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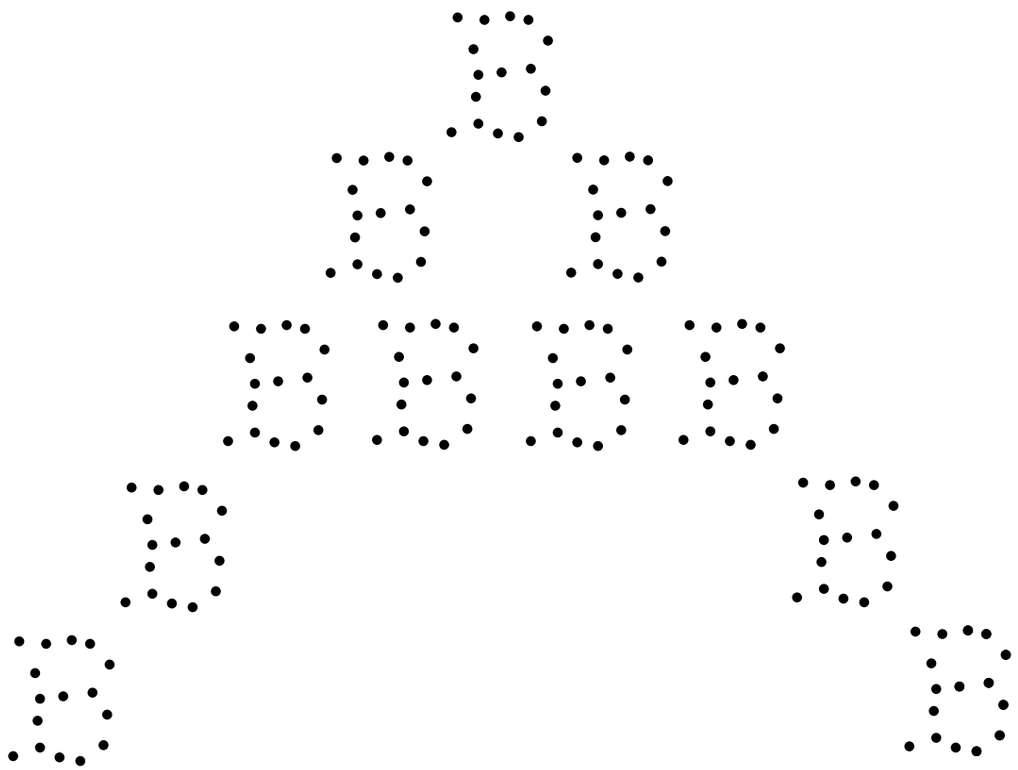

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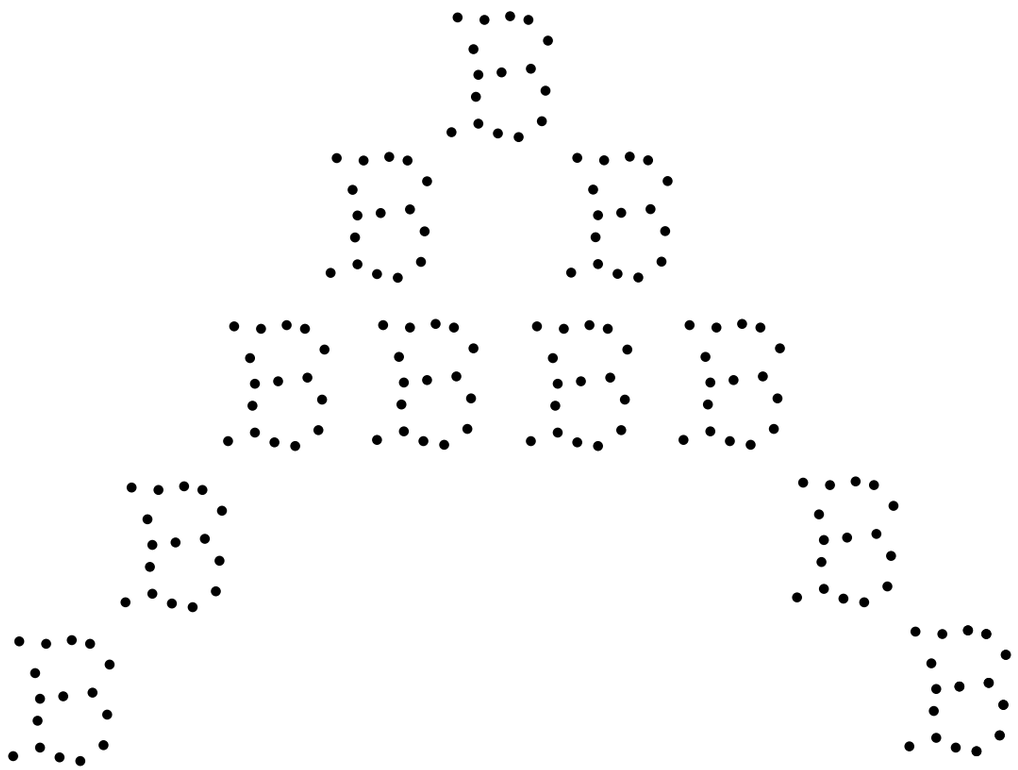

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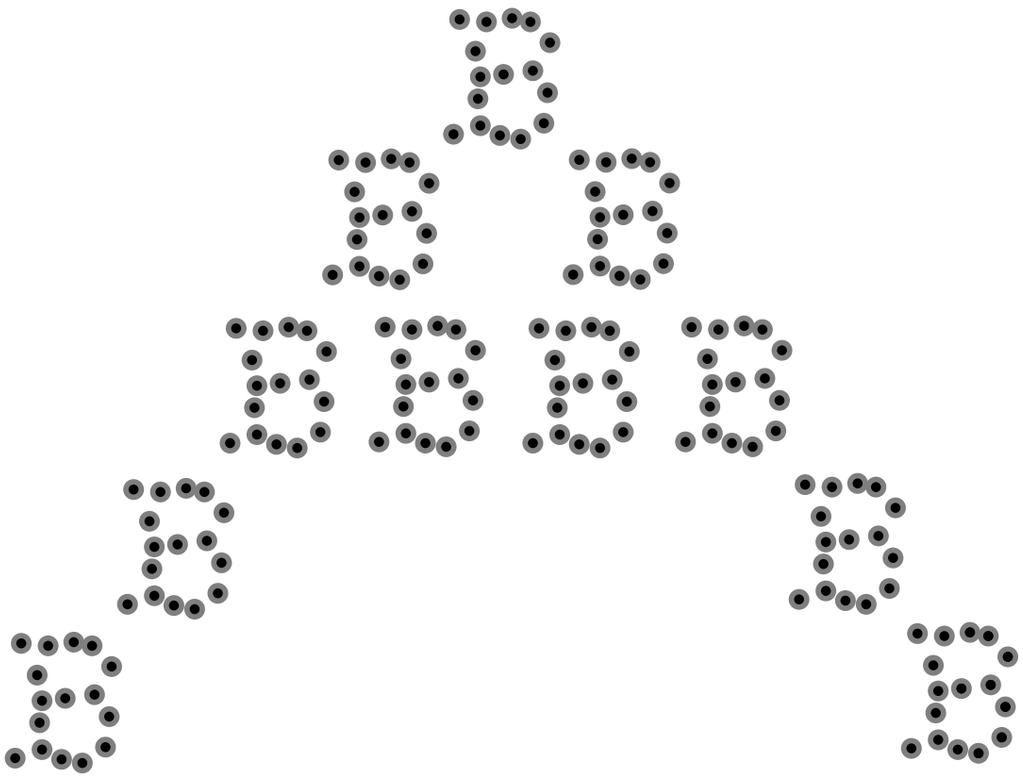

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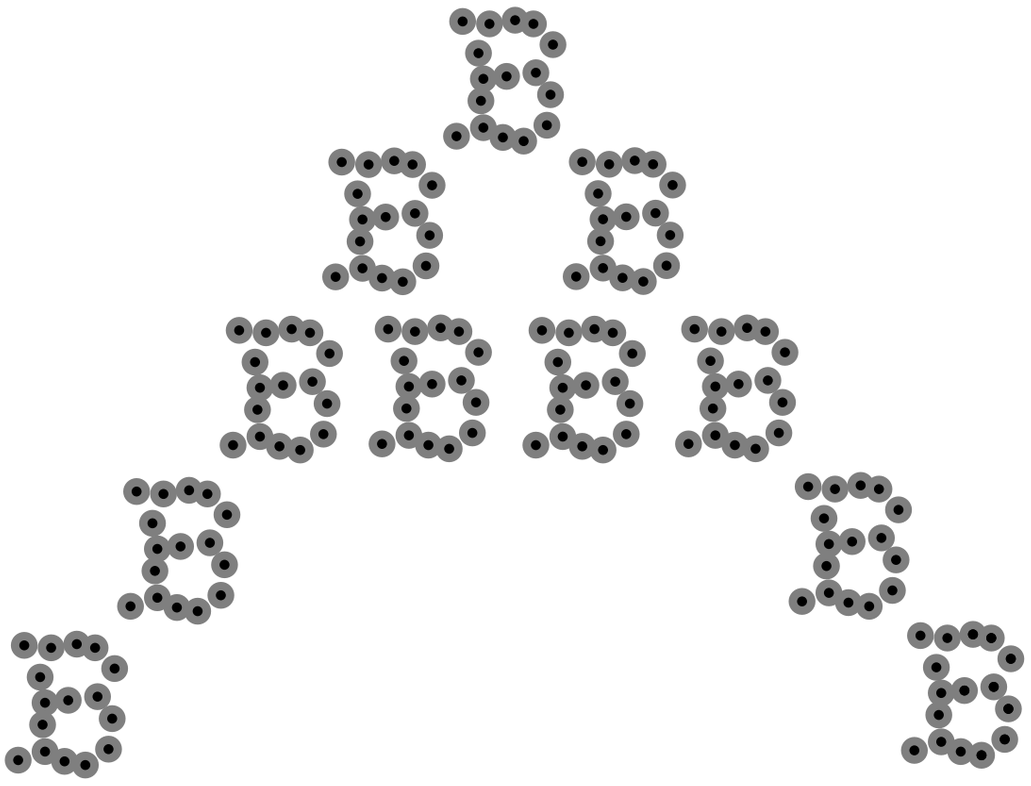

