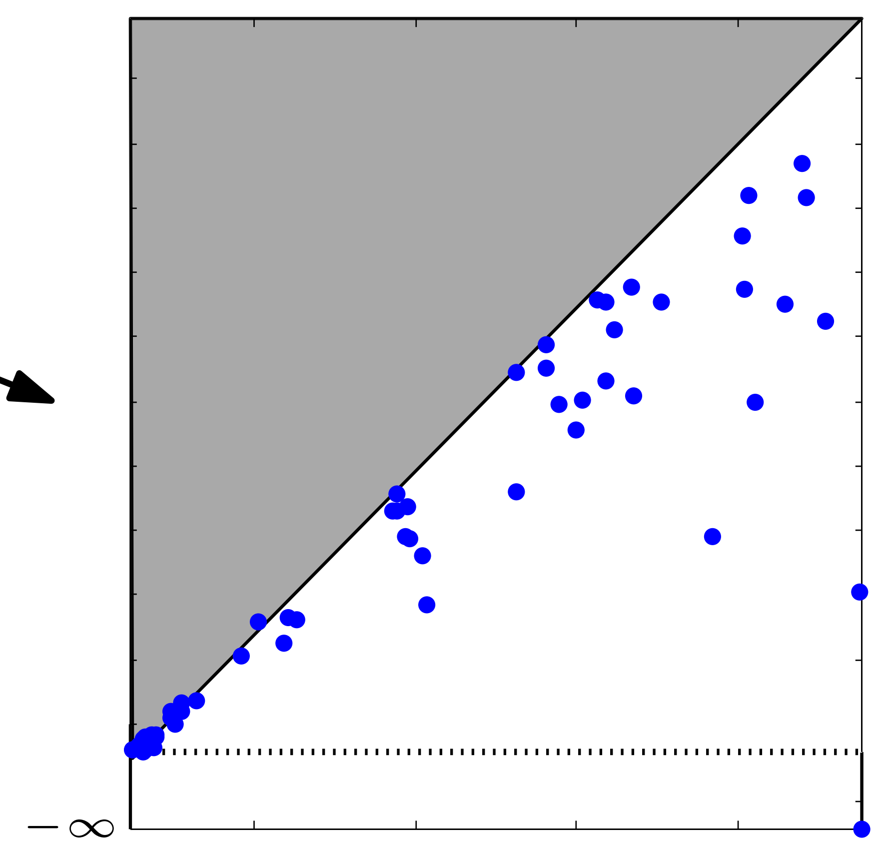


$\tau = 0$

ToMATo





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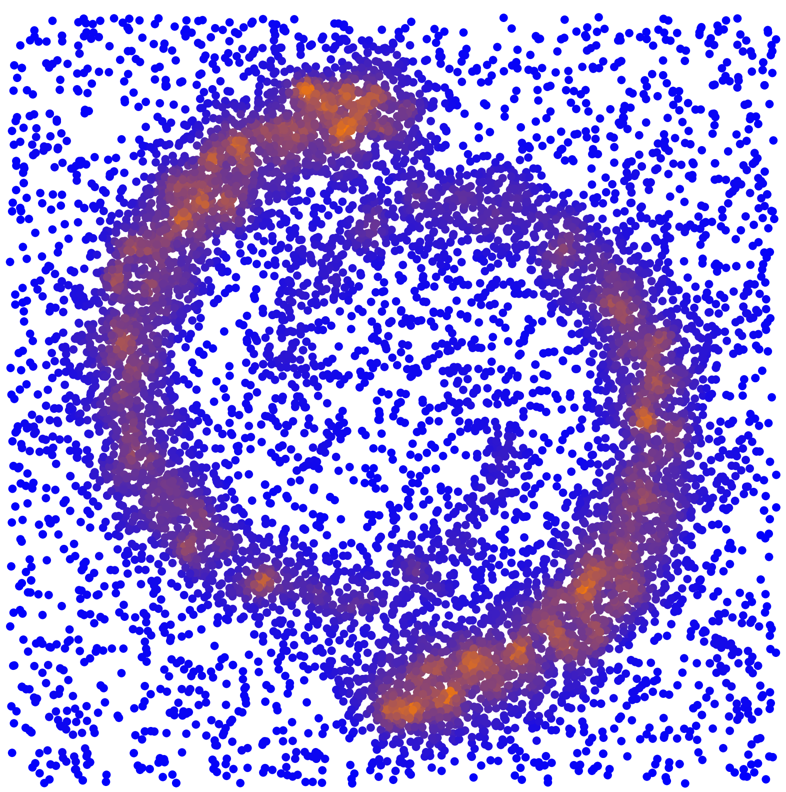

