Foundations of Geometric Methods in Data Analysis
2017-18

Clustering algorithms and introduction to persistent homology

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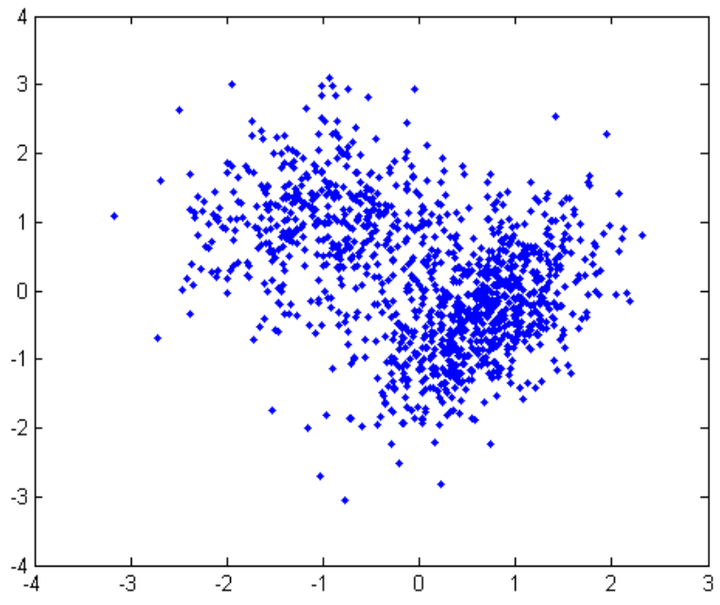
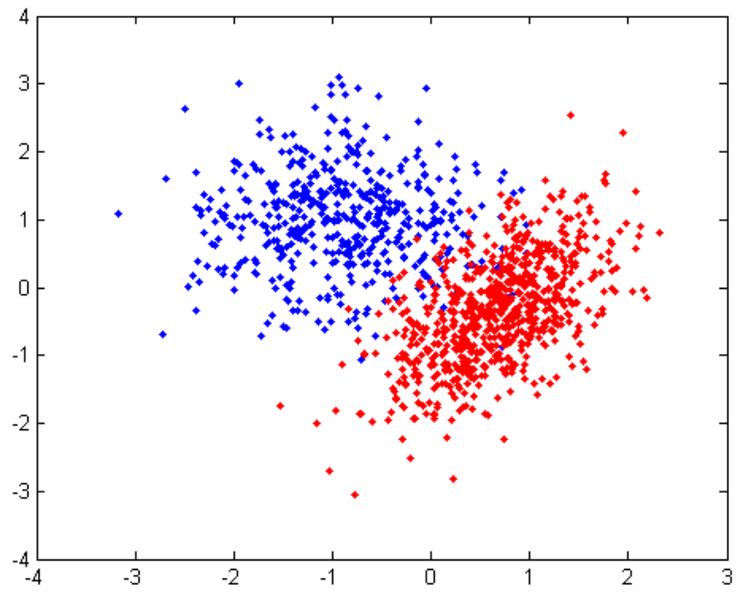
Introduction

Clustering: A partition of data into groups of similar observations. The observations in each group (cluster) are similar to each other and dissimilar to observations from other groups.

Input: a finite set of observations: point cloud embedded in an Euclidean space (with coordinates) or a more general metric space (pairwise distance/similarity) matrix.





Goal: partition the data into a relevant family of subsets (clusters).

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Not a single/universal notion of cluster.

A wealth of approaches:

- Variational
- Spectral
- Density based
- Hierarchical
- etc...

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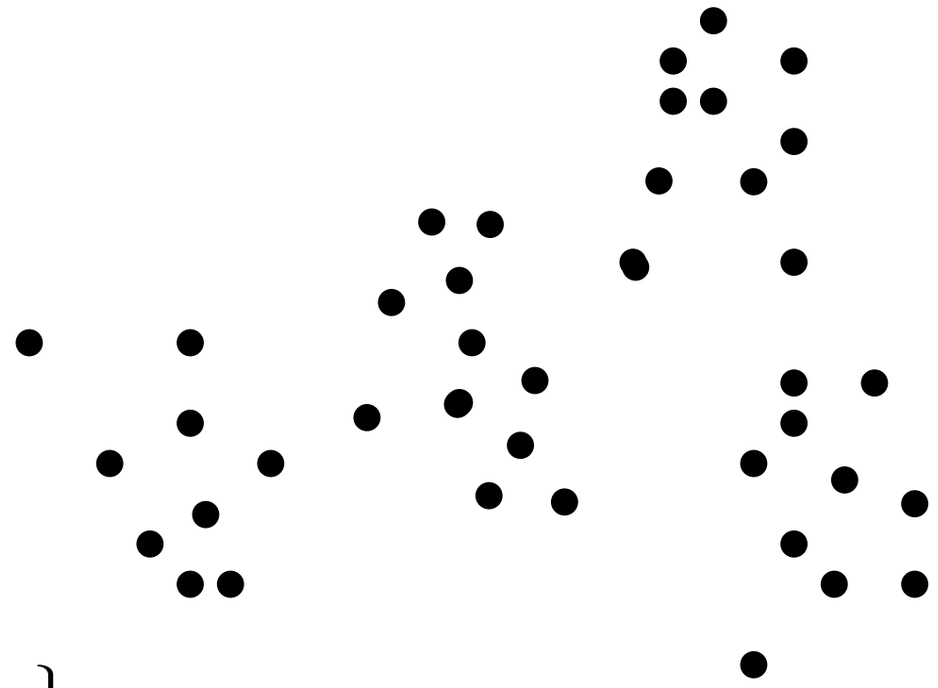
In this lecture:

- a few basic classical "algorithms" motivating and bringing us to the introduction of persistent homology.

The k-means algorithm

Input: A (large) set of N points X and an integer $k < N$.



Goal: Find a set of k points $L = \{y_1, \cdots y_k\}$ that minimizes

$$E = \sum_{i=1}^{N} d(x_i, L)^2$$

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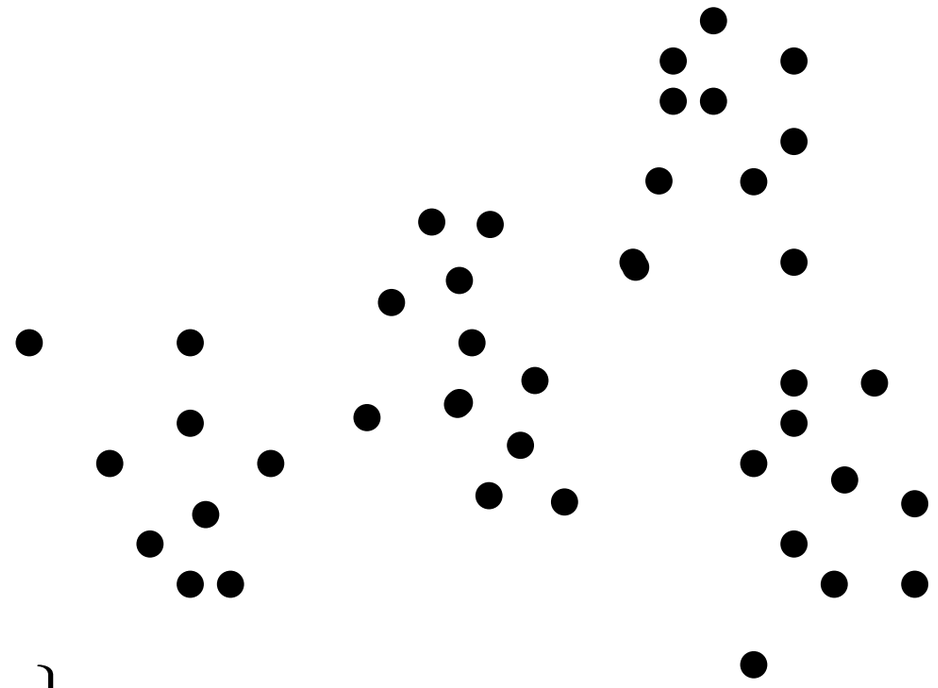

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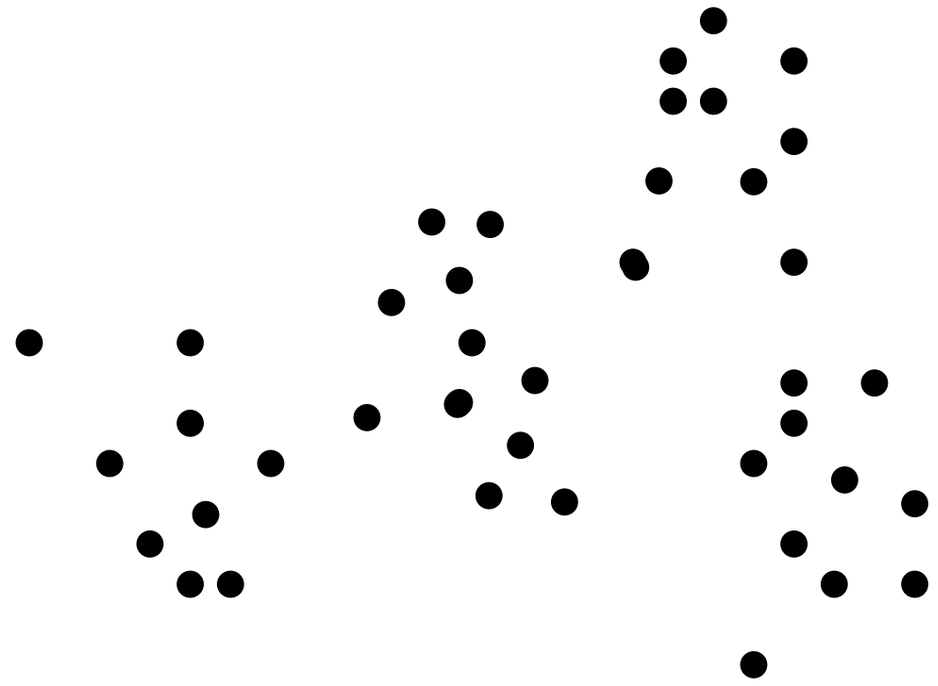
This is a NP hard problem!

The Lloyd's algorithm: a very simple local search algorithm $\rightarrow$ local minimum.

The k-means algorithm

The Lloyd's algorithm



- Select $L^1 = \{y_1^1, \cdots y_k^1\}$ initial "seeds";
- $i = 1$;
- Repeat
  - For $(j = 1; j \leq k; j++)$ $S_j^i = \{x \in X : d(x, y_j^i) = d(x, L^i)\}$;
  - For $(j = 1; j \leq k; j++)$

$$y_j^{i+1} = \frac{1}{|S_j^i|} \sum_{x \in S_j^i} x$$

  - $i++$;
- Until convergence

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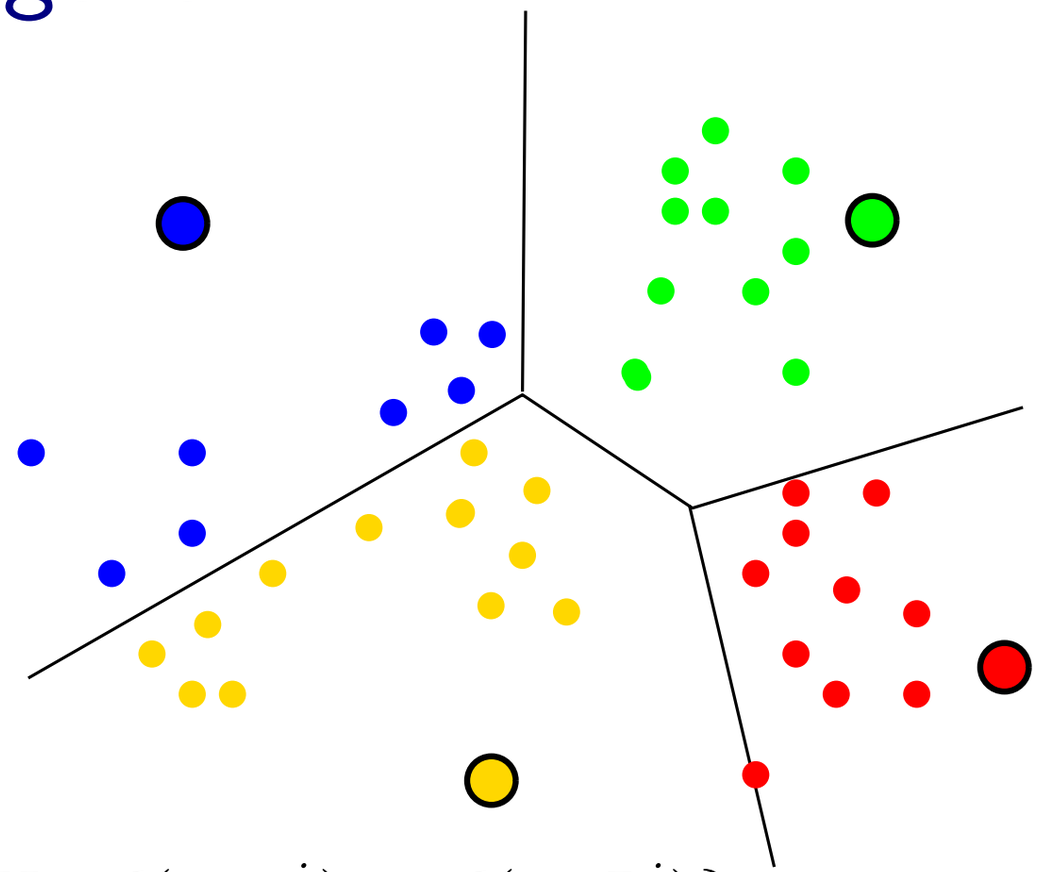

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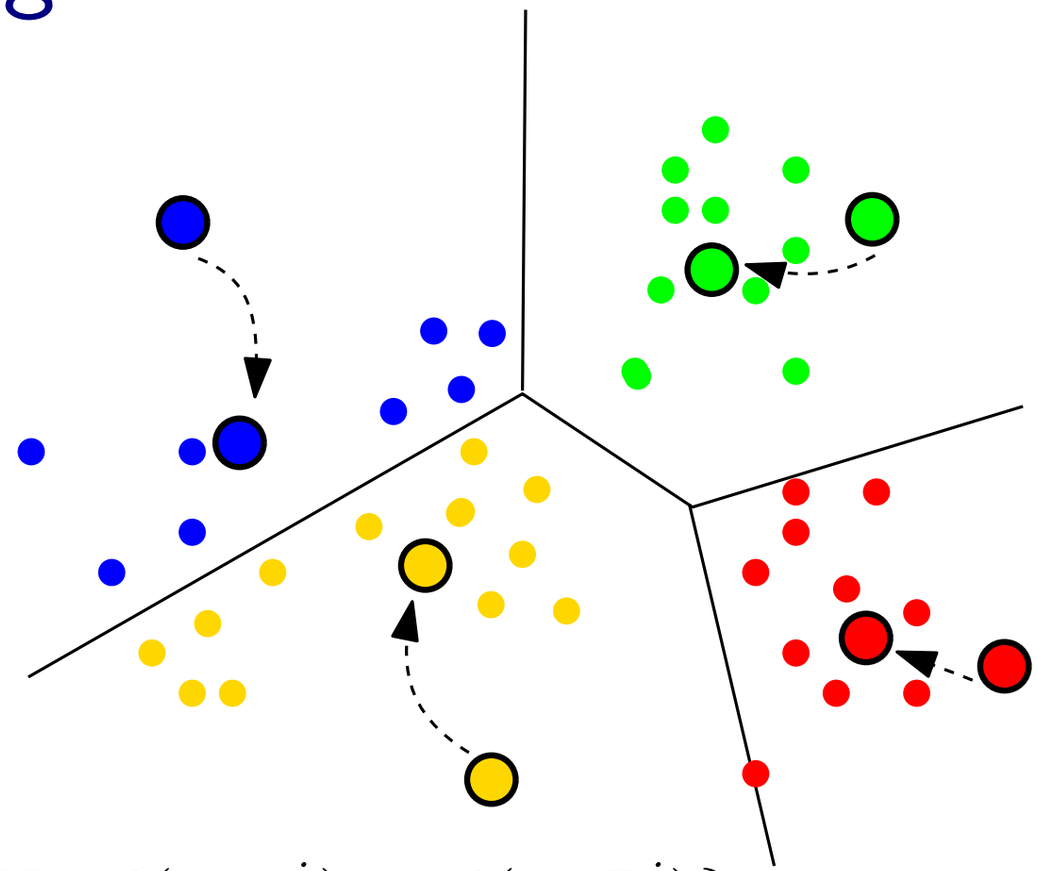

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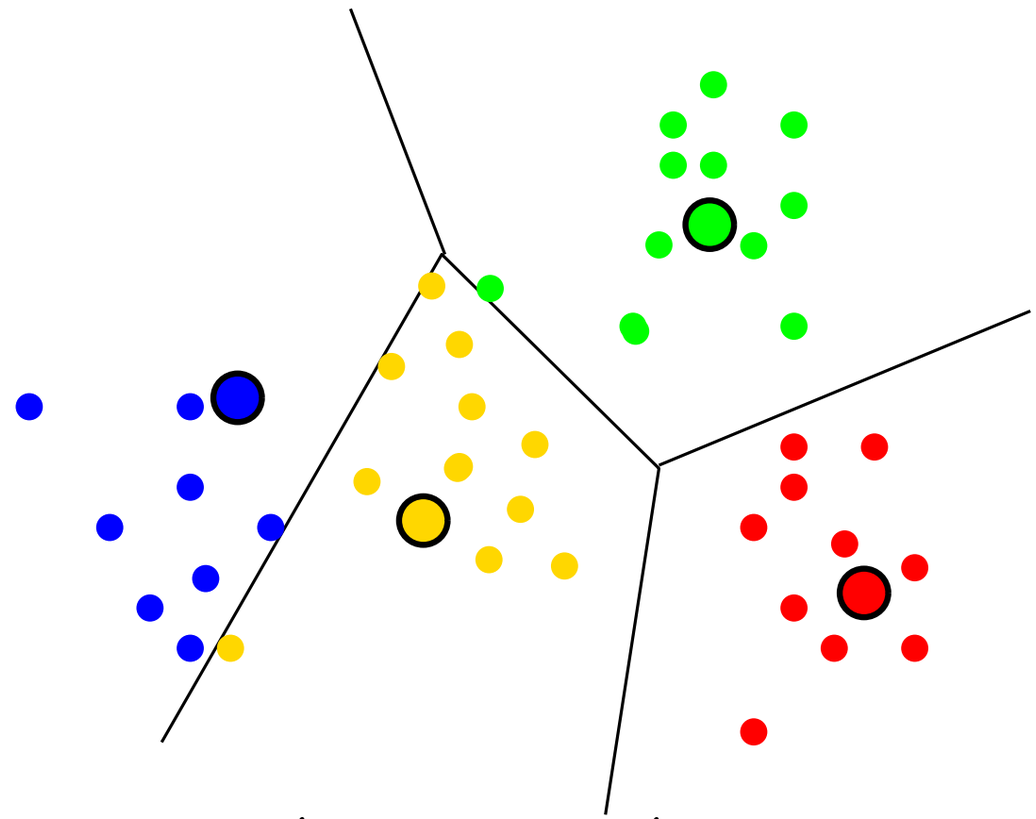

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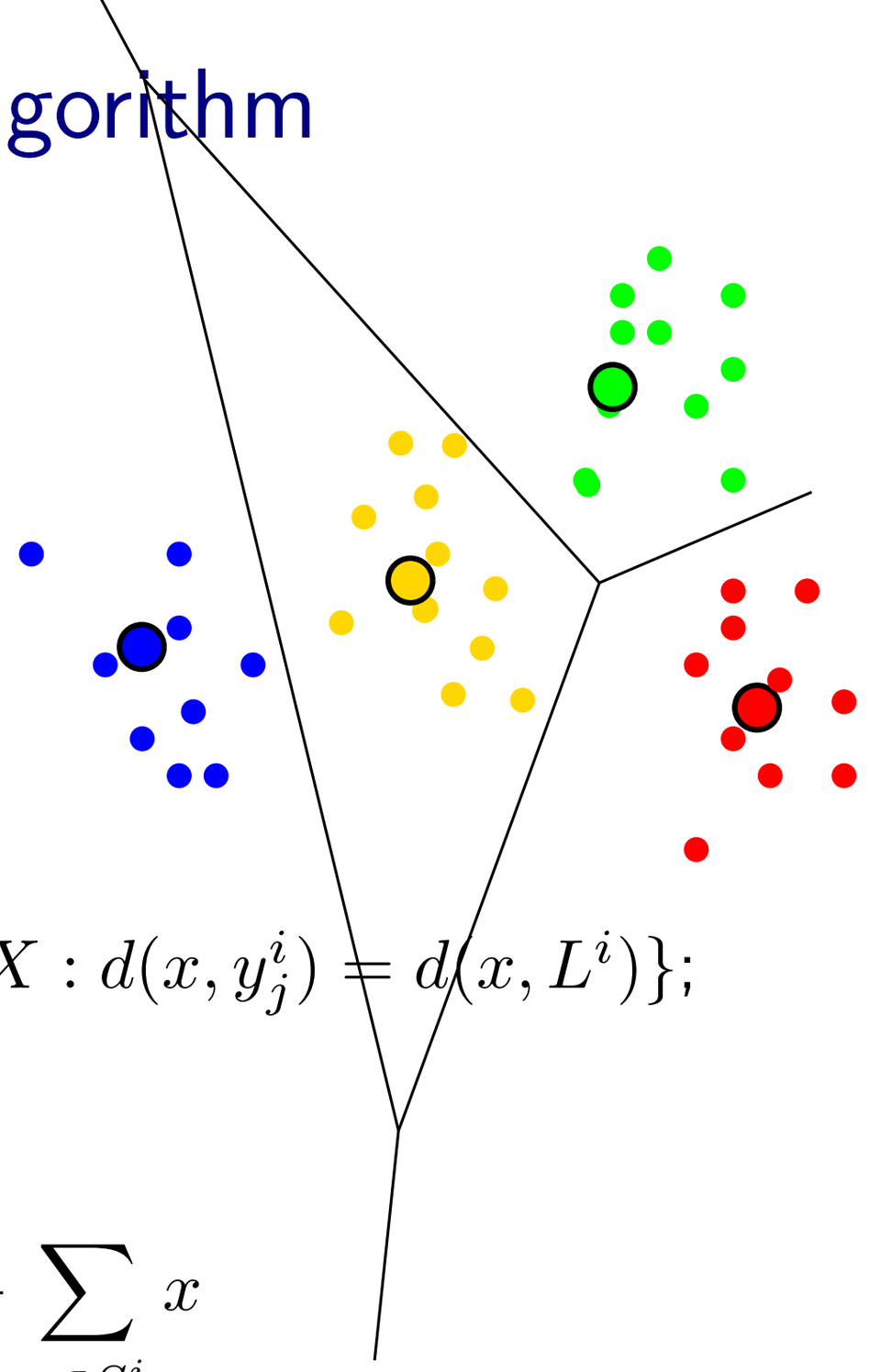

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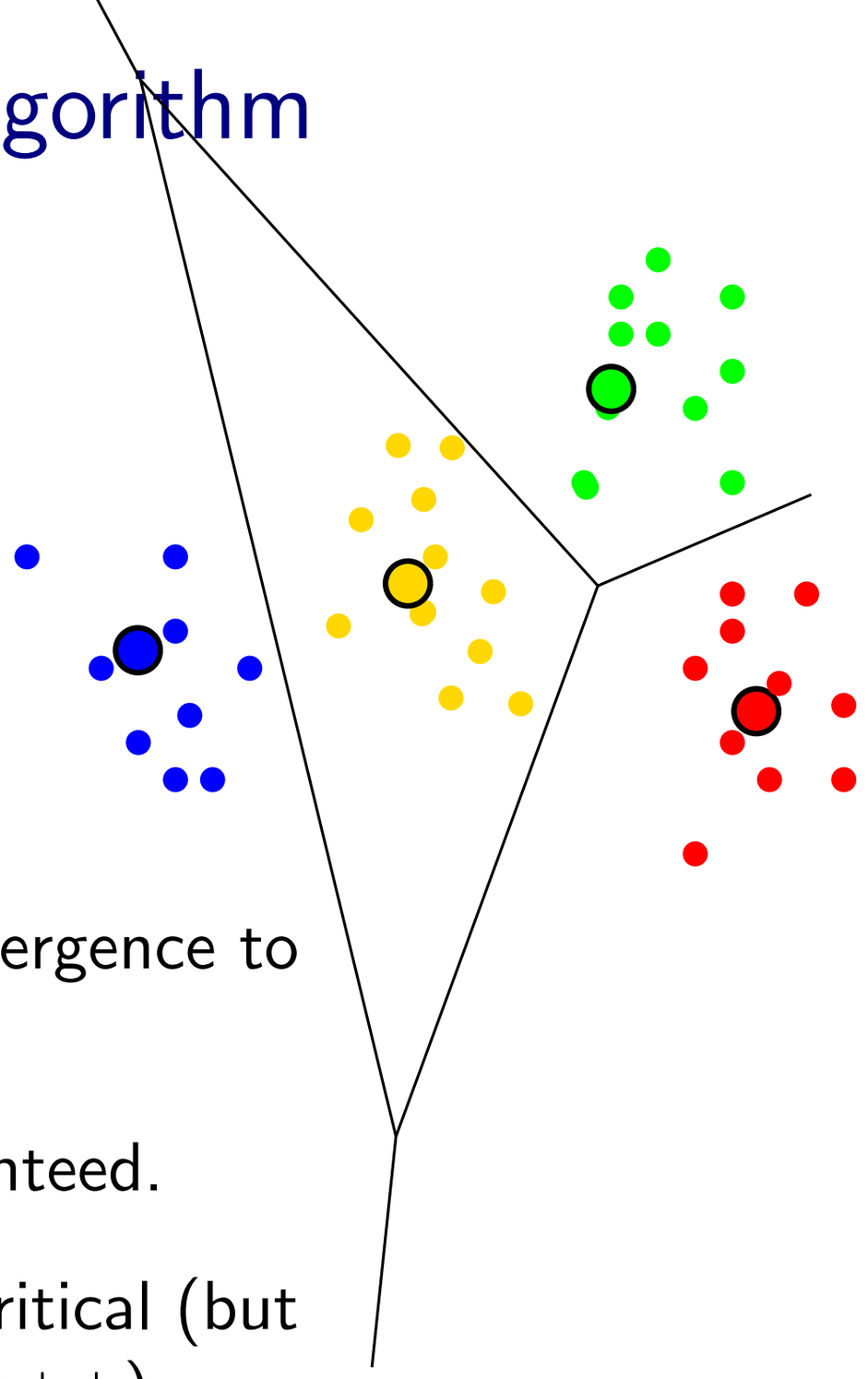

Warning:

- Lloyd's algorithm does not ensure convergence to a global minimum!
- The speed of convergence is not guaranteed.
- the choice of the initial seeds may be critical (but there exists some strategies $\rightarrow$ k-means++).

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Build a hierarchy of clusters (nested family of clustering partitions)

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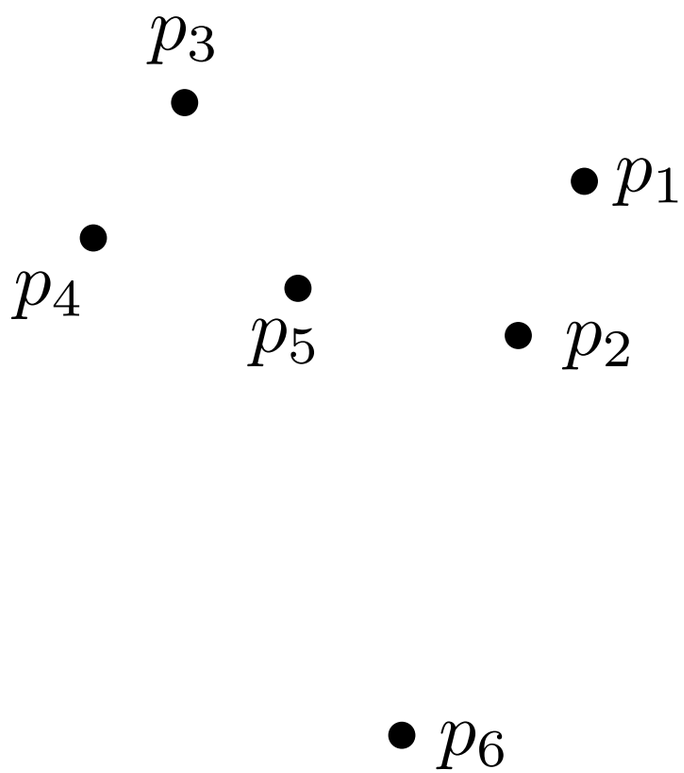
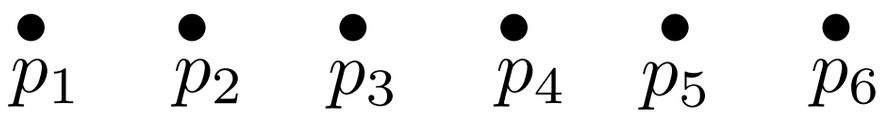
Start with single point cluster and recursively merge the most similar clusters to one parent cluster until reaching a stopping criterion (e.g. number of clusters).





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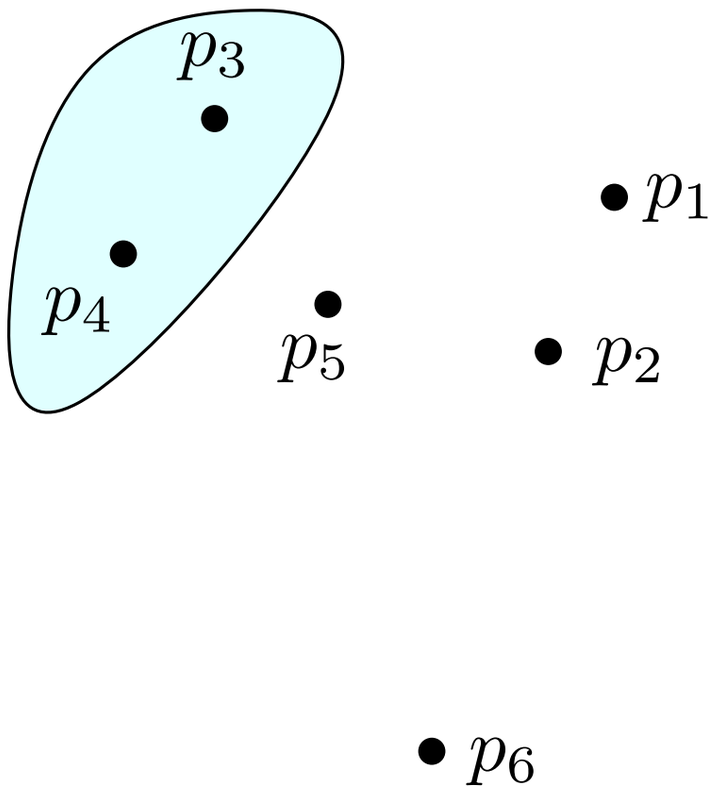

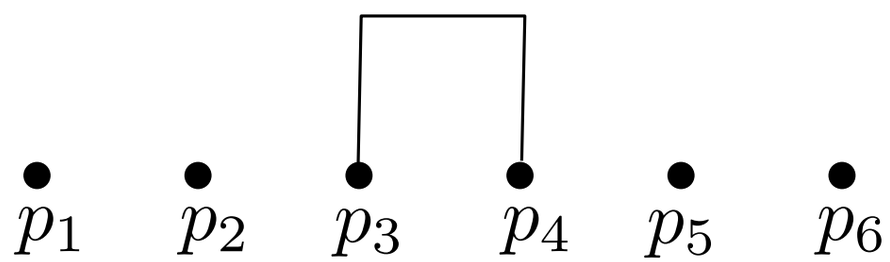

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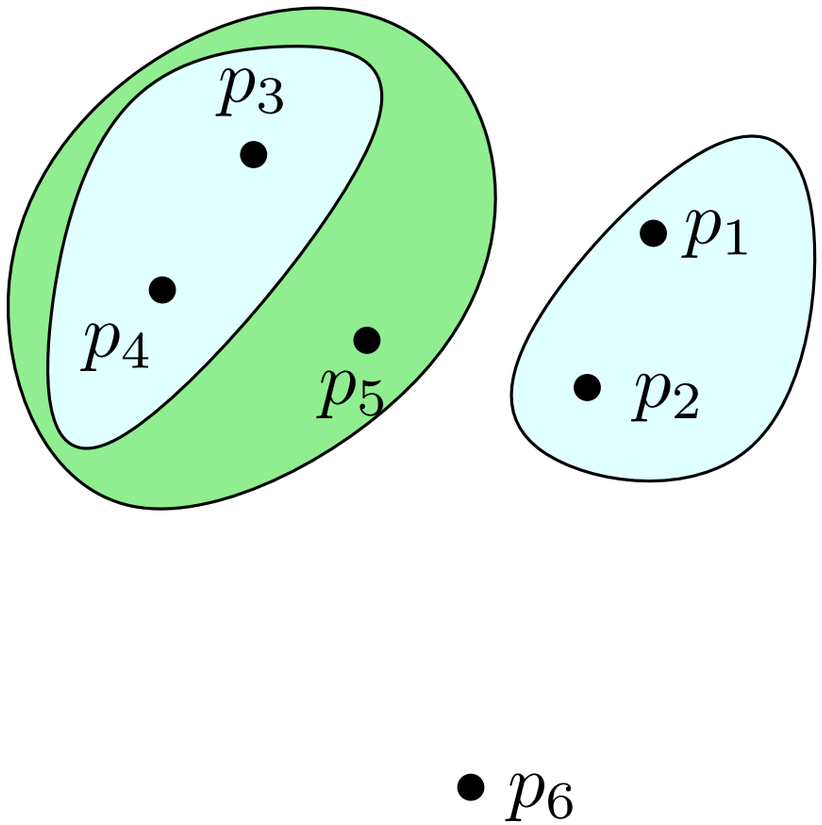

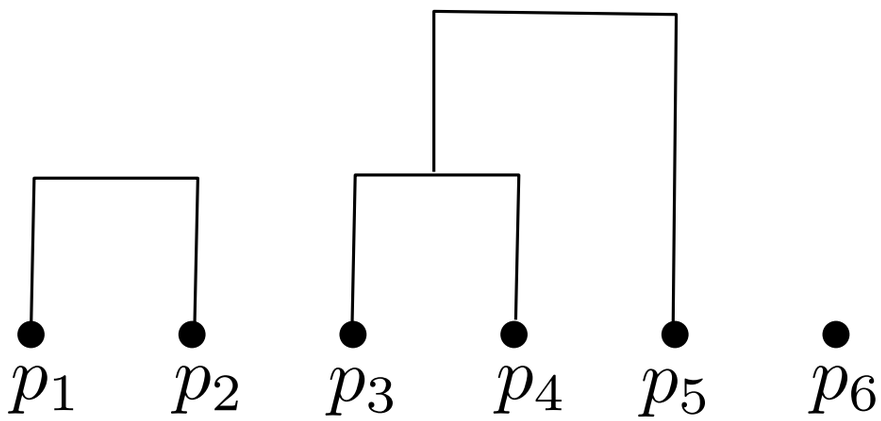

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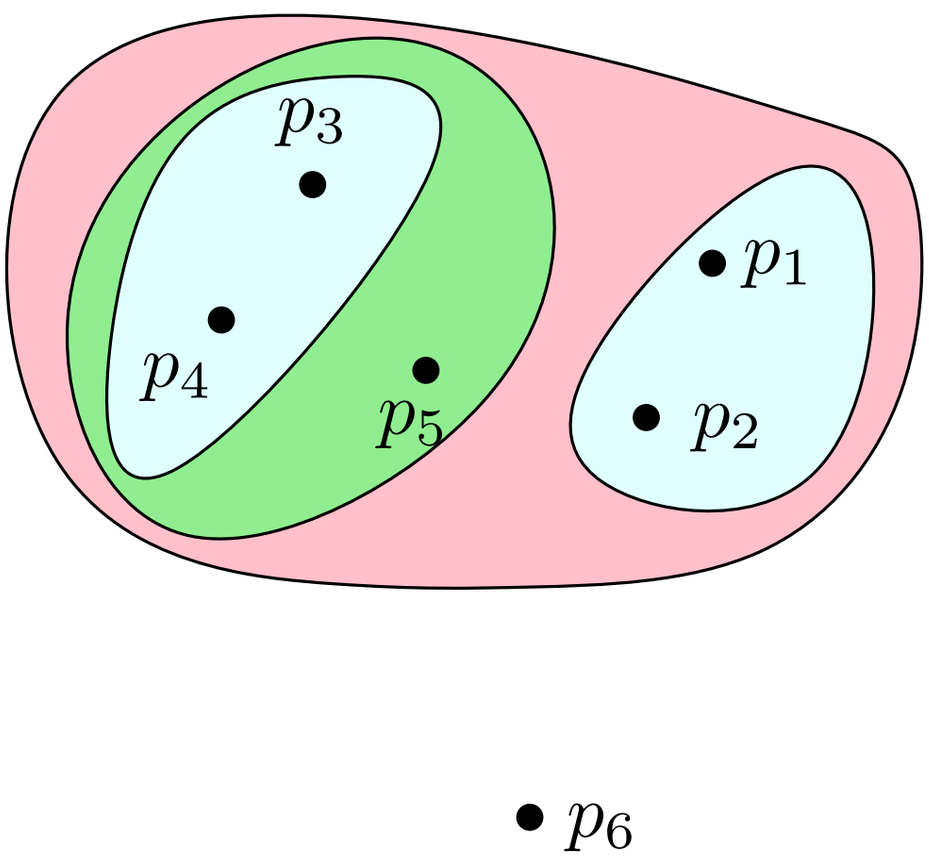