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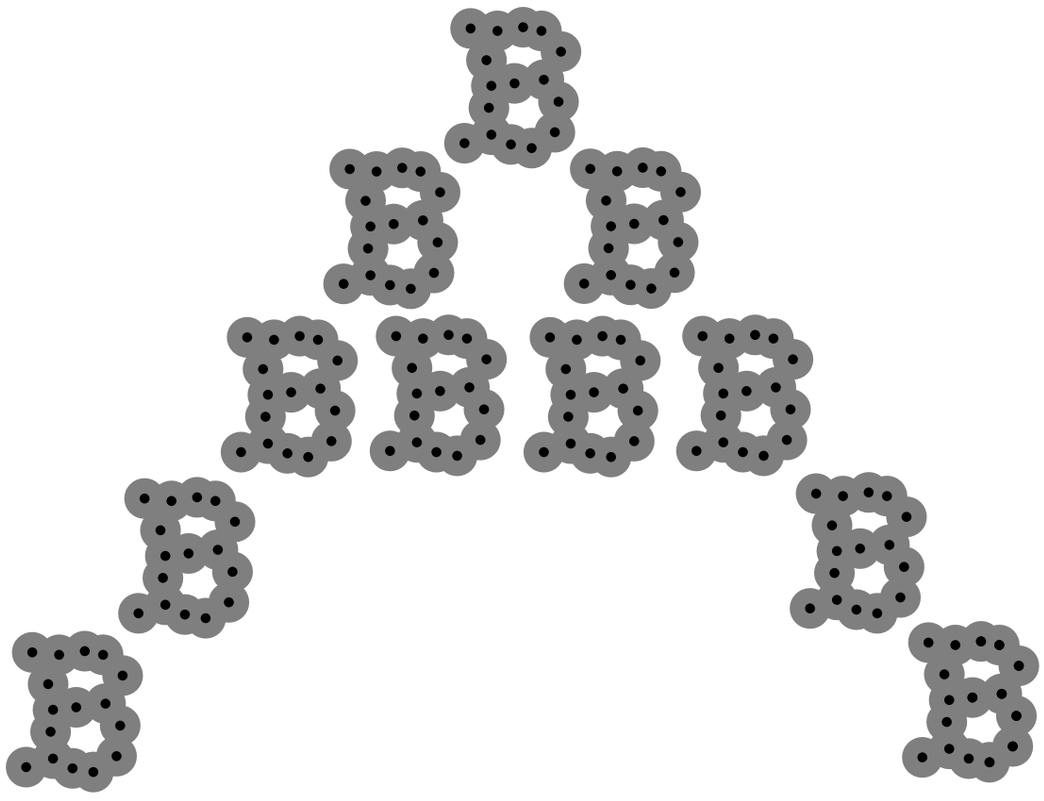

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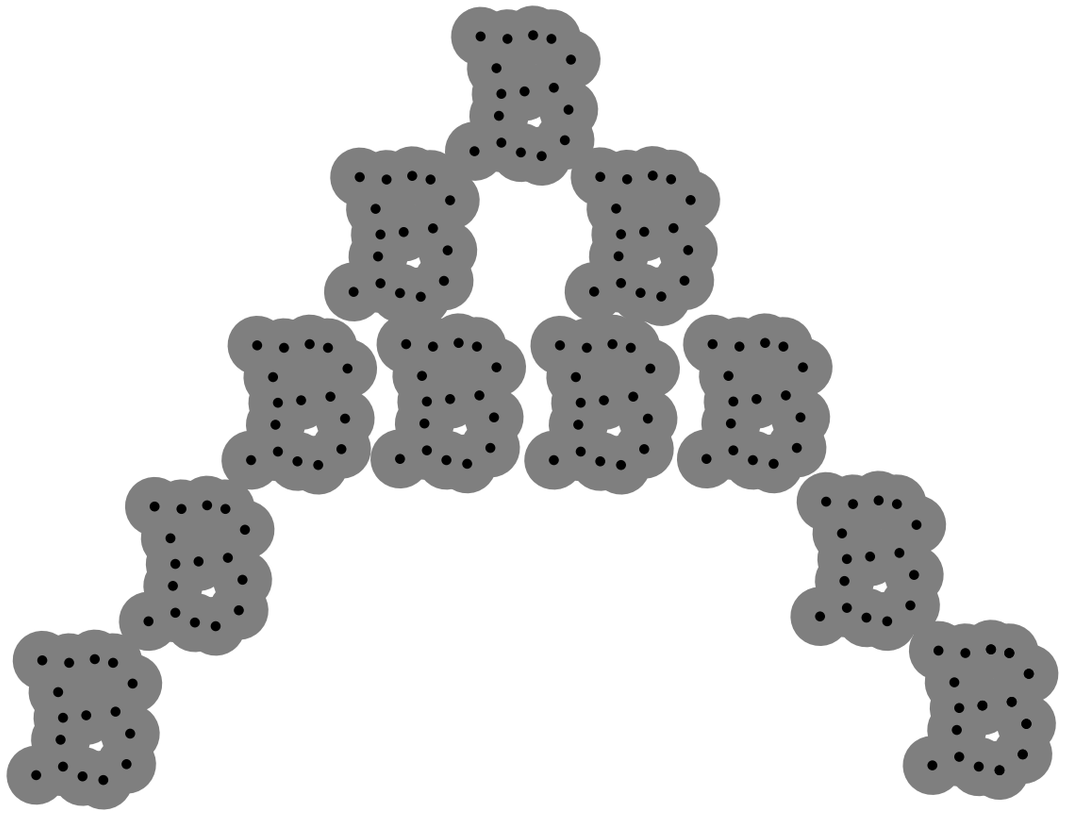

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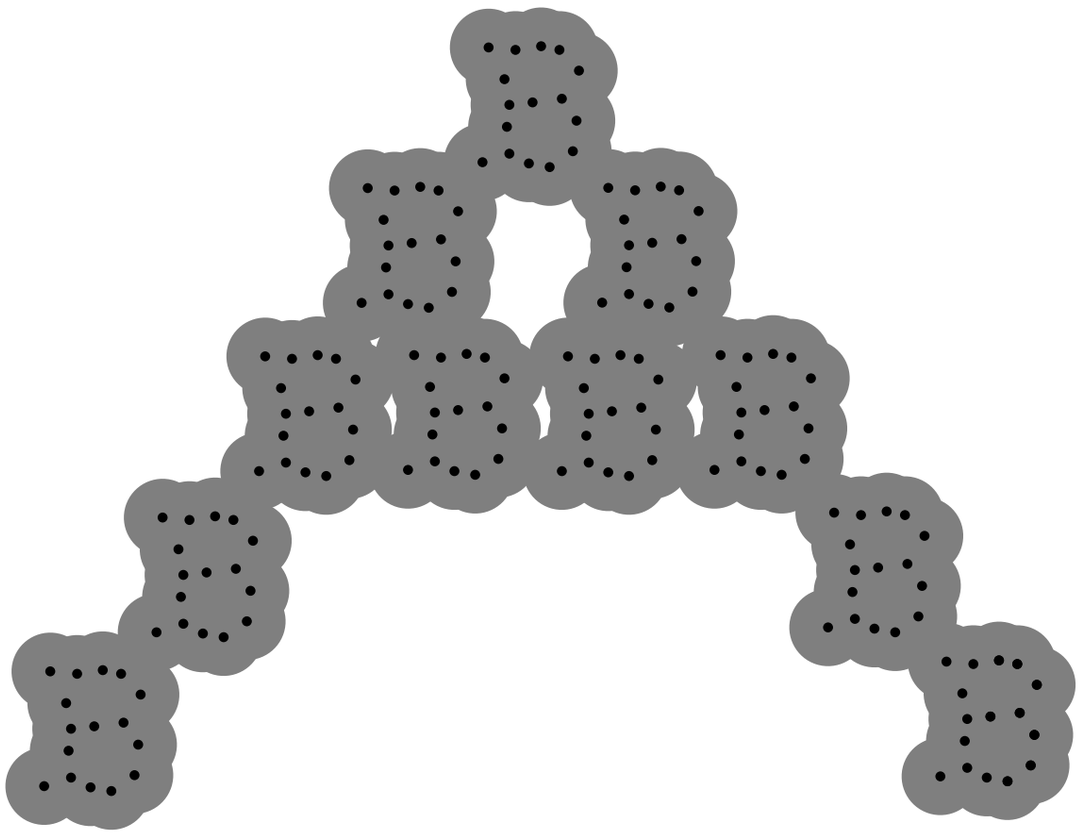

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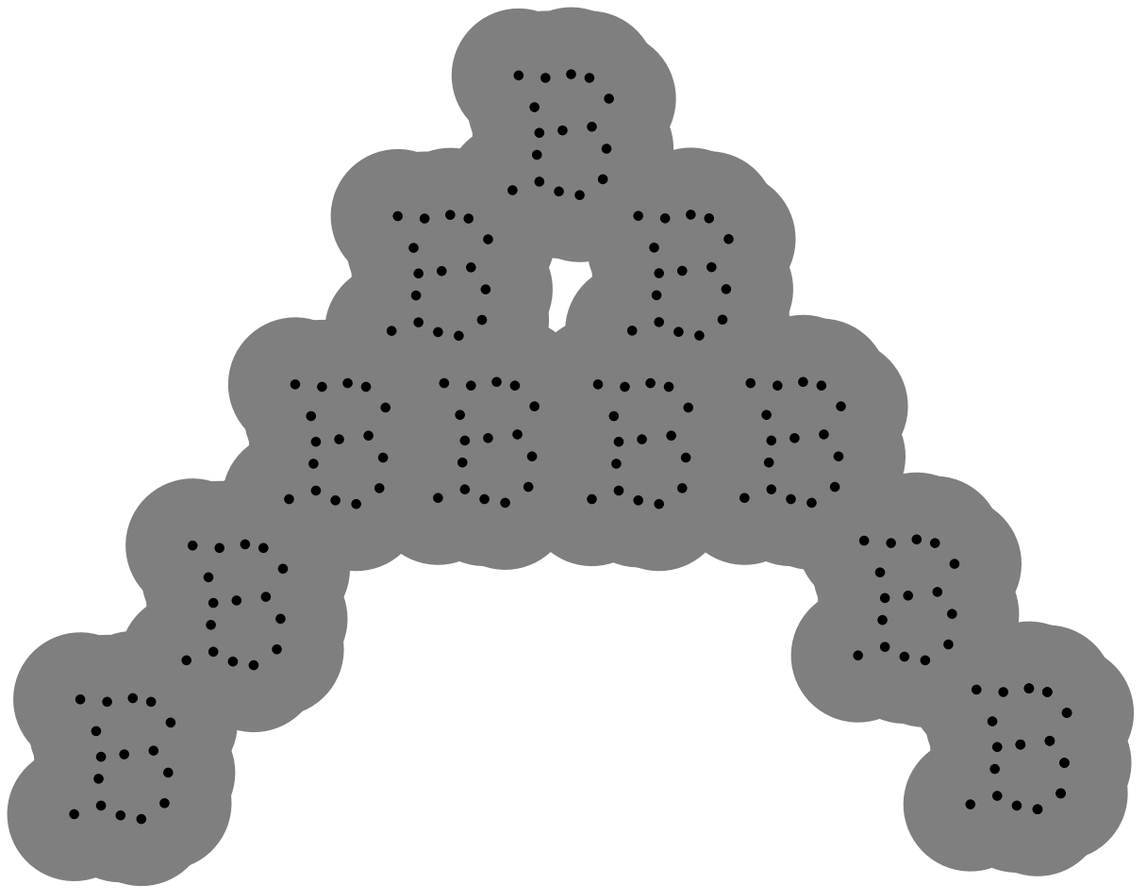