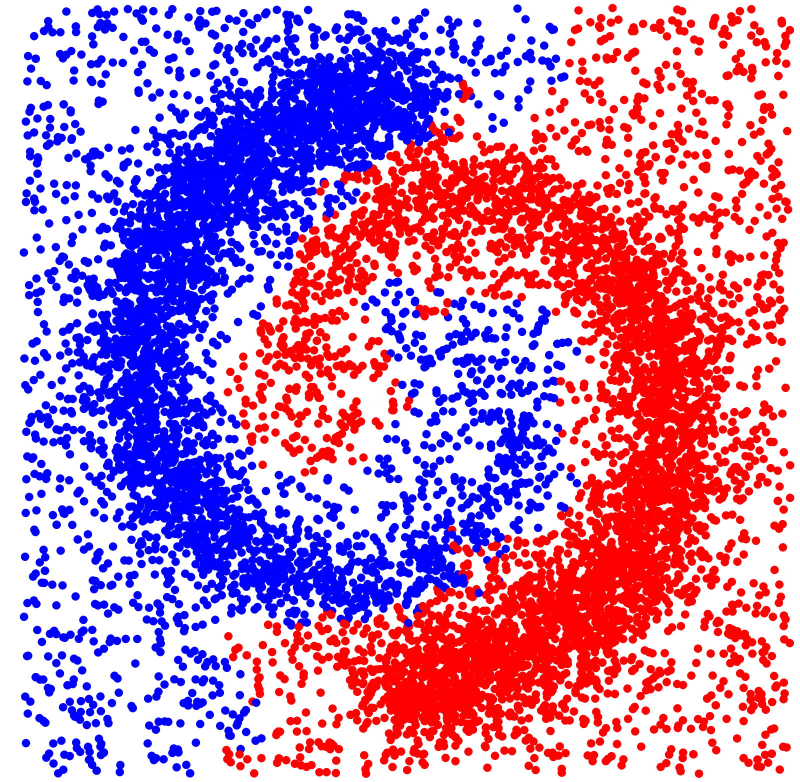

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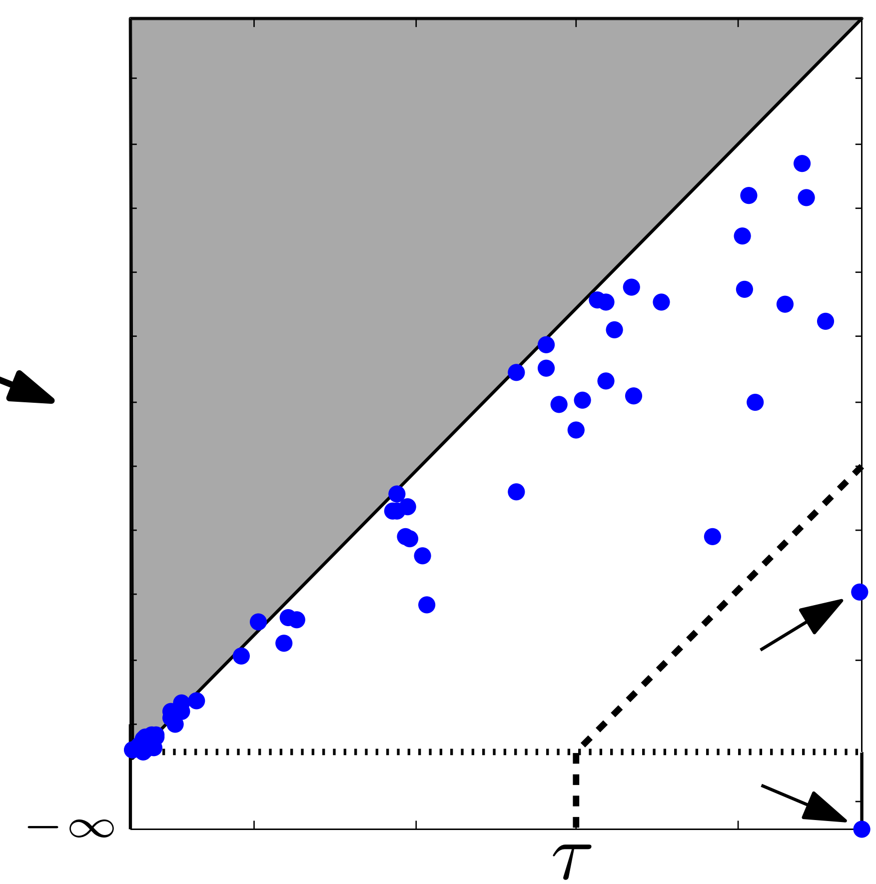