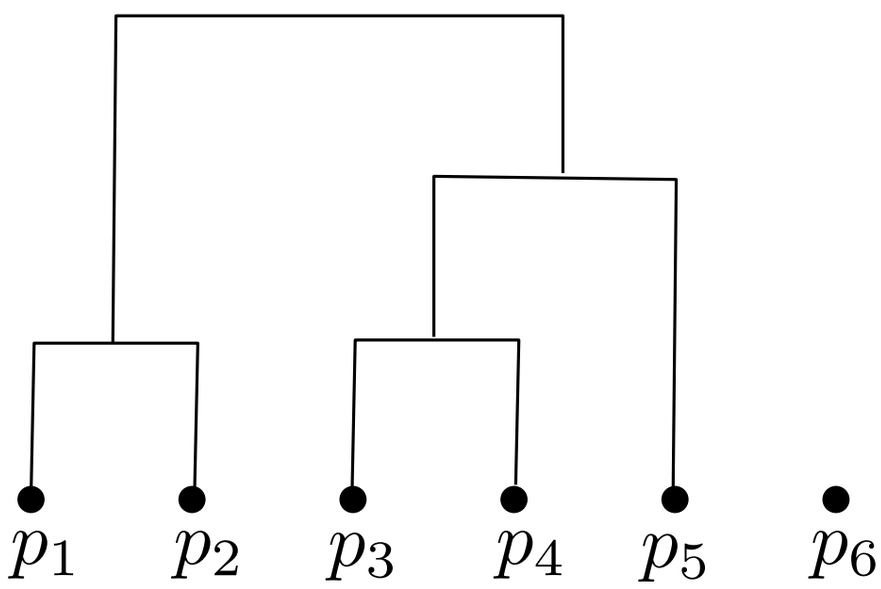

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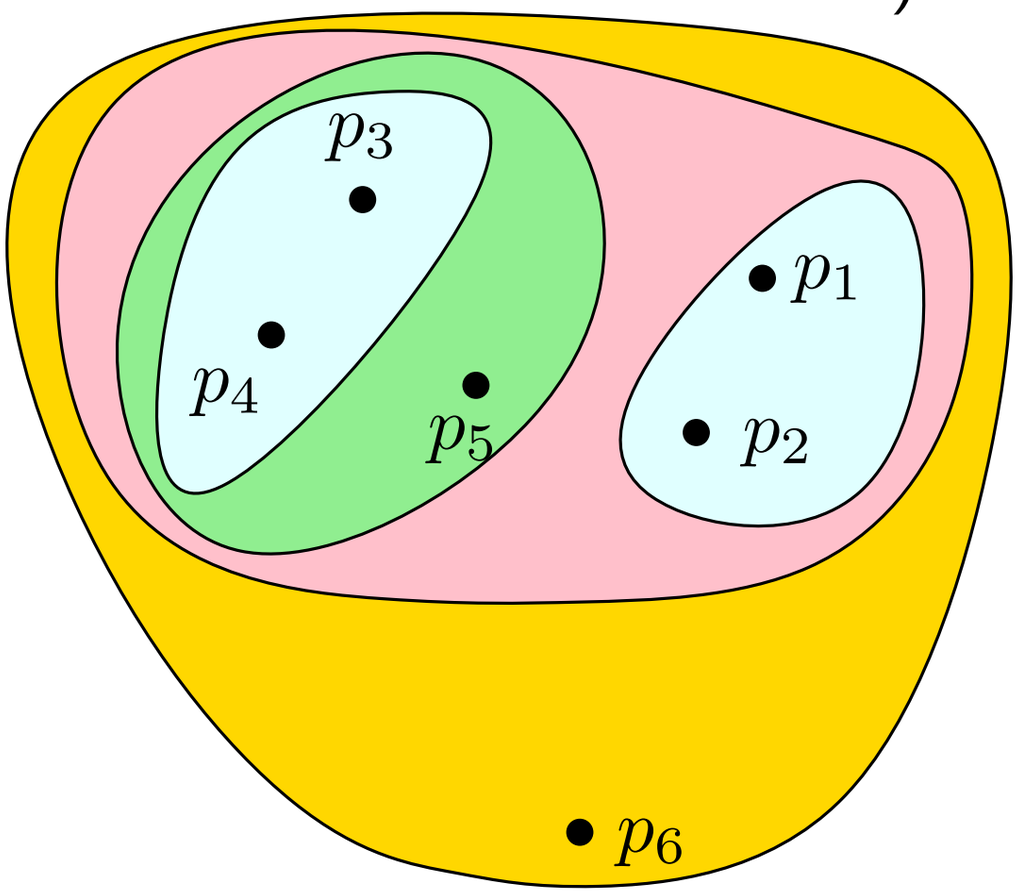

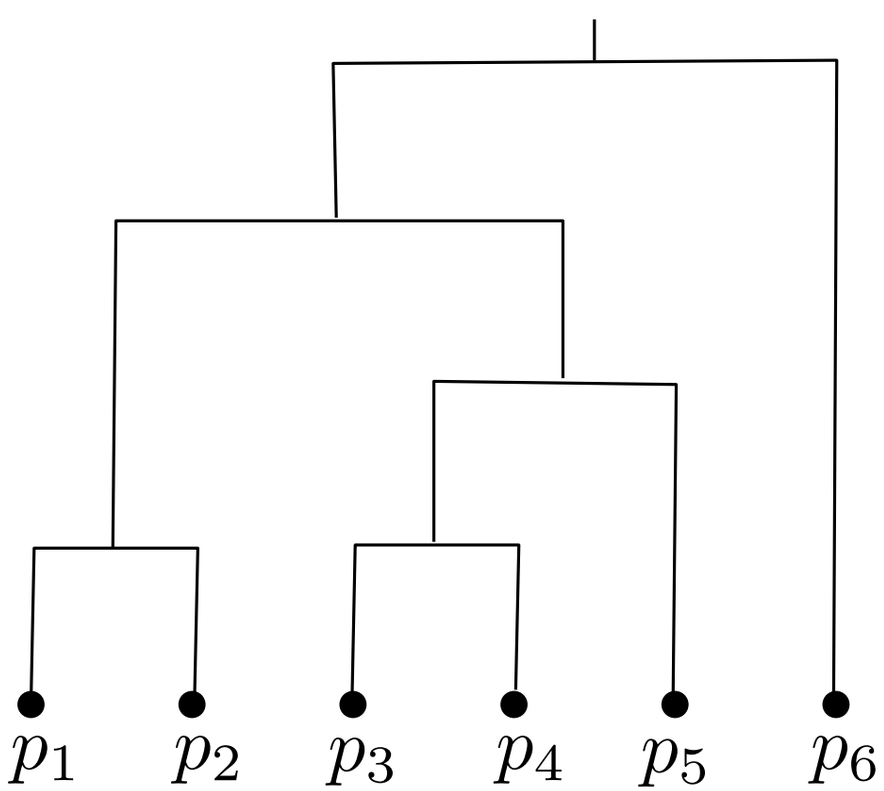

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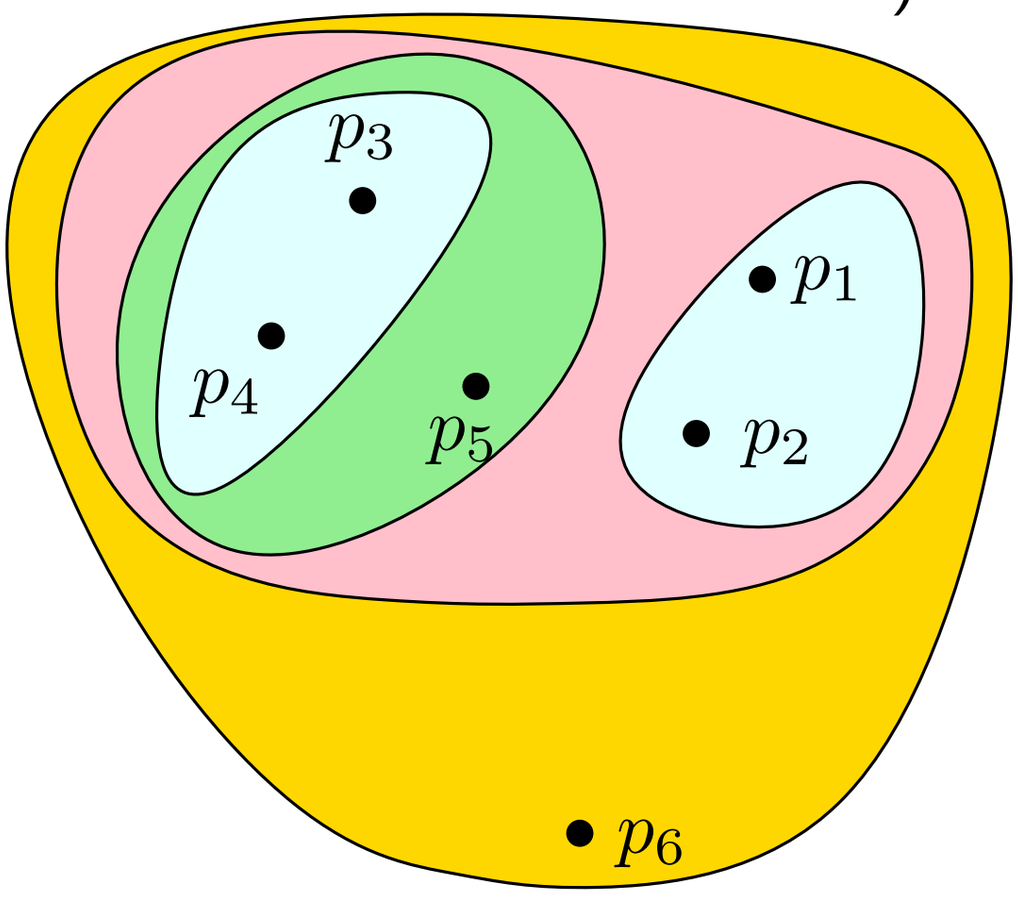
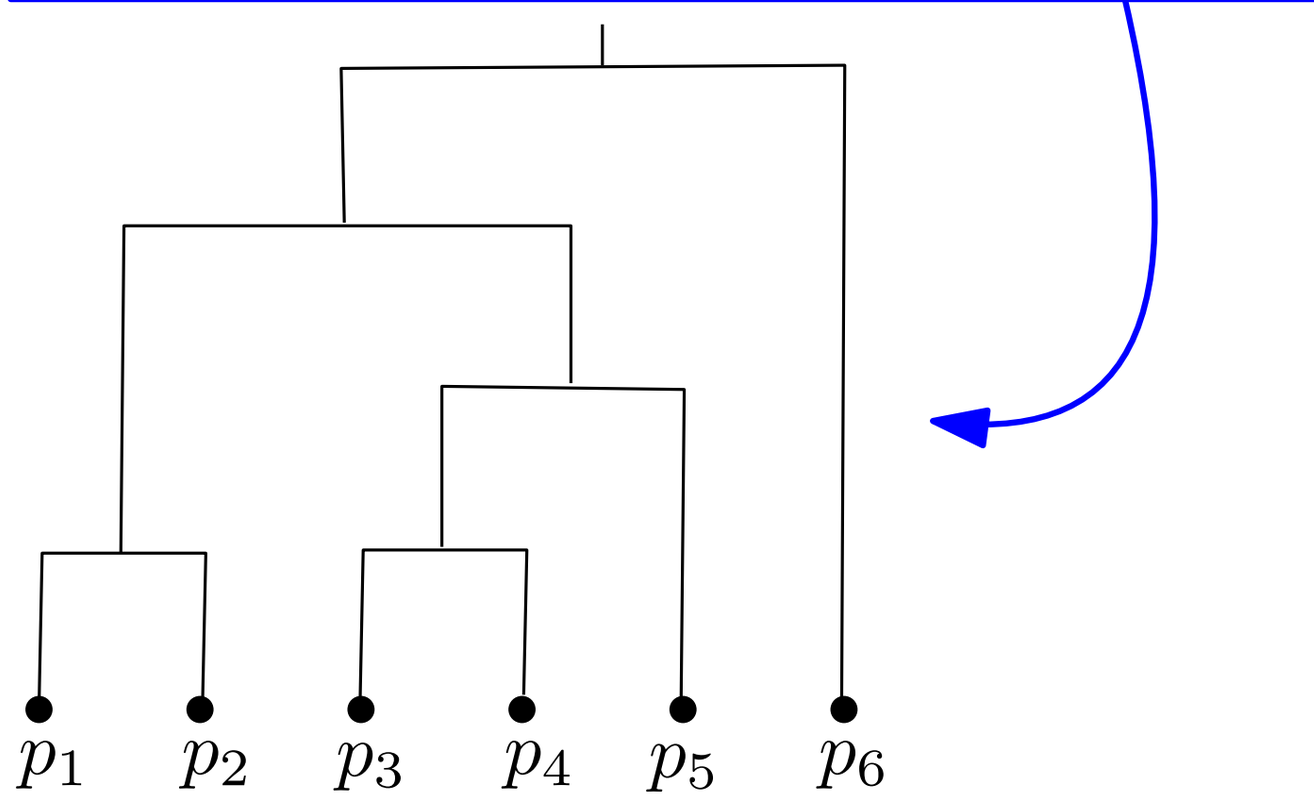


Dendogram, i;e. a tree such that:
- each leaf node is a singleton,
- each node represent a cluster,
- the root node contains the whole data,
- each internal node has two daughters, corresponding to the clusters that were merged to obtain it.



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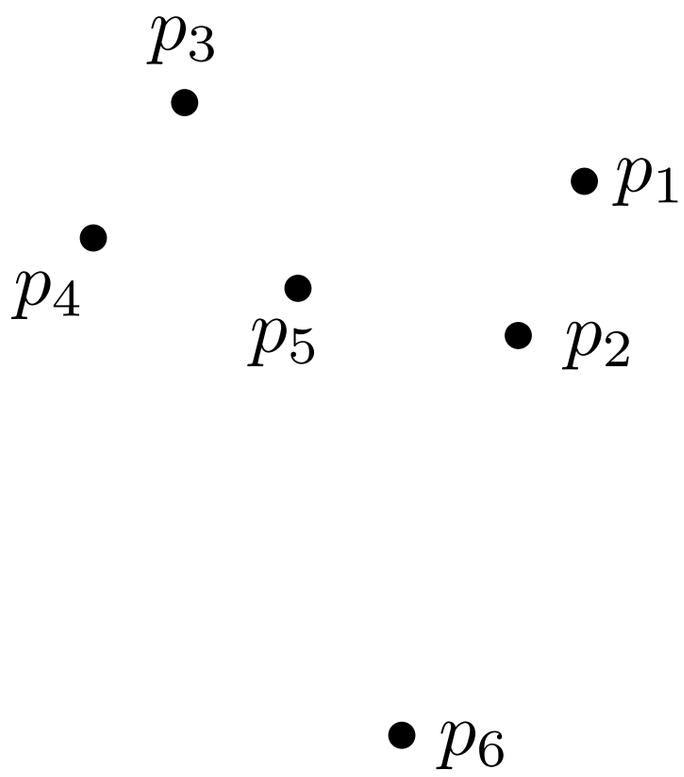
Start with single point cluster and recursively merge the most similar clusters to one parent cluster until reaching a stopping criterion (e.g. number of clusters).

Dividing (top-down)

Start with a single global cluster and recursively split each cluster until reaching a stopping criterion.



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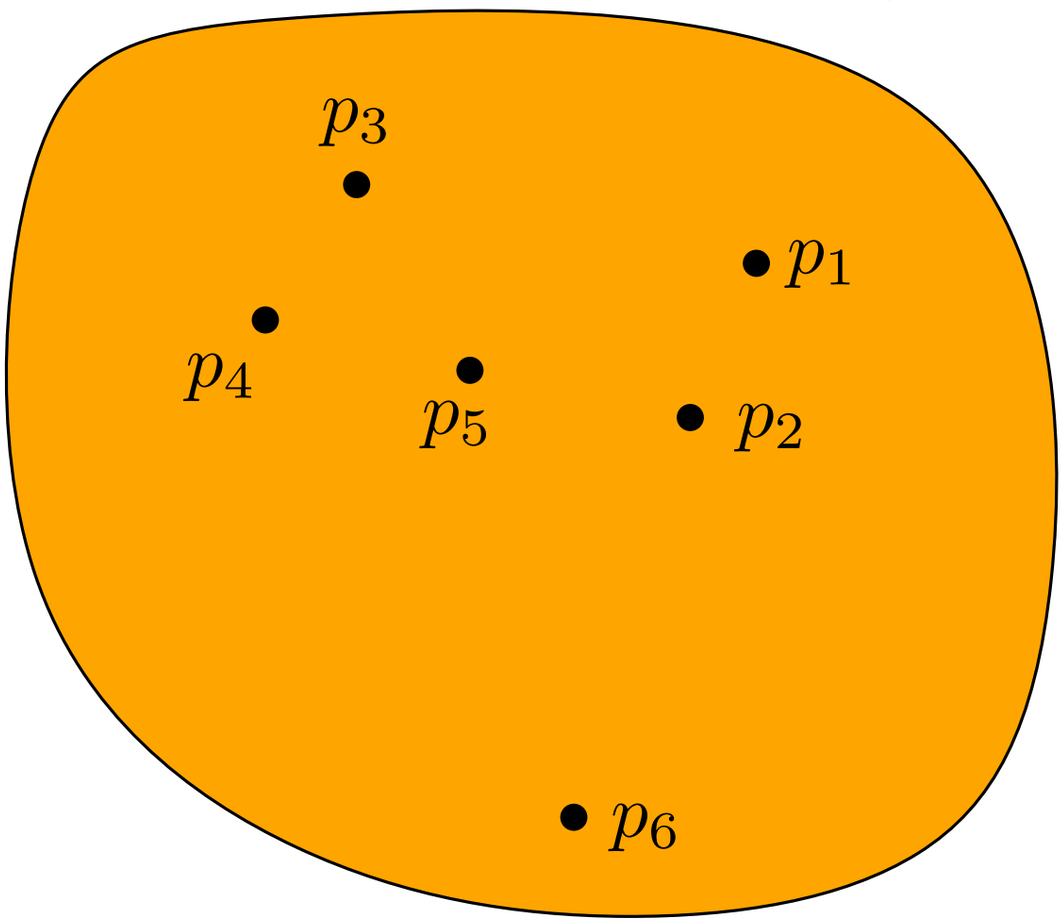

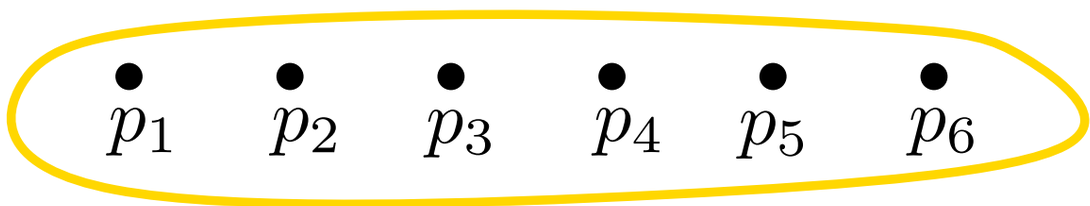

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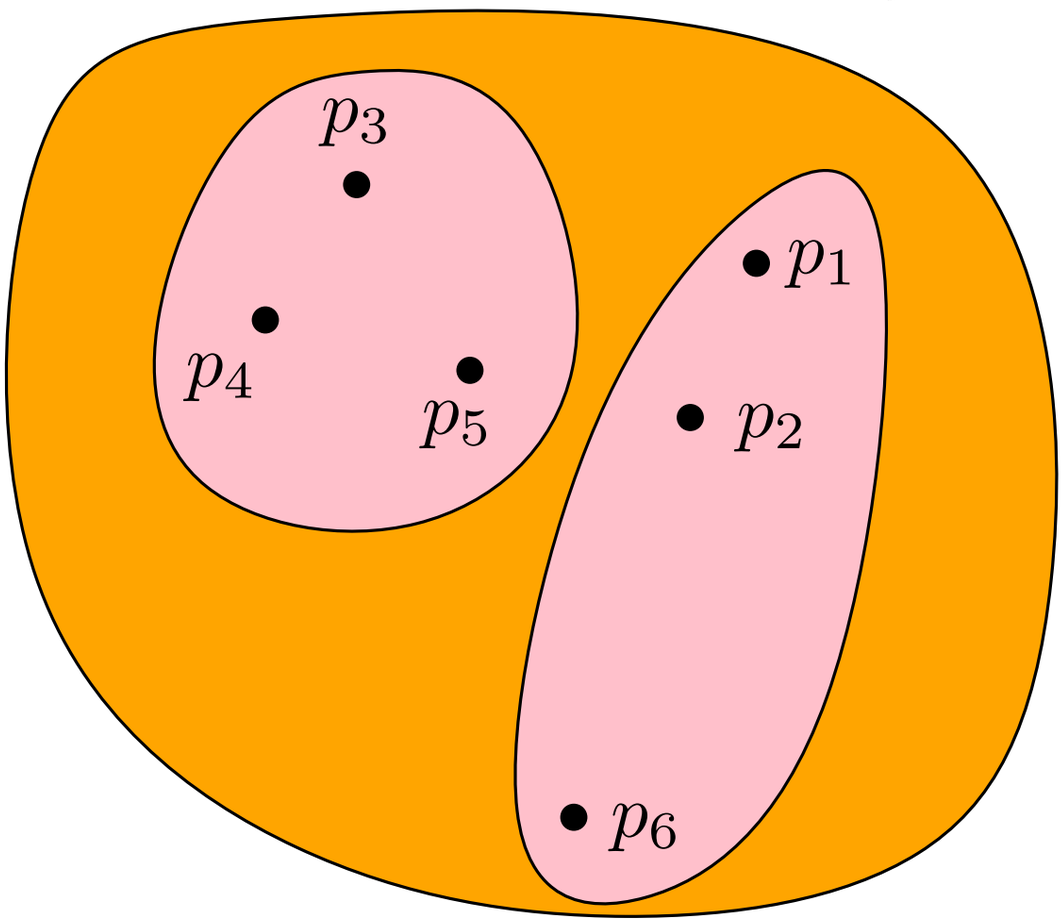

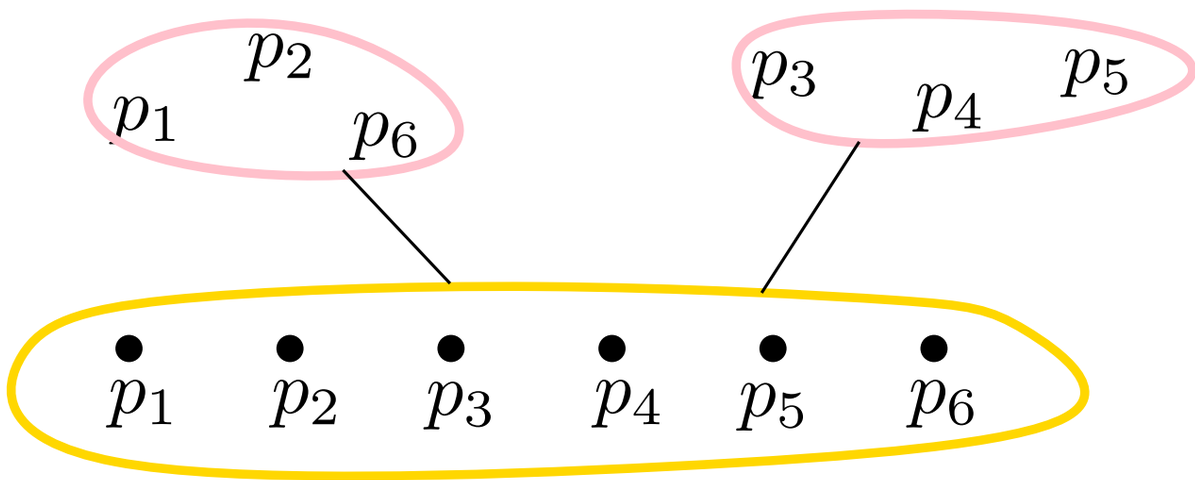

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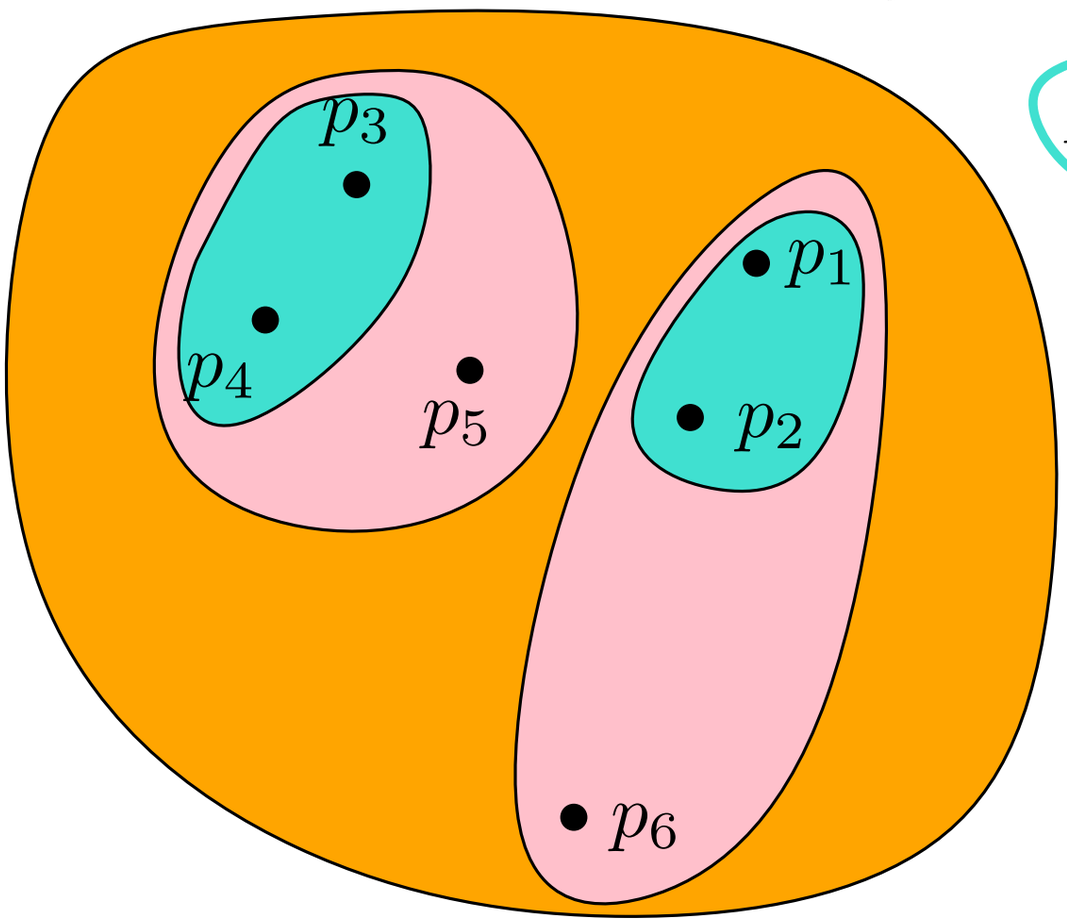

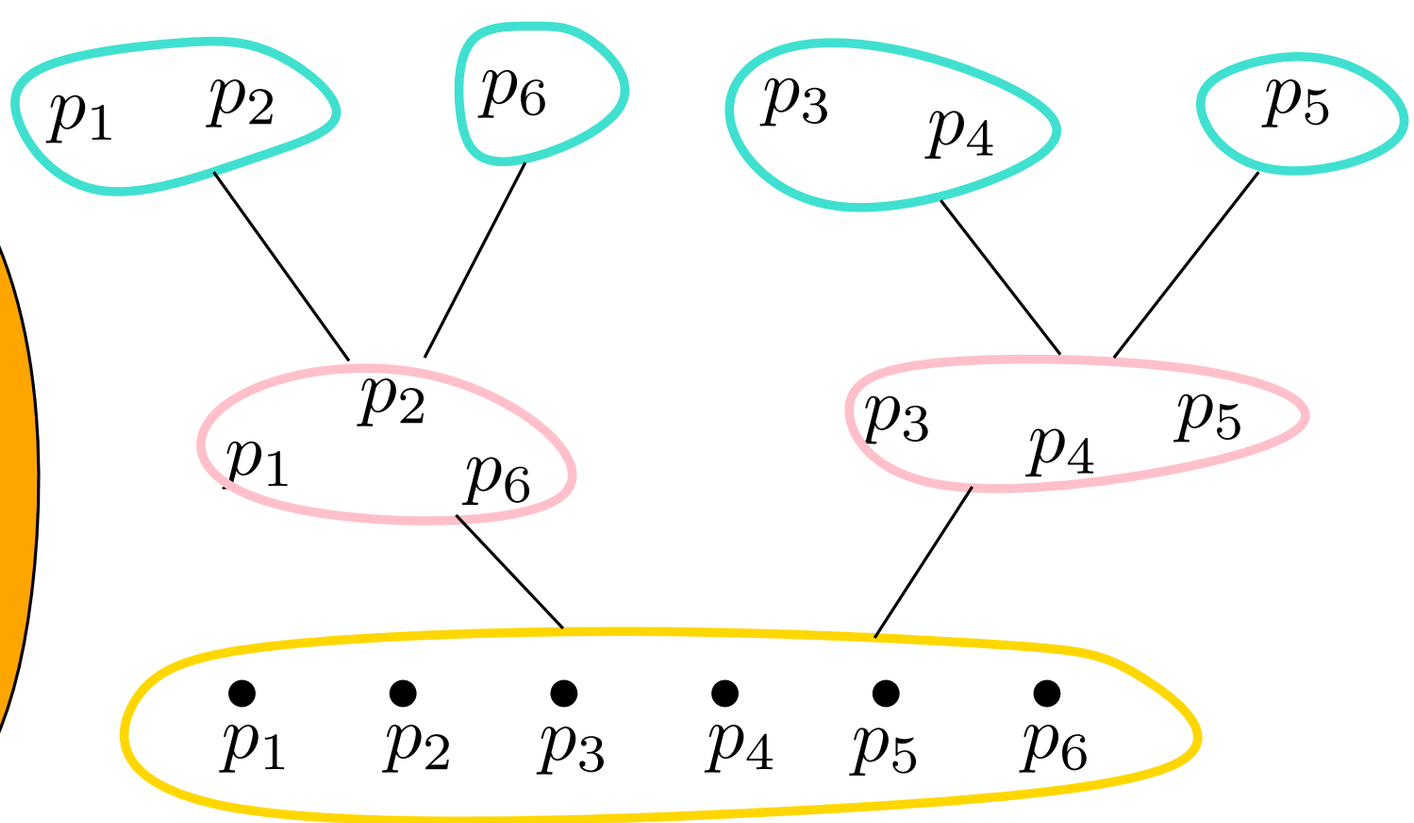

Single linkage clustering

Input: A set $X_n = \{x_1, \cdots, x_n\}$ in a metric space (X, d) (or just a matrix of pairwise dissimilarities $(d_{i,j})$).

Given two clusters $C, C' \subseteq X_n$ let

$$d(C, C') = \inf_{x \in C, x' \in C'} d(x, x')$$

1. Start with a clustering where each x_i is a cluster.

2. At each step, merge the two closest clusters until it remains a single cluster (containing all data points).

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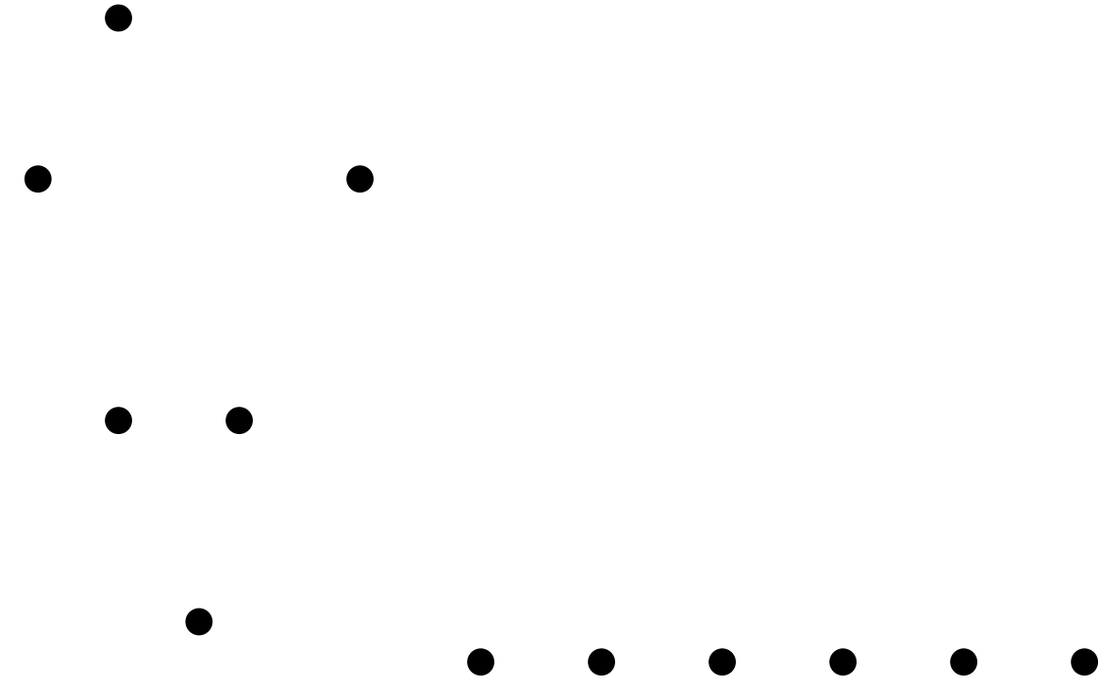

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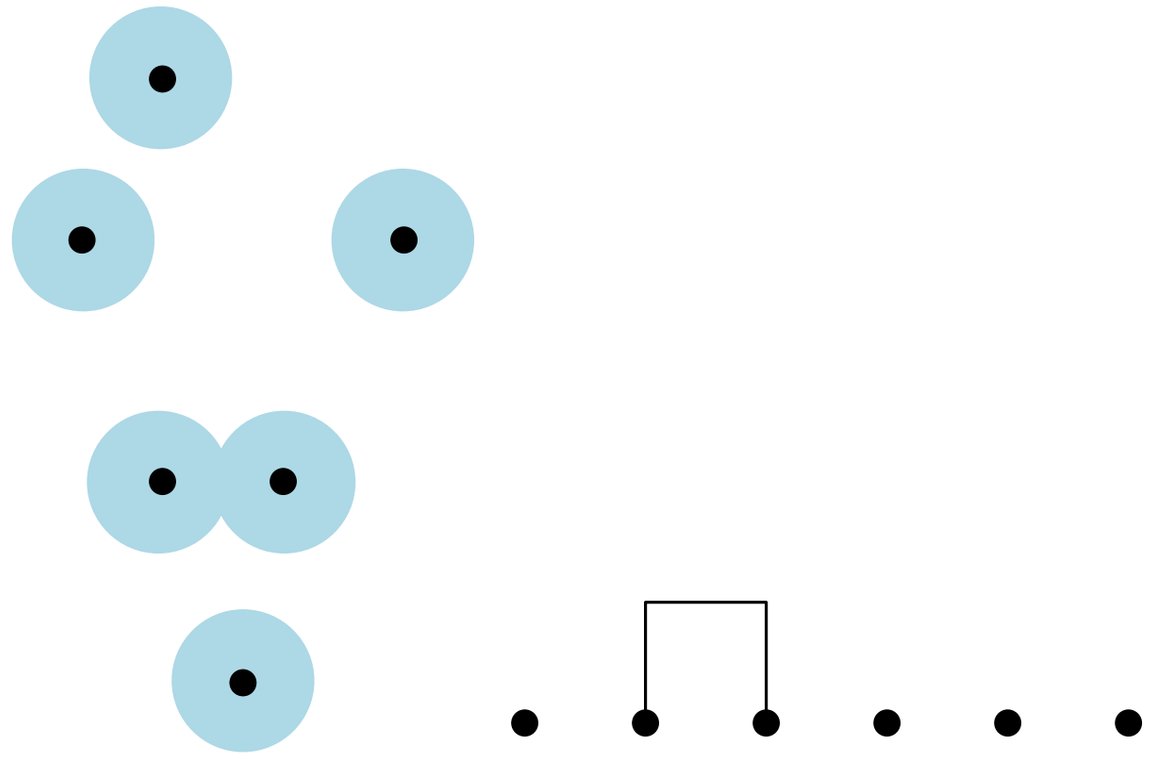

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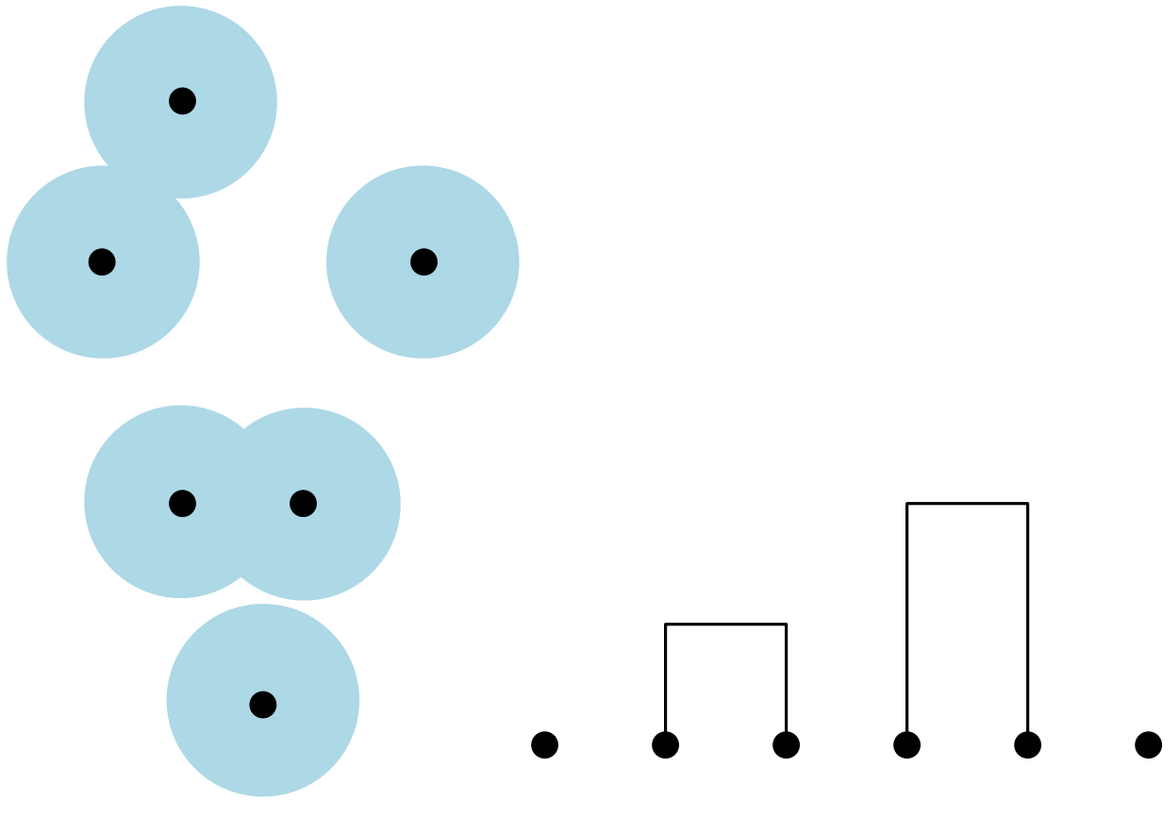