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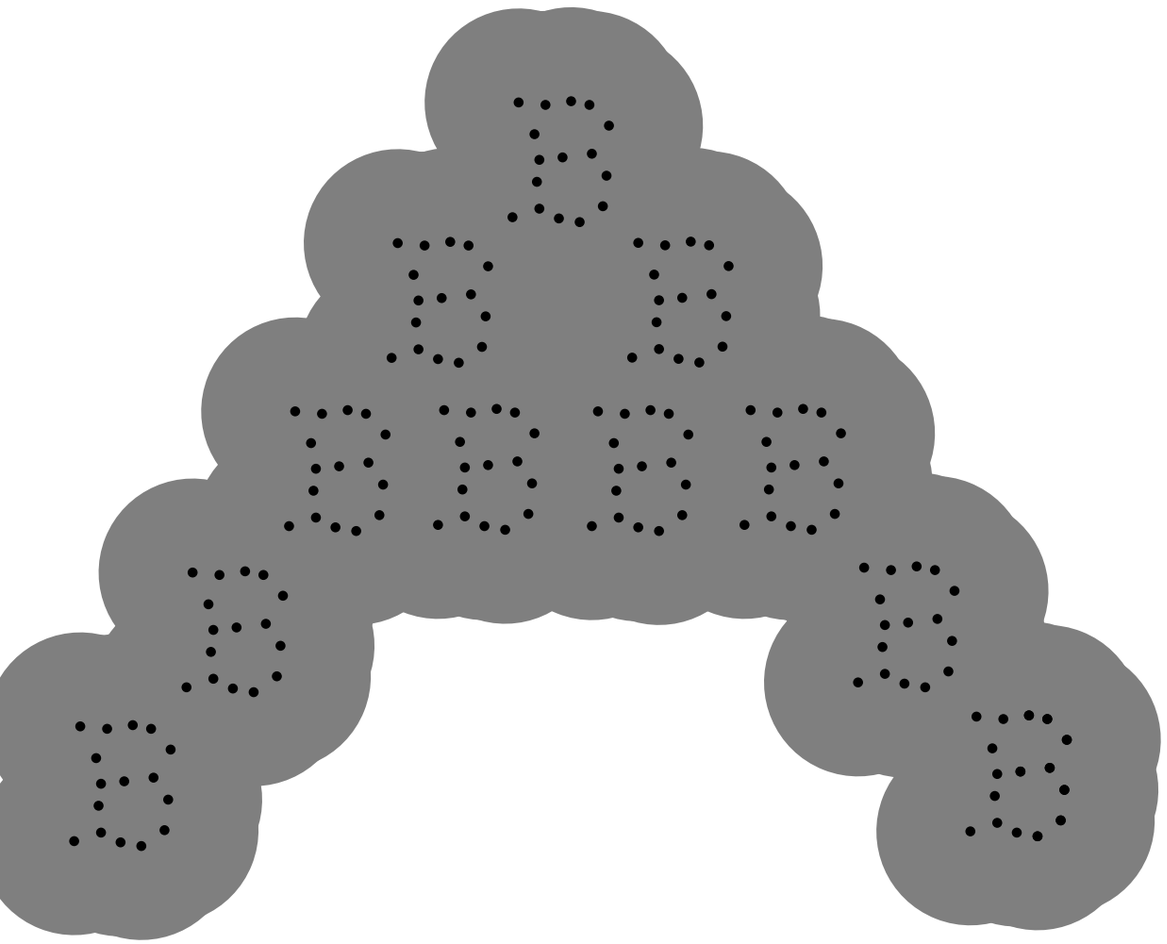

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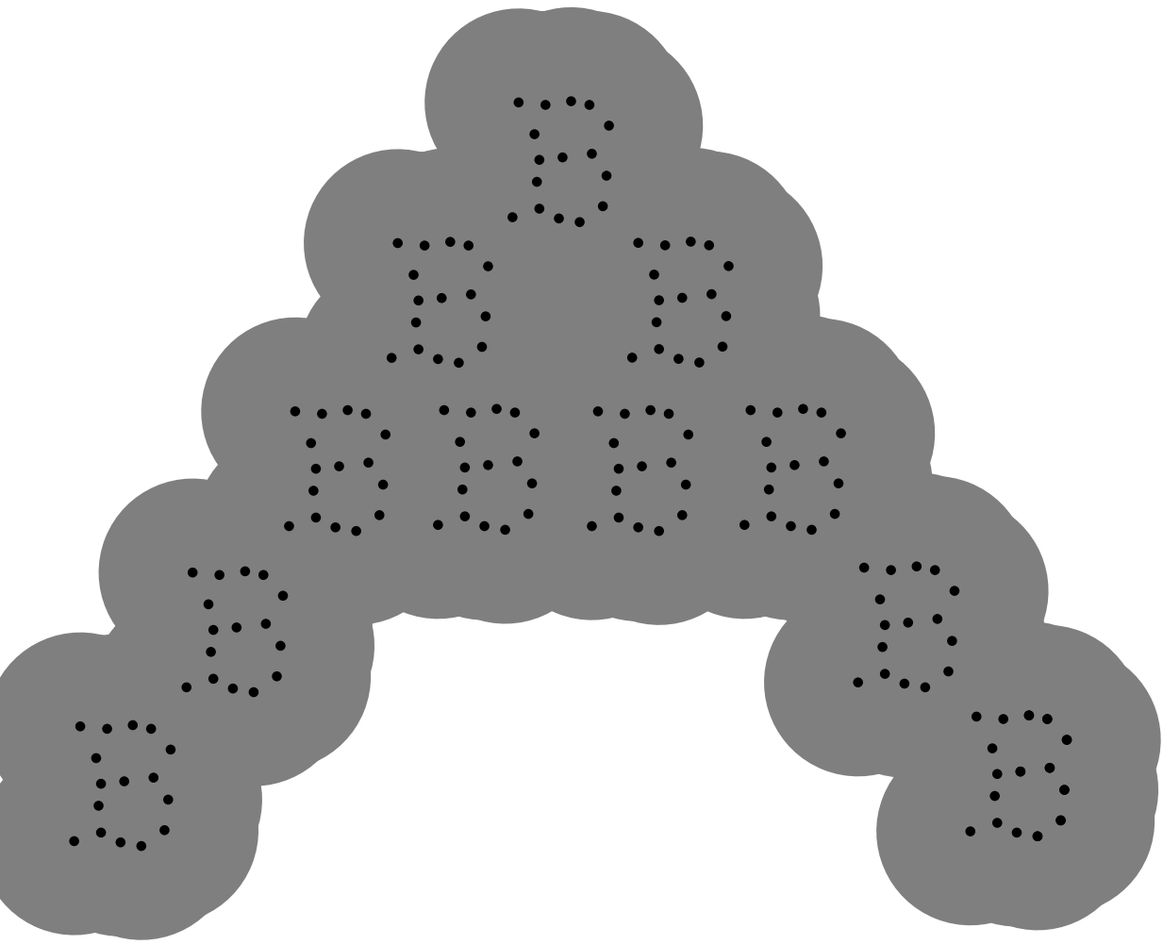

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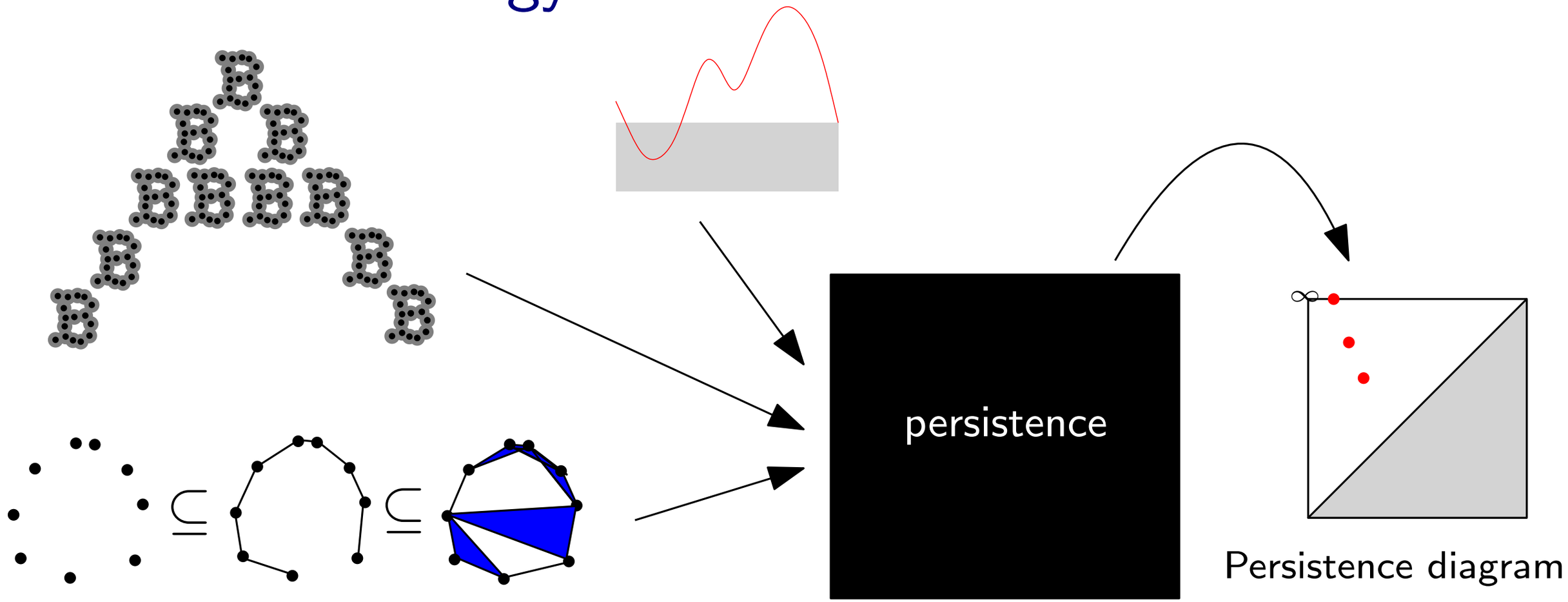
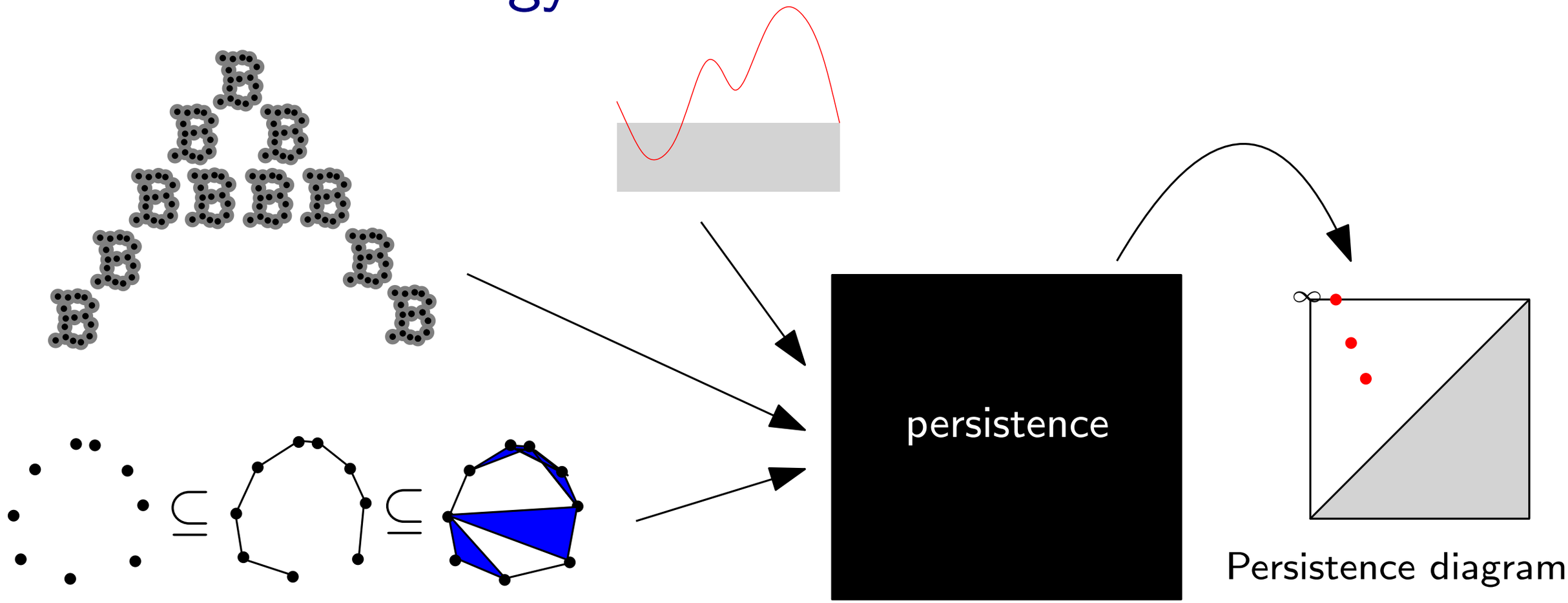
Persistent homology aims at encoding the homology of the complex at *all possible scales* into a compact descriptor.