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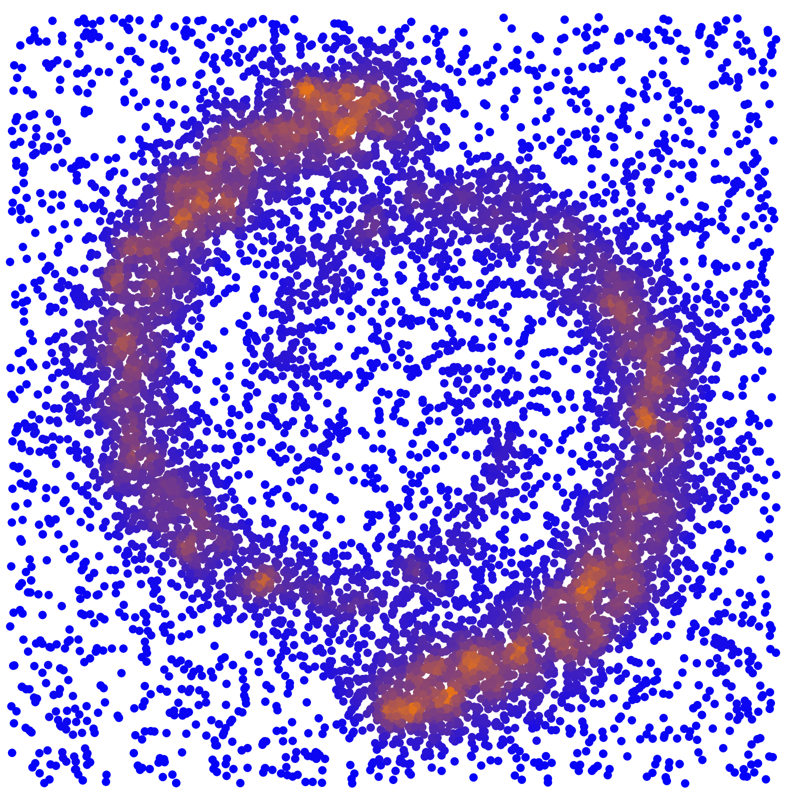