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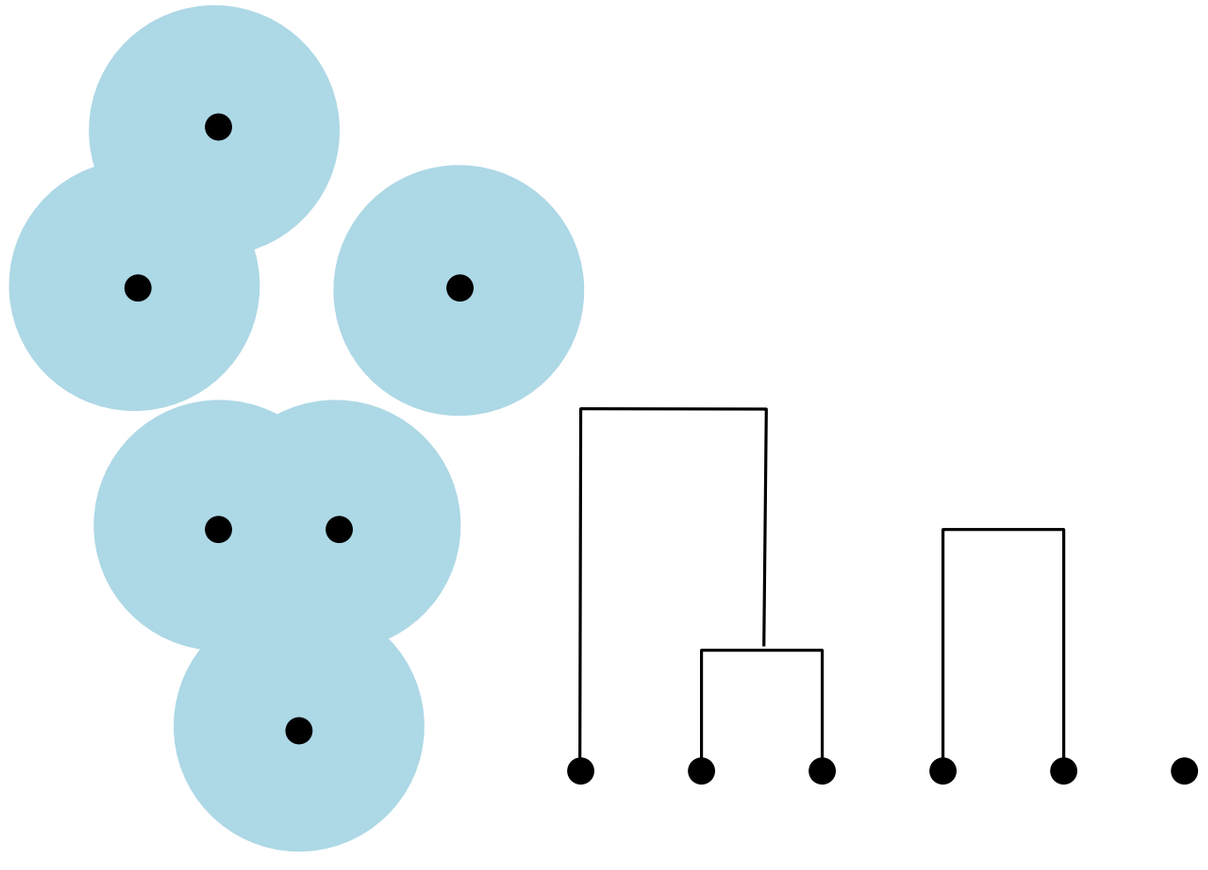

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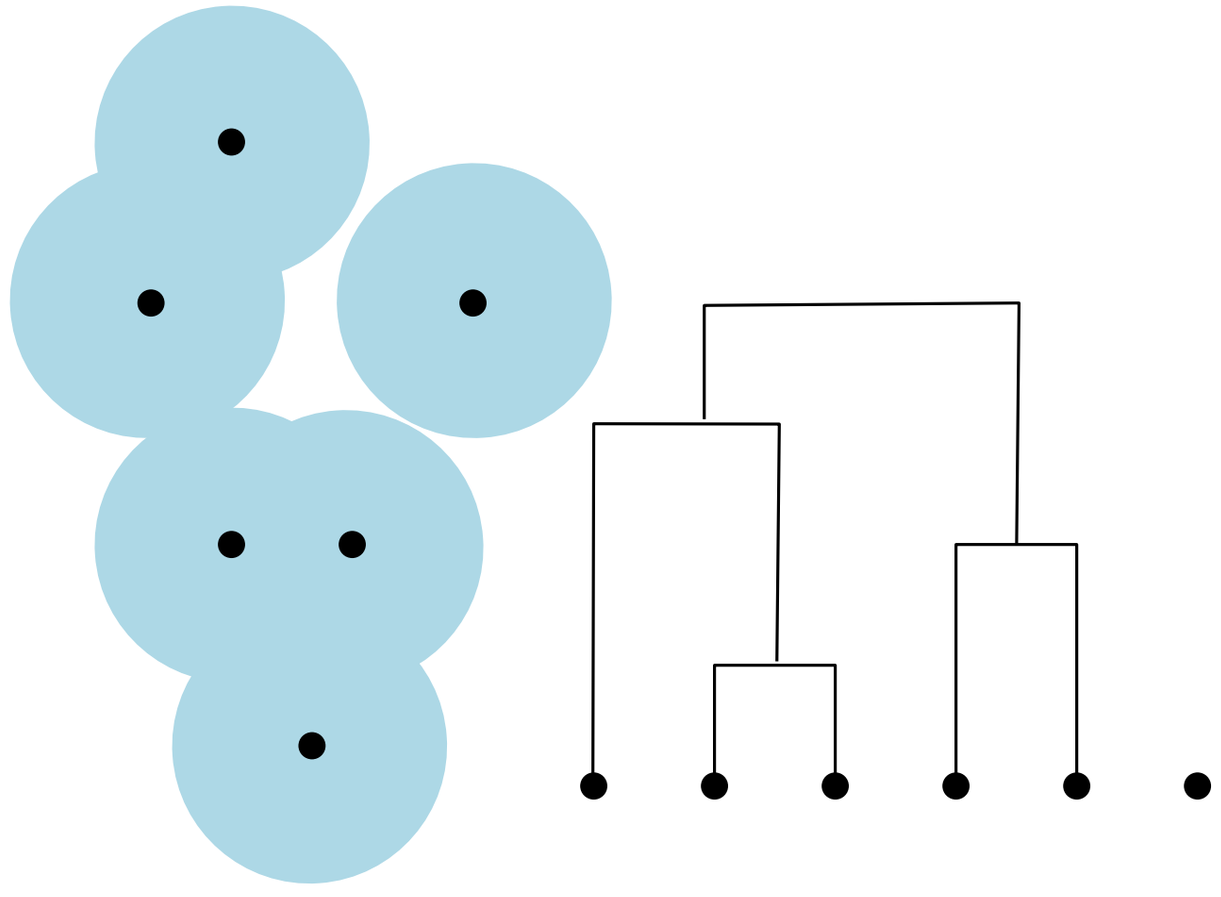

Output:: the resulting dendogram

Single linkage clustering

Input: A set $X_n = \{x_1, \cdots, x_n\}$ in a metric space (X, d) (or just a matrix of pairwise dissimilarities $(d_{i,j})$).

Given two clusters $C, C' \subseteq X_n$ let

$$d(C, C') = \inf_{x \in C, x' \in C'} d(x, x')$$

1. Start with a clustering where each x_i is a cluster.

2. At each step, merge the two closest clusters until it remains a single cluster (containing all data points).

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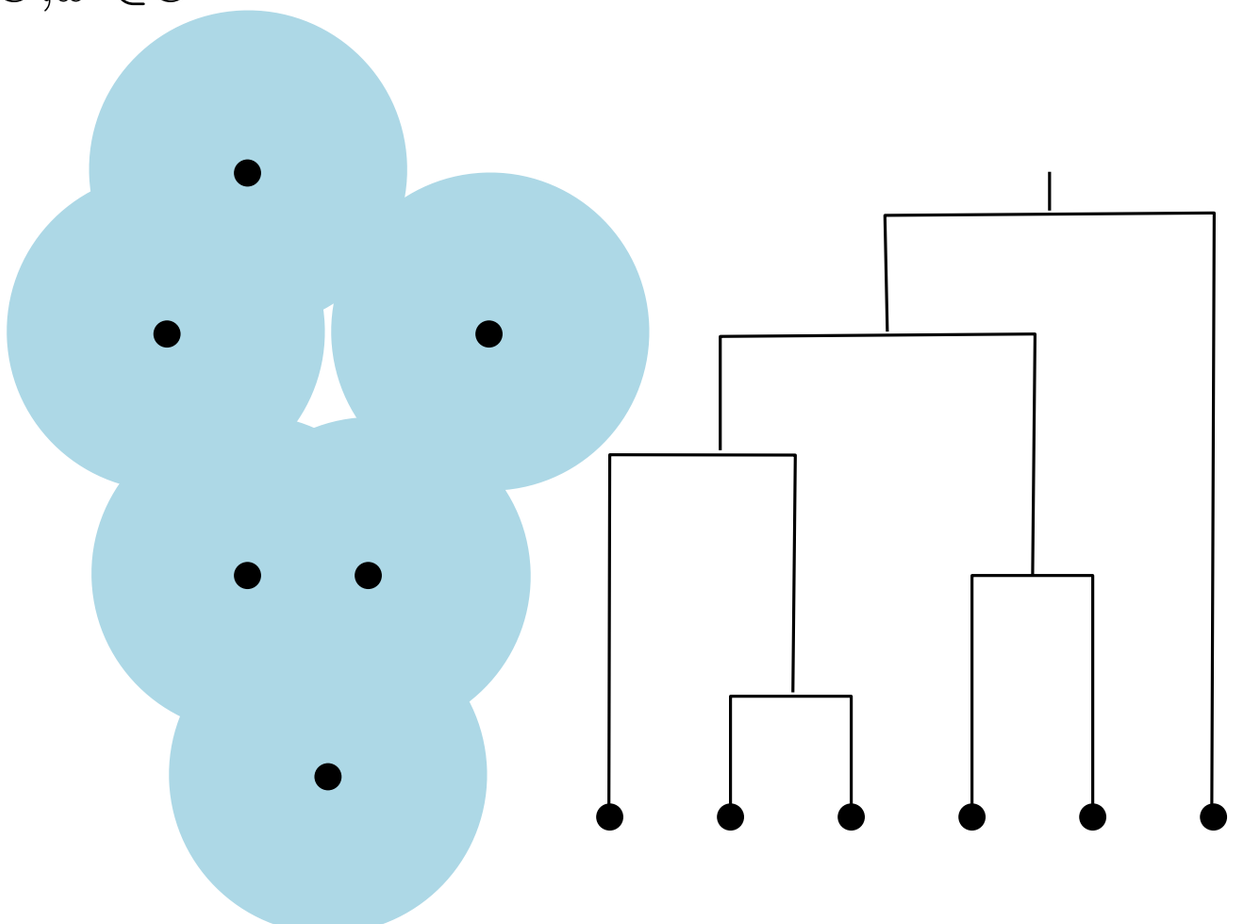

The unstability of dendograms

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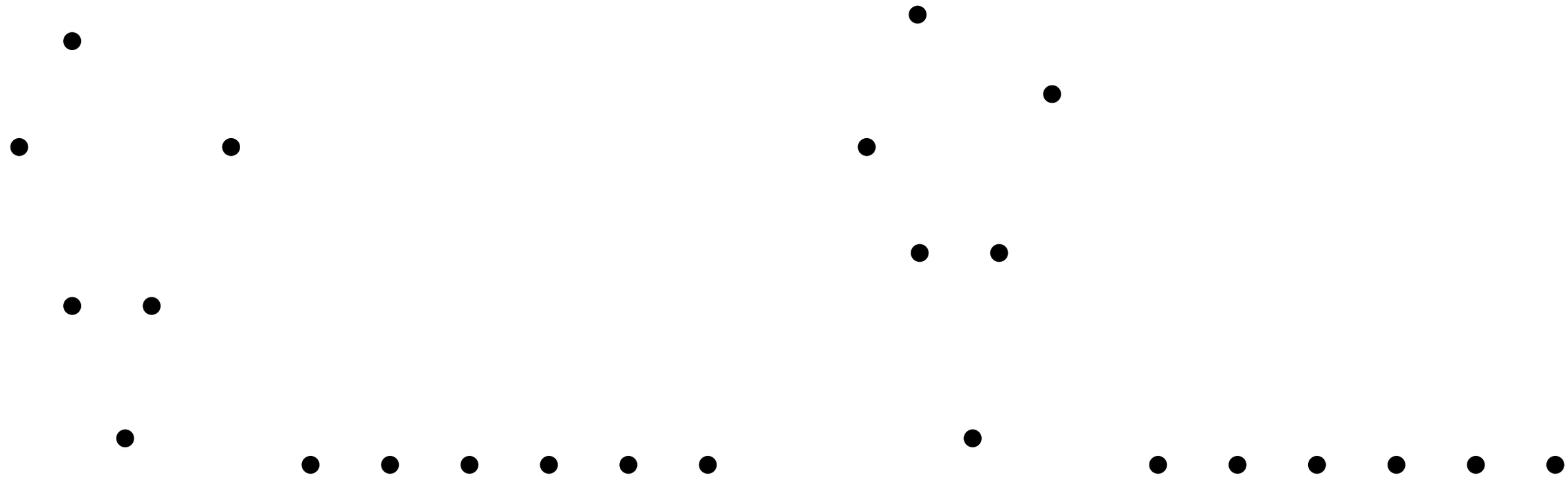

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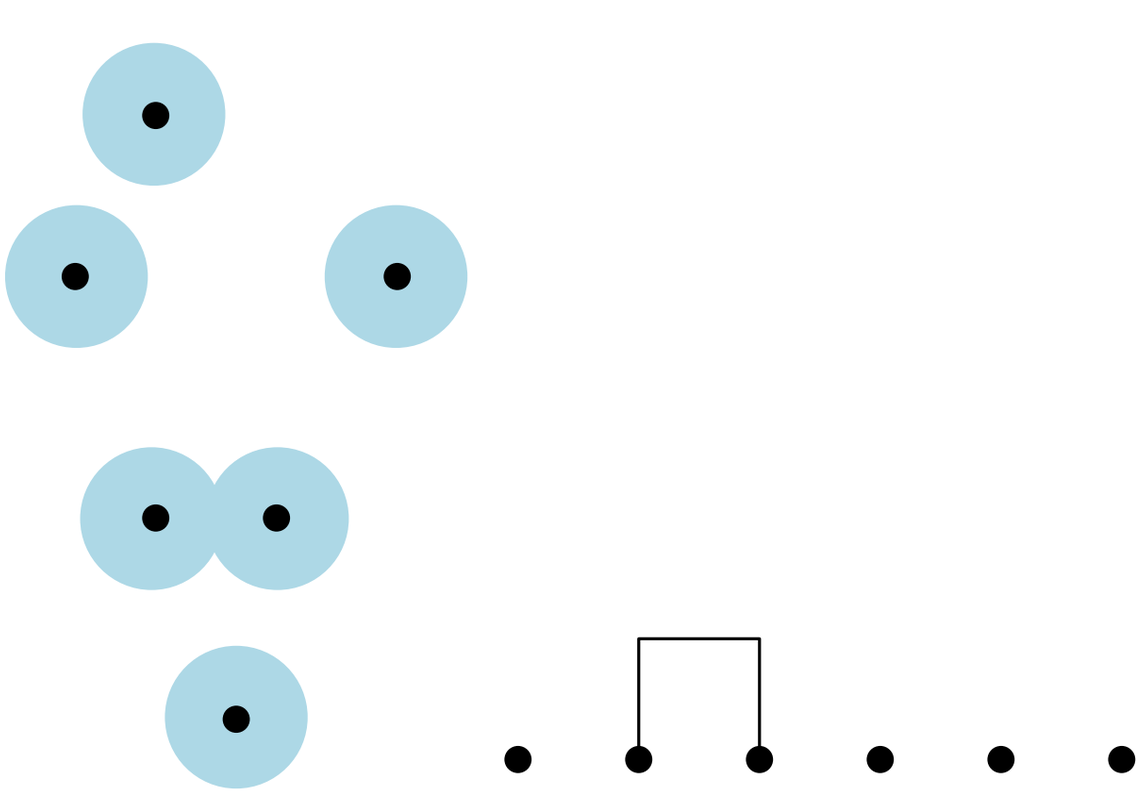

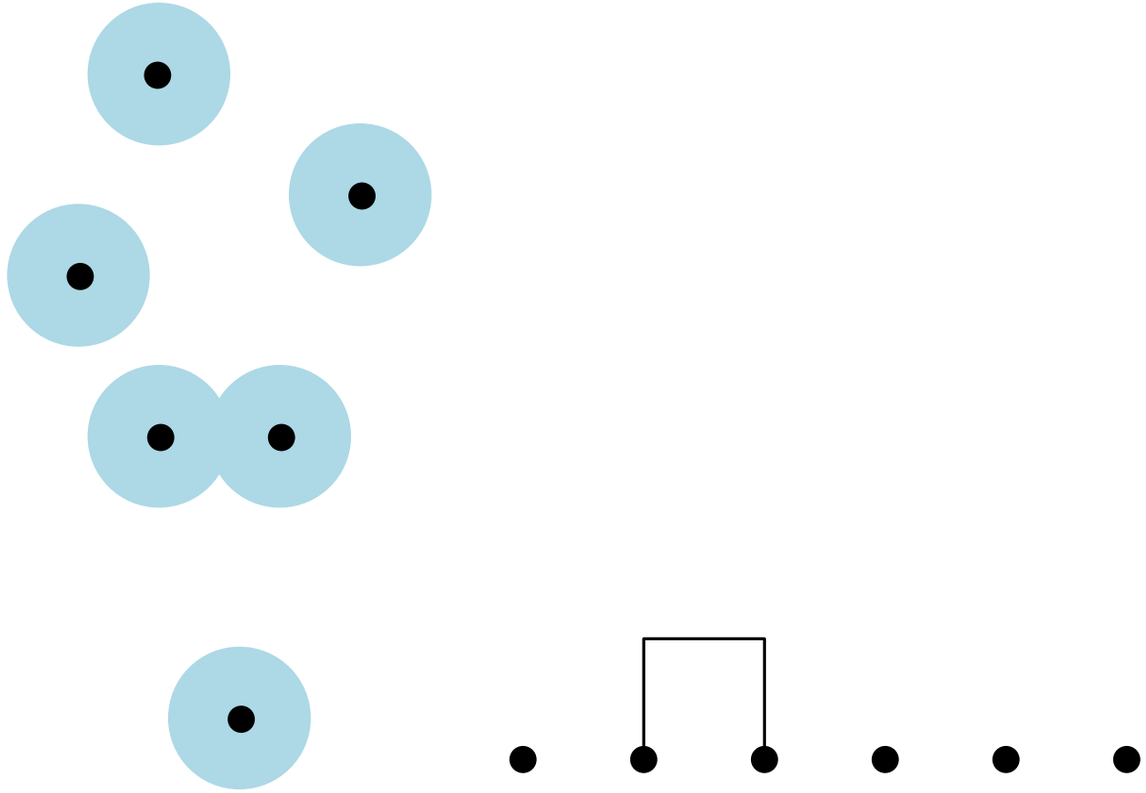

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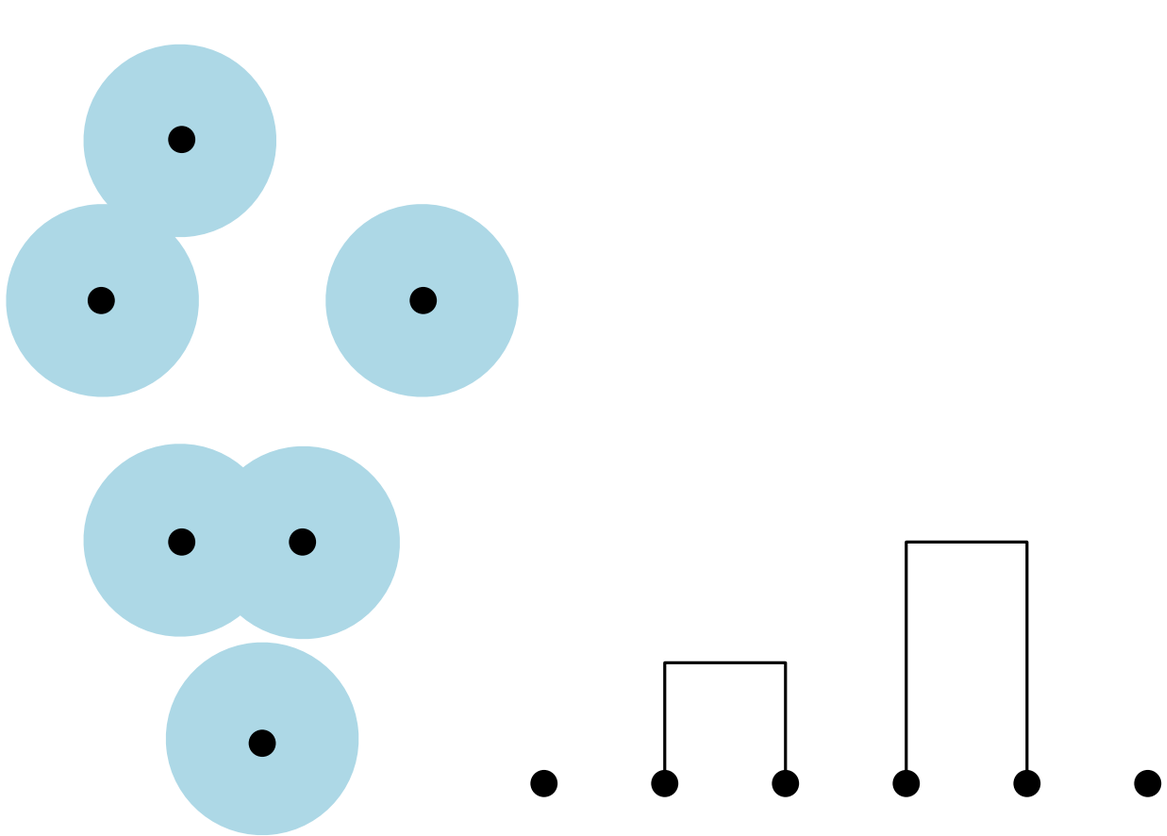

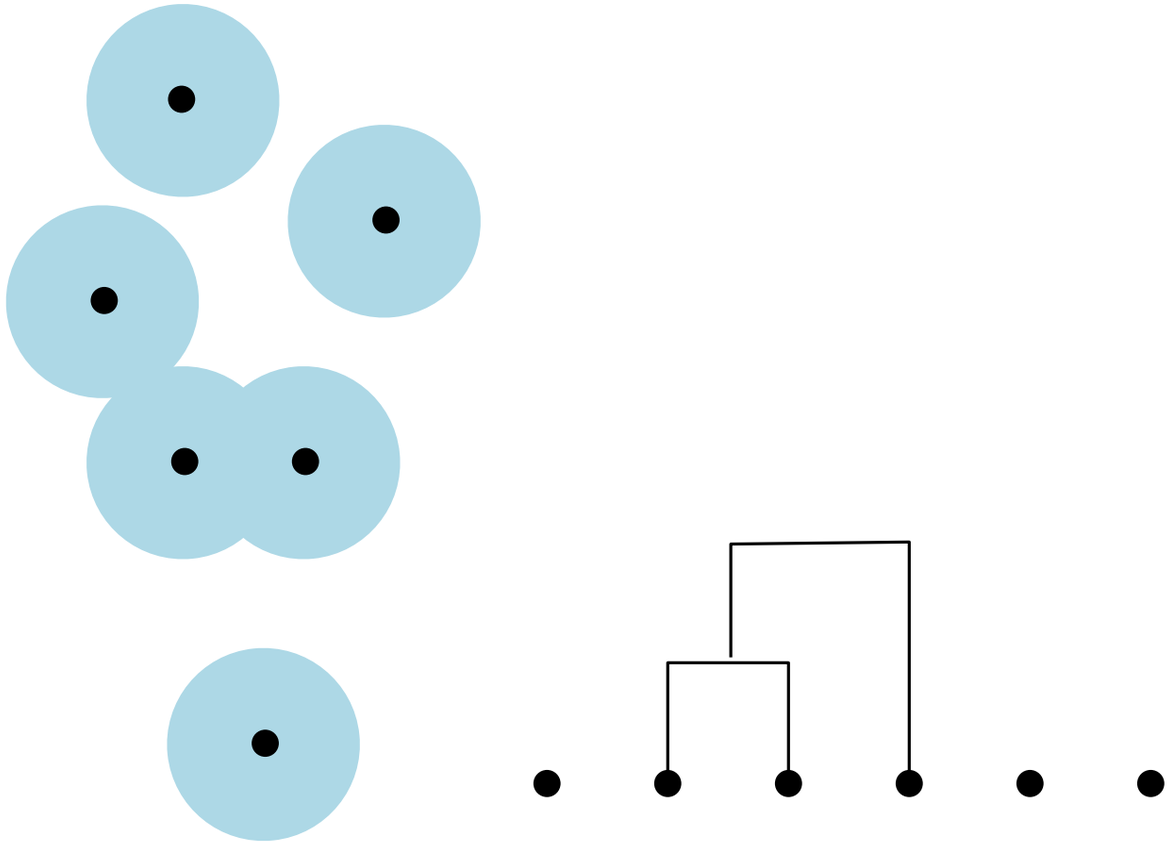

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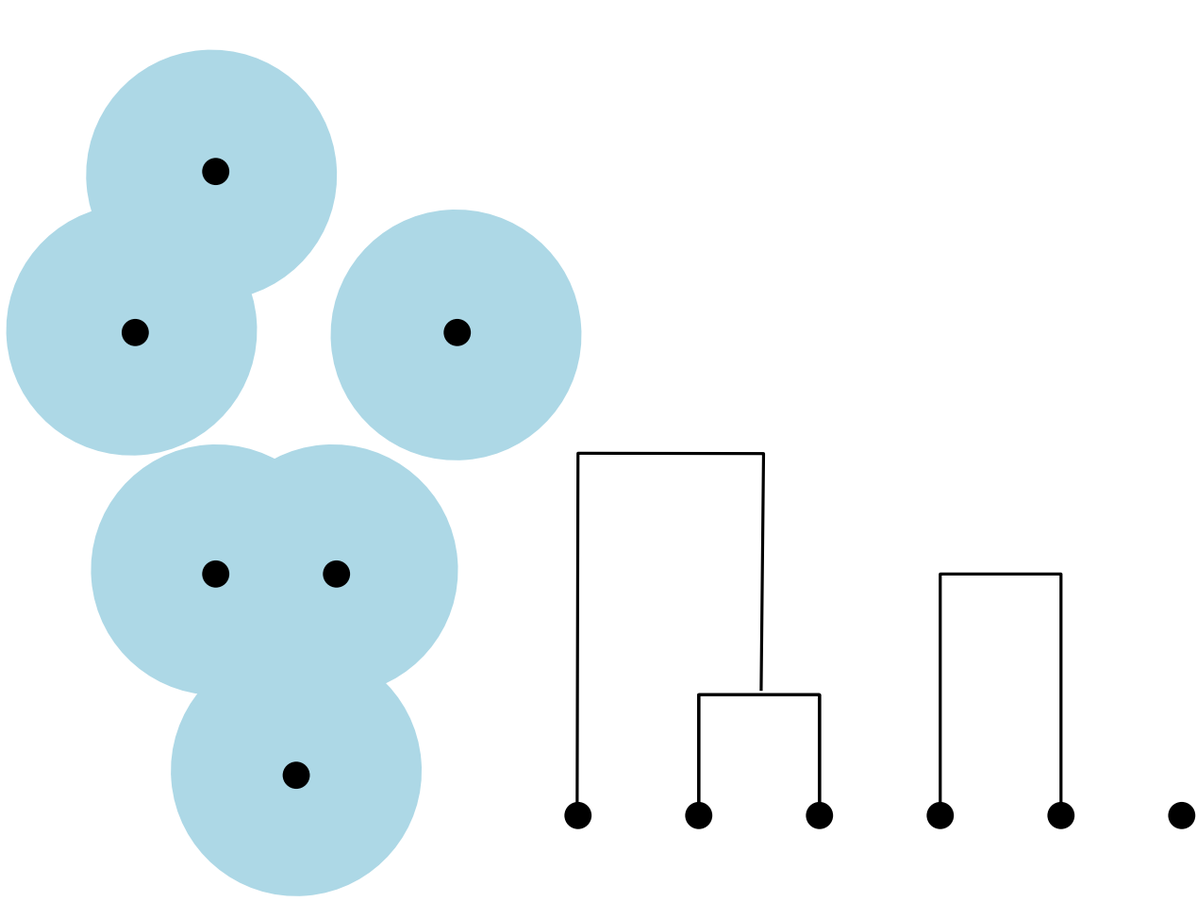

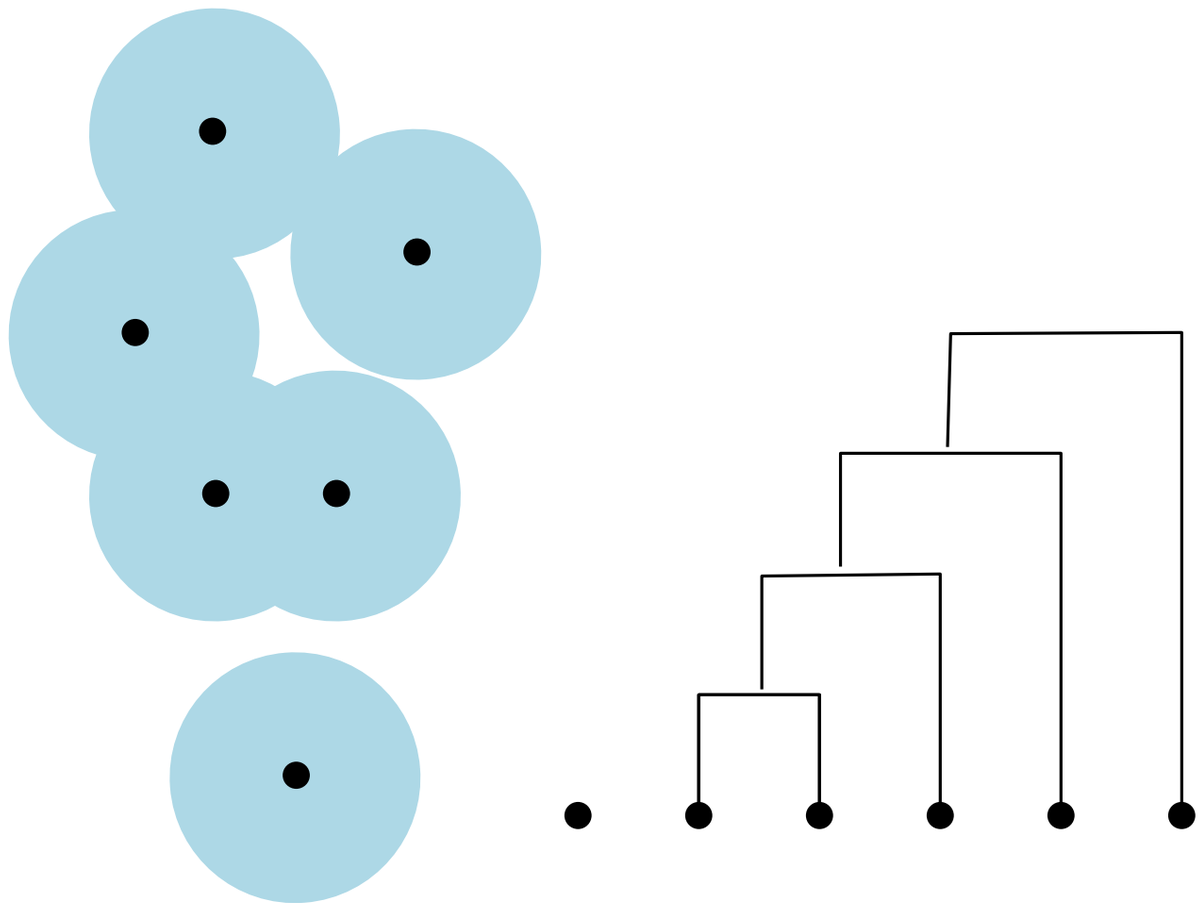

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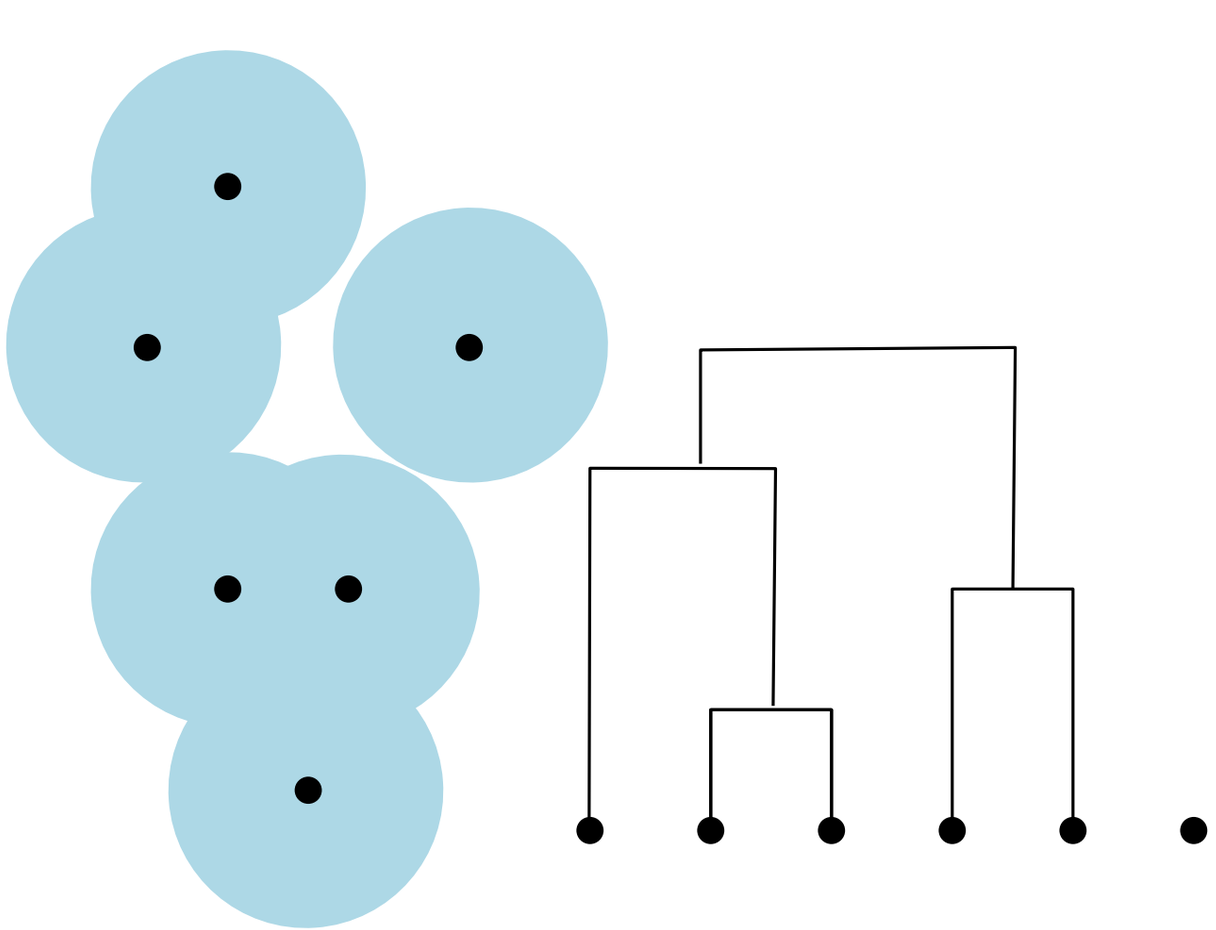