Persistent homology



What is persistent homology?

Persistent homology

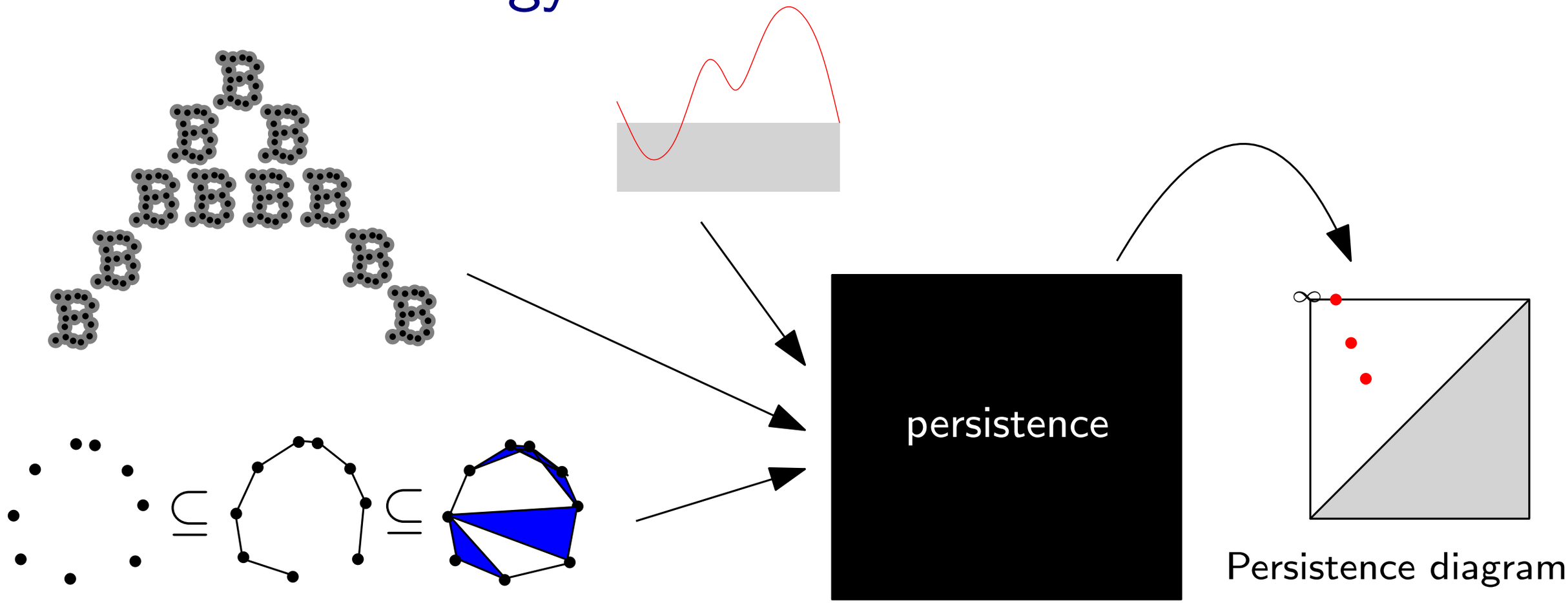


What is persistent homology?

$\rightarrow$ a mathematical framework for encoding the evolution of the homology of filtrations of simplicial complexes (it also works for general filtered spaces).

$\rightarrow$ formalized by H. Edelsbrunner et al. (2002) and G. Carlsson et al. (2005) with wide developments during the last decade.

Persistent homology



What is persistent homology?

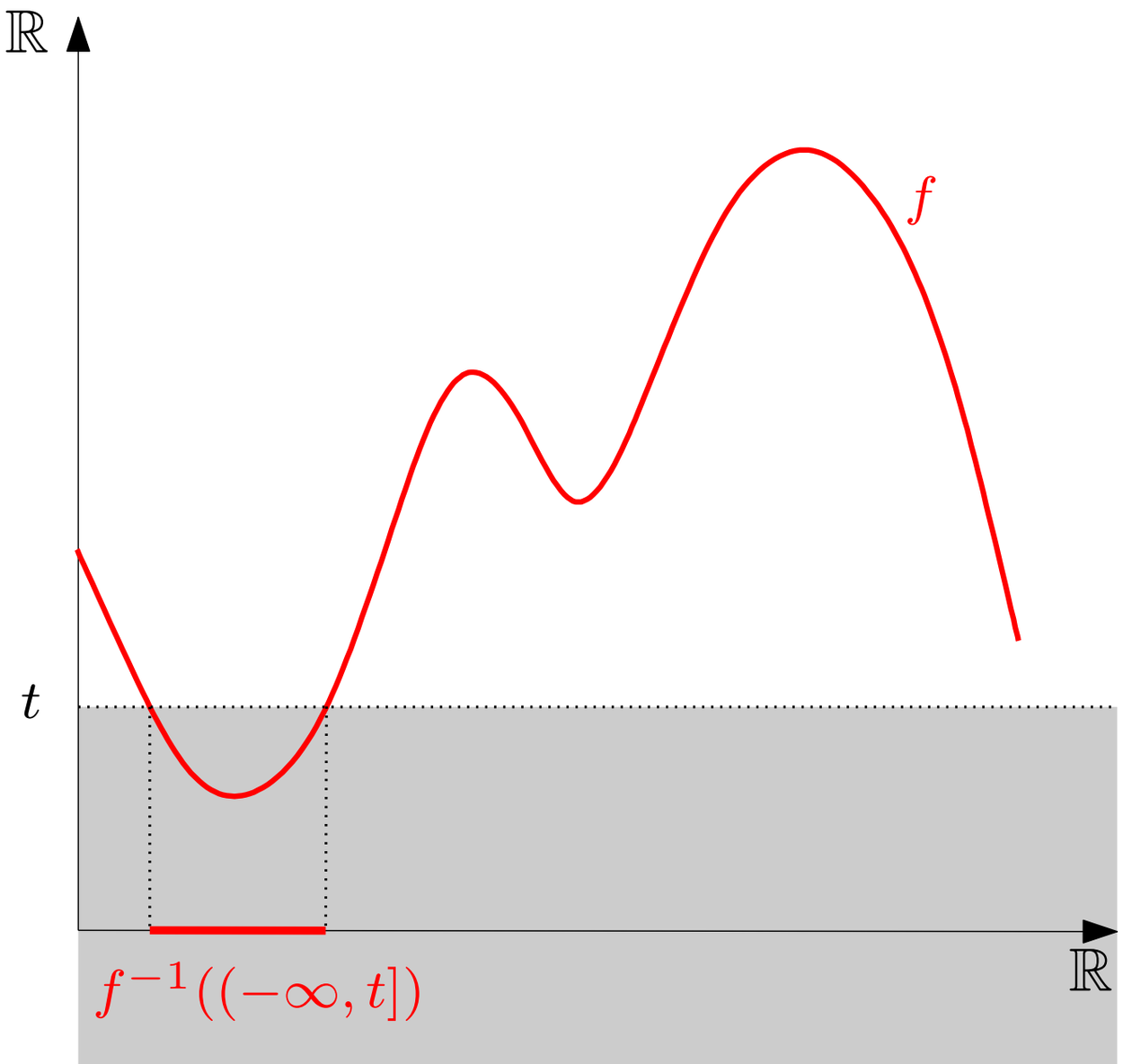
$\rightarrow$ barcodes/persistence diagrams can be efficiently computed.

$\rightarrow$ multiscale topological information.

$\rightarrow$ stability properties.

Example: persistence of sublevel sets of function

- input: *filtration* = nested family of sublevel-sets $f^{-1}((-\infty, t])$ for t ranging over $\mathbb{R}$
- track the evolution of the topology (homology) throughout the family