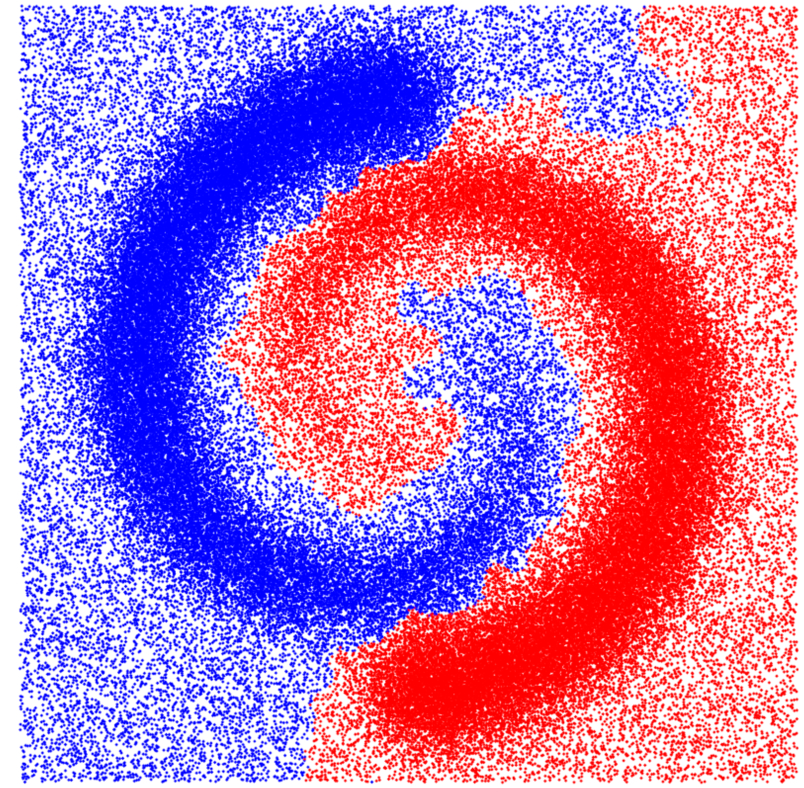
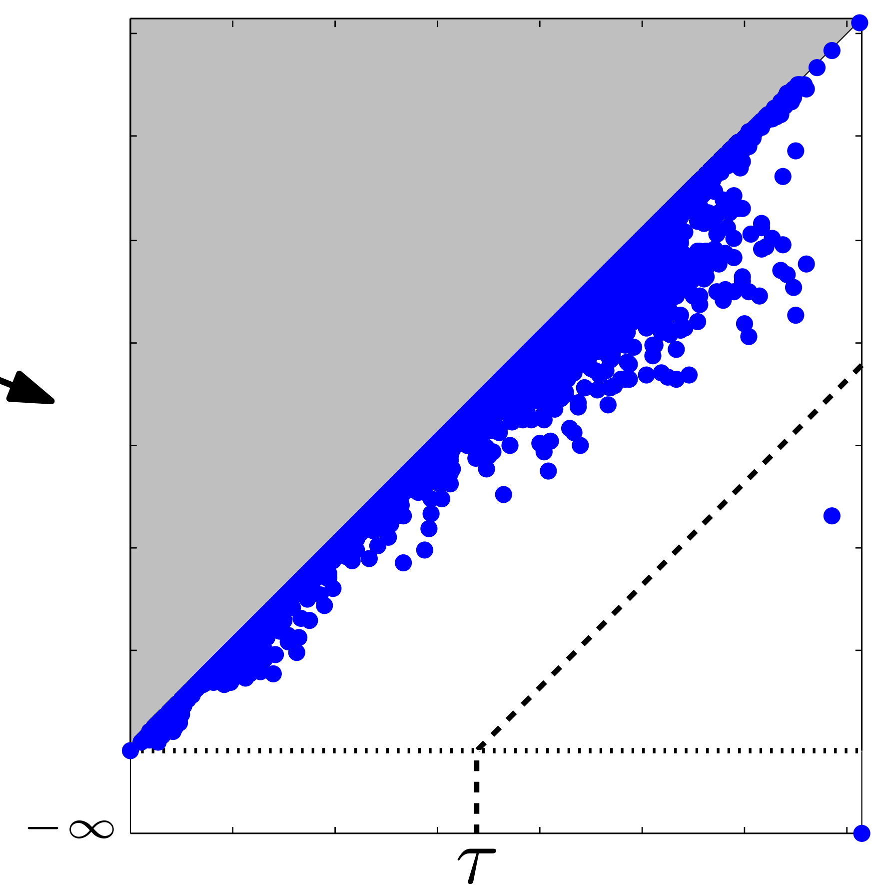