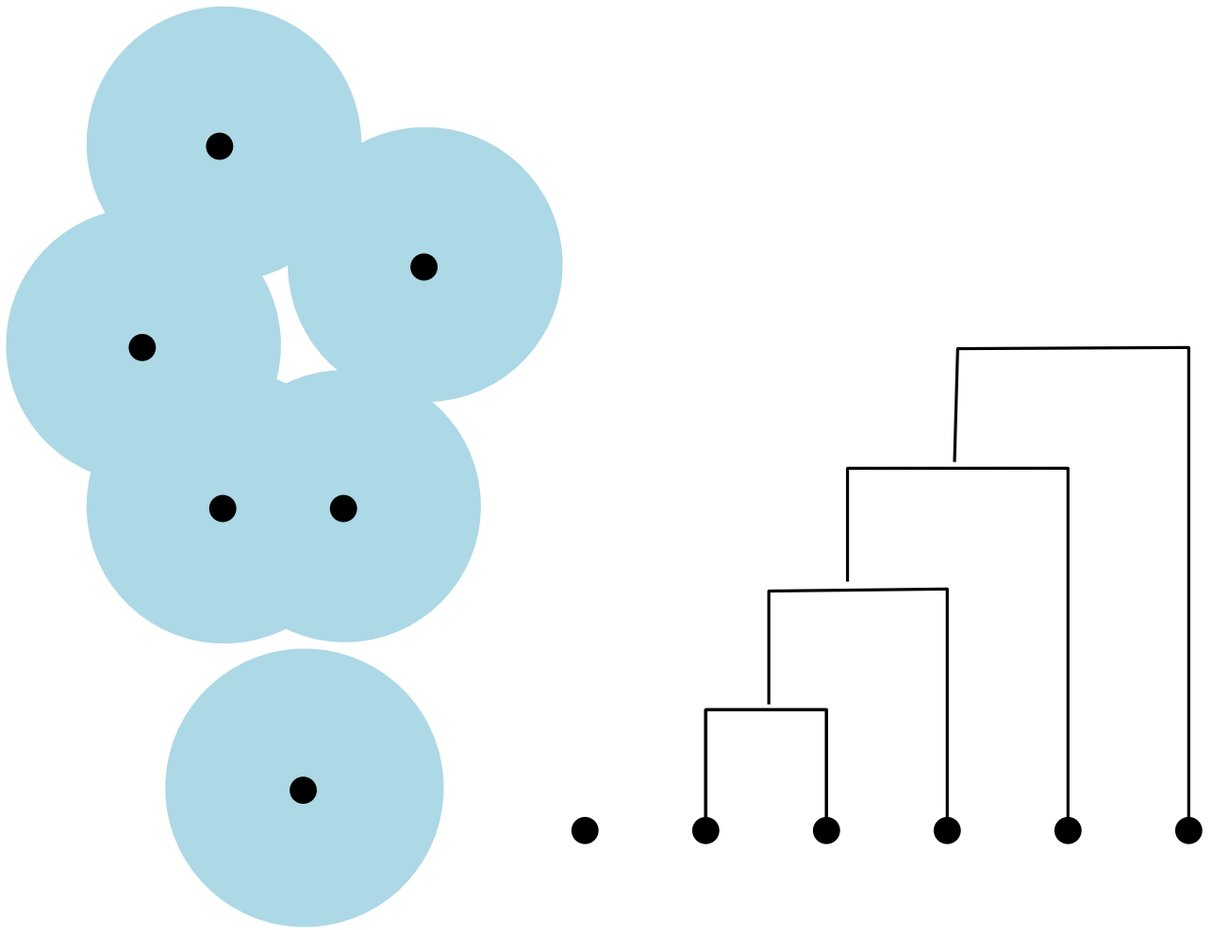

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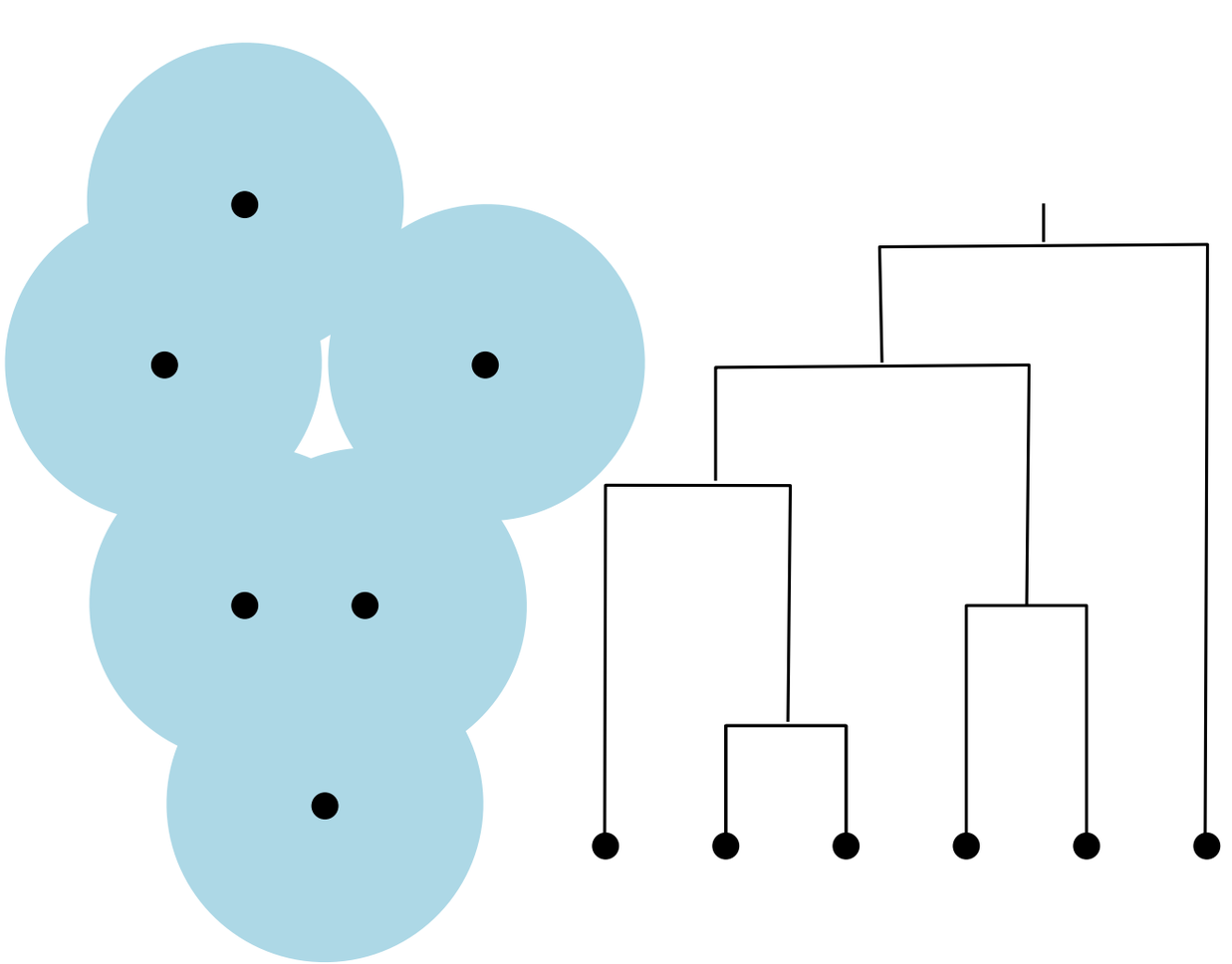

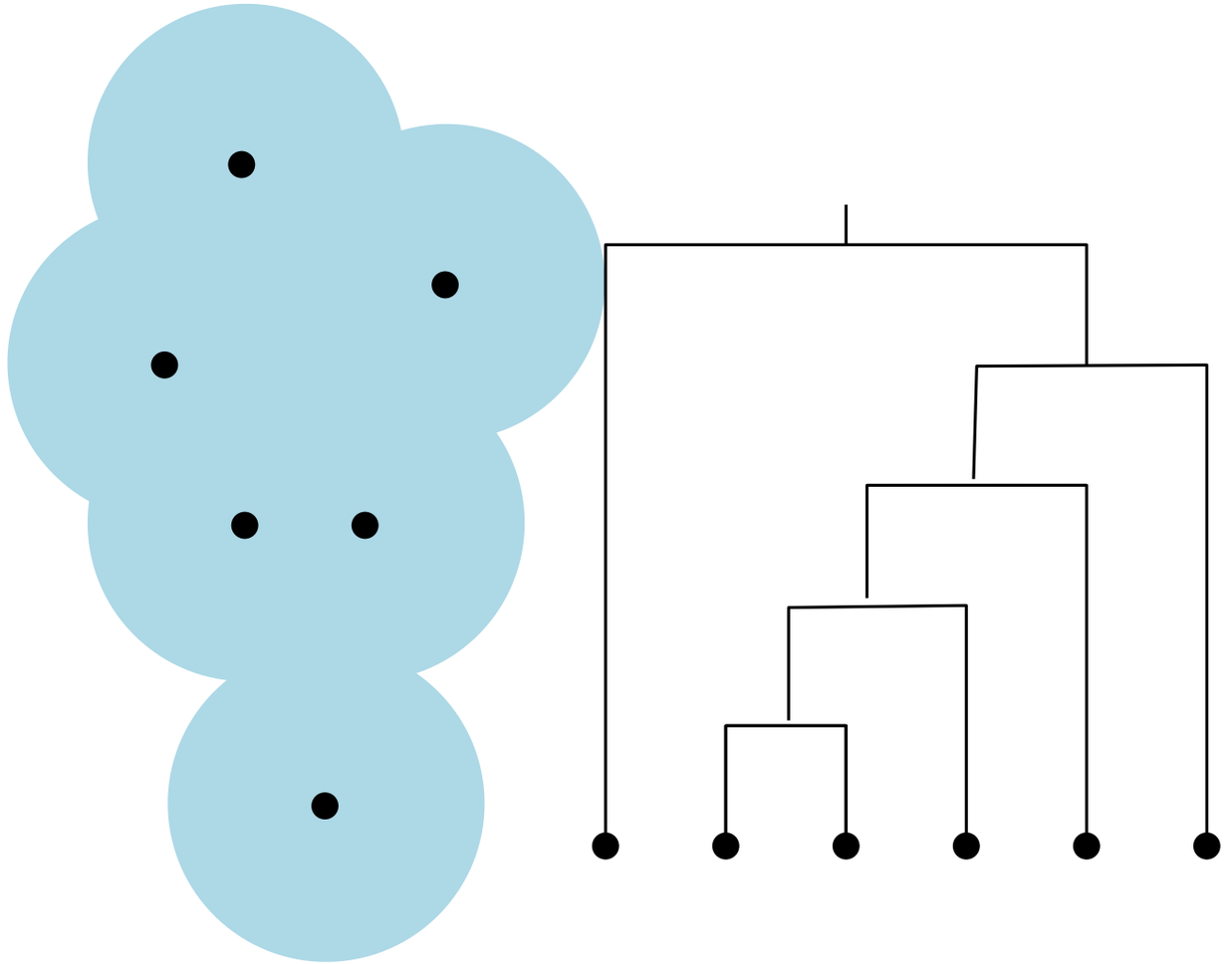

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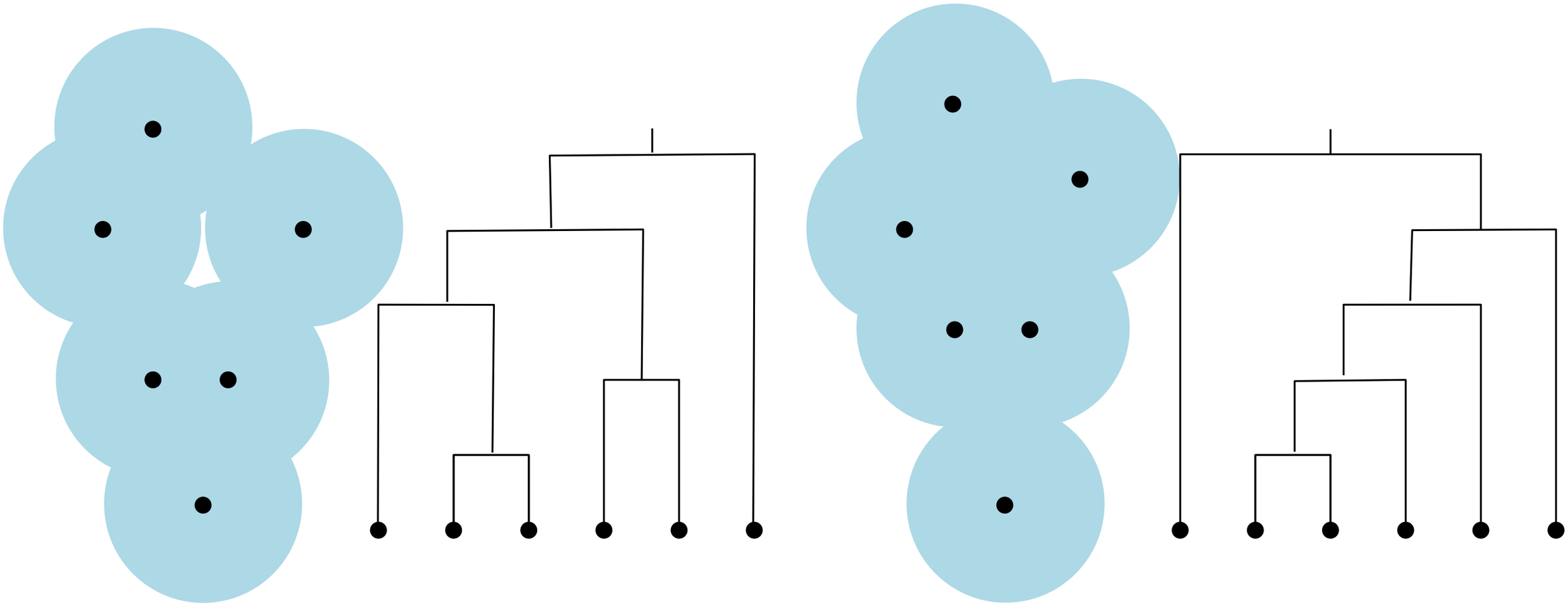
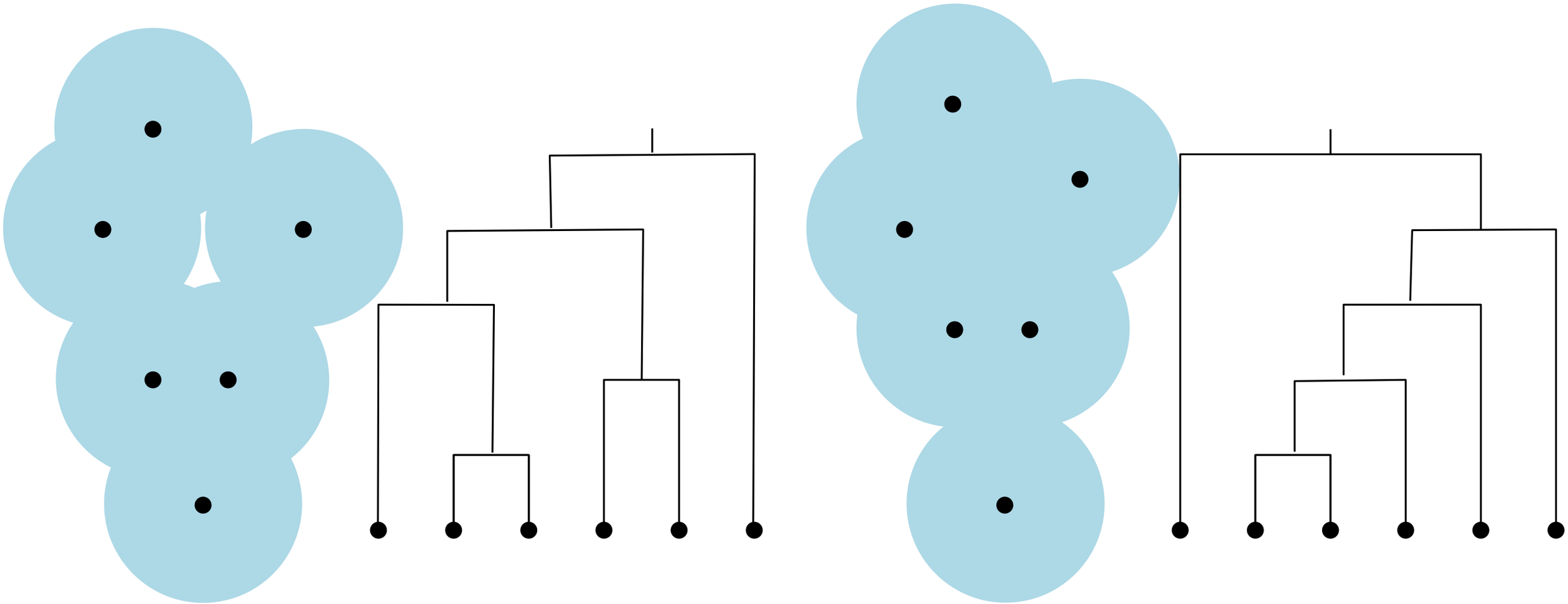


- Small perturbations on the input data may lead to wide change in the structure of the trees.
- However, the "merging times" remain stable.
- (For Euclidean data), the single linkage clustering keeps track of the evolution of the connected components of the distance function to the data.

The unstability of dendograms



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Persistent homology!

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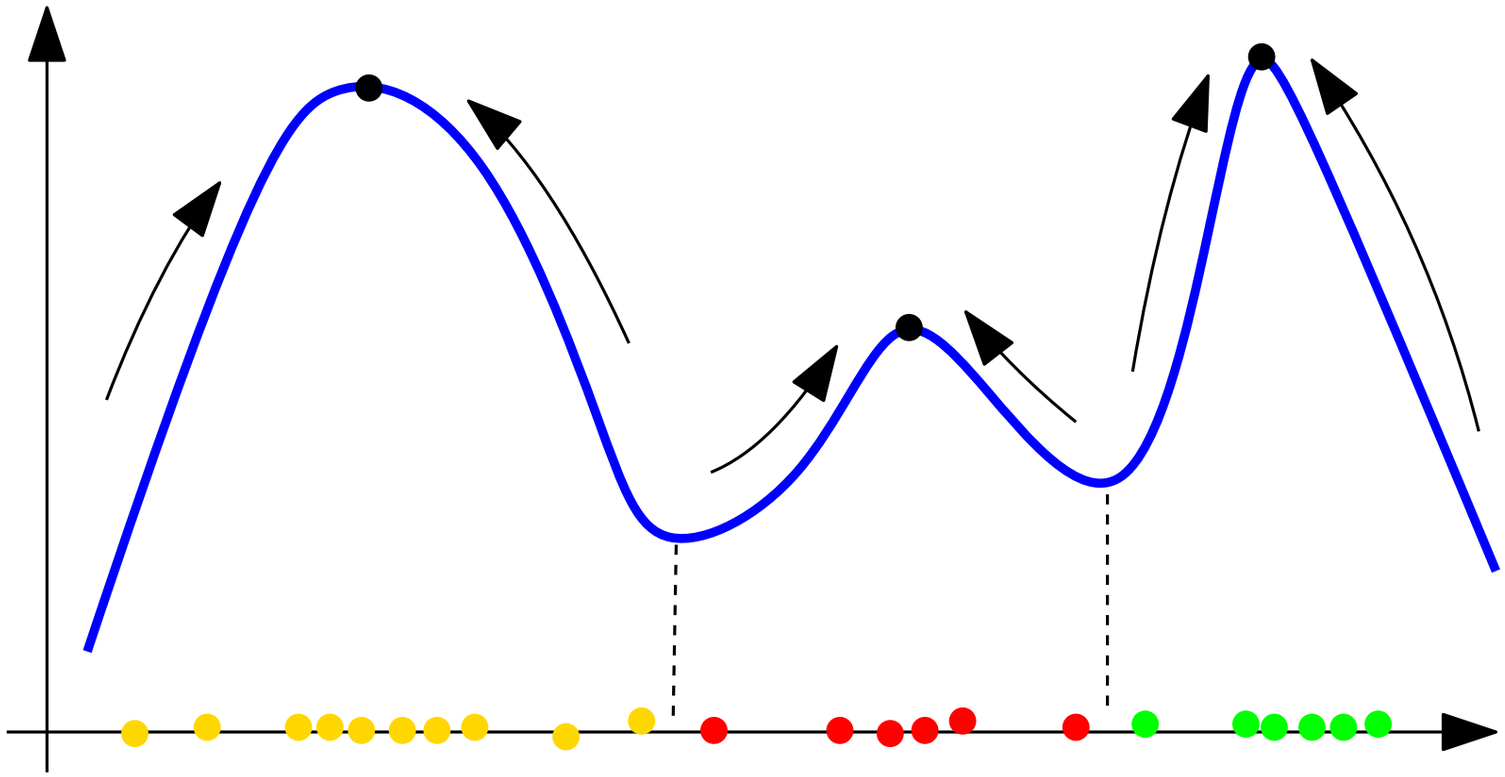
Mode seeking clustering

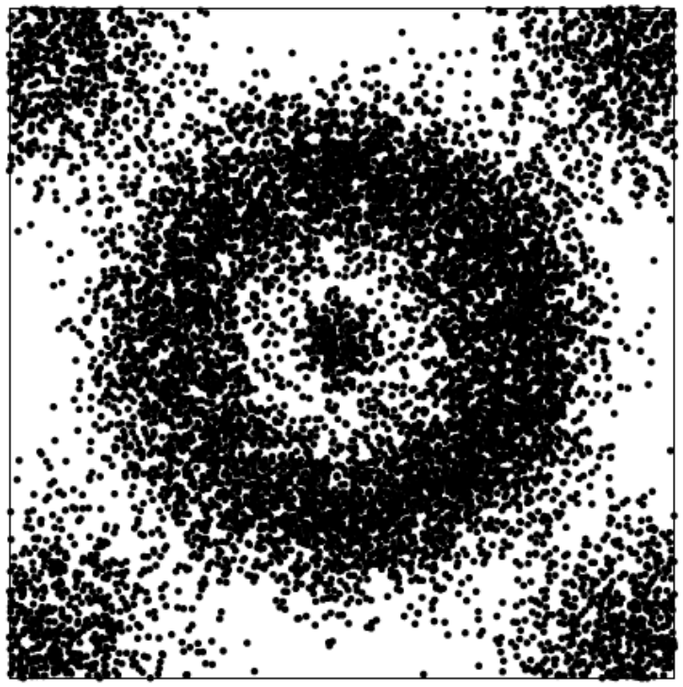


- Data points are sampled according to some (unknown) probability density.
- Clusters = the basins of attractions of the density

Two approaches:

- **Iterative**, such as, e.g., Mean Shift [Comaniciu et al, IEEE Trans. on Pattern Analysis and Machine Intelligence, 2002].
- **Graph-based**, such as, e.g., [Koontz et al, IEEE Trans. on Computers 1976].

The Koonz, Narendra and Fukunaga algorithm (1976)



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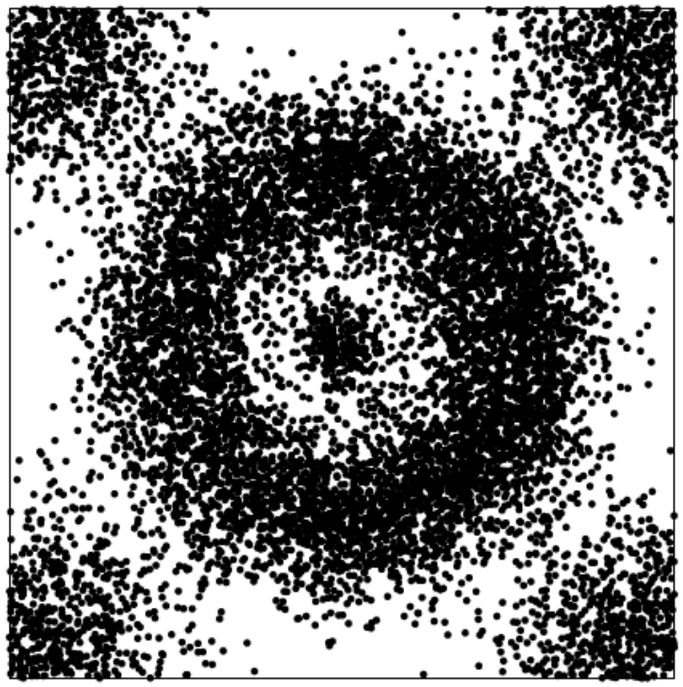
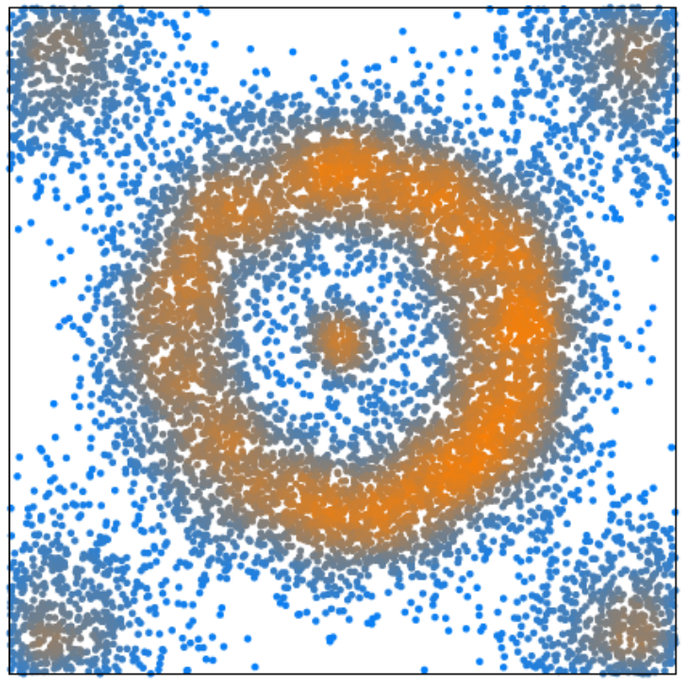


Density estimation



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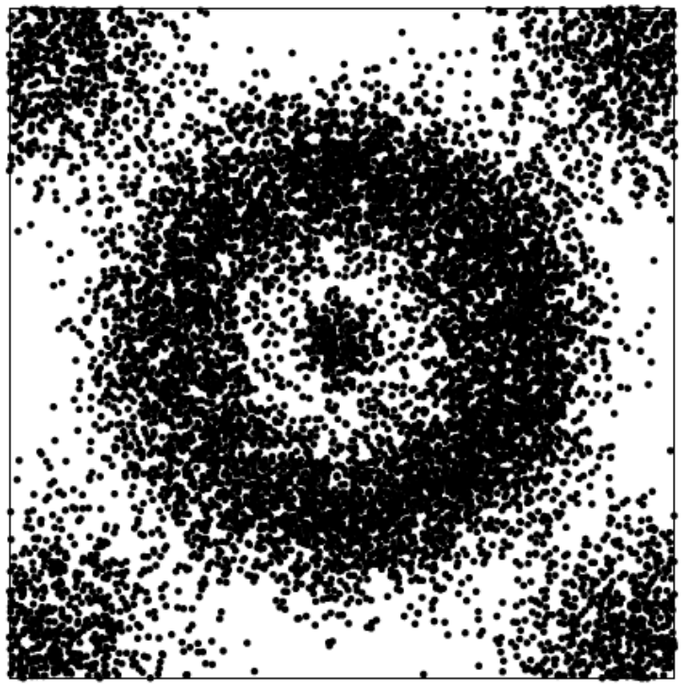

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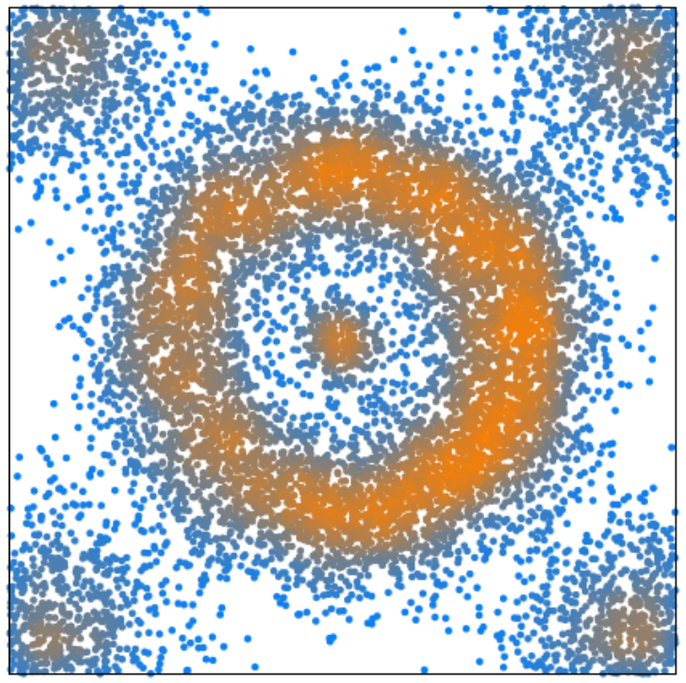
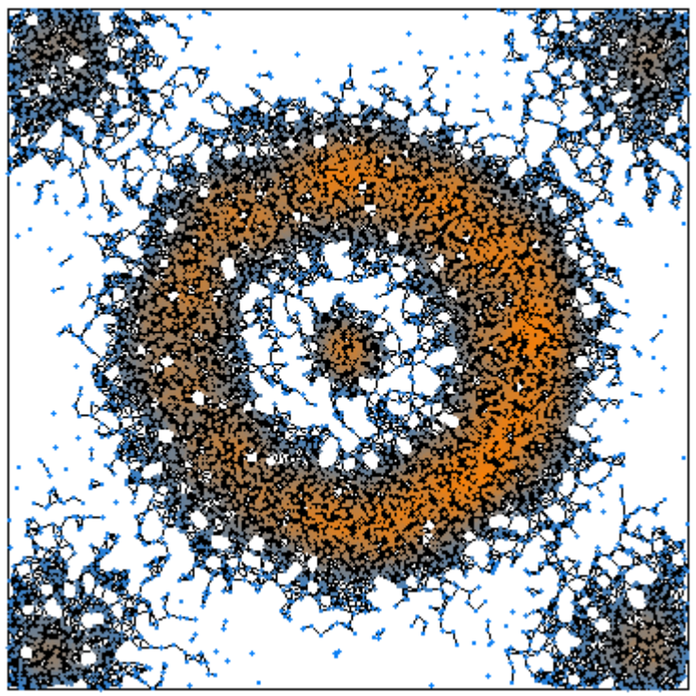


Neighborhood graph



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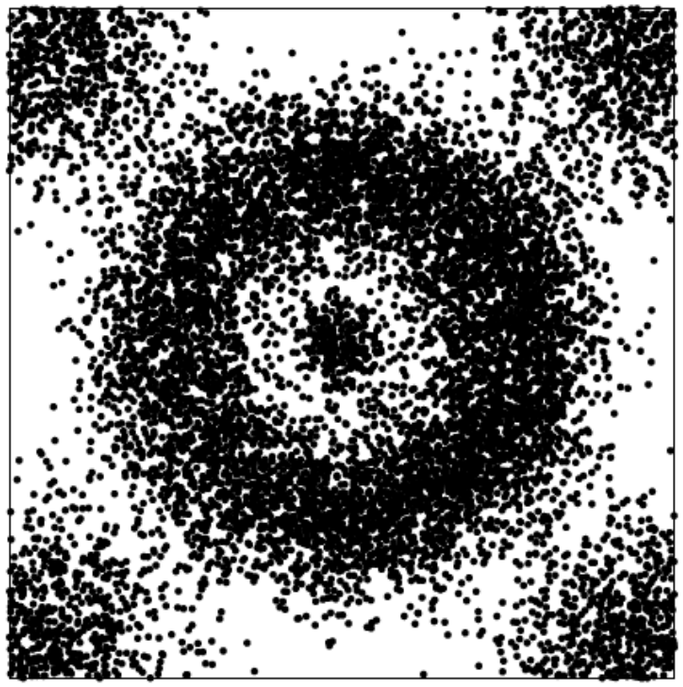

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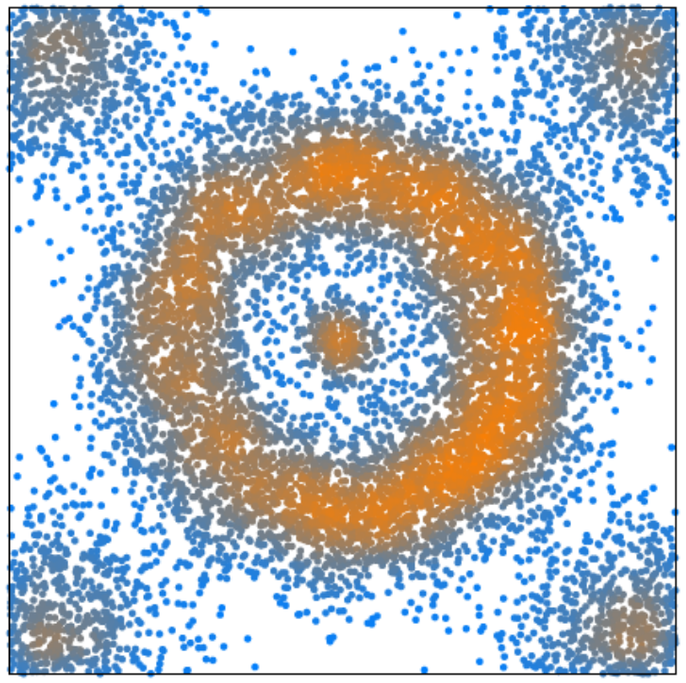

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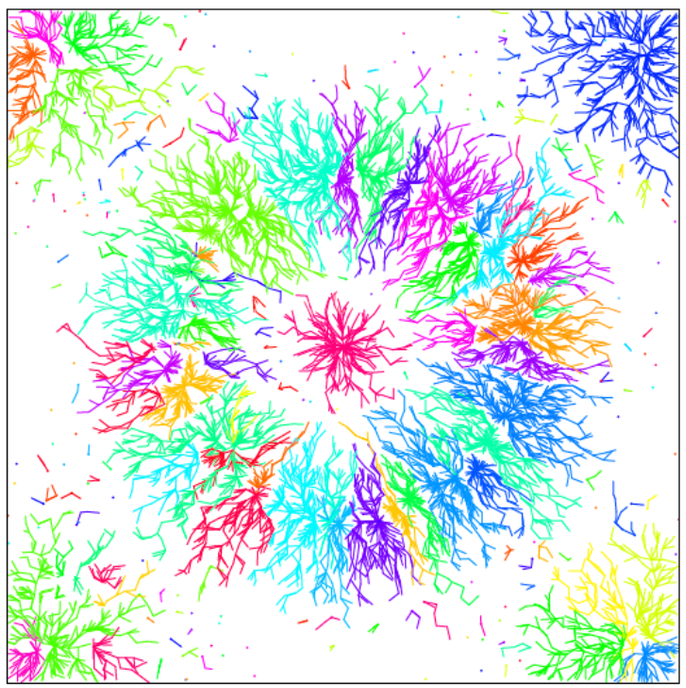
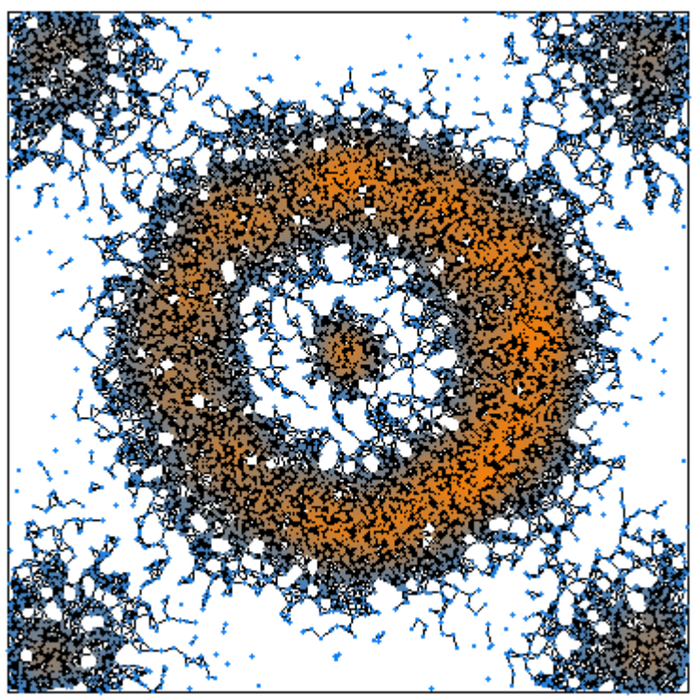


Discrete approximation of the gradient; for each vertex v, a gradient edge is selected among the edges adjacent to v.