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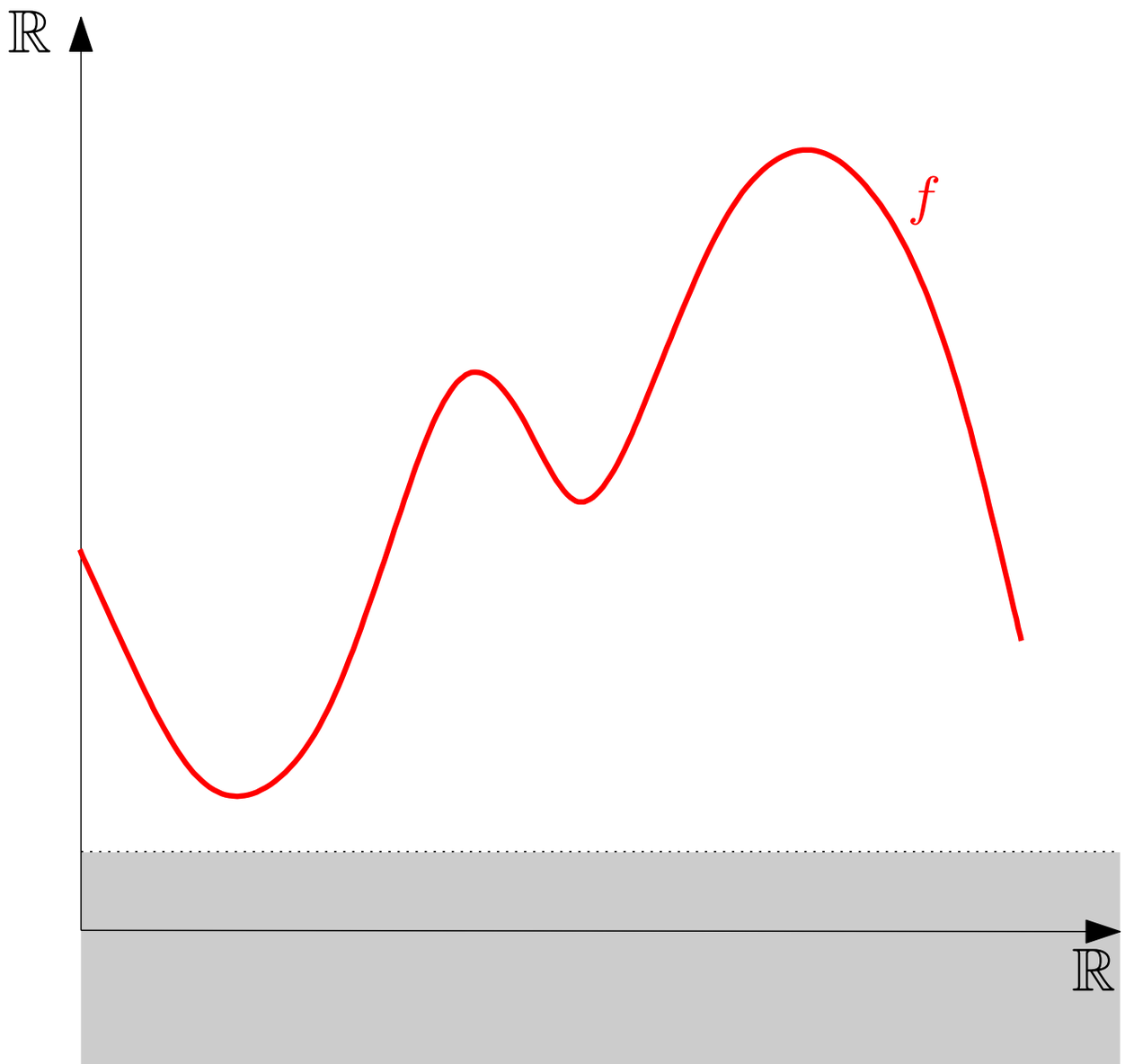

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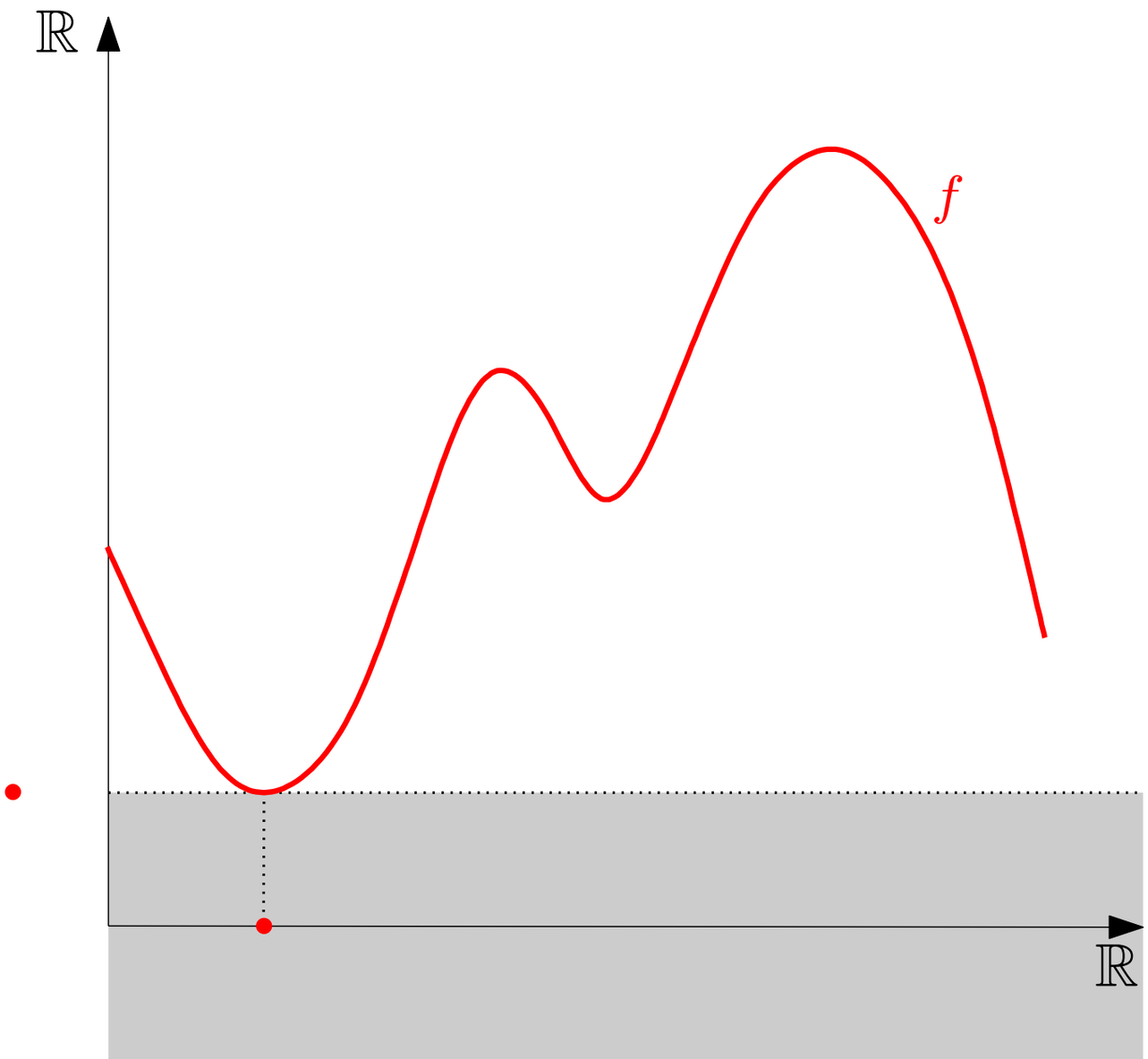

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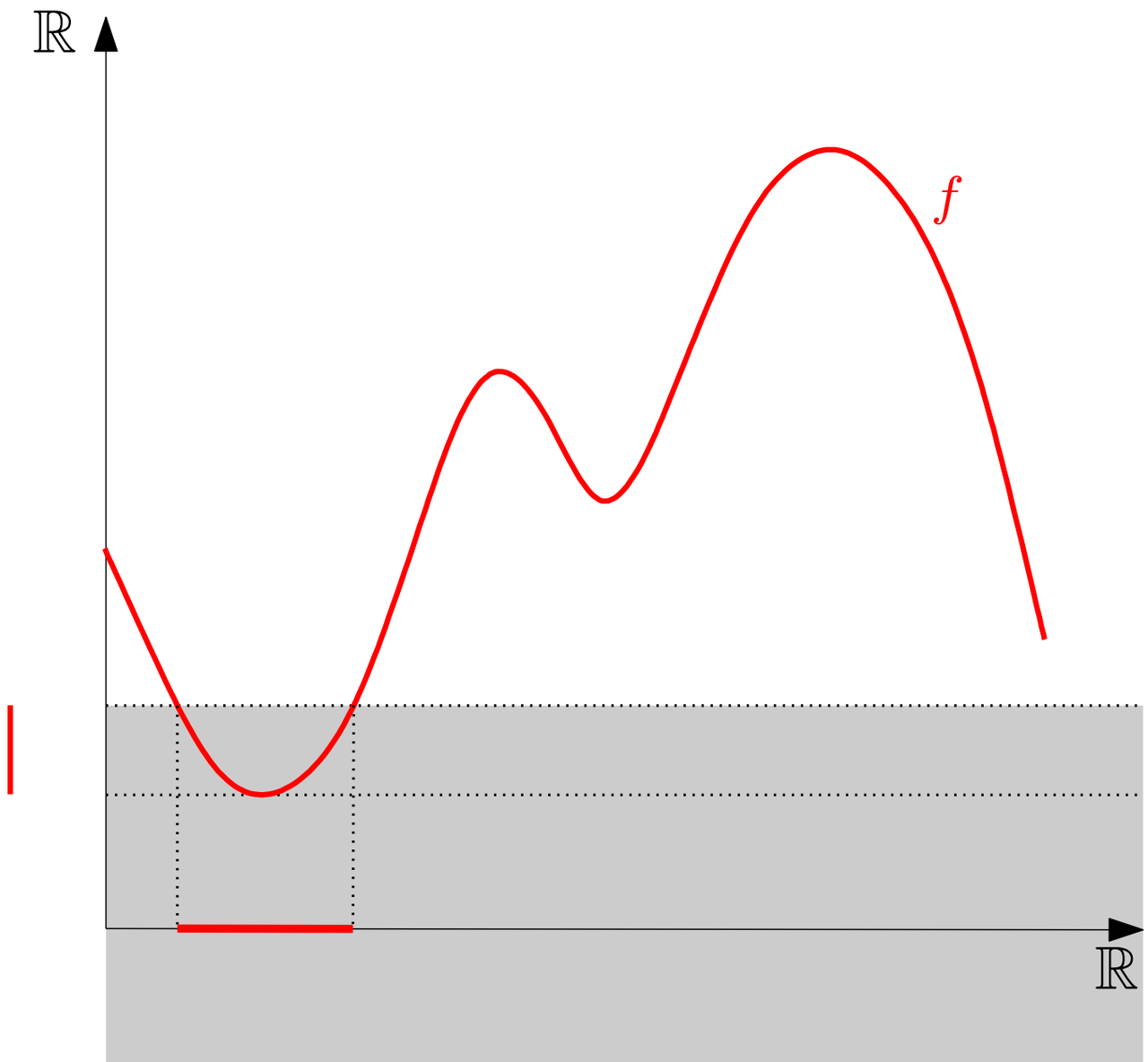