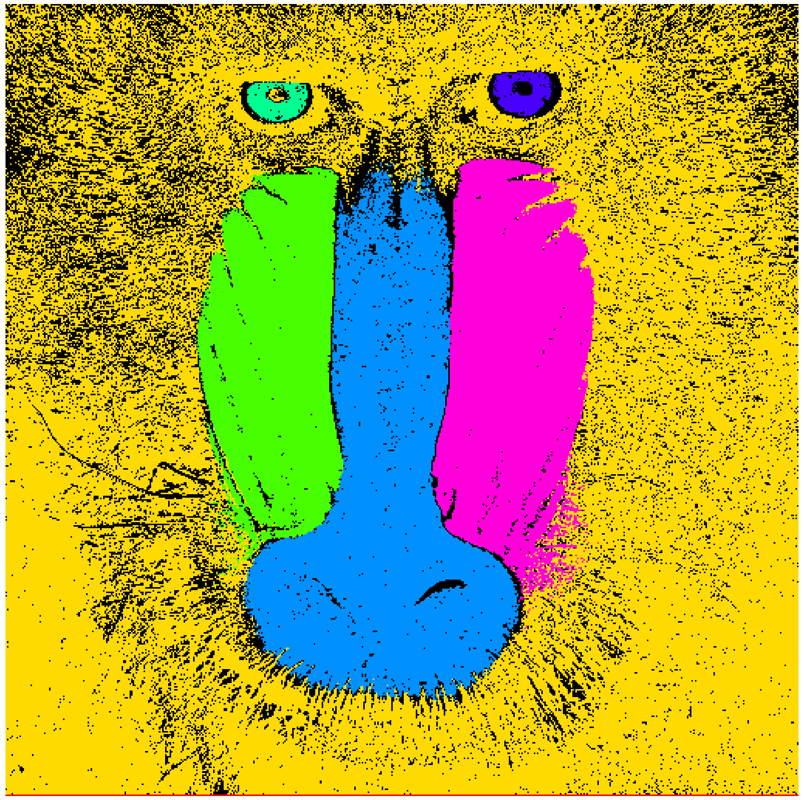


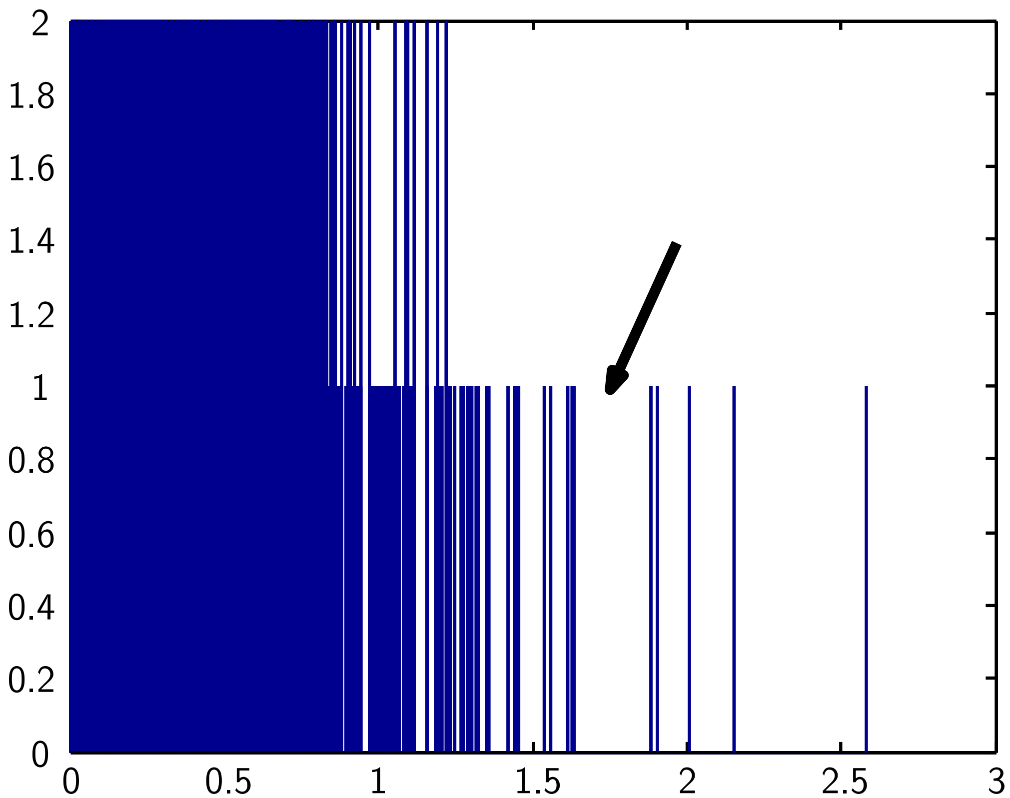
Experimental Results

Image Segmentation

Density is estimated in 3D color space (Luv)