The Koonz, Narendra and Fukunaga algorithm (1976)

The algorithm:

Input: neighborhood graph G with n vertices (the data points) and a n-dimensional vector $\hat{f}$ (density estimate)

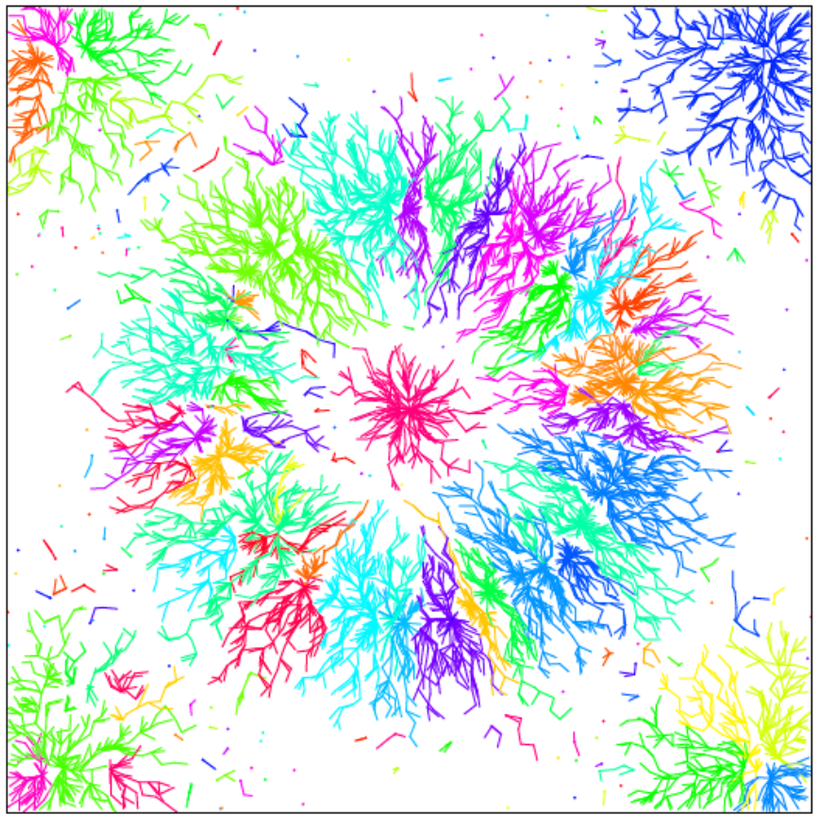
Sort the vertex indices $\{1, 2, \cdots, n\}$ in decreasing order: $\hat{f}(1) \geq \hat{f}(2) \geq \cdots \geq \hat{f}(n)$;
Initialize a union-find data structure (disjoint-set forest) $\mathcal{U}$ and two vectors g, r of size n;

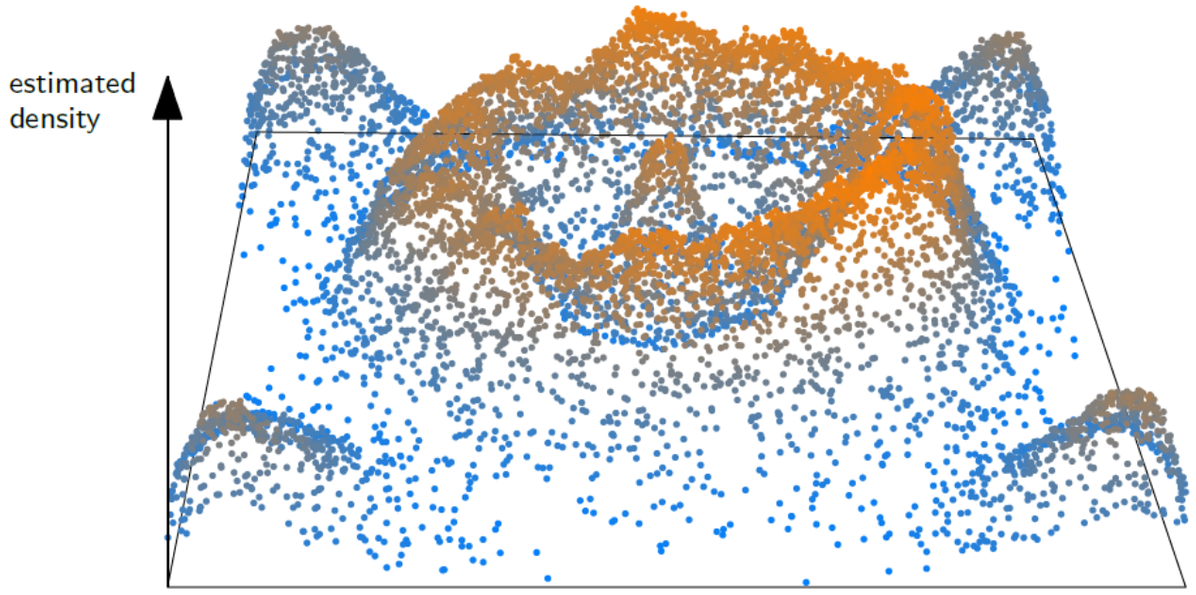
for $i = 1$ to n **do**
    Let N be the set of neighbors of i in G that have indices higher than i;
    if $N = \emptyset$
        Create a new entry e in $\mathcal{U}$ and attach vertex i to it;
        $r(e) \leftarrow i$ *// $r(e)$ stores the root vertex associated with the entry e*
    else
   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

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

The Koonz, Narendra and Fukunaga algorithm (1976)

Drawbacks:





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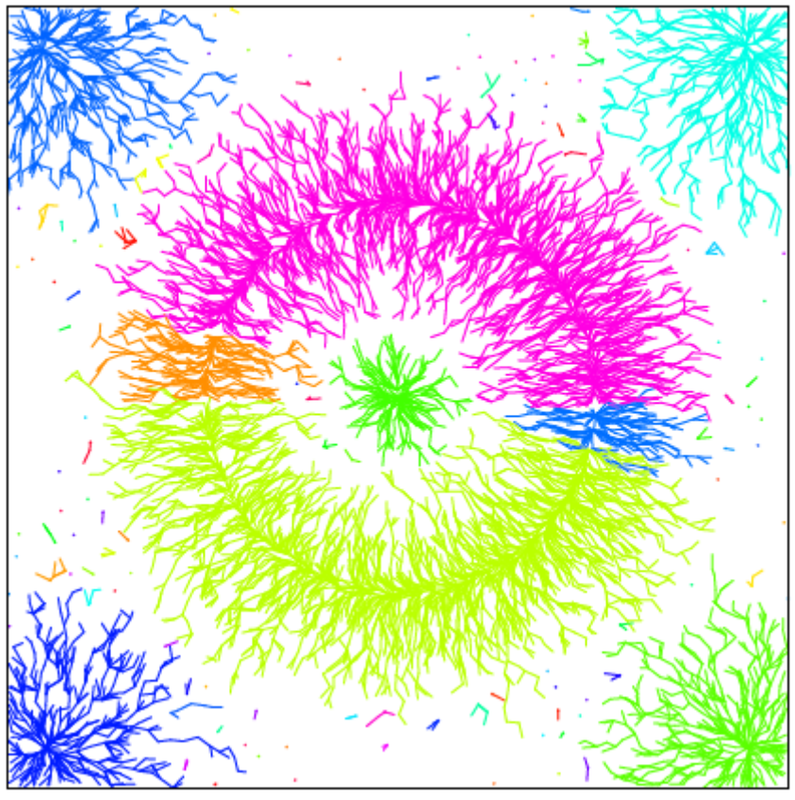

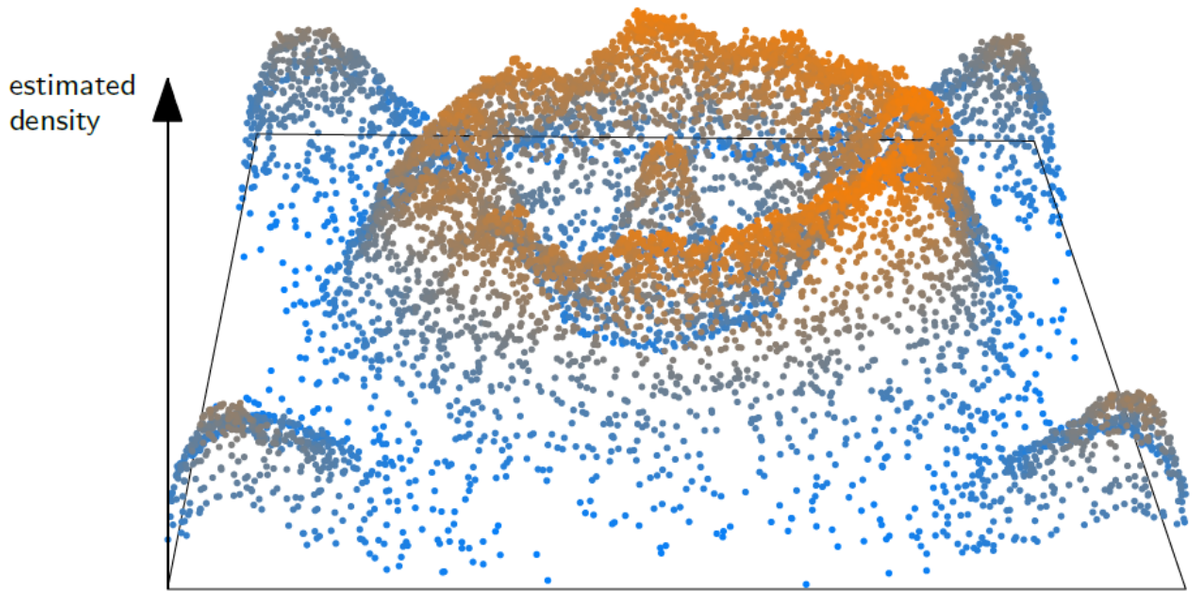

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- The choice of the neighborhood graph may result in wide changes in the output.

The Koonz, Narendra and Fukunaga algorithm (1976)

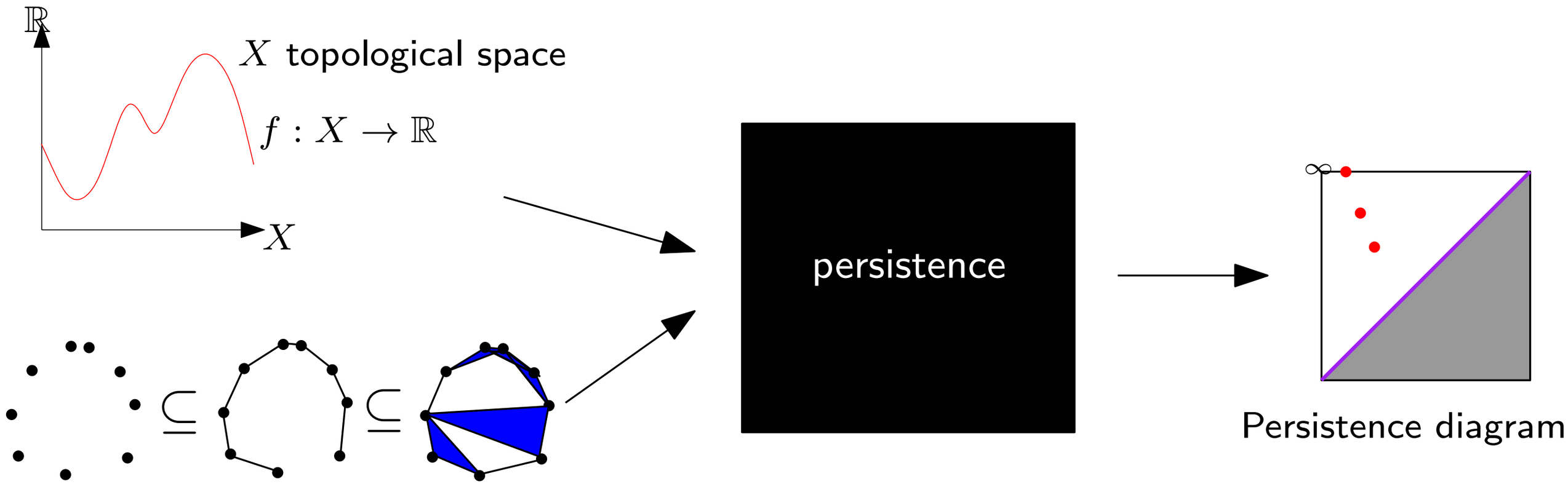
Drawbacks:

- As many clusters as local maxima of the density estimate $\rightarrow$ sensitivity to noise!
- The choice of the neighborhood graph may result in wide changes in the output.

Approaches to overcome these issues:

- Smooth out the density estimate (e.g. mean-shift)... But pb of choice of a smoothing param.
- Merge clusters: various way to do that. In the following: use persistent homology!

Persistent homology

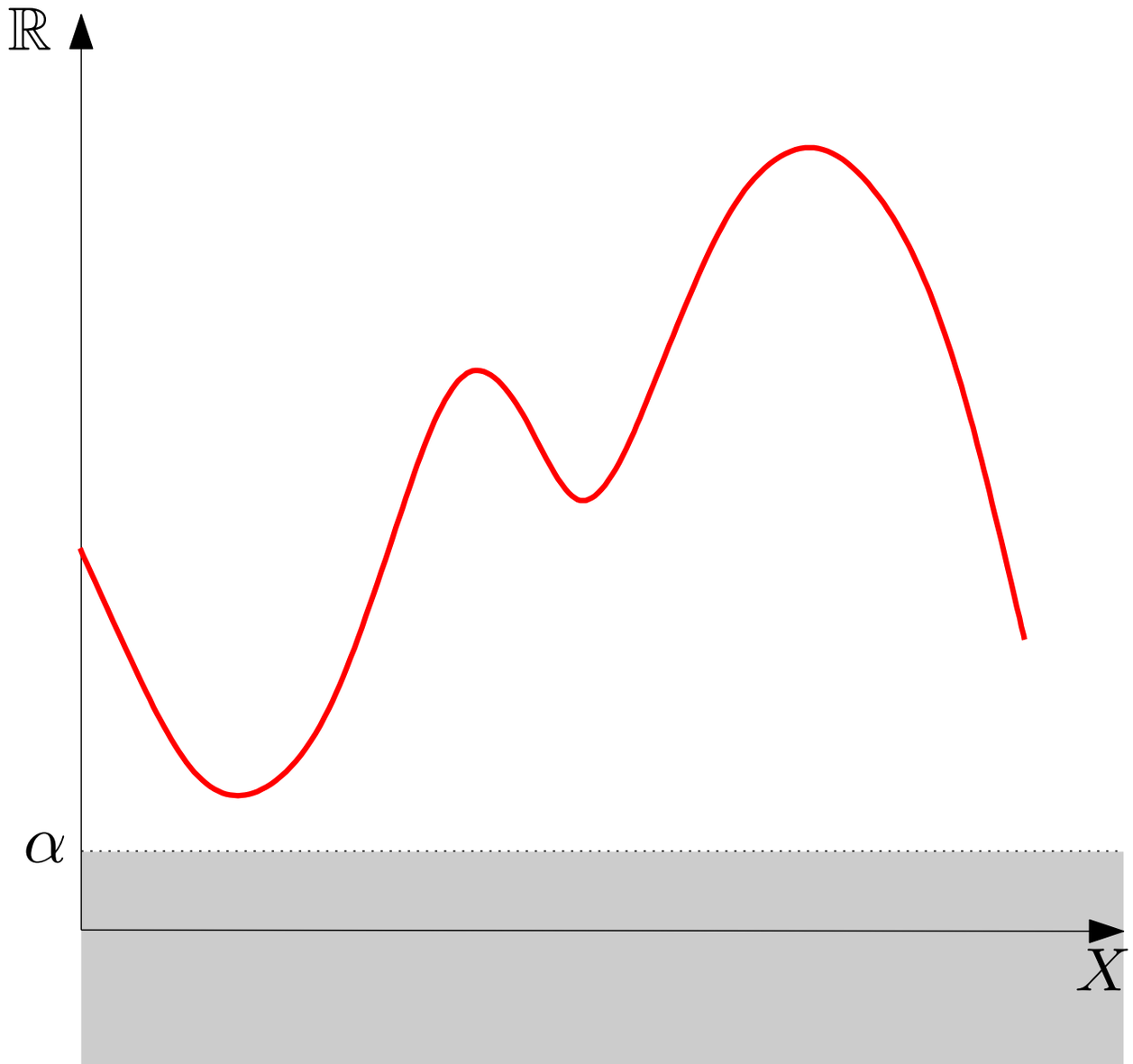


Nested spaces

- A general mathematical framework to encode the evolution of the topology (homology) of families of nested spaces (filtered complex, sublevel sets,...).
- Formalized by H. Edelsbrunner (2002) et al and G. Carlsson et al (2005) - wide development during the last decade.
- Multiscale topological information.
- Barcodes/persistence diagrams can be efficiently computed.
- Stability properties

(0-dimensional) persistent homology for functions

- Nested family (filtration) of sublevel-sets $f^{-1}((-\infty, \alpha])$ for $\alpha = -\infty$ to $+\infty$.
- Track evolution of connectedness throughout the family.



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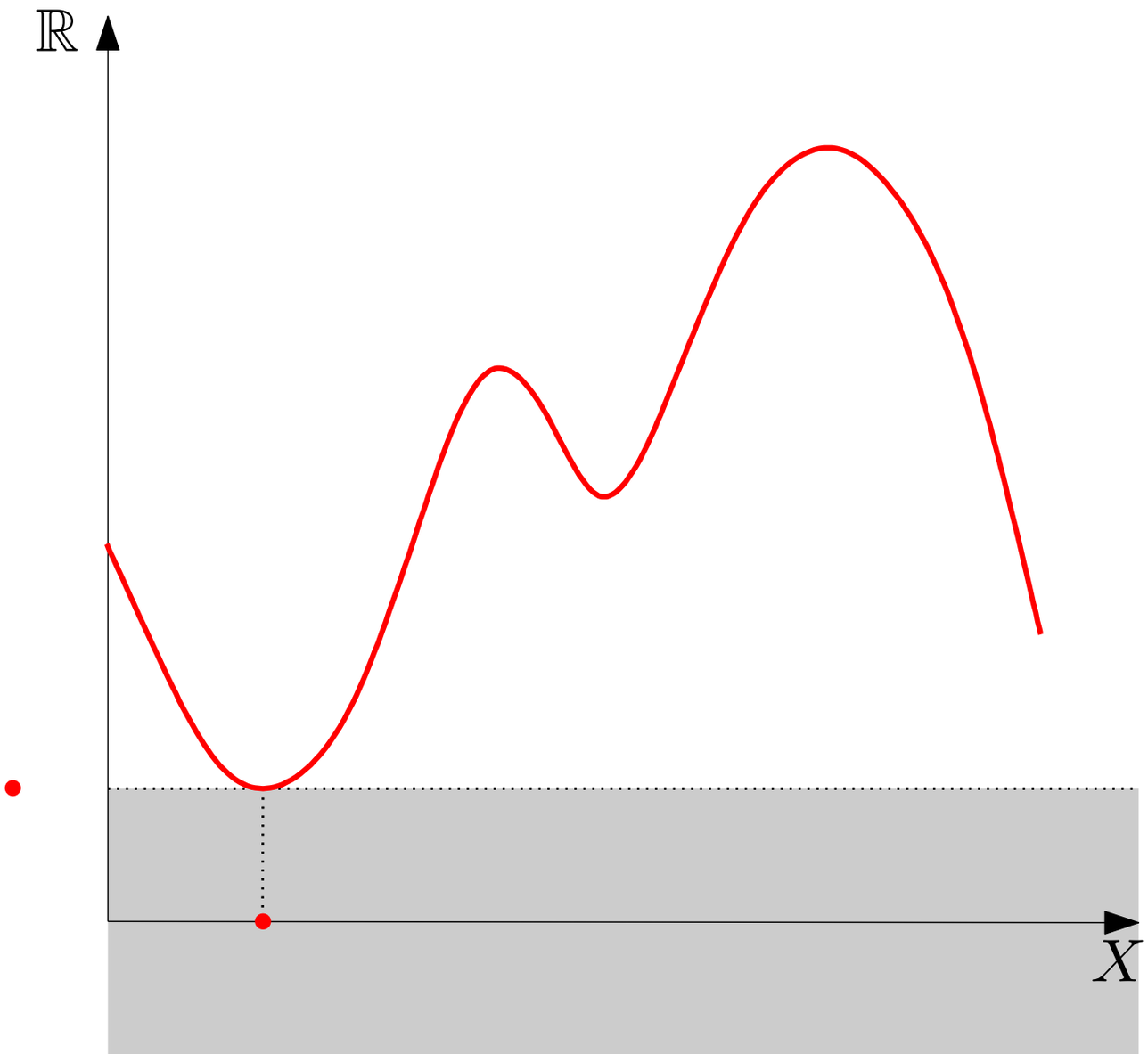

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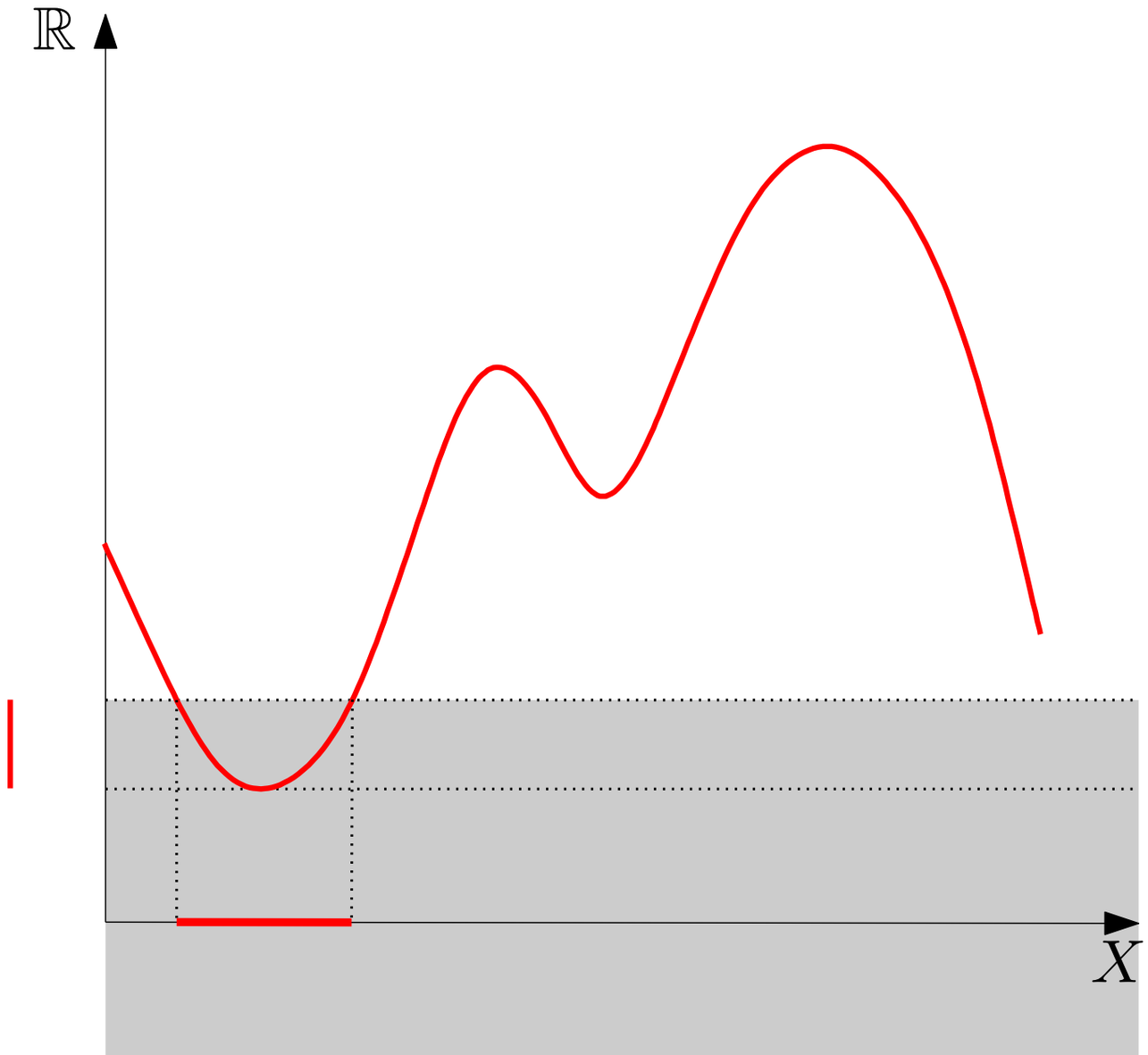

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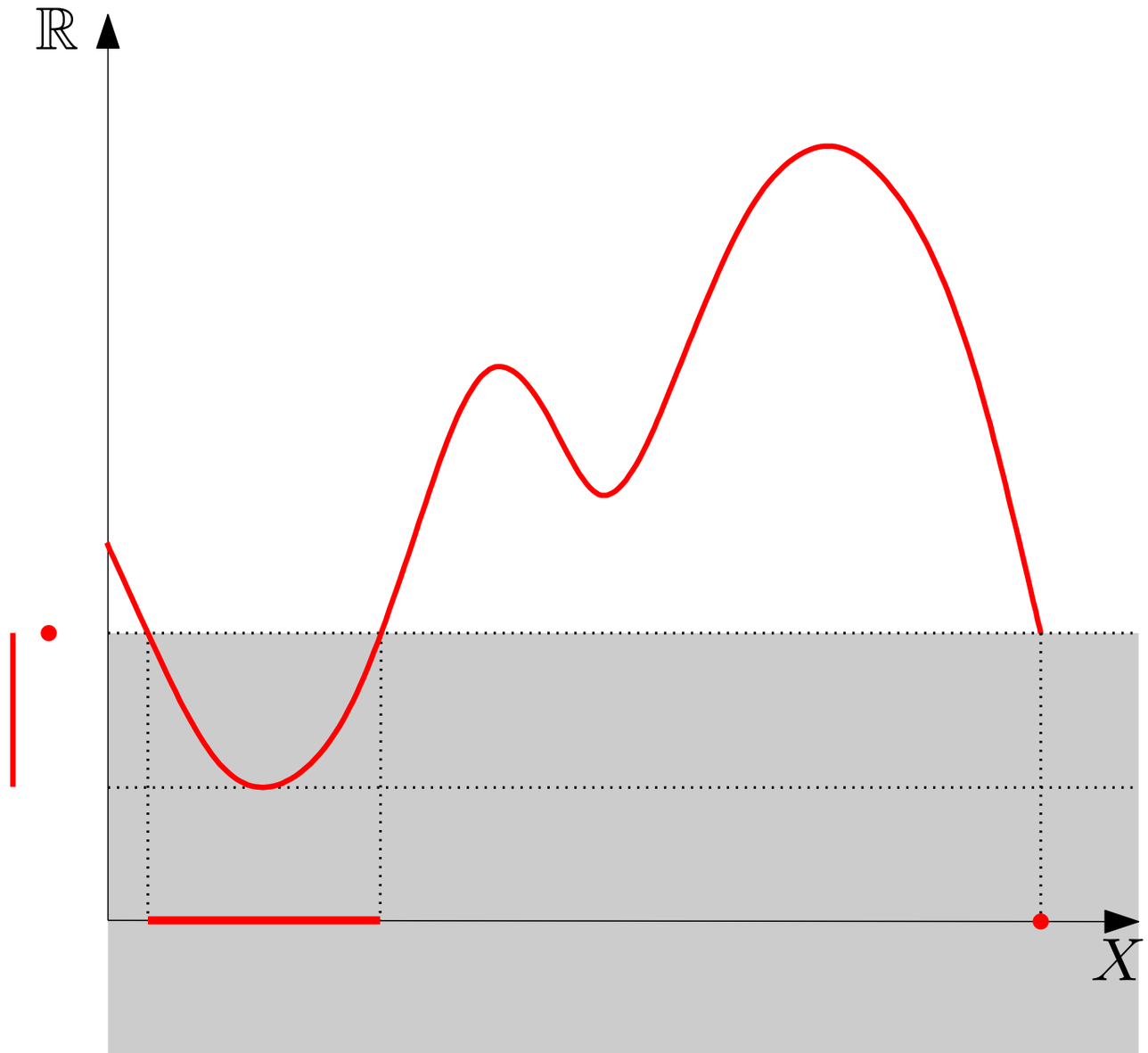

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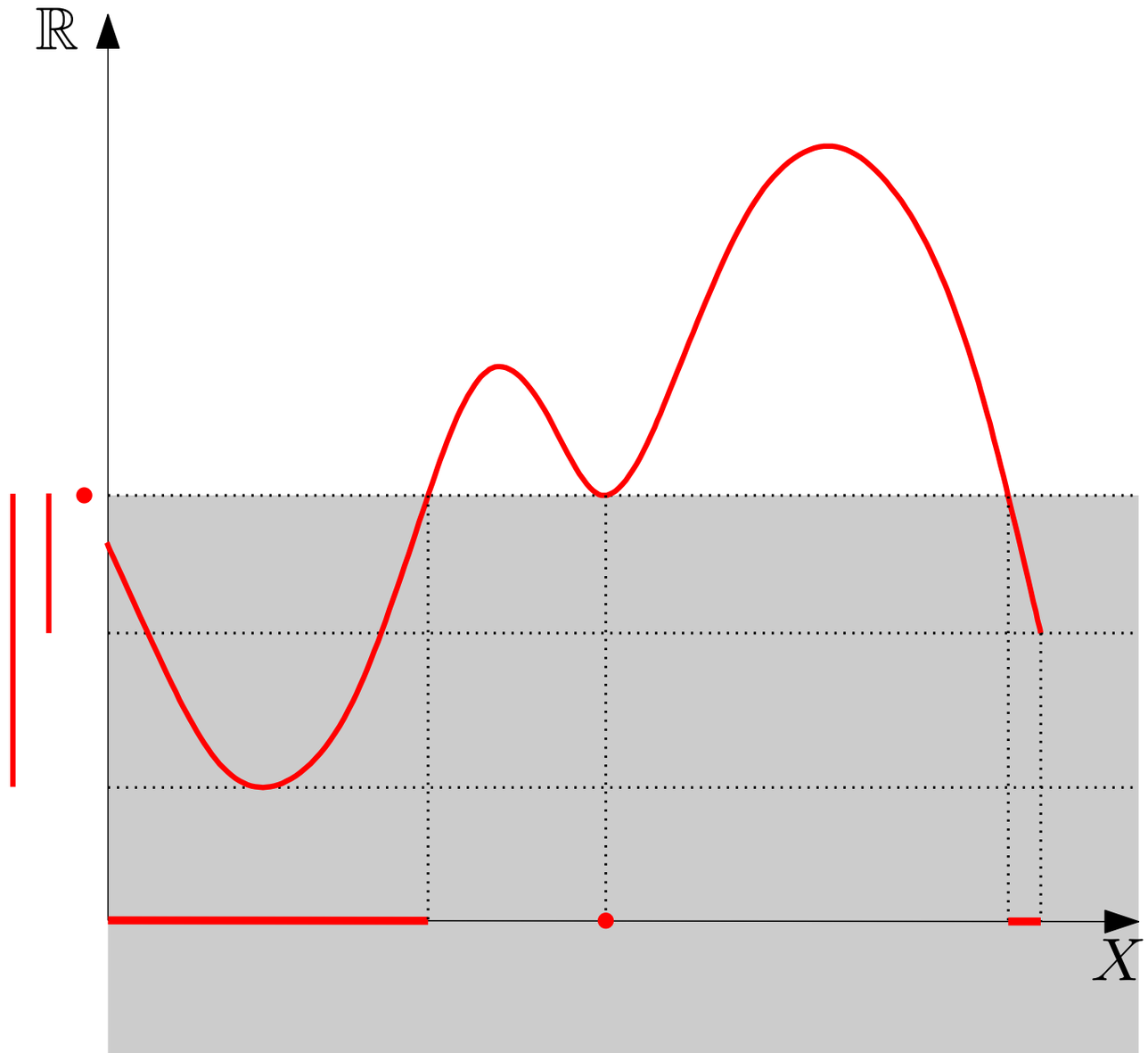

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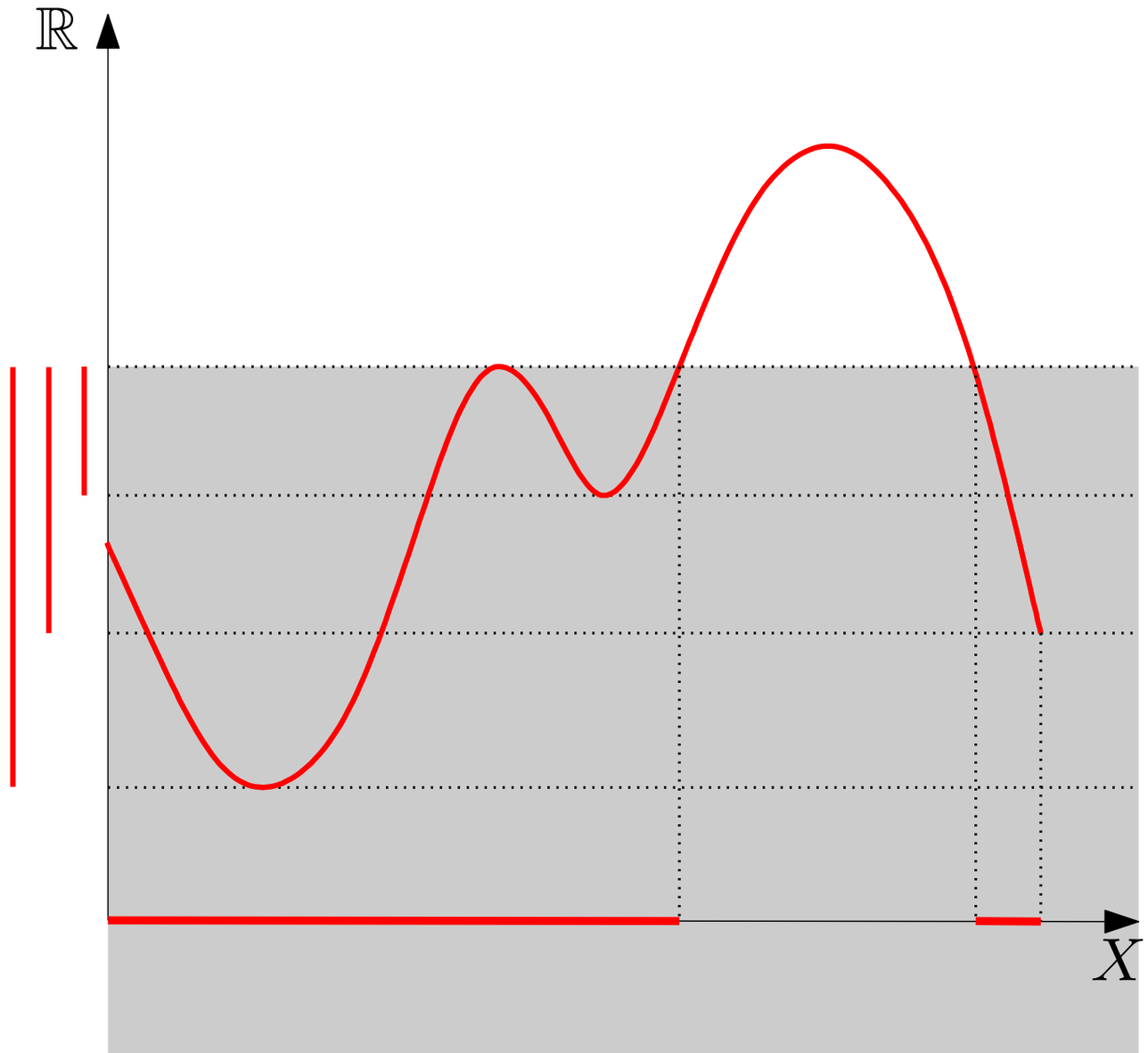

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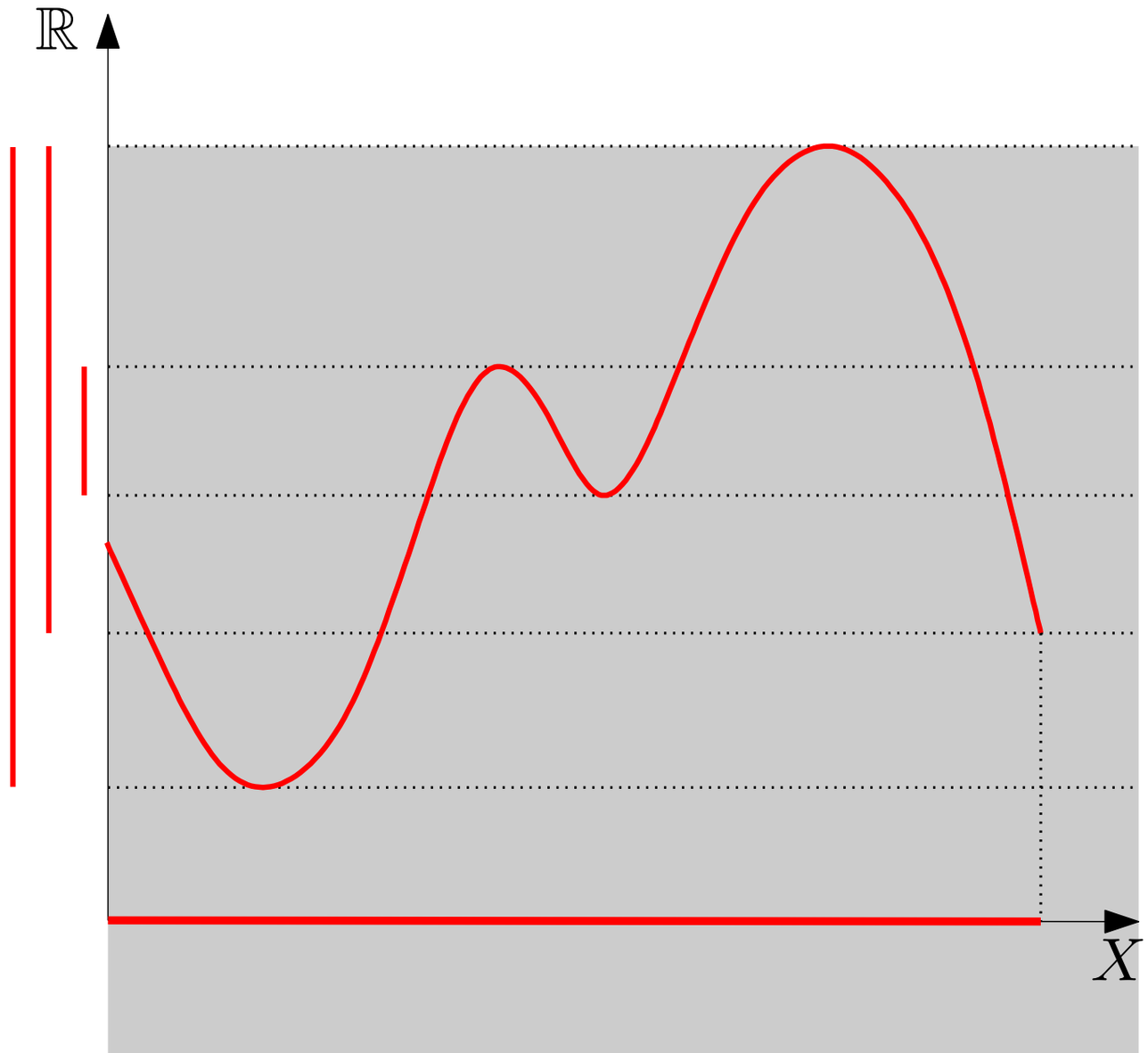

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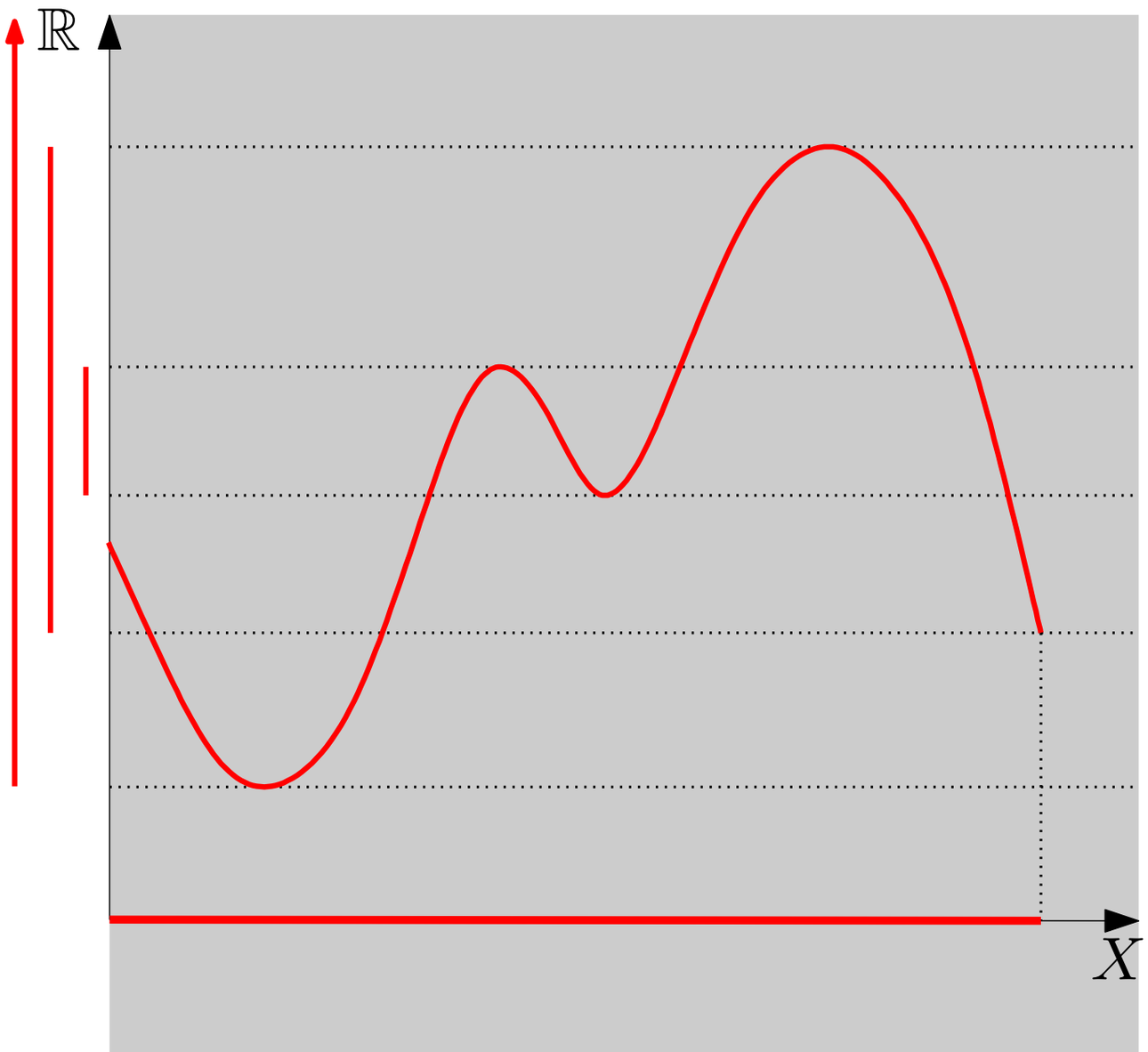