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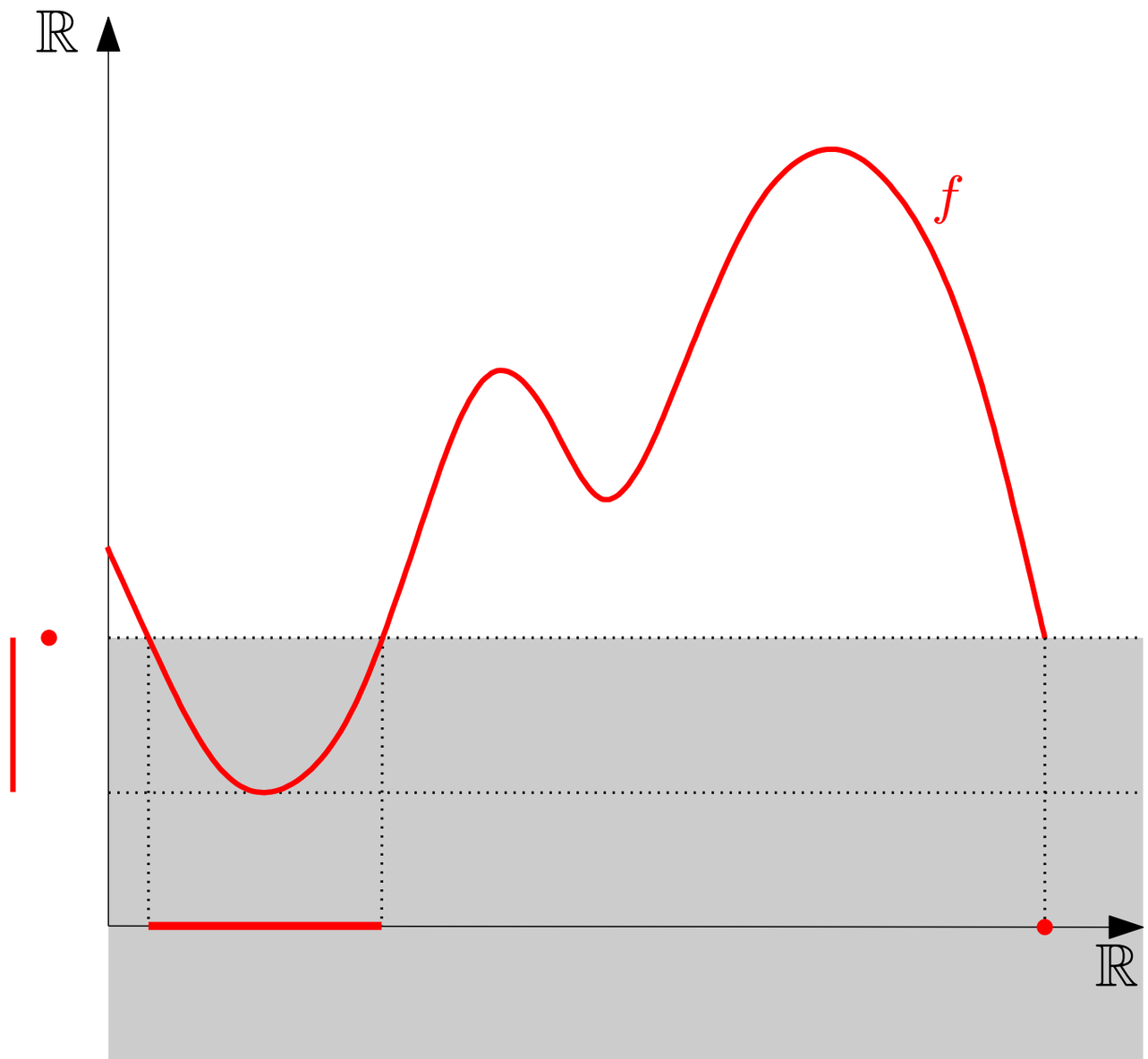

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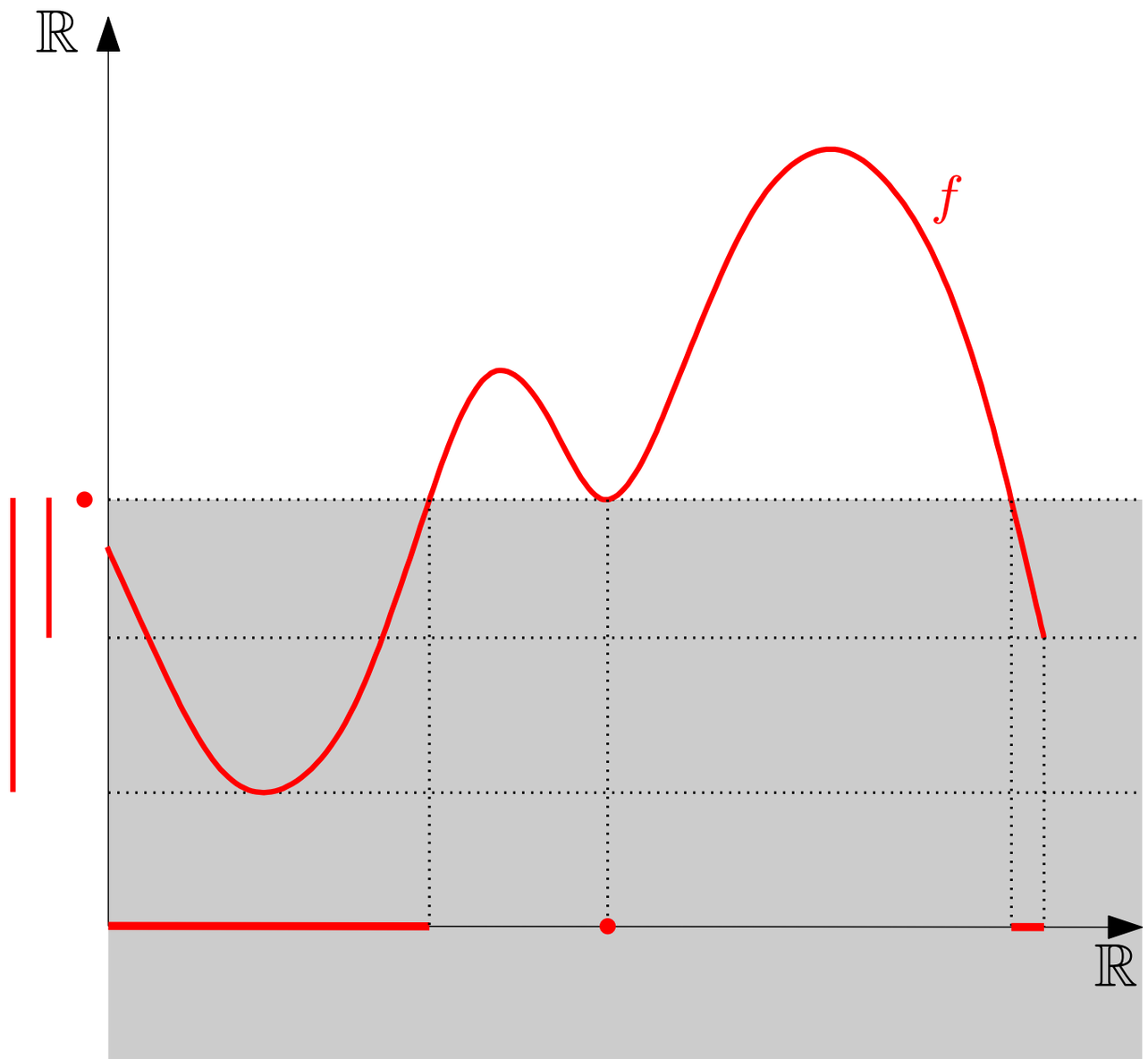

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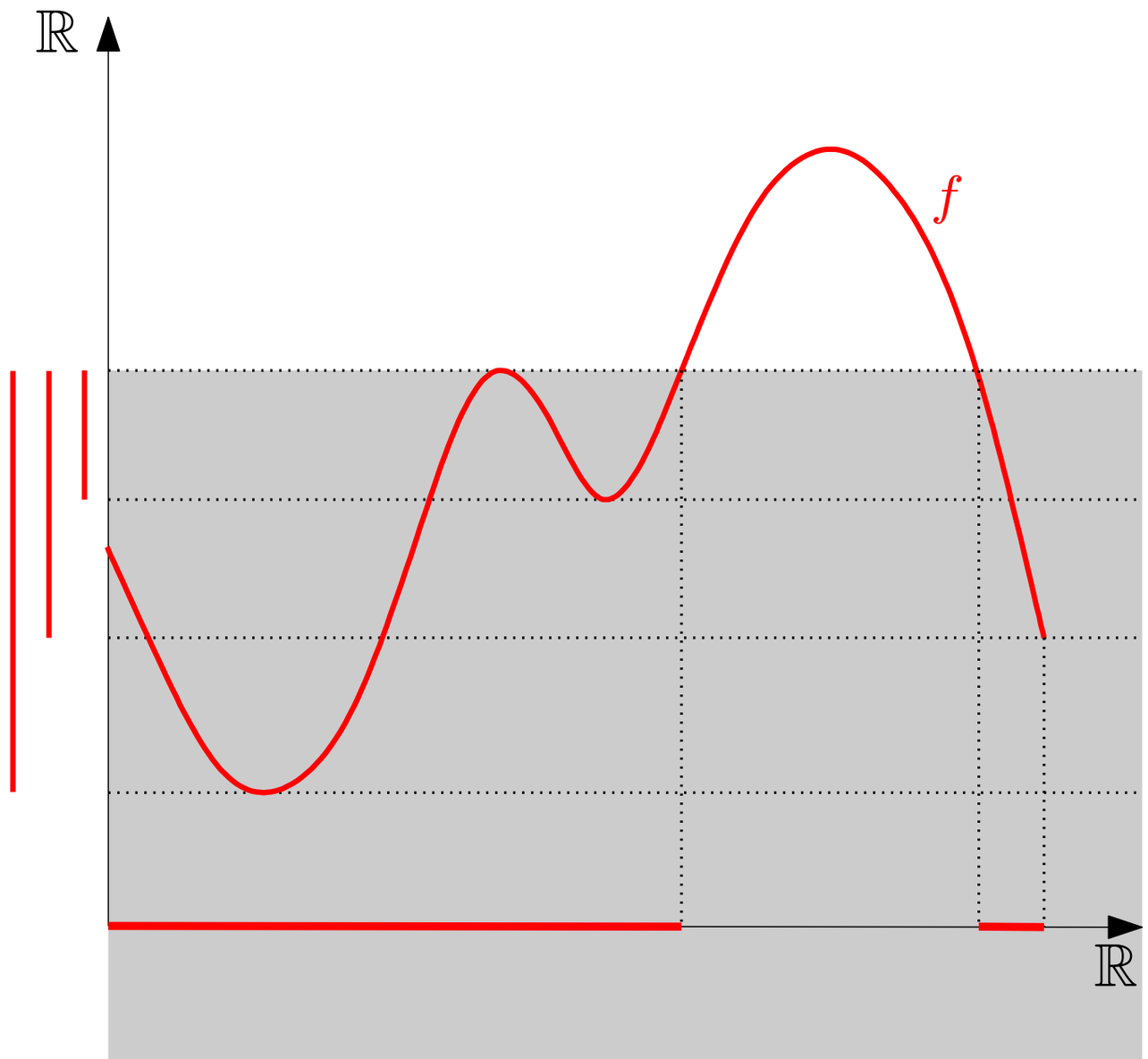