Neighborhood graph is built in image domain





Distribution of prominences does not usually show a clear unique gap

Still, relationship between choice of τ and number of obtained clusters remains explicit

Estimating the Correct Number of Clusters

Hypotheses:

- $f : \mathbb{X} \to \mathbb{R}$ a c-Lipschitz probability density function,
- P a finite set of n points of $\mathbb{X}$ sampled i.i.d. according to f,
- $\hat{f} : P \to \mathbb{R}$ a density estimator such that $\eta := \max_{p \in P} |\hat{f}(p) - f(p)| < \Pi/5$,
- $G = (P, E)$ the δ-neighborhood graph for some positive $\delta < \frac{\Pi - 5\eta}{5c}$.

Note: Π is the prominence of the least prominent peak of f

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Conclusion:

For any choice of τ such that $2(c\delta + \eta) < \tau < \Pi - 3(c\delta + \eta)$, the number of clusters computed by the algorithm is equal to the number of peaks of f with probability at least $1 - e^{-\Omega(n)}$.

(the Ω notation hides factors depending on c, δ)

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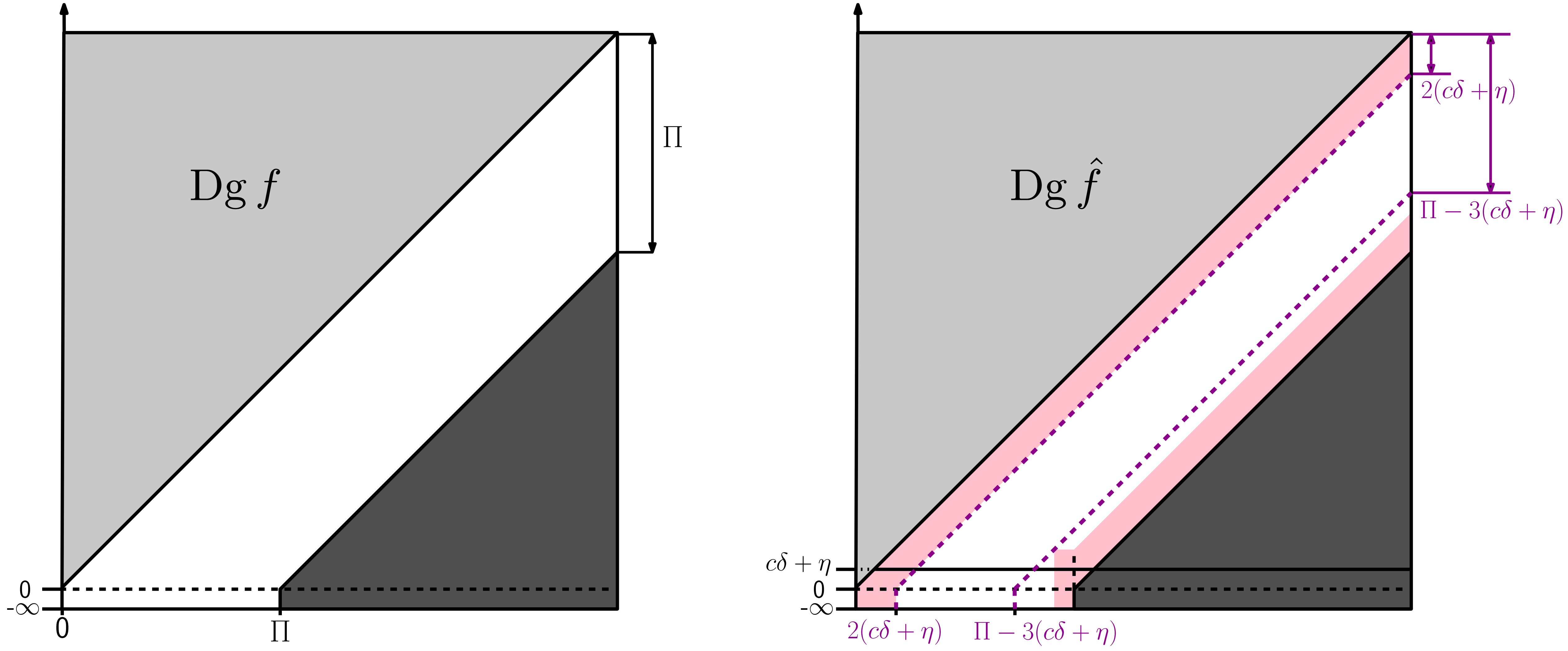