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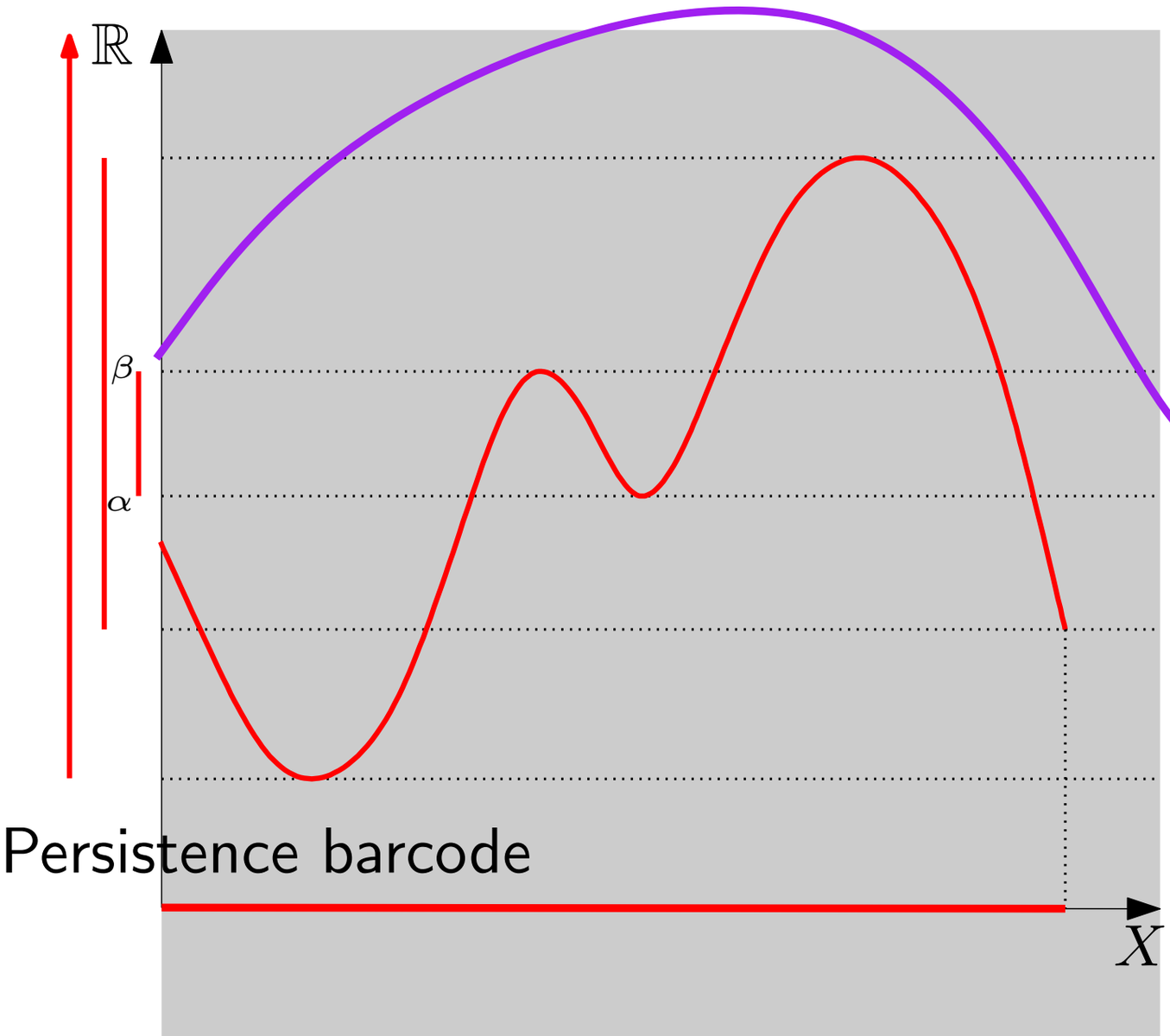
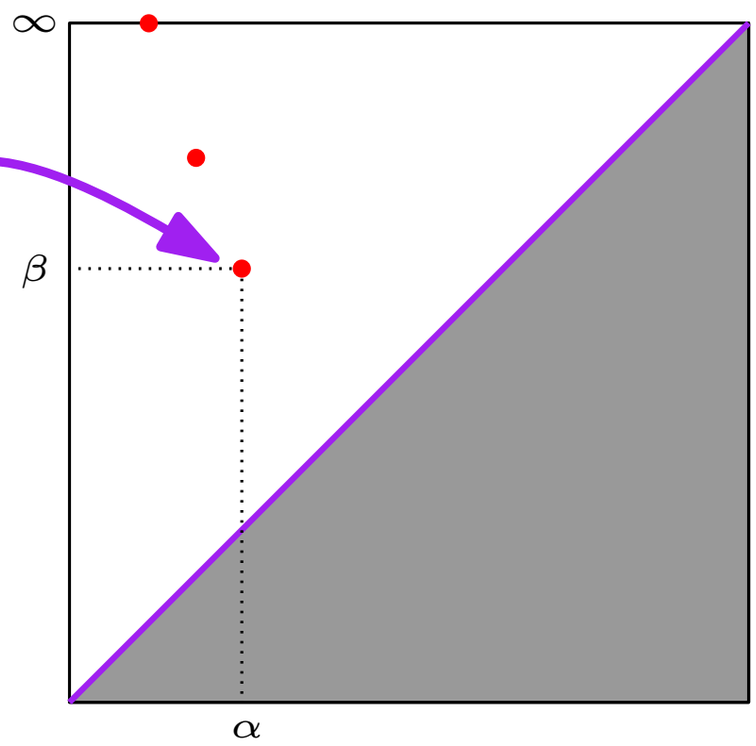


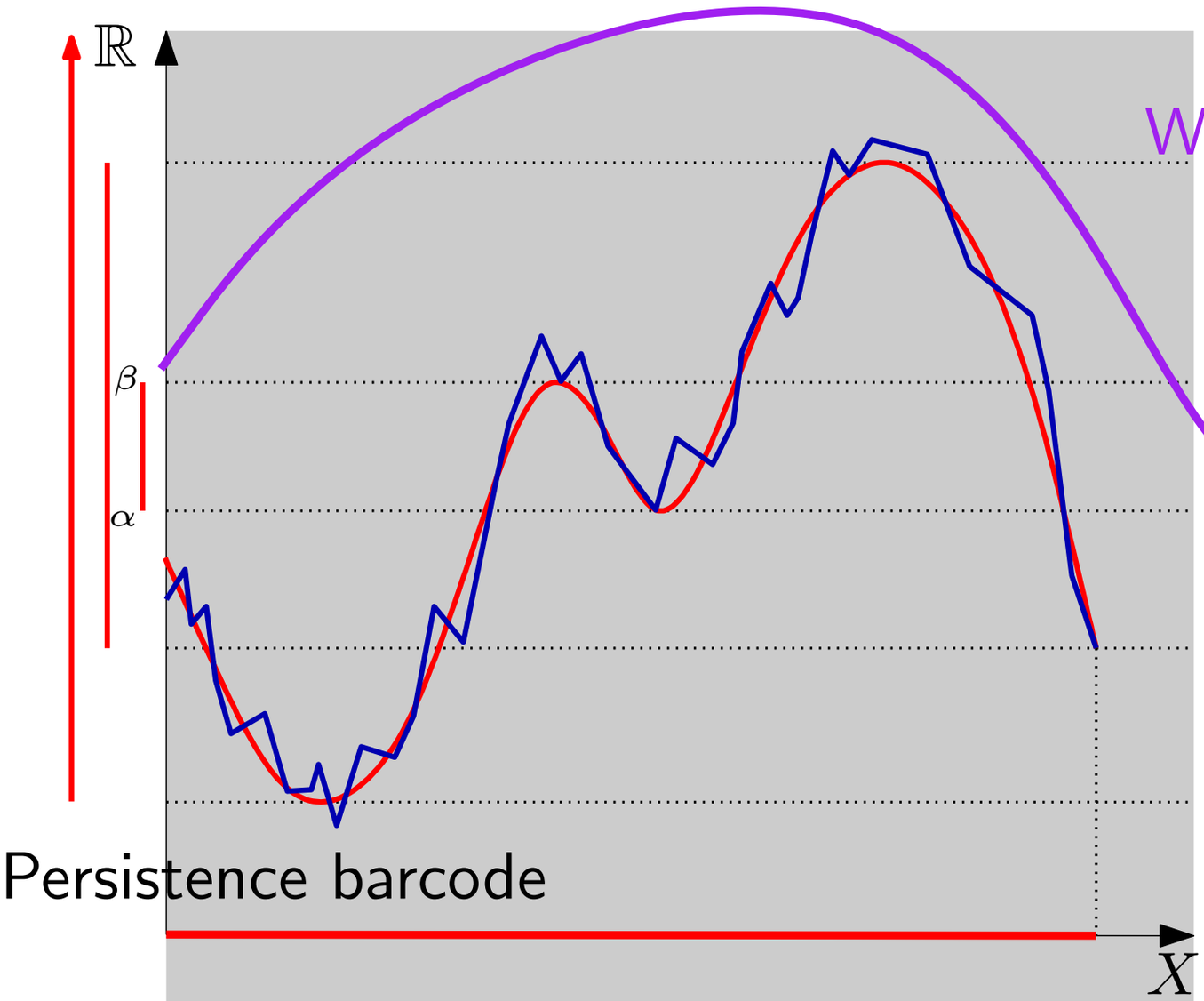


Persistence diagram

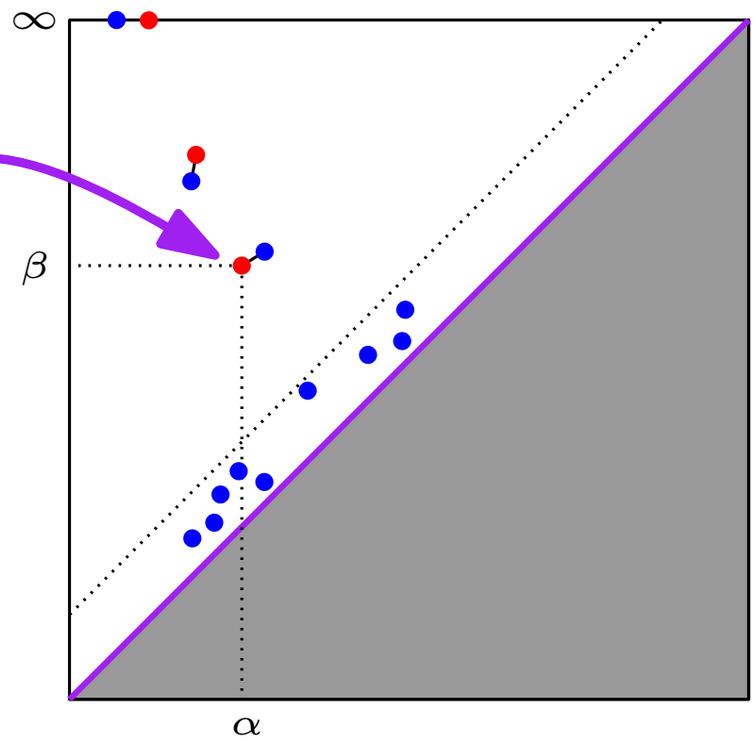
(0-dimensional) persistent homology for functions

Theorem (Stability):
For any *tame* functions $f, g : \mathbb{X} \to \mathbb{R}$, $\mathrm{d}(\mathrm{D}_f, \mathrm{D}_g) \leq \|f - g\|_\infty$.

[Cohen-Steiner, Edelsbrunner, Harer 05], [C., Cohen-Steiner, Glisse, Guibas, Oudot 09], [C., de Silva, Glisse, Oudot 12]

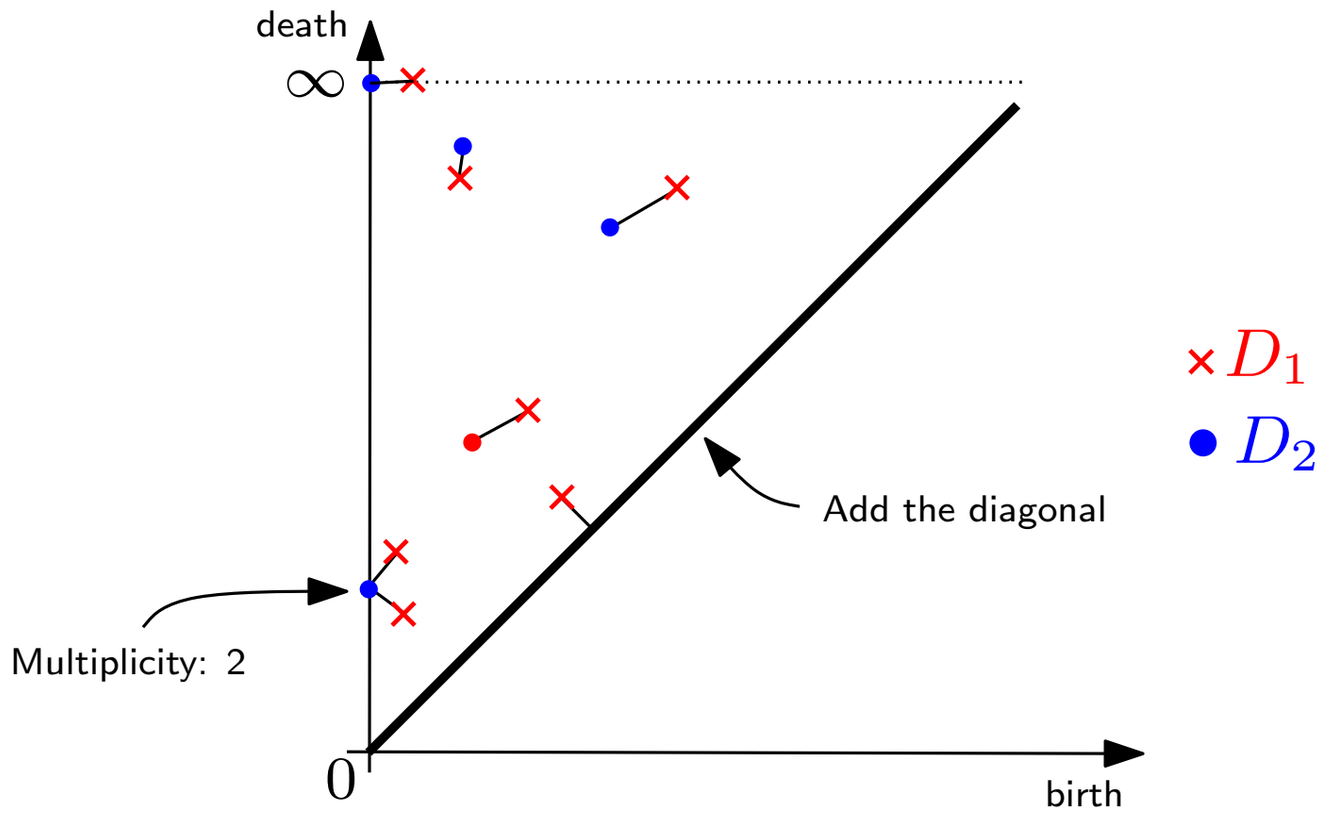


What if f is slightly perturbed?



Persistence diagram

Distance between persistence diagrams



The bottleneck distance between two diagrams D_1 and D_2 is

$$d_B(D_1, D_2) = \inf_{\gamma \in \Gamma} \sup_{p \in D_1} \|p - \gamma(p)\|_\infty$$

where Γ is the set of all the bijections between D_1 and D_2 and $\|p - q\|_\infty = \max(|x_p - x_q|, |y_p - y_q|)$.

The example of distance functions

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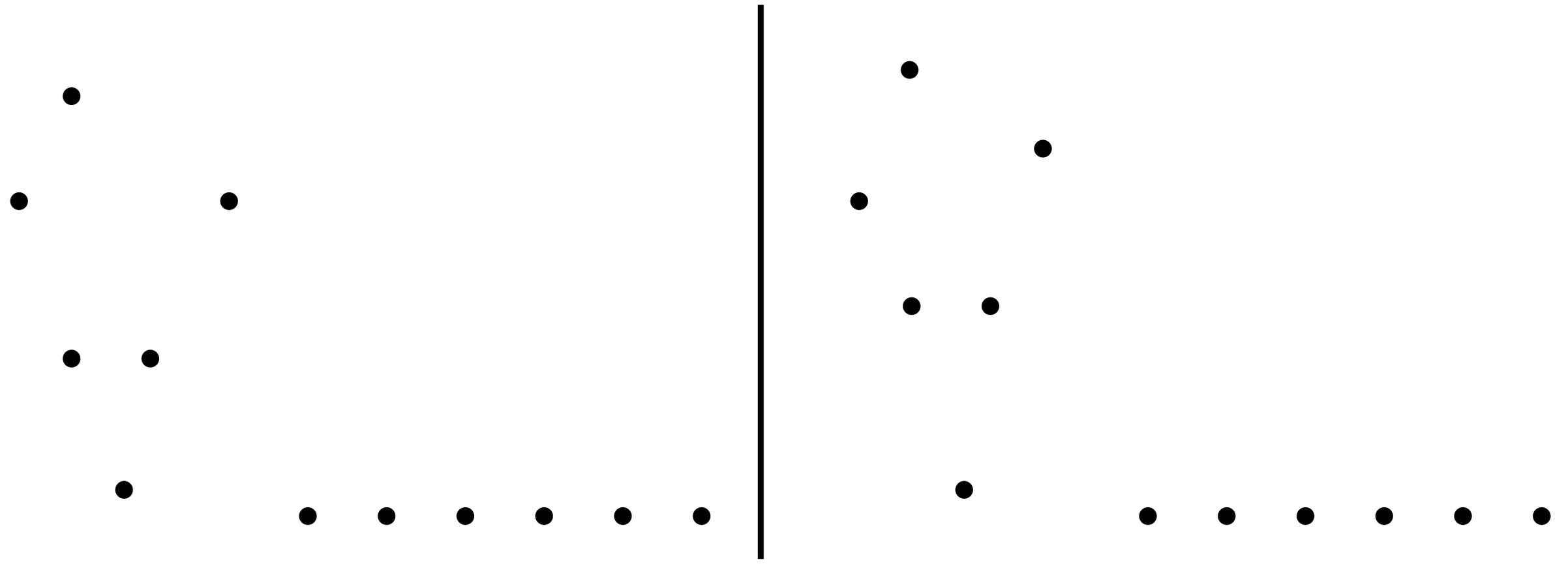
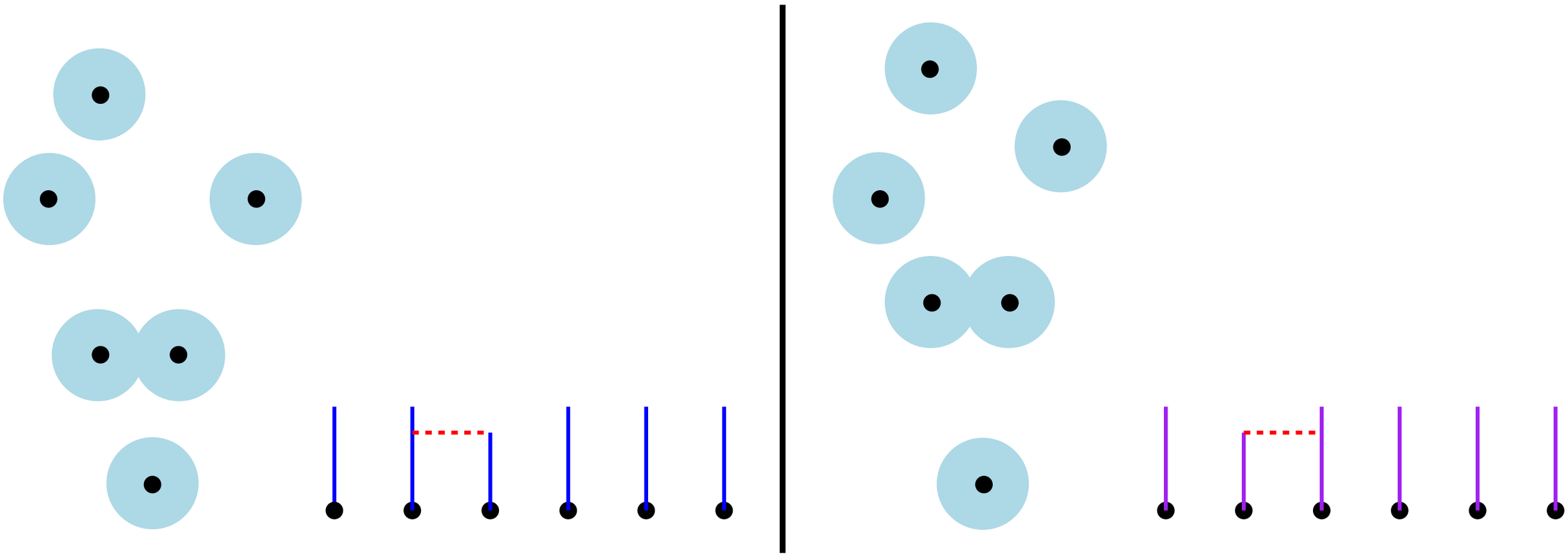


$$f_P : \quad \mathbb{R}^2 \to \mathbb{R}$$
$$x \mapsto \min_{p \in P} \|x - p\|_2$$

Link with single linkage clustering

The example of distance functions



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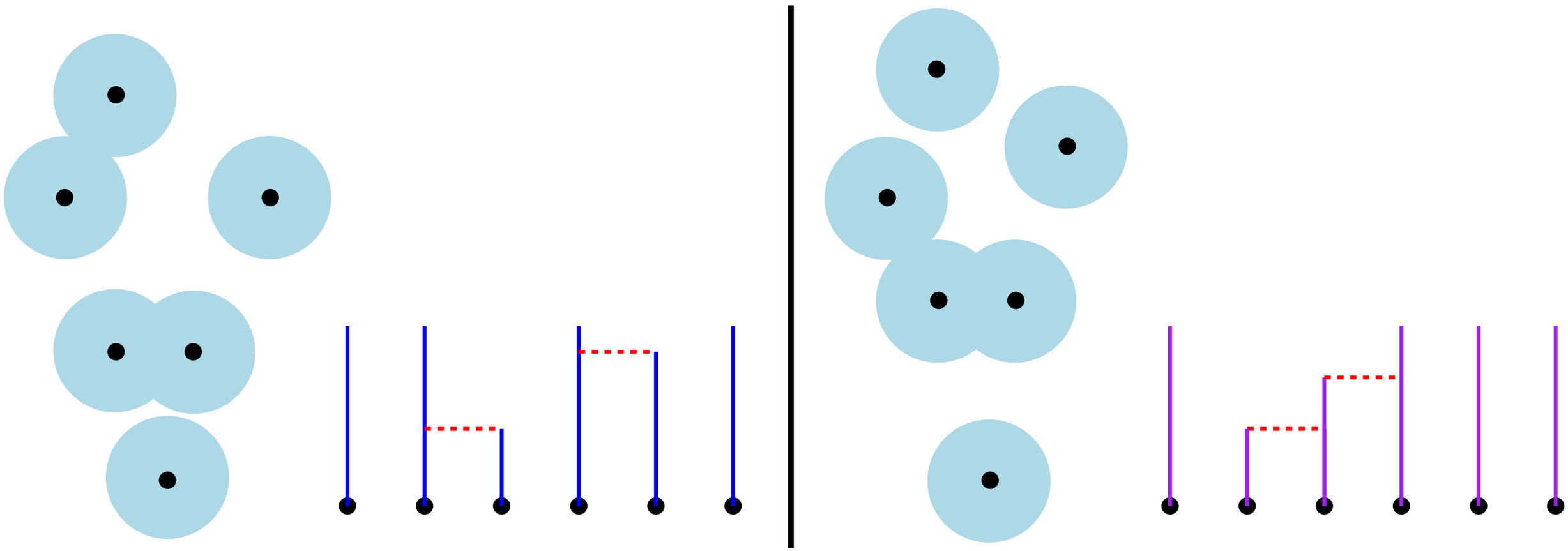

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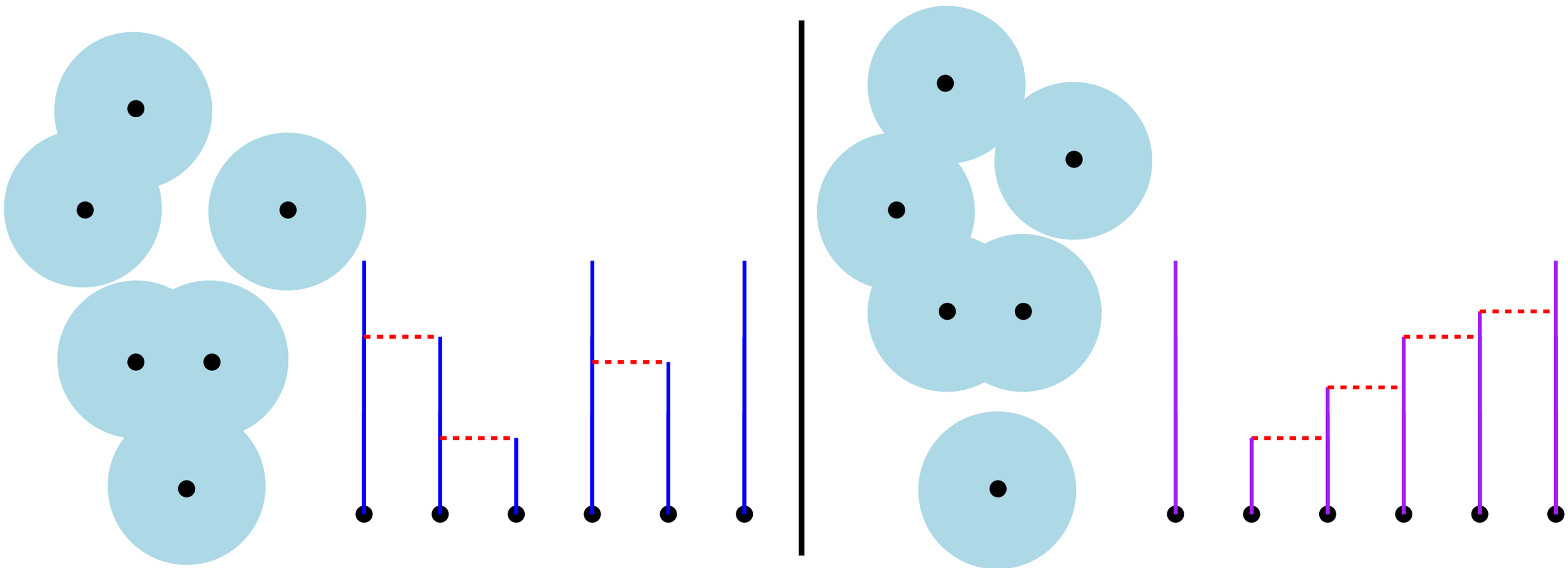

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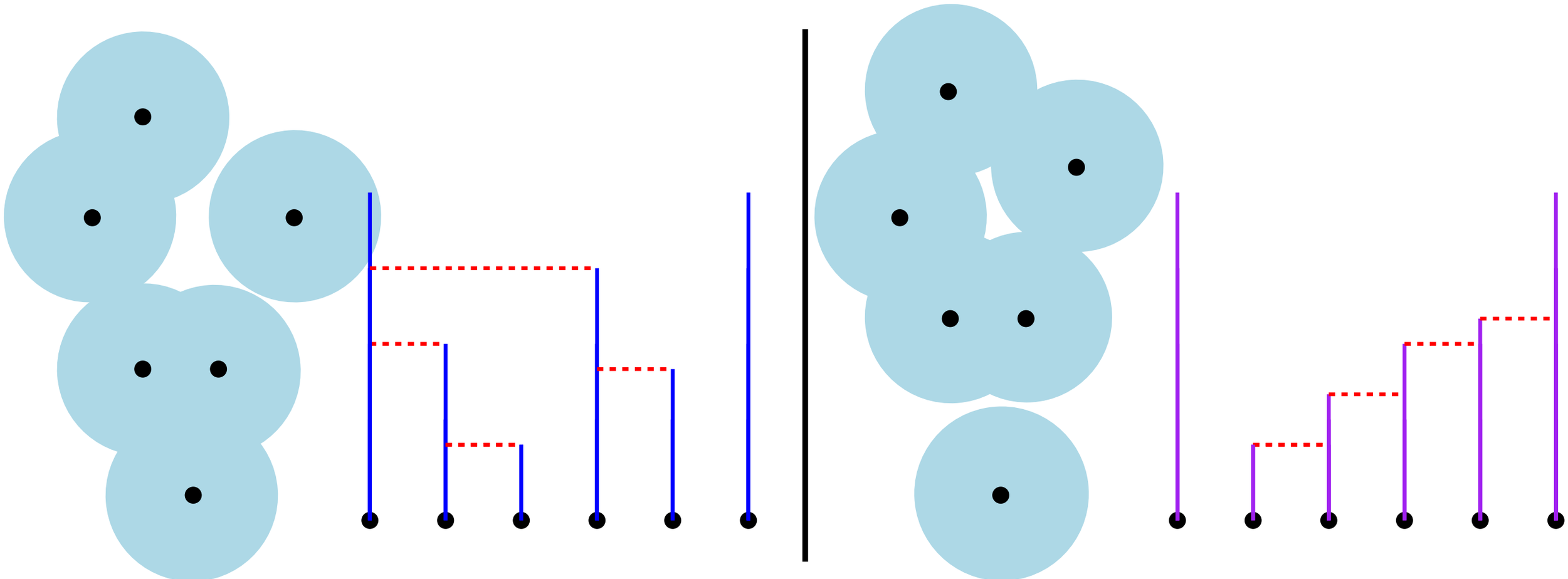

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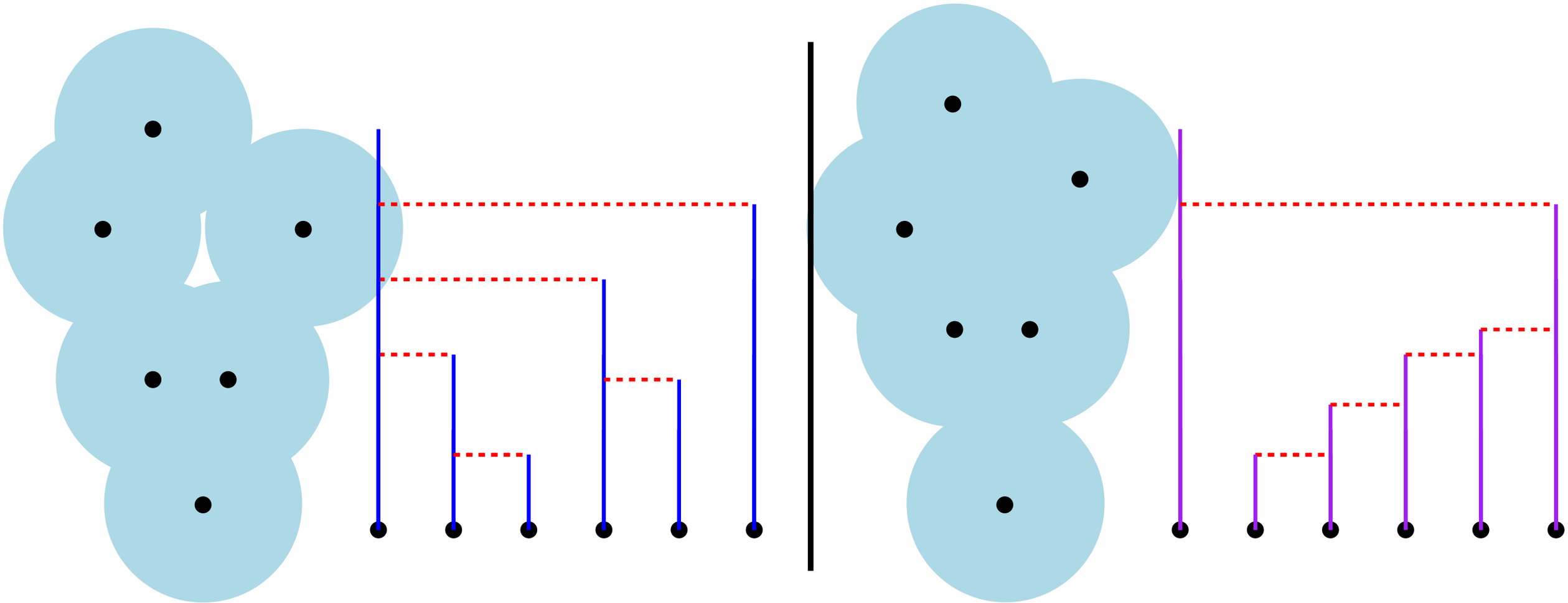

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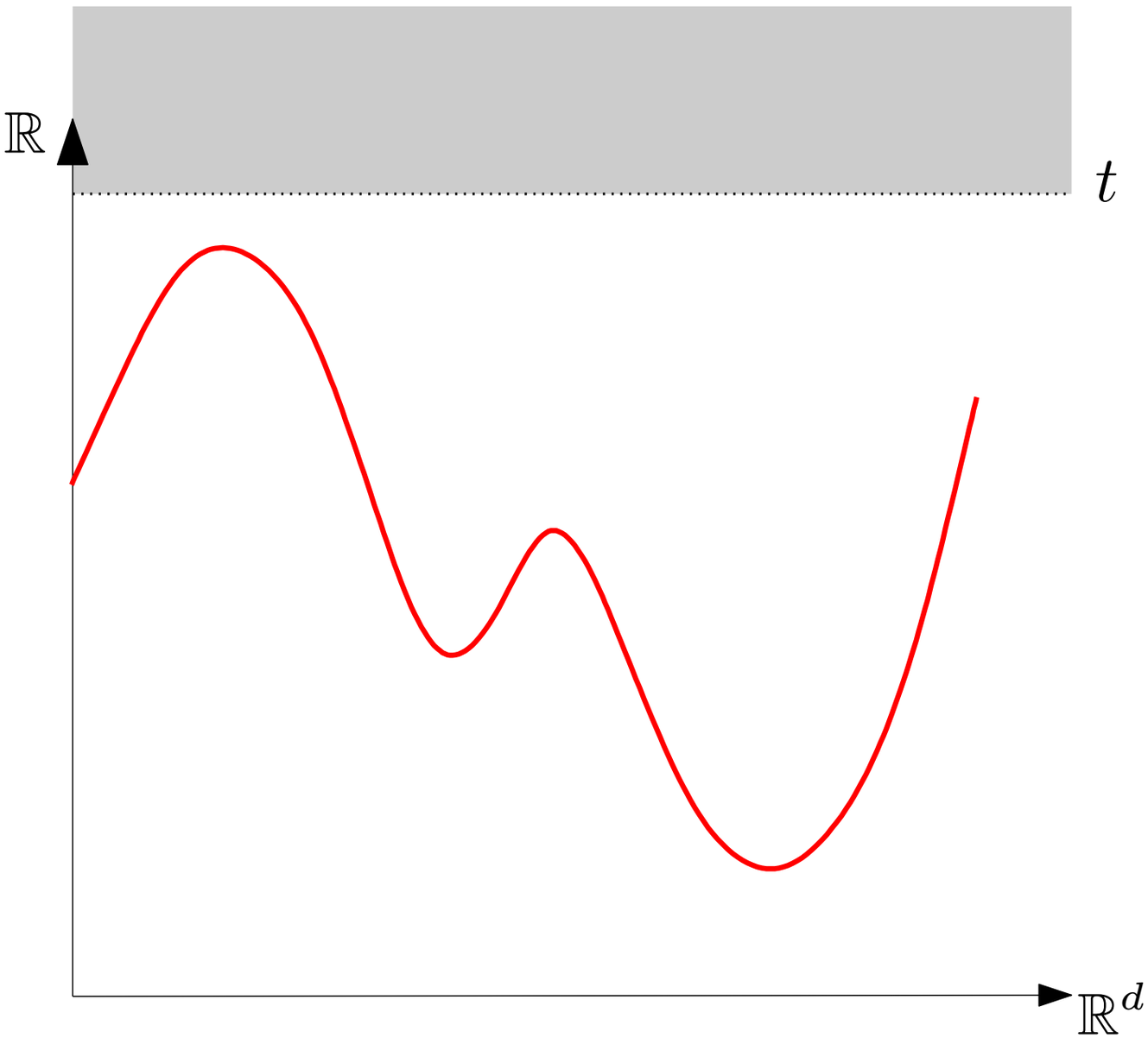
Link with single linkage clustering

The case of density and back to mode seeking

Given a probability density f:

- Consider the superlevel-sets filtration $f^{-1}([t, +\infty))$ for t from $+\infty$ to $-\infty$, instead of the sublevel-sets filtration.
- Persistence is defined in the same way