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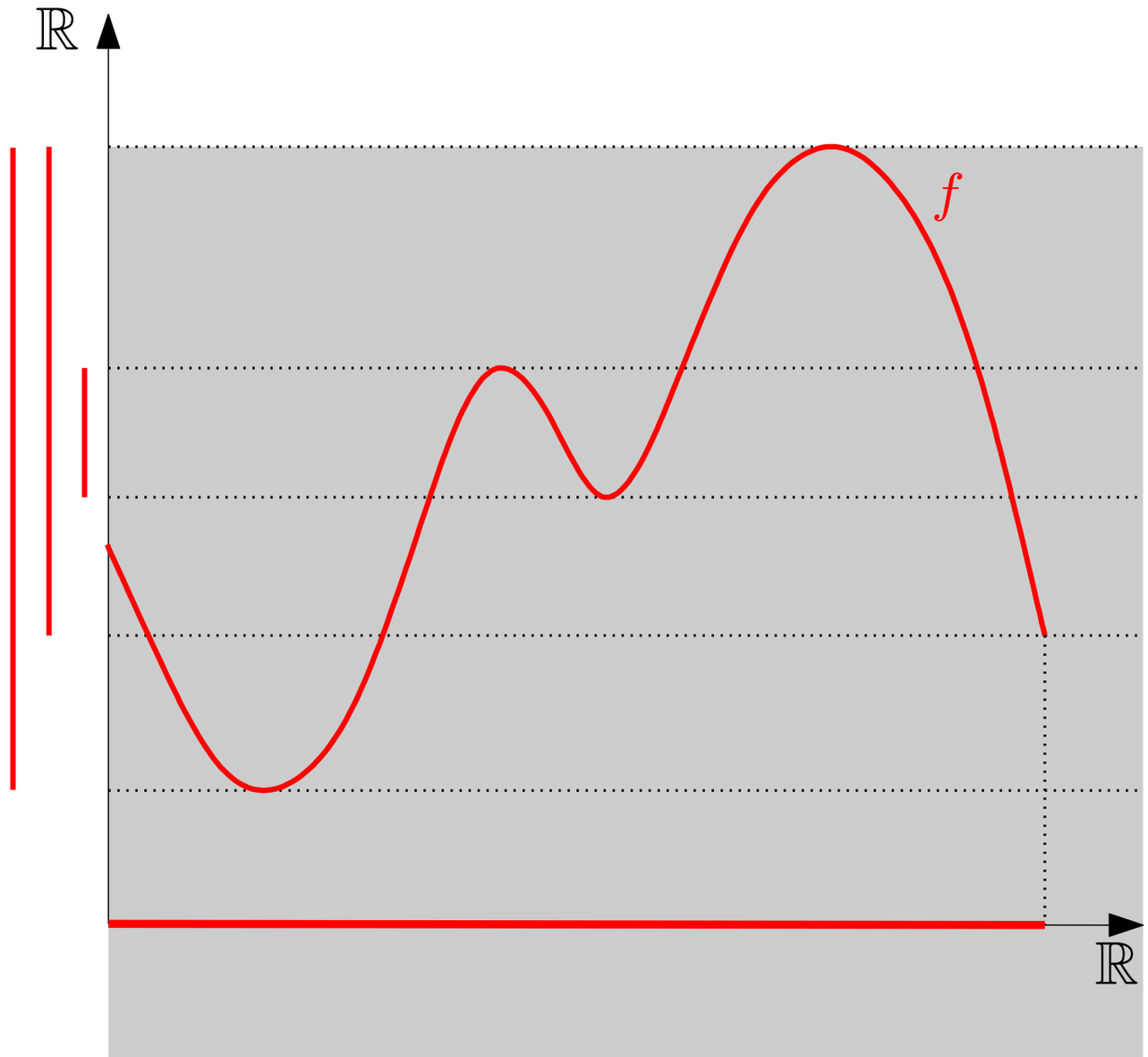

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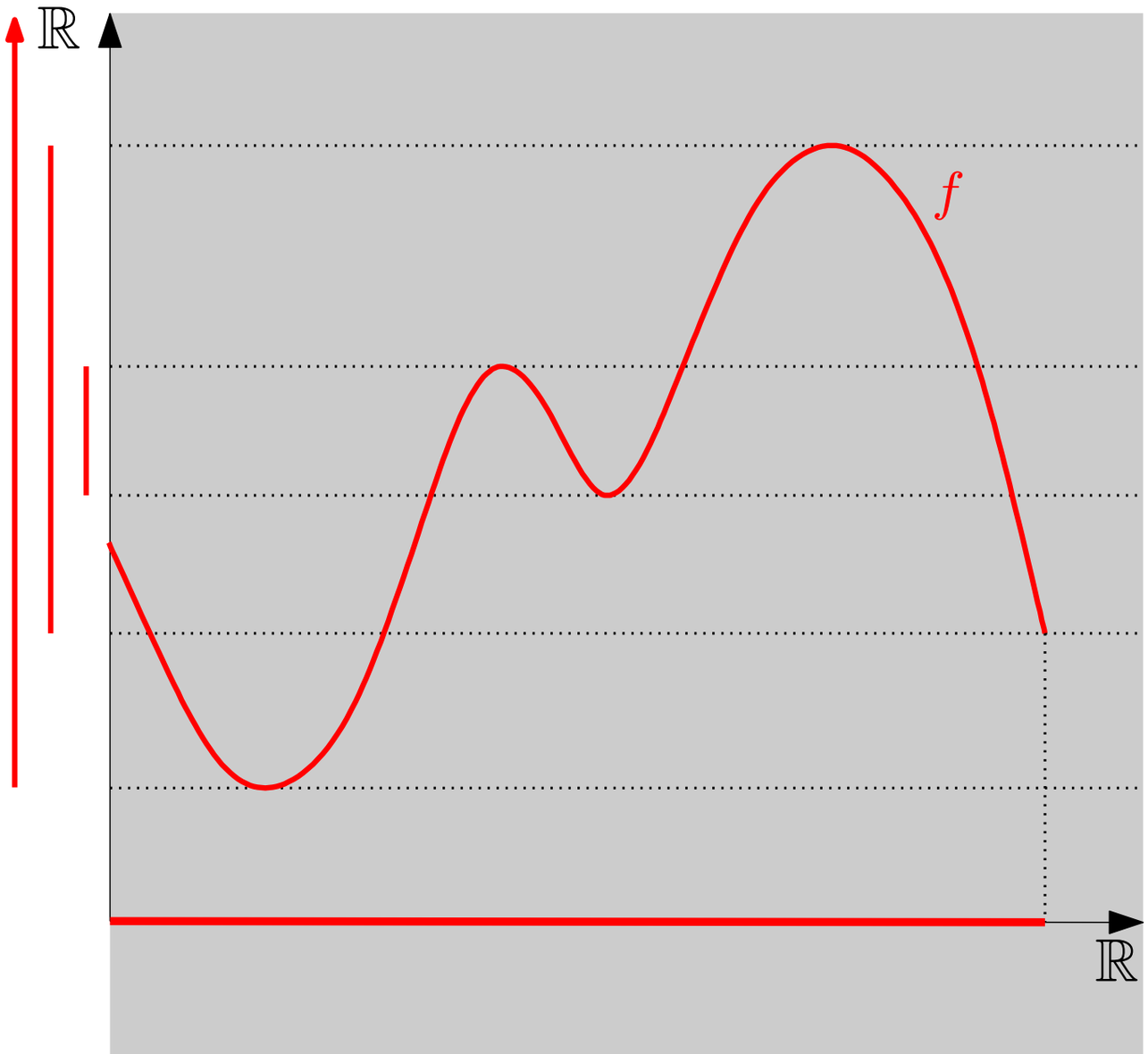

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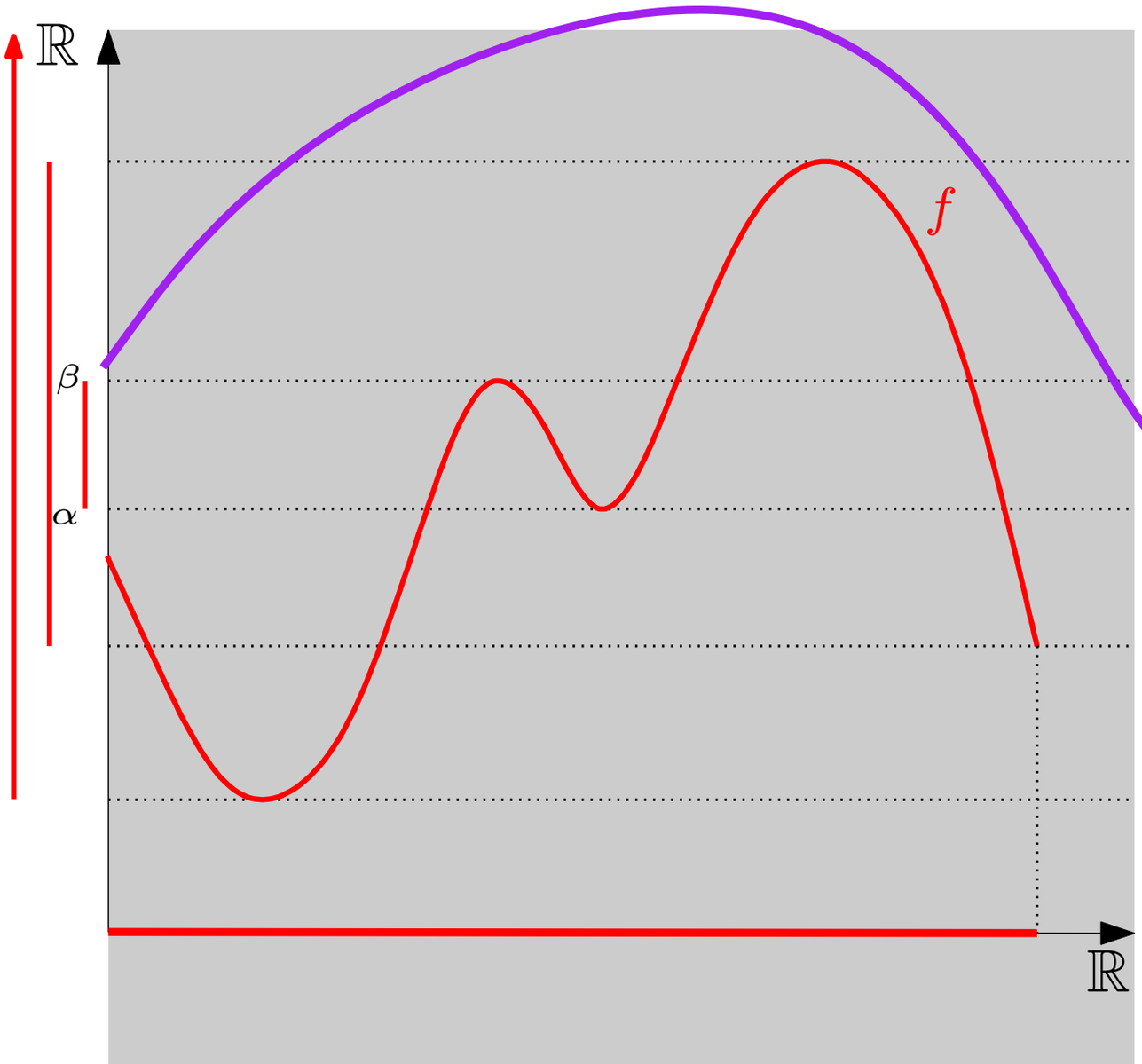
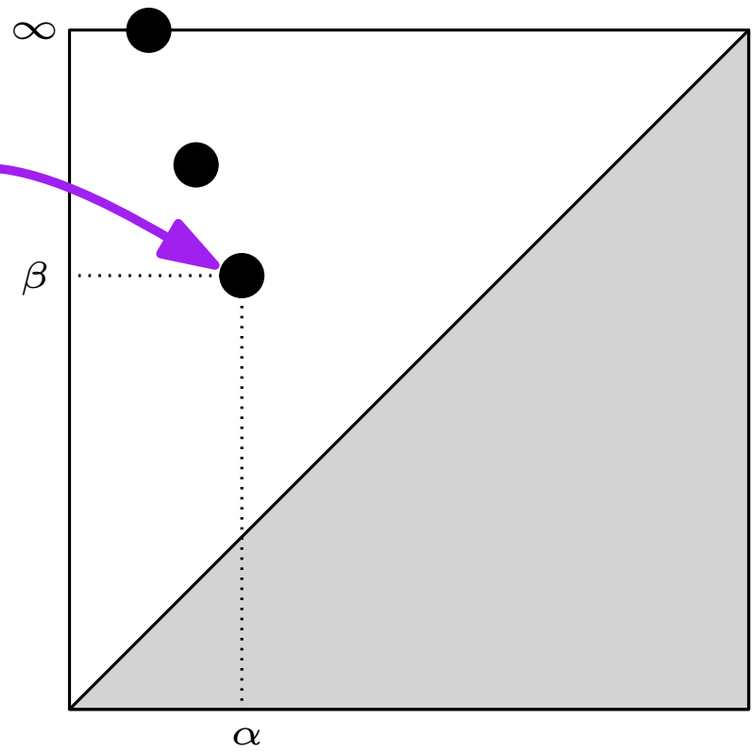


- alternate representation as a (multi-) set of points in the plane (*persistence diagram*).