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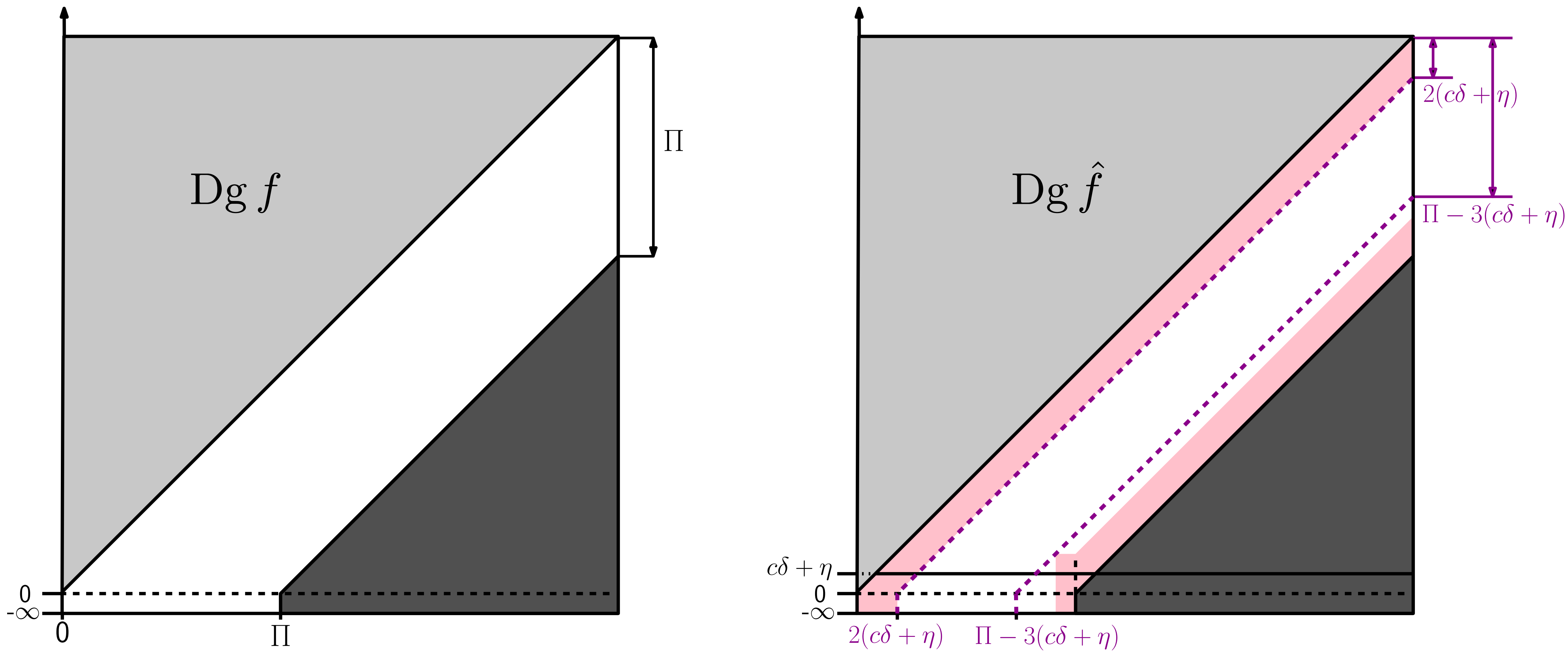

Proof's main ingredient: stability theorem for persistence diagrams

Note: $f, \hat{f}$ are not defined over the same domain