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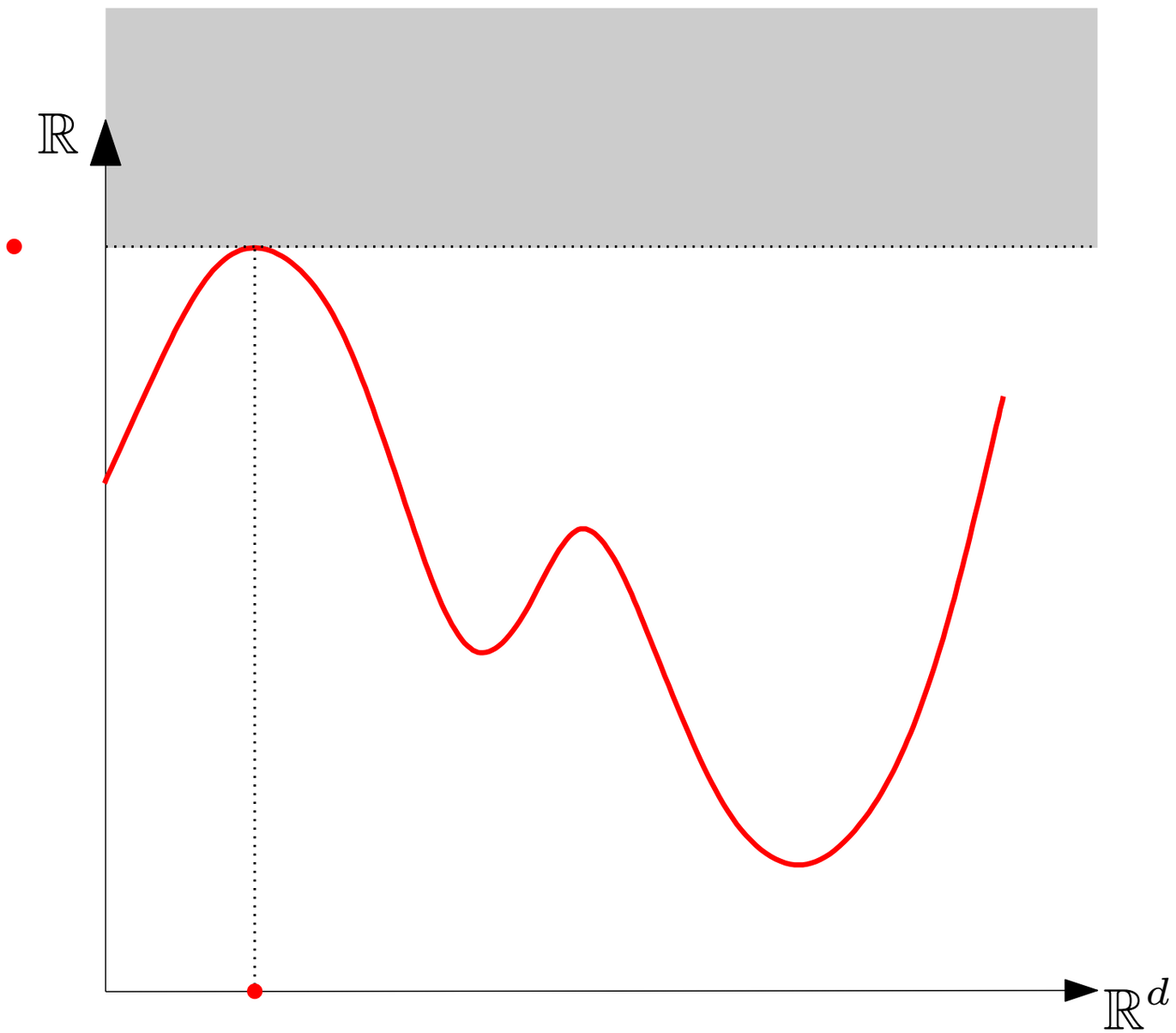

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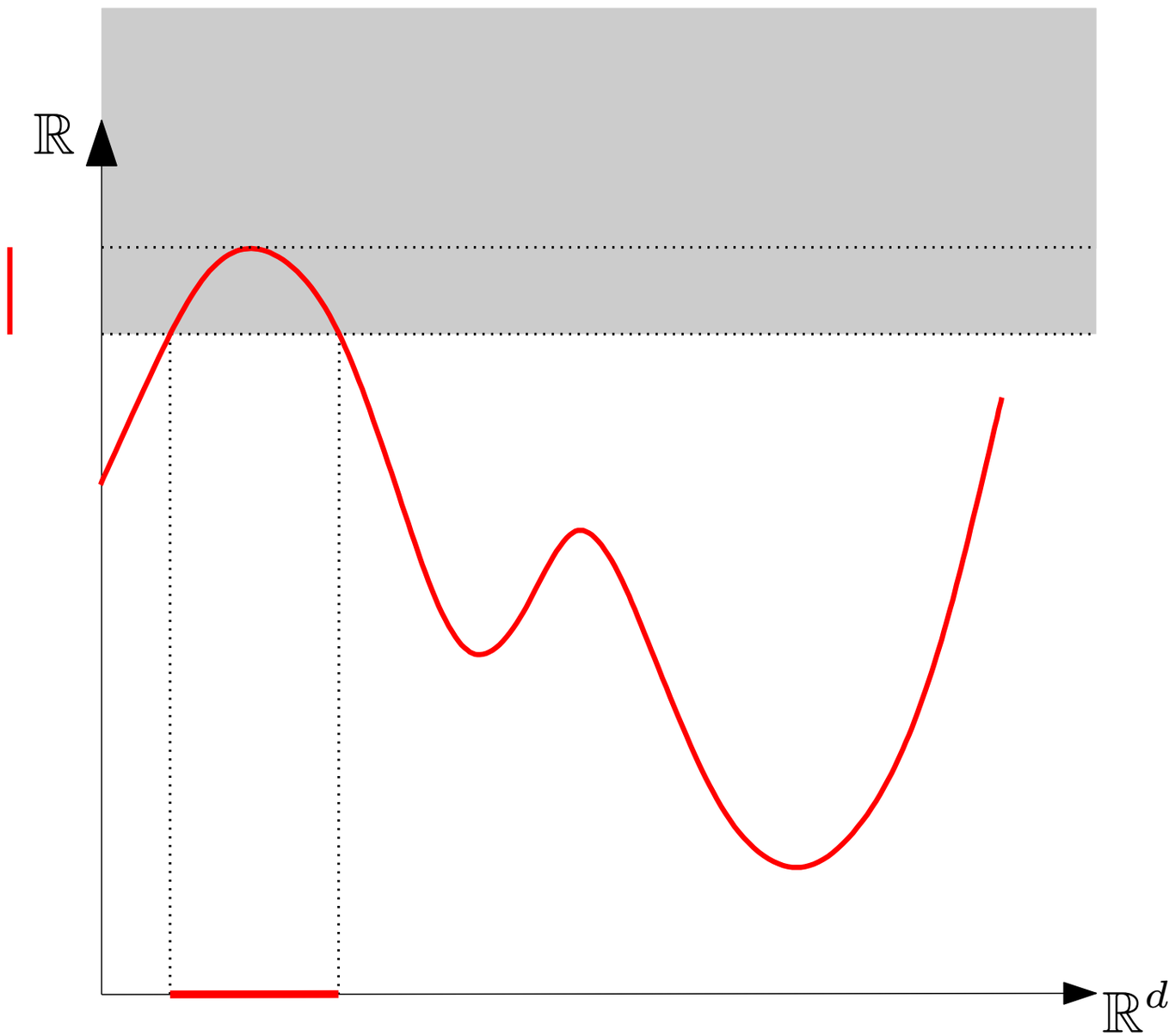

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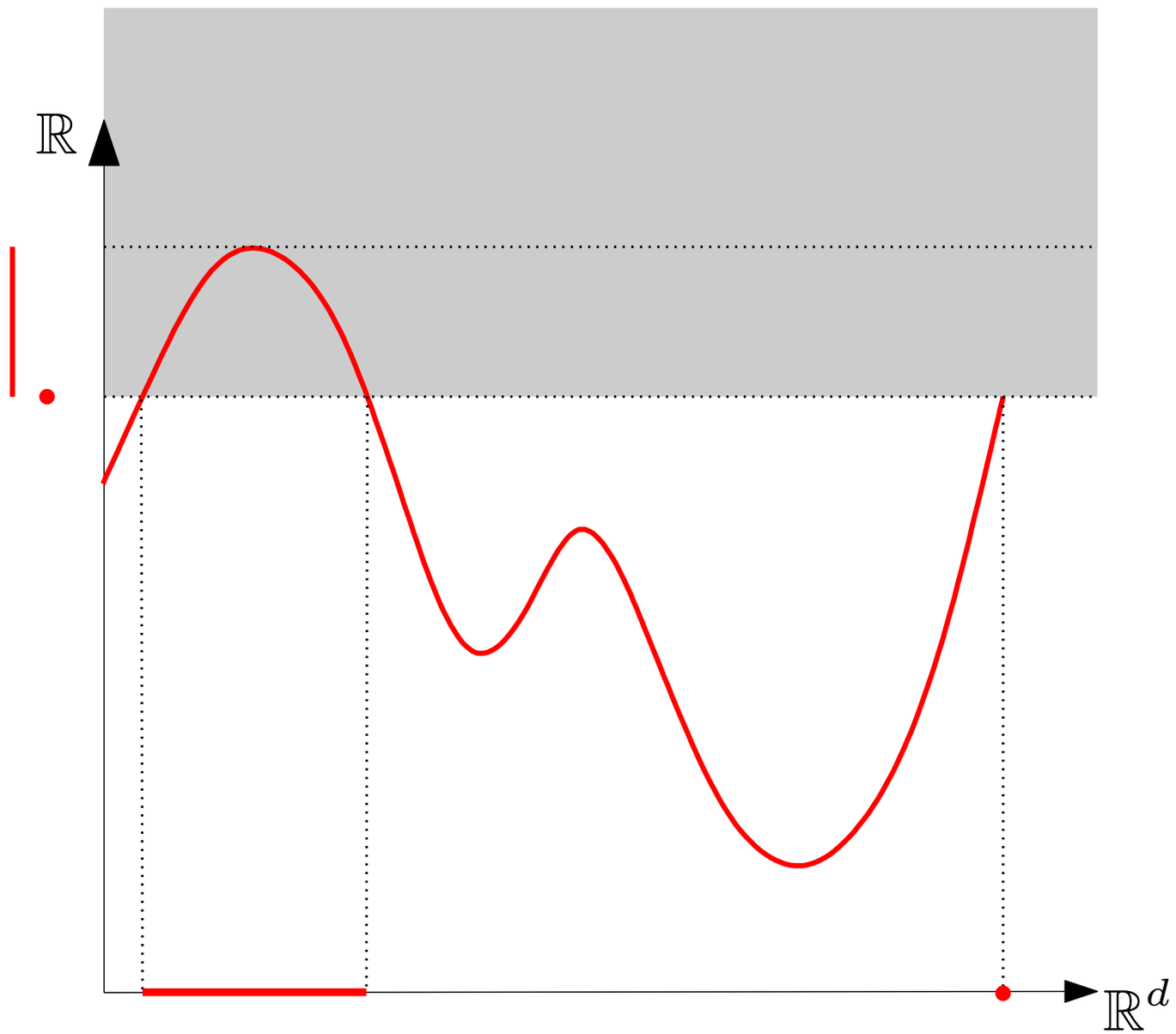

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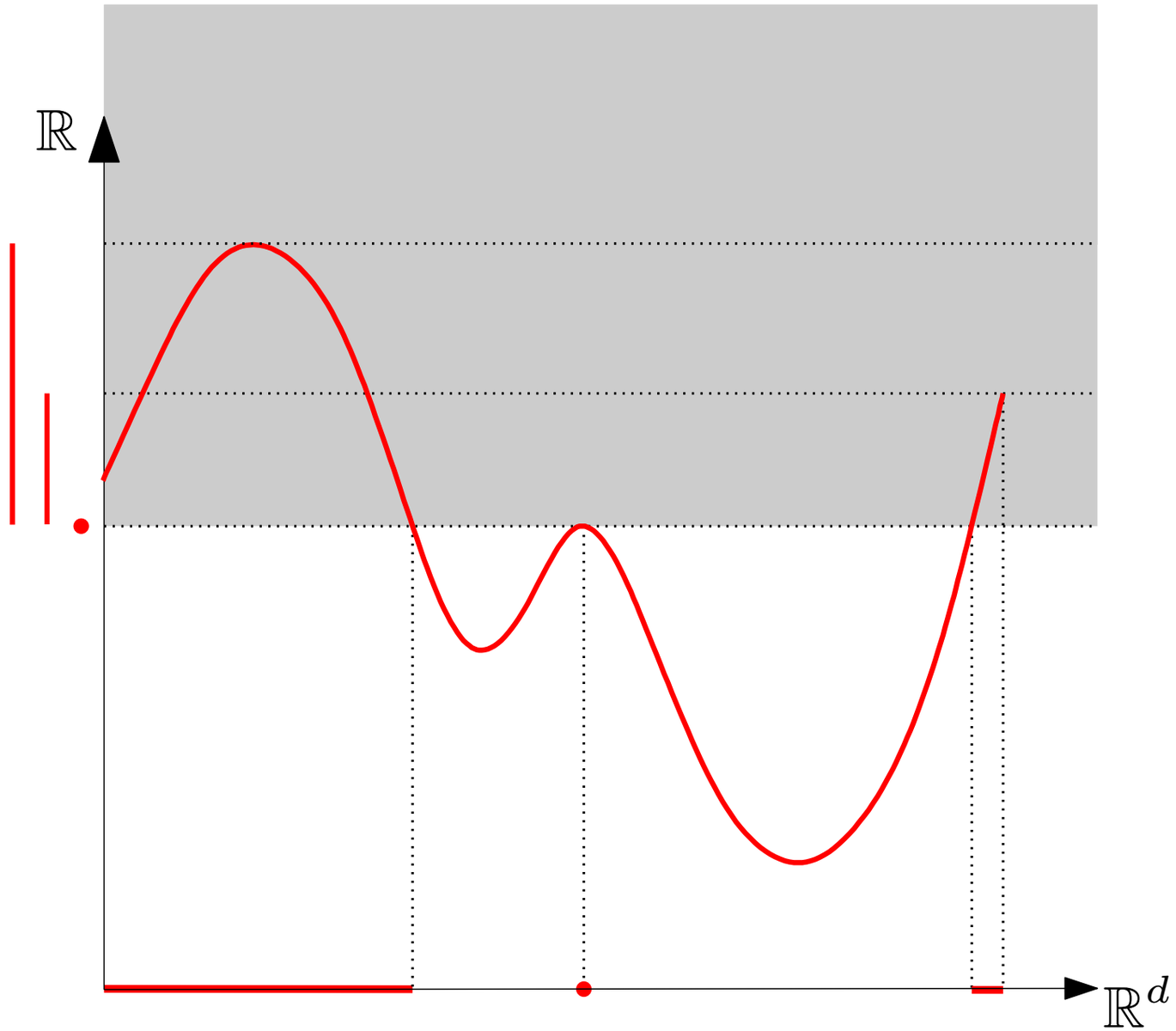

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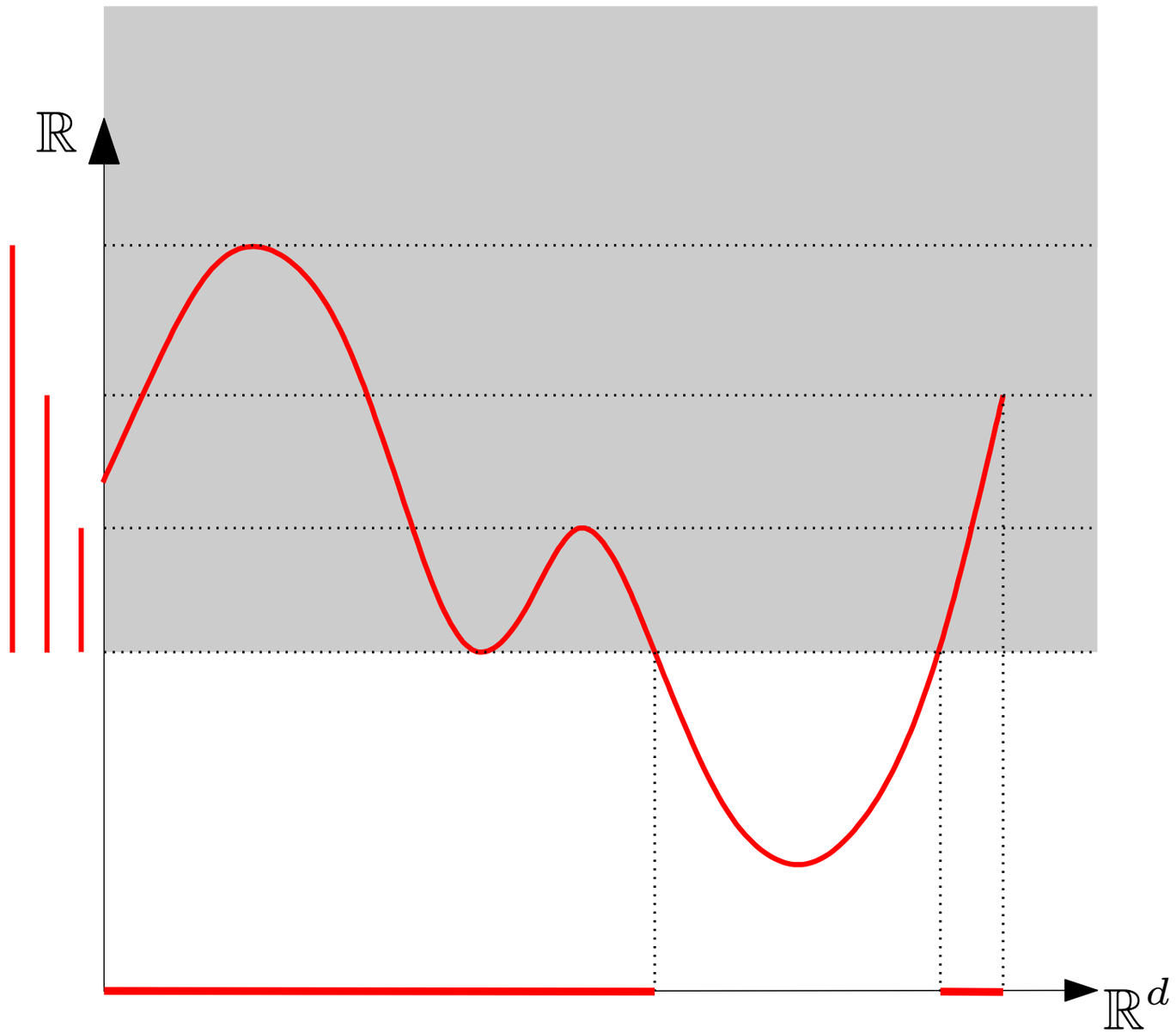

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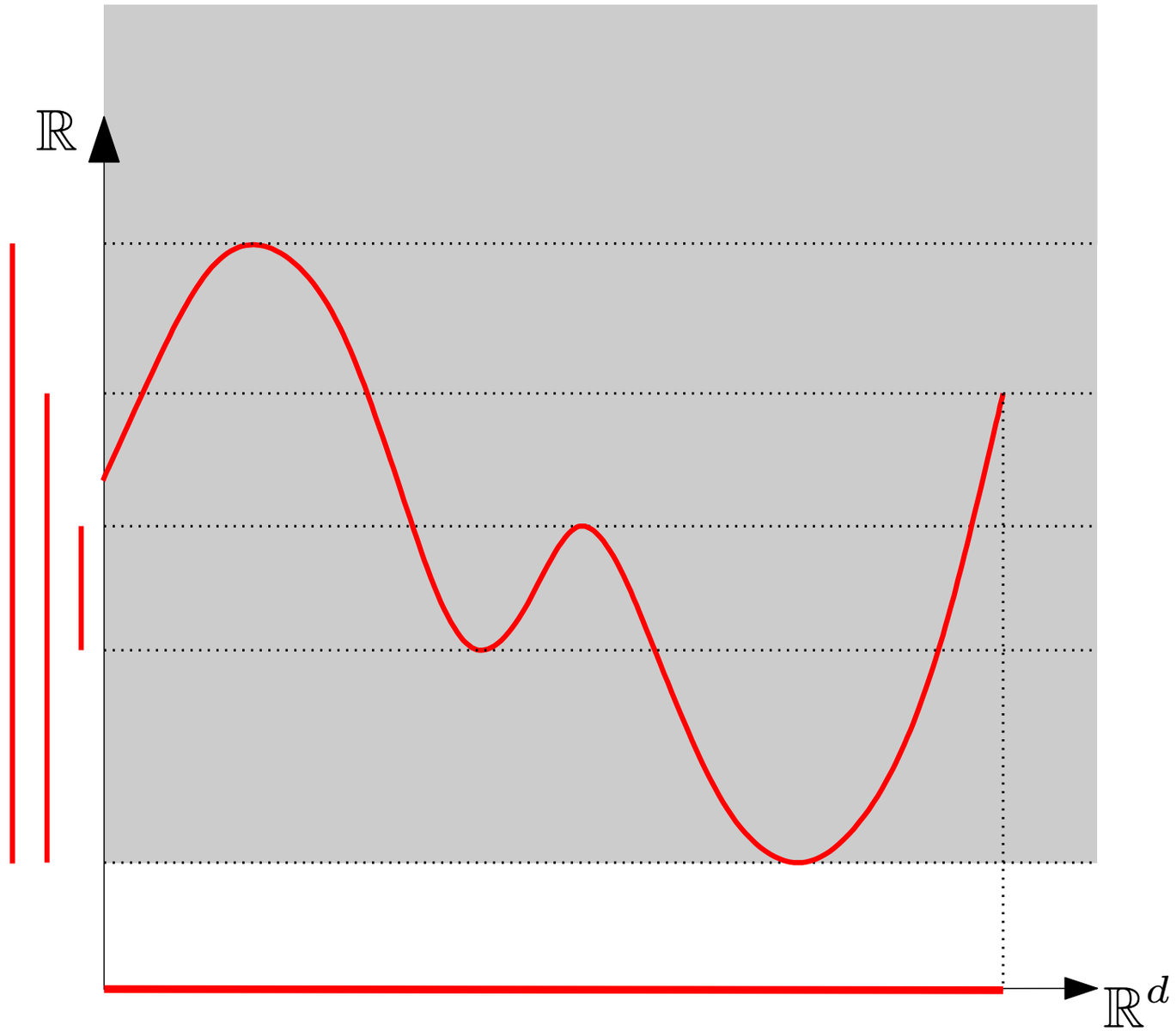

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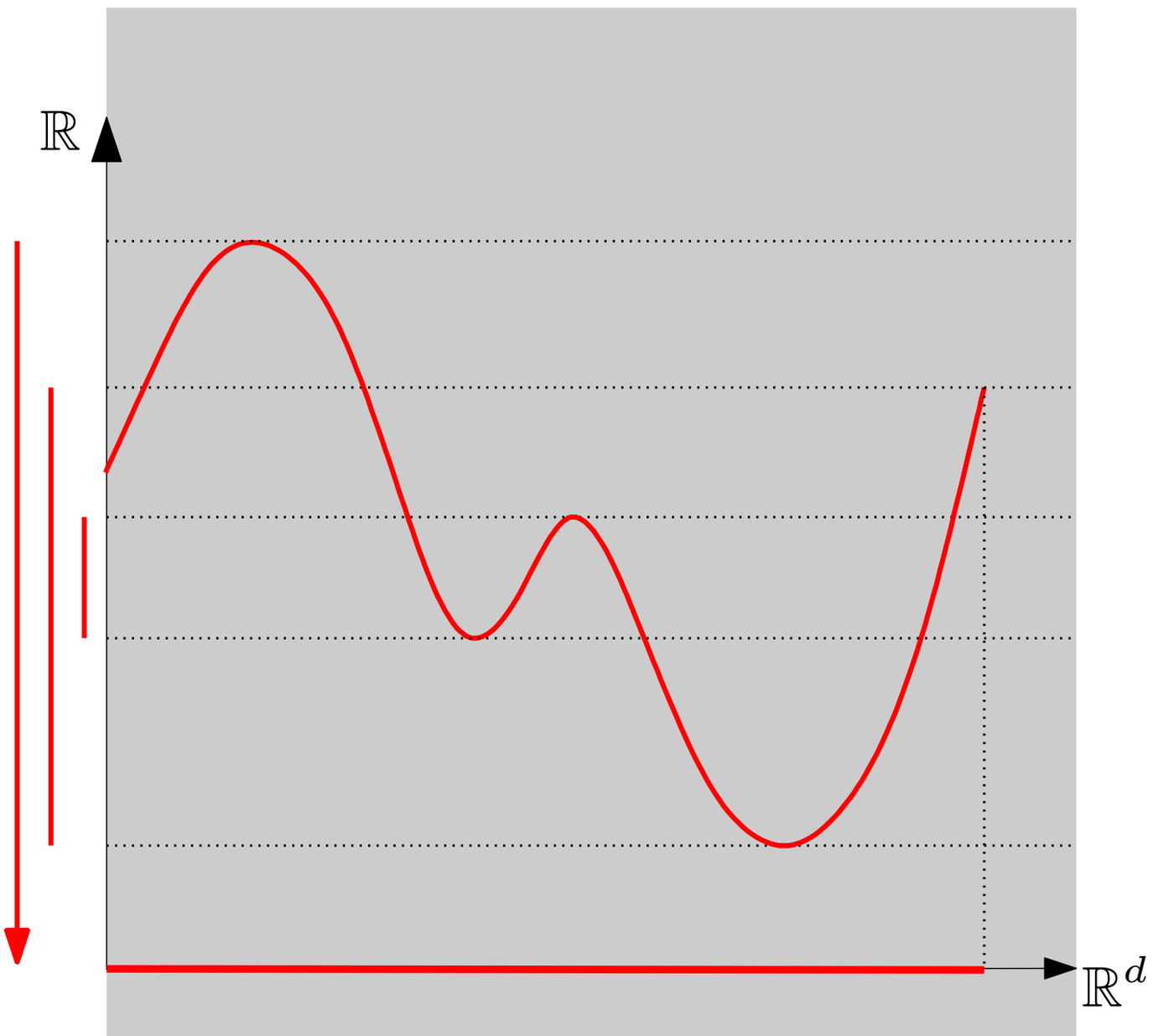

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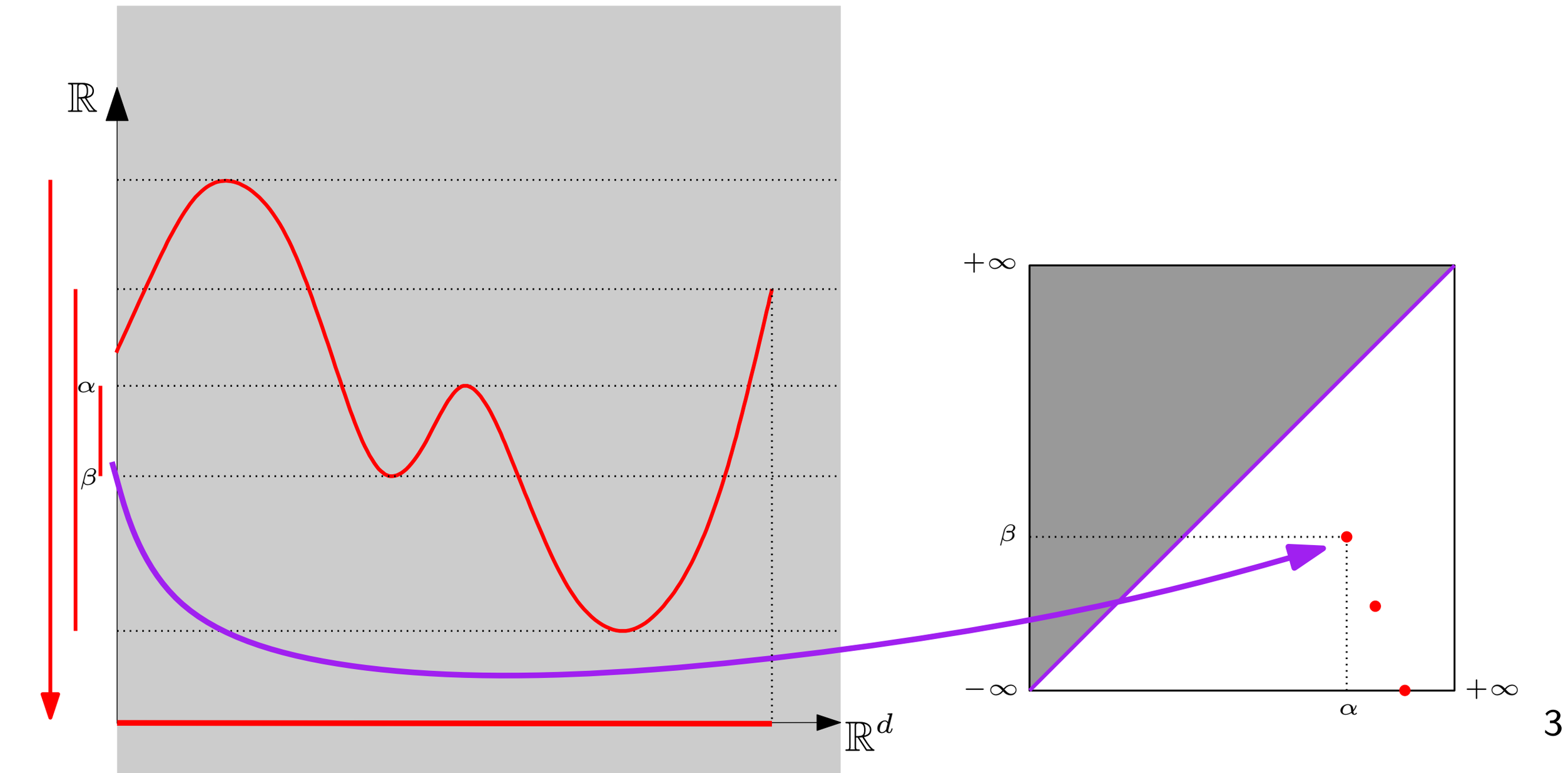
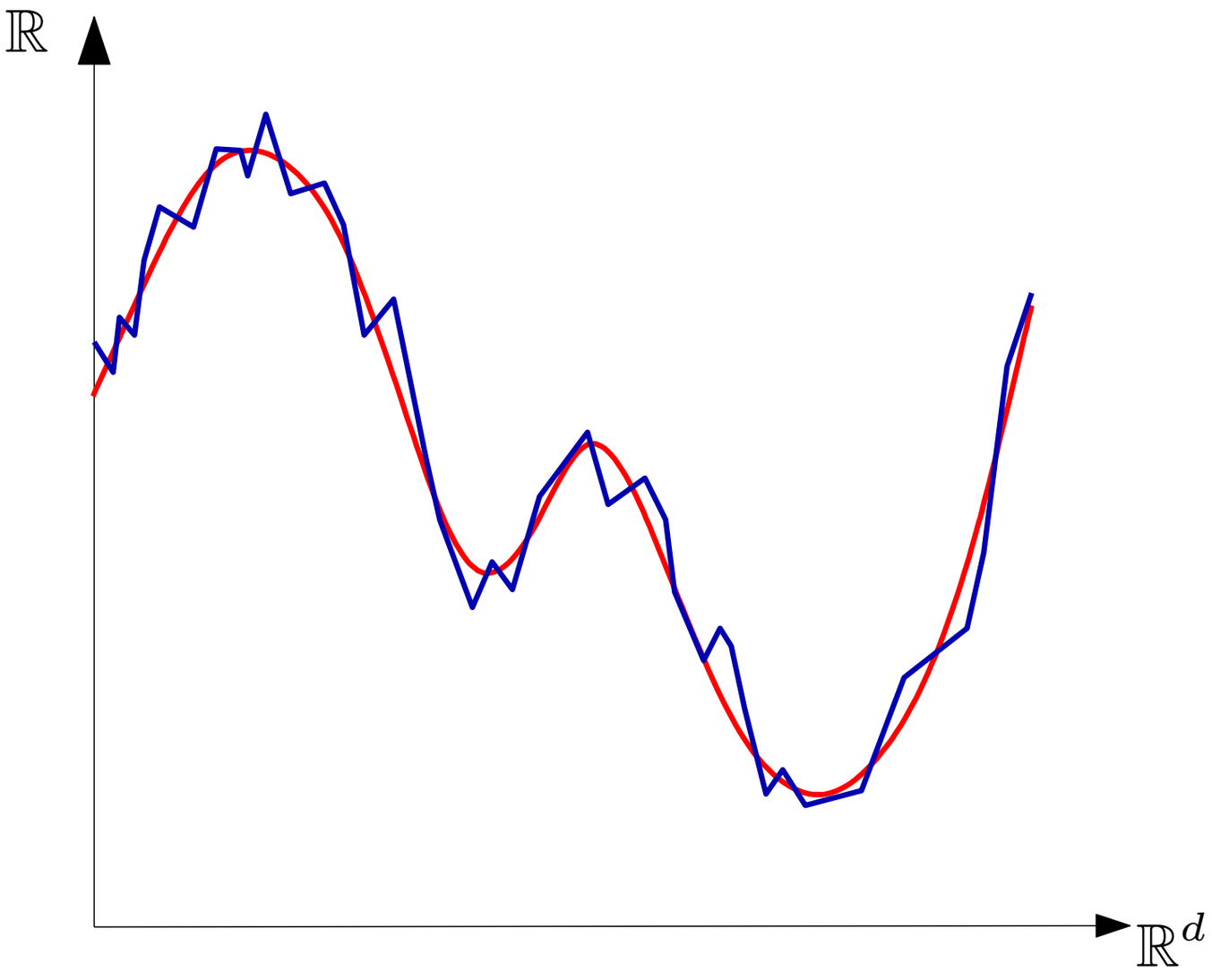
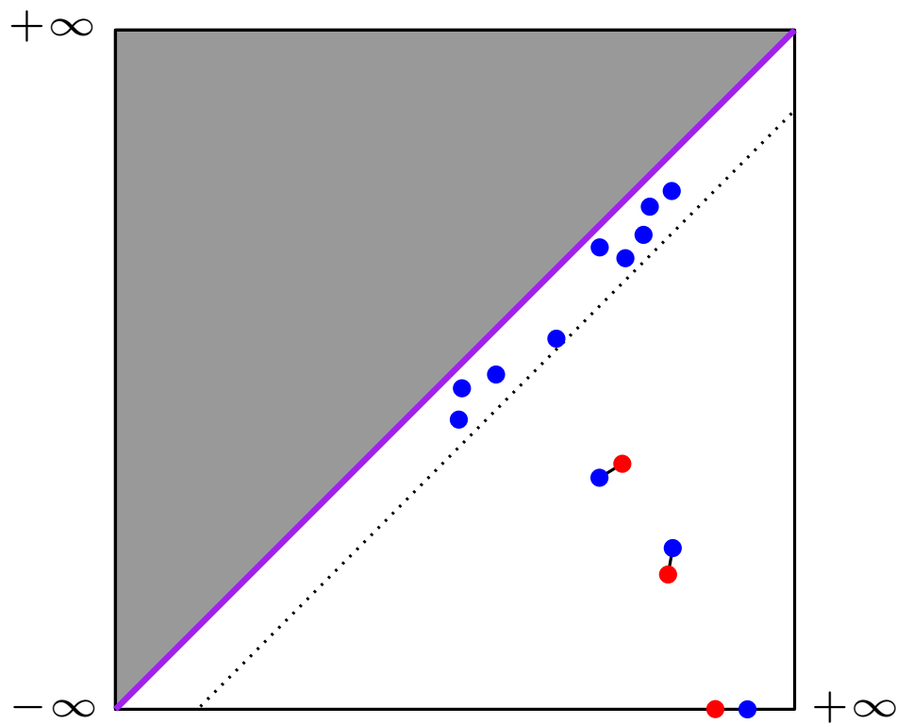


The case of density and back to mode seeking

Given an estimator $\hat{f}$:

Stability Theorem $\Rightarrow d_B(Df, D\hat{f}) \leq \|f - \hat{f}\|_\infty$.

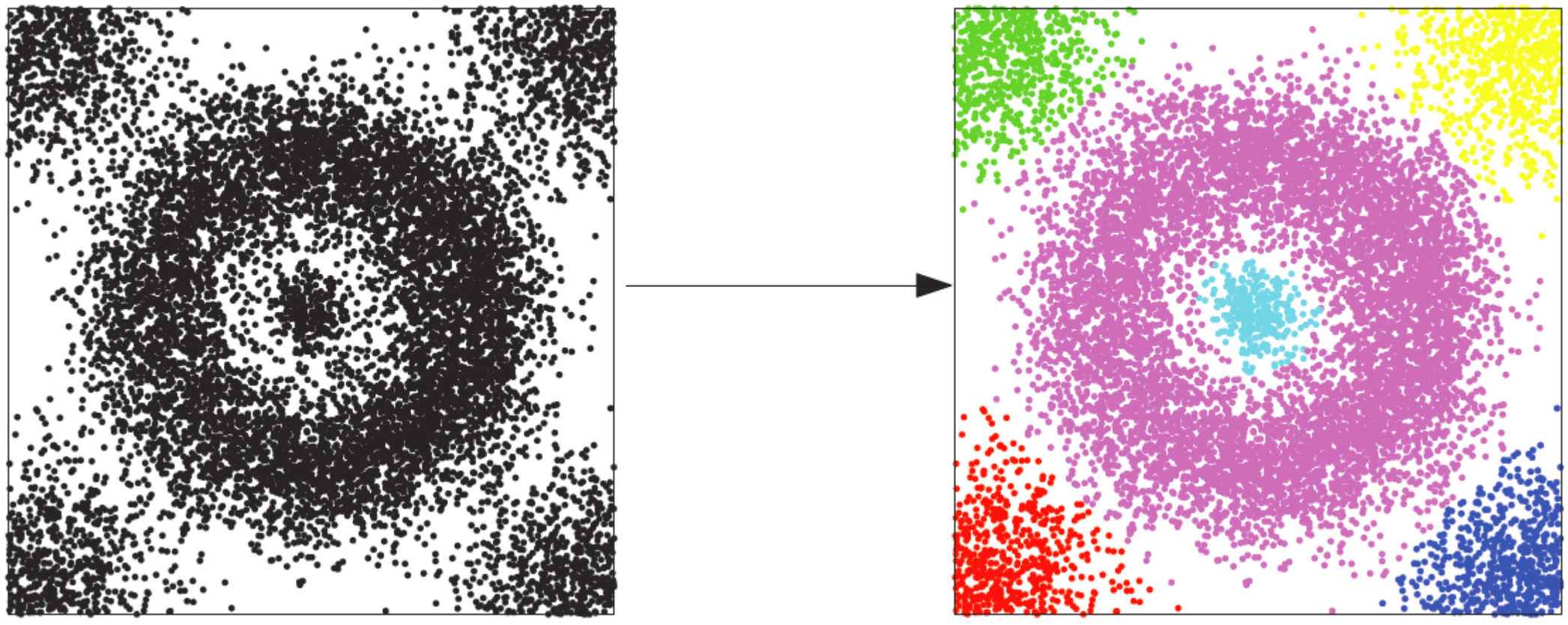




Persistence-based clustering

Combine a mode seeking approach with (0-dim) persistence computation.