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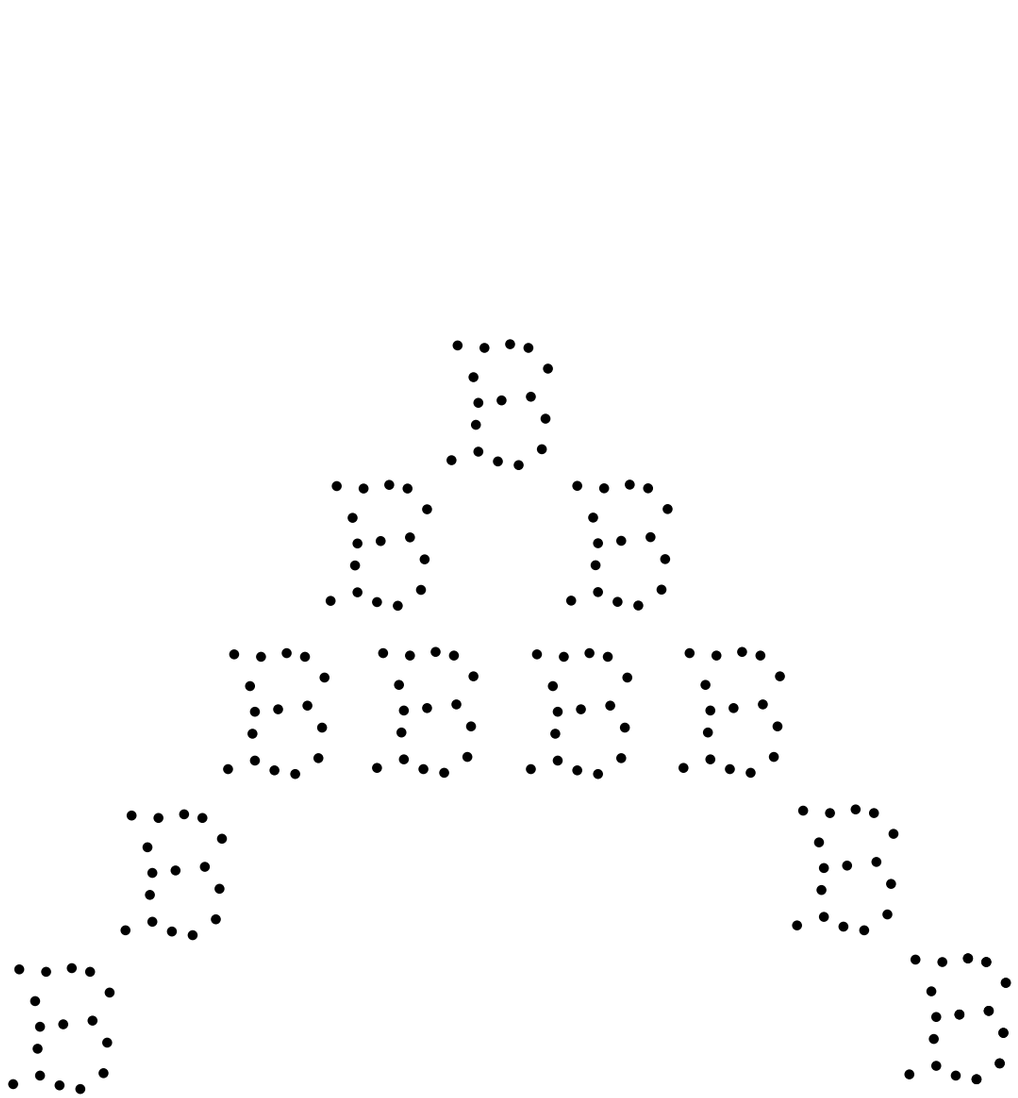

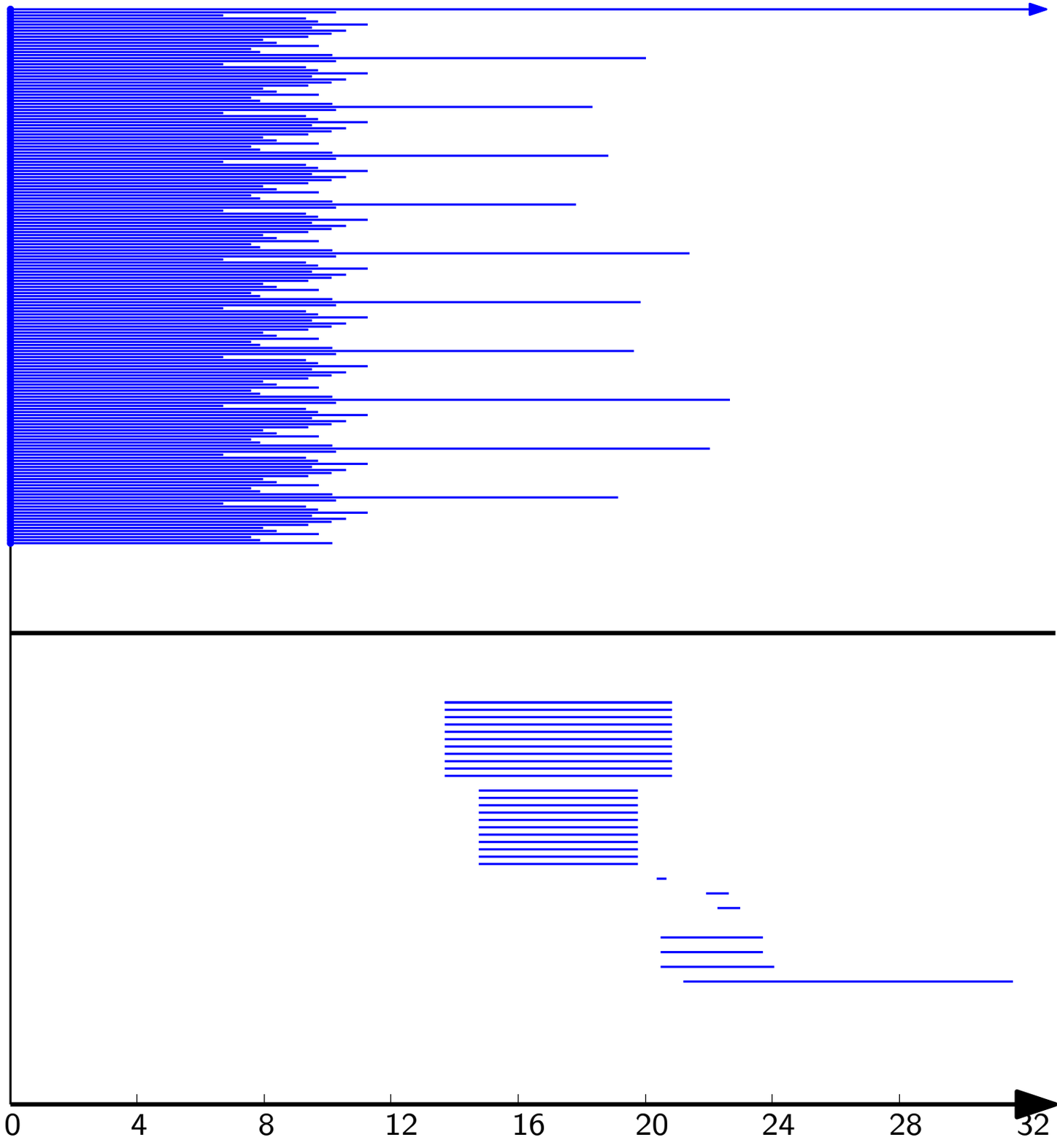

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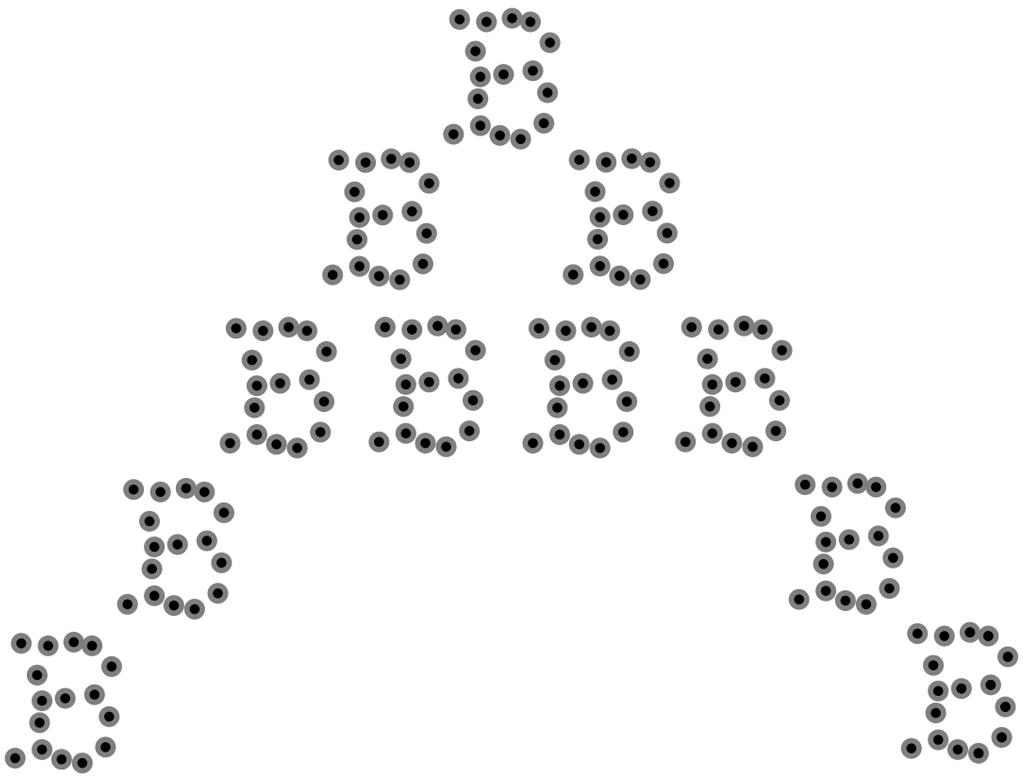