[C.,Guibas,Oudot,Skraba - J. ACM 2013]



Input:

1. A finite set X of observations (point cloud with coordinates or pairwise distance matrix),
2. A real valued function f defined on the observations (e.g. density estimate).

Goal: Partition the data according to the basins of attraction of the peaks of f

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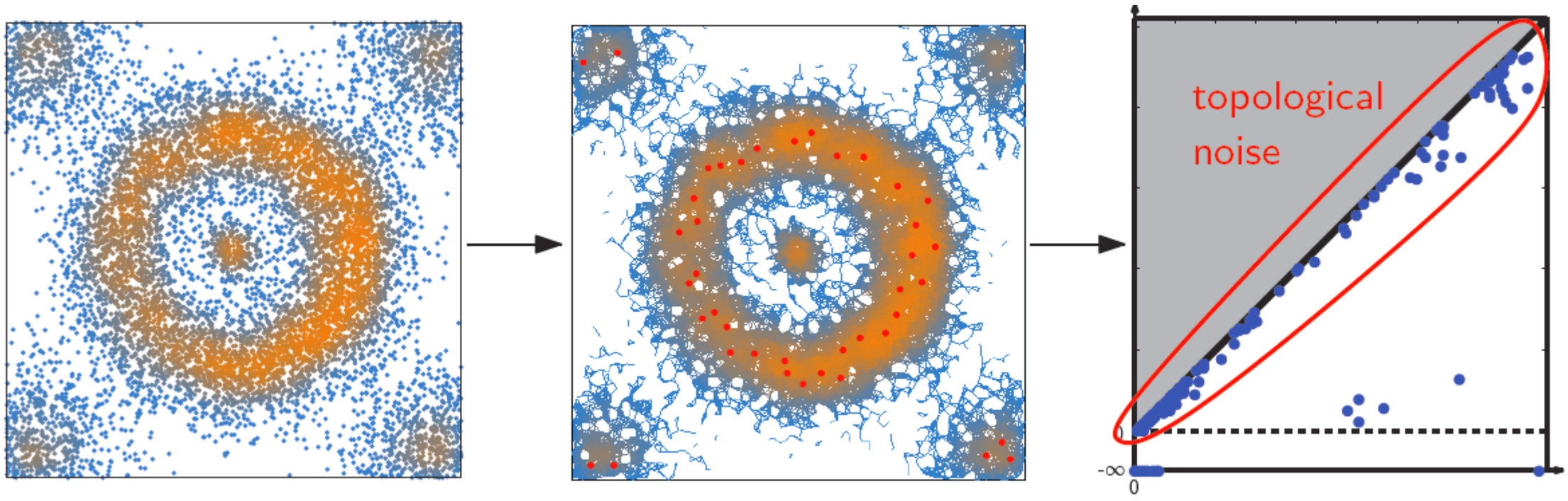

1. Build a neighborhing graph G on top of X.

2. Compute the (0-dim) persistence of f to identify prominent peaks $\rightarrow$ number of clusters (union-find algorithm).

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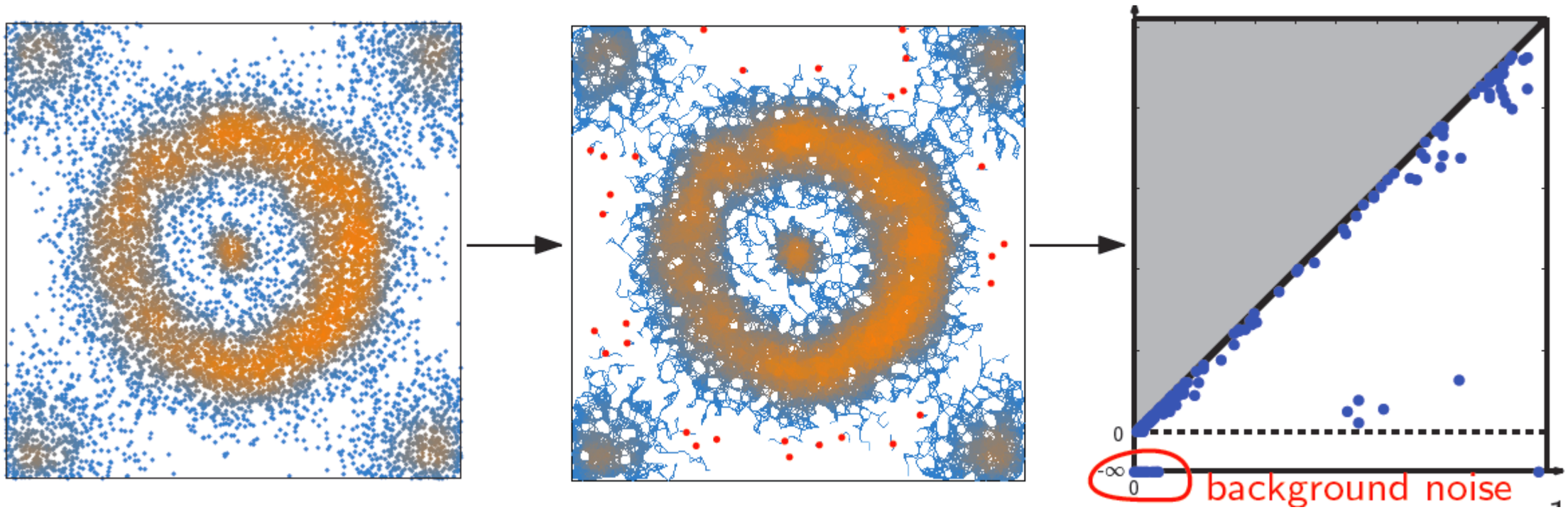

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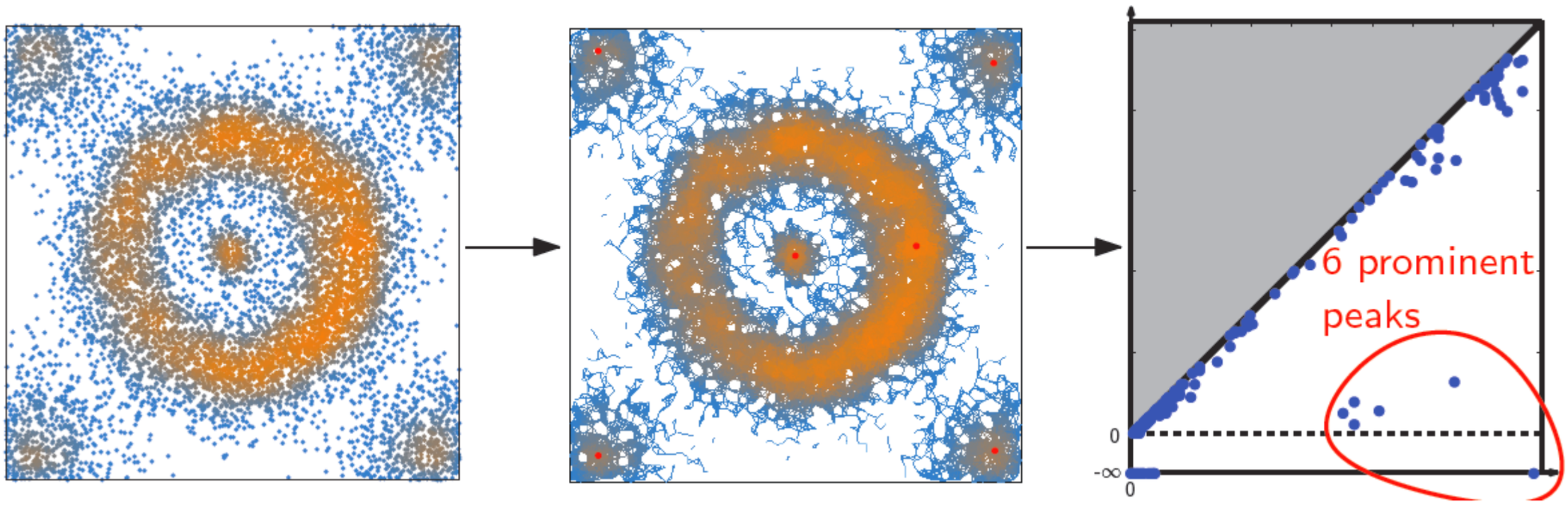

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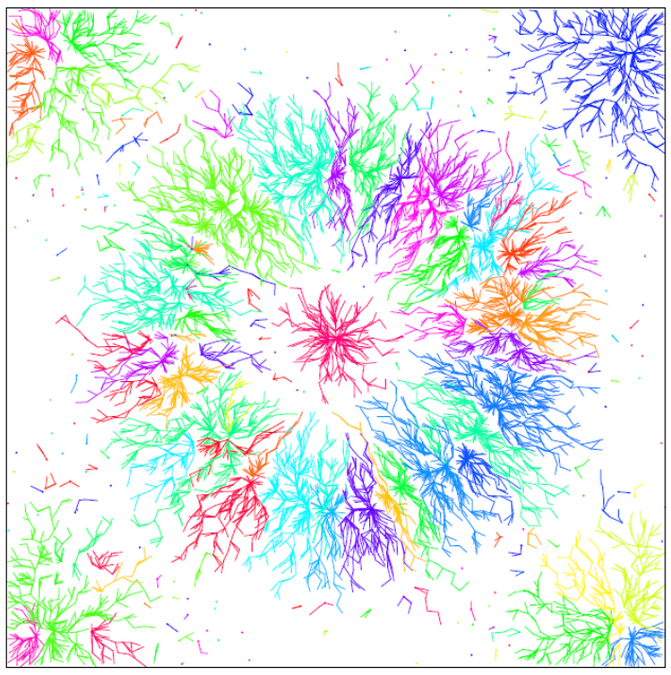
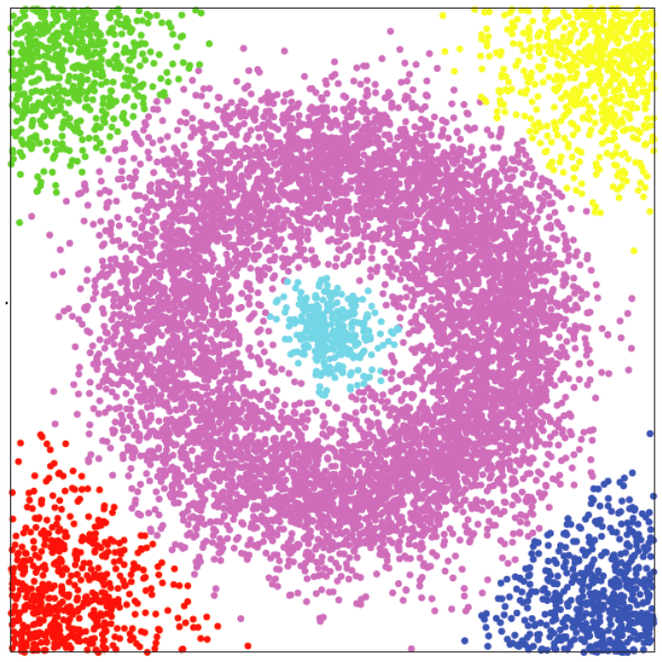
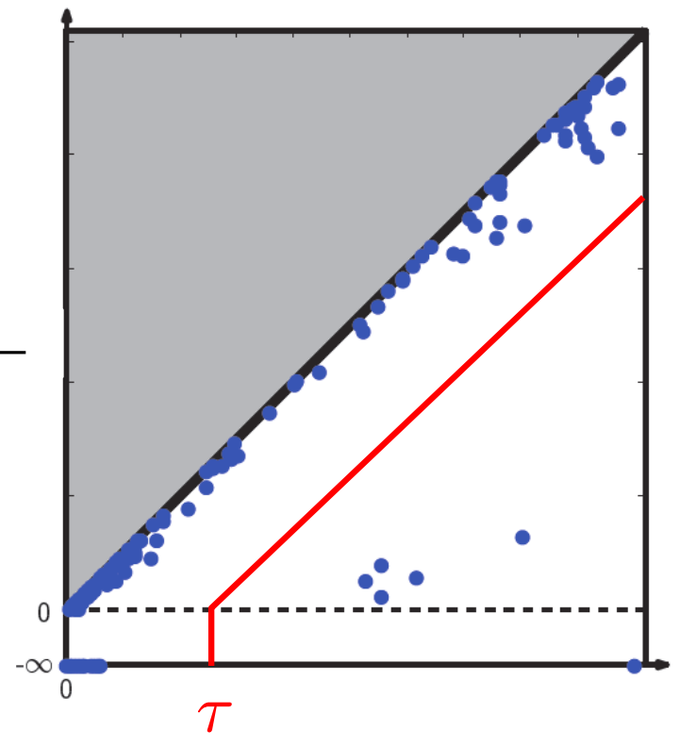


$\tau = 0$





1. Build a neighborhing graph G on top of X.

2. Compute the (0-dim) persistence of f to identify prominent peaks $\rightarrow$ number of clusters (union-find algorithm).

3. Chose a threshold $\tau > 0$ and use the persistence algorithm to merge components with prominence less than τ.

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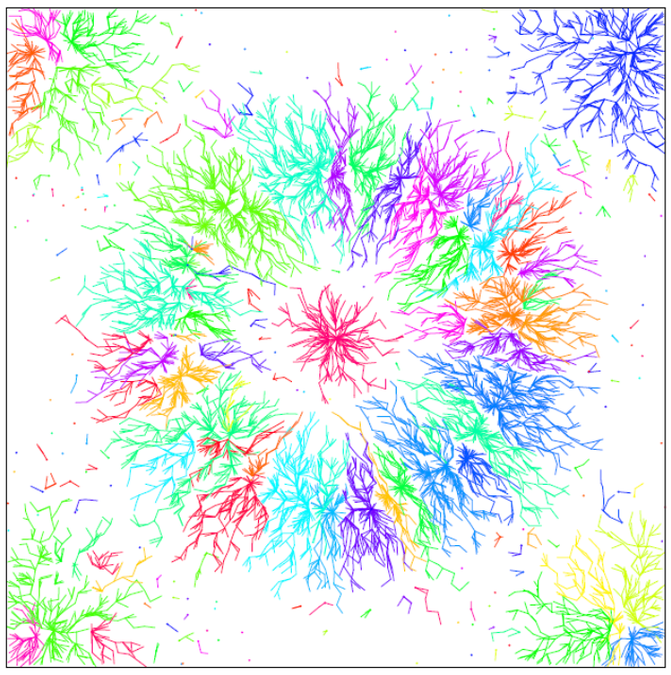
[C.,Guibas,Oudot,Skraba - J. ACM 2013]



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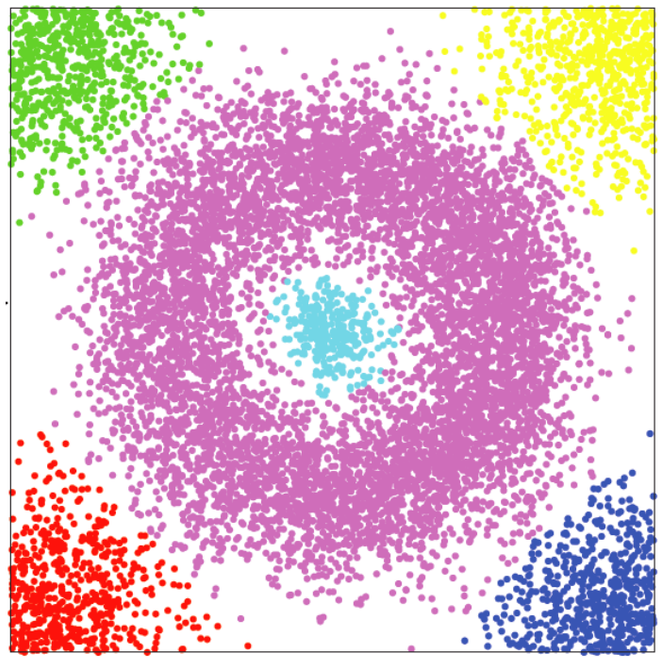
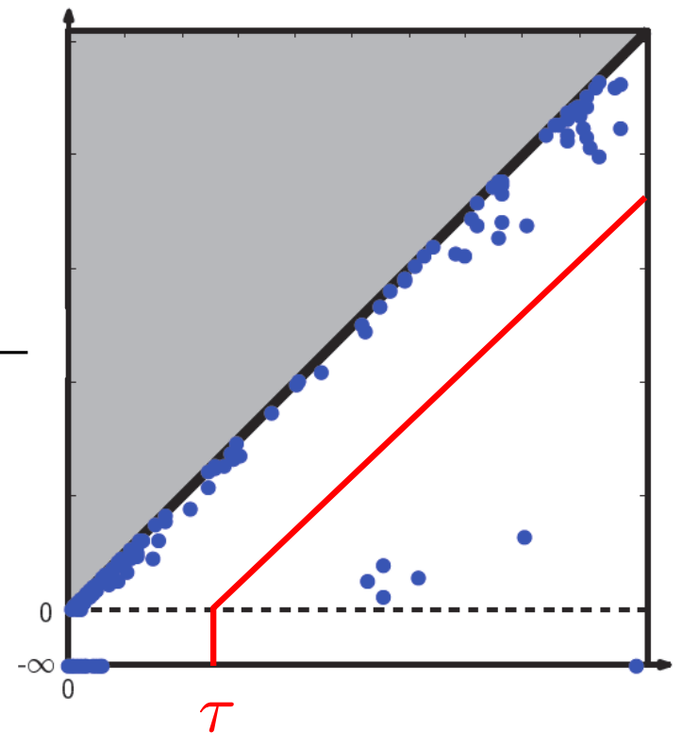




Complexity of the algorithm: $\mathrm{O}(n \log n)$

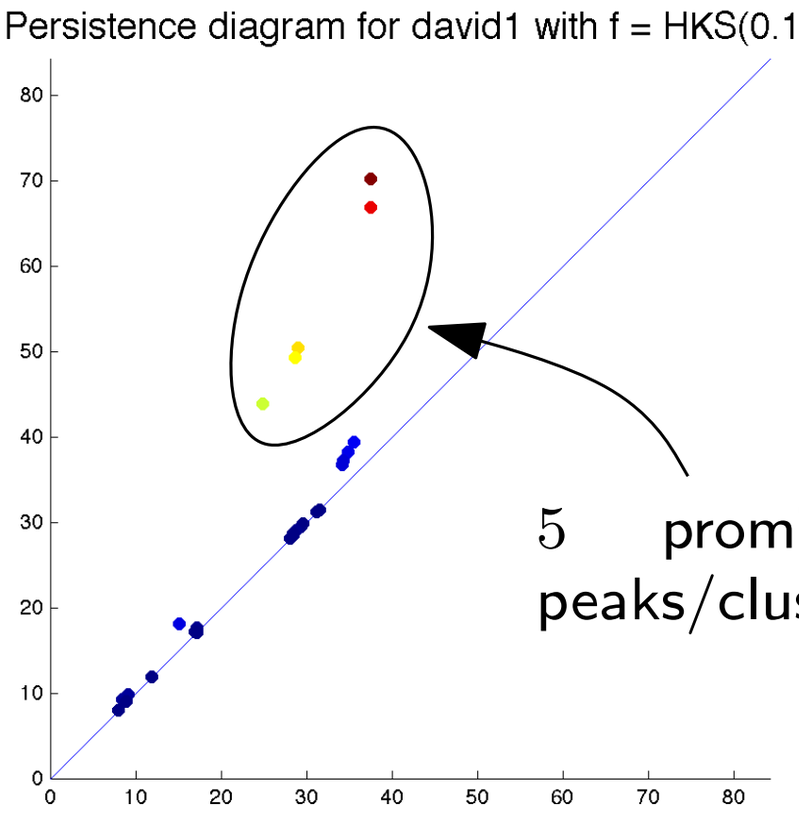
Theoretical guarantees:

- Stability of the number of clusters (w.r.t. perturbations of X and f).
- Partial stability of clusters: well identified stable parts in each cluster.

"soft " clustering

Application to non-rigid shape segmentation

[Skraba, Ovsjanikov, C.,Guibas, NORDIA 10]



X : a 3D shape

f = HKS function on X

Problem: some part of clusters are unstable $\rightarrow$ dirty segments

Application to non-rigid shape segmentation

[Skraba, Ovsjanikov, C.,Guibas, NORDIA 10]

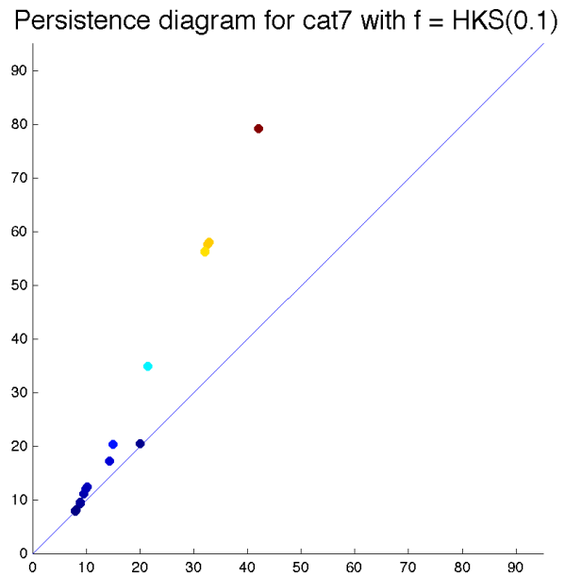
Problem: some part of clusters are unstable $\rightarrow$ dirty segments

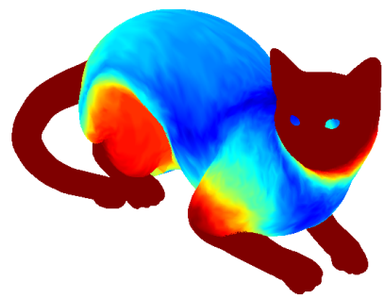
Idea:

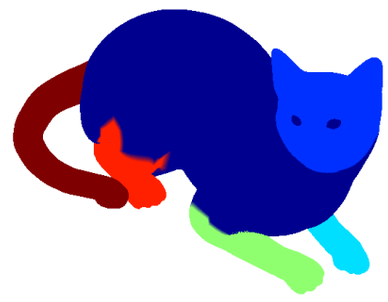
- Run the persistence based algorithm several times on random perturbations of f (size bounded by the "persistence" gap).
- Partial stability of clusters allows to establish correspondences between clusters across the different runs $\rightarrow$ for any $x \in X$, a vector giving the probability for x to belong to each cluster.

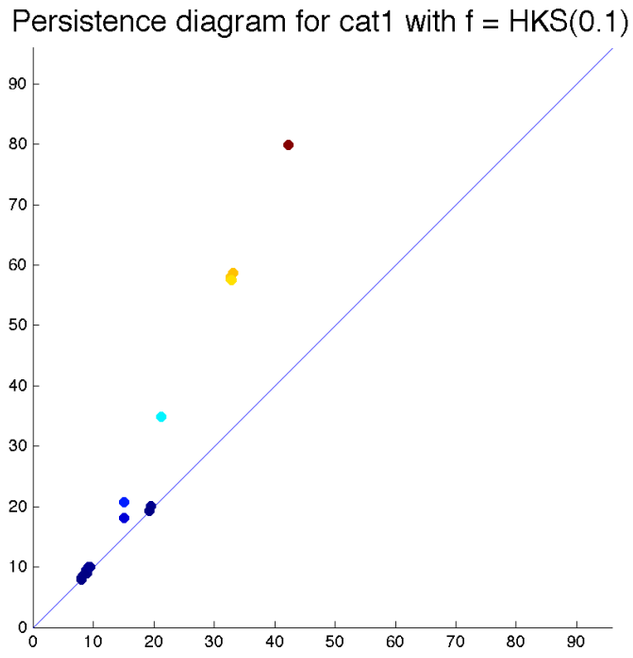
Application to non-rigid shape segmentation

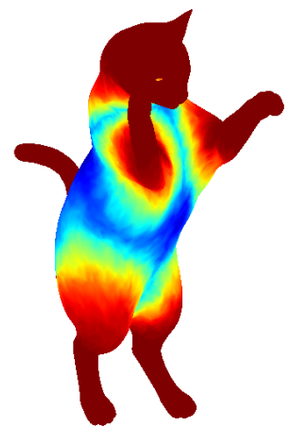
[Skraba, Ovsjanikov, C.,Guibas, NORDIA 10]







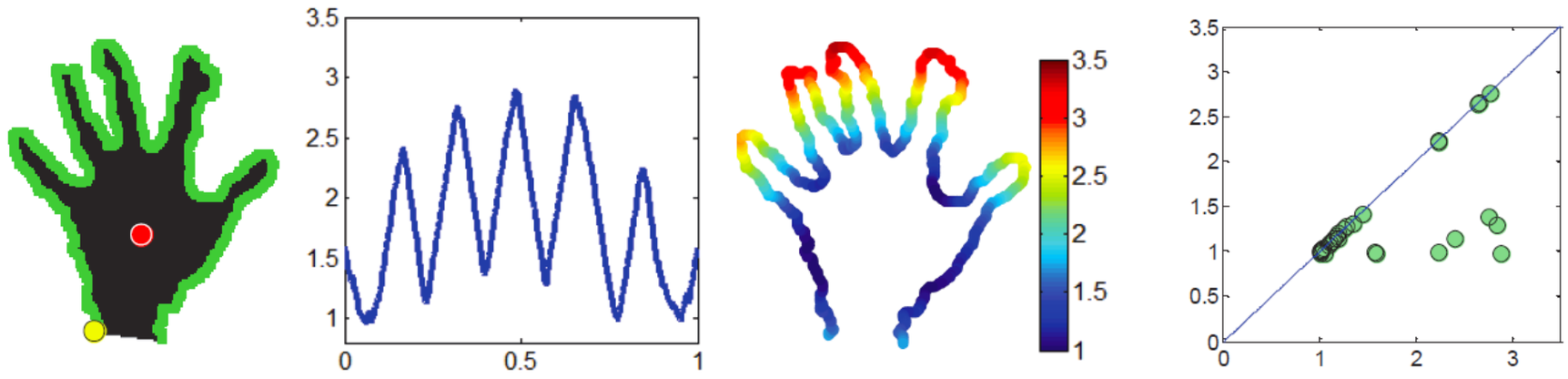




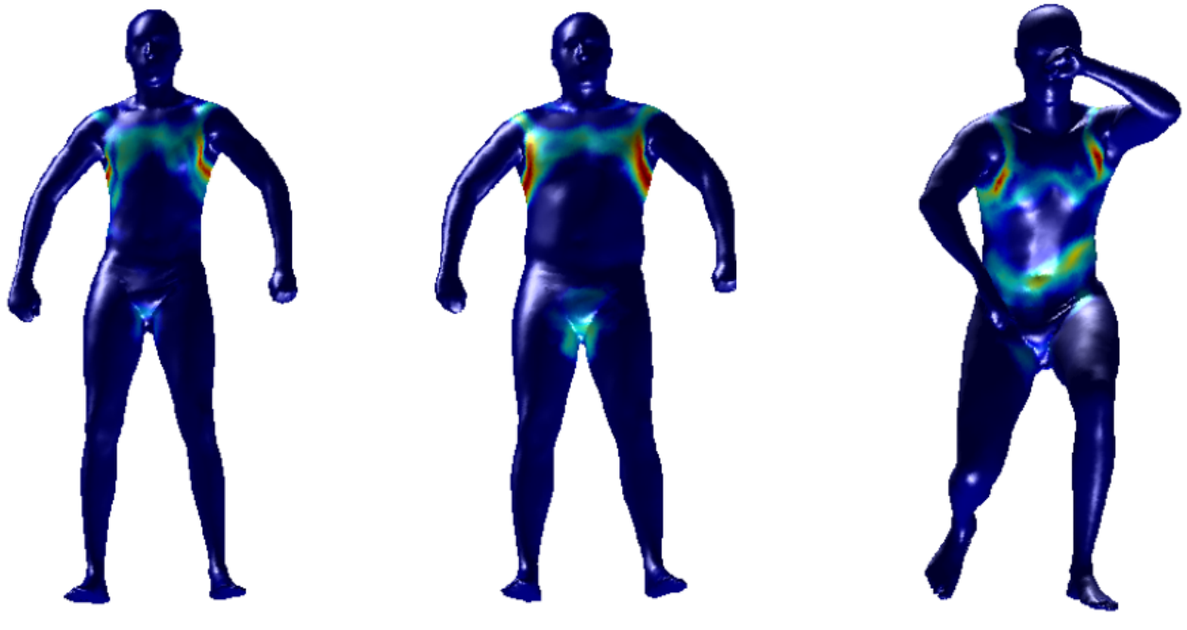
Other applications: classification, object recognition

Examples:

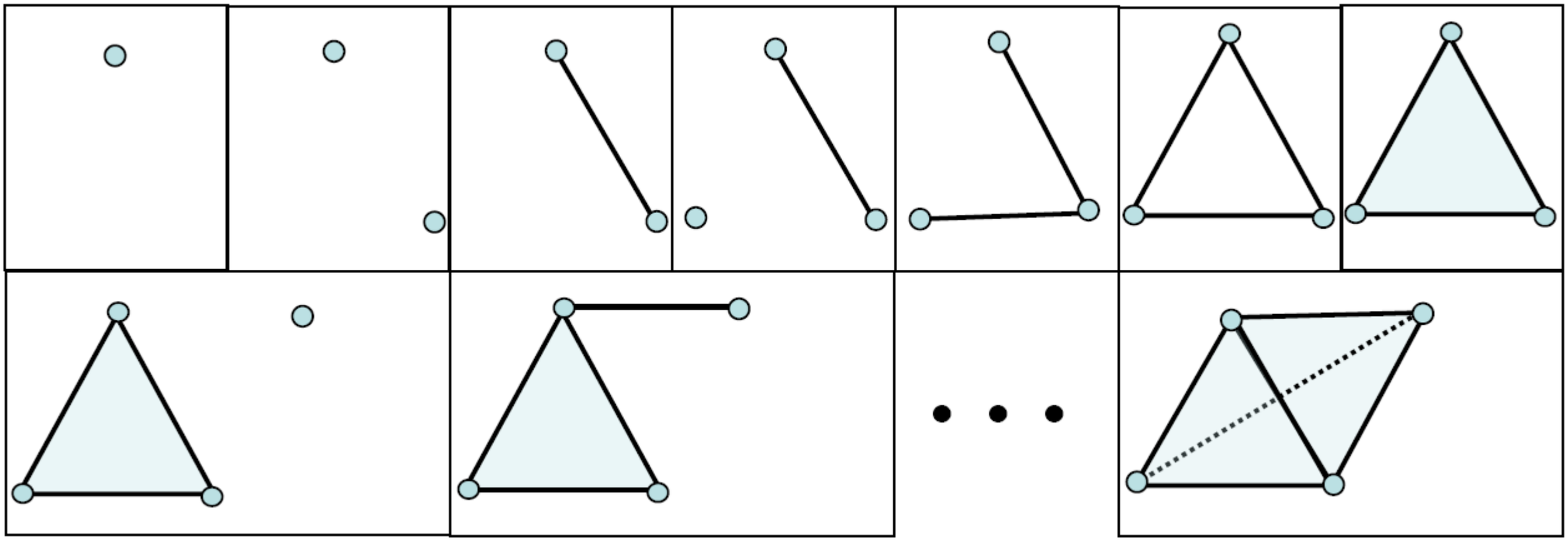
- Hand gesture recognition [Li, Ovsjanikov, C. - CVPR'14]



- Persistence-based pooling for shape recognition [Bonis, Ovsjanikov, Oudot, C. 2015]



Filtrations of simplicial complexes



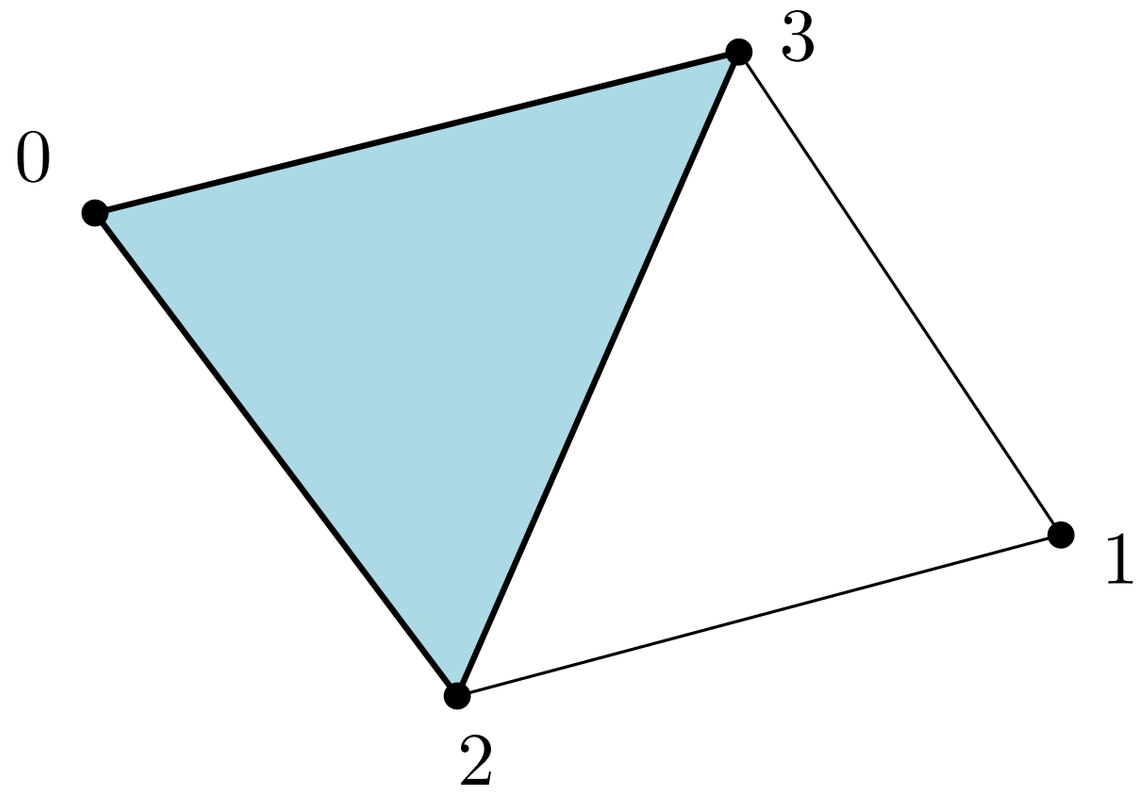
A filtration of a (finite) simplicial complex K is a sequence of subcomplexes such that

i) $\emptyset = K^0 \subset K^1 \subset \cdots \subset K^m = K$,

ii) $K^{i+1} = K^i \cup \sigma^{i+1}$ where σ^{i+1} is a simplex of K.

There are many ways to build filtrations - see the following of the course.

Sublevel set filtration associated to a function



- f a real valued function defined on the vertices of K
- For $\sigma = [v_0, \cdots, v_k] \in K$, $f(\sigma) = \max_{i=0,\cdots,k} f(v_i)$
- The simplices of K are ordered according increasing f values (and dimension in case of equal values on different simplices).

Exercise: show that this is a filtration

General case: if $f : X \to \mathbb{R}$, X a topological space, $\forall t \leq t' \in \mathbb{R}$, $f^{-1}((-\infty, t]) \subseteq f^{-1}((-\infty, t']) \to$ filtration of X by the sublevel sets of f.

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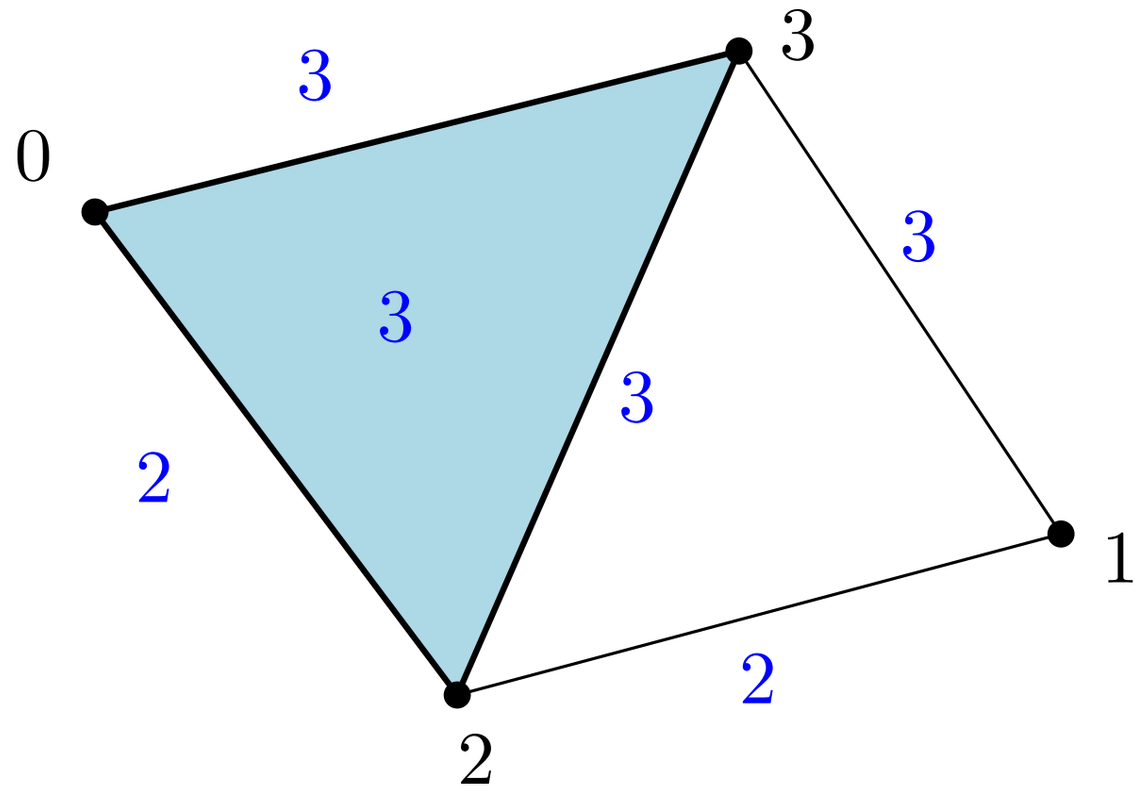

Note: the upper level set filtration is defined similarly

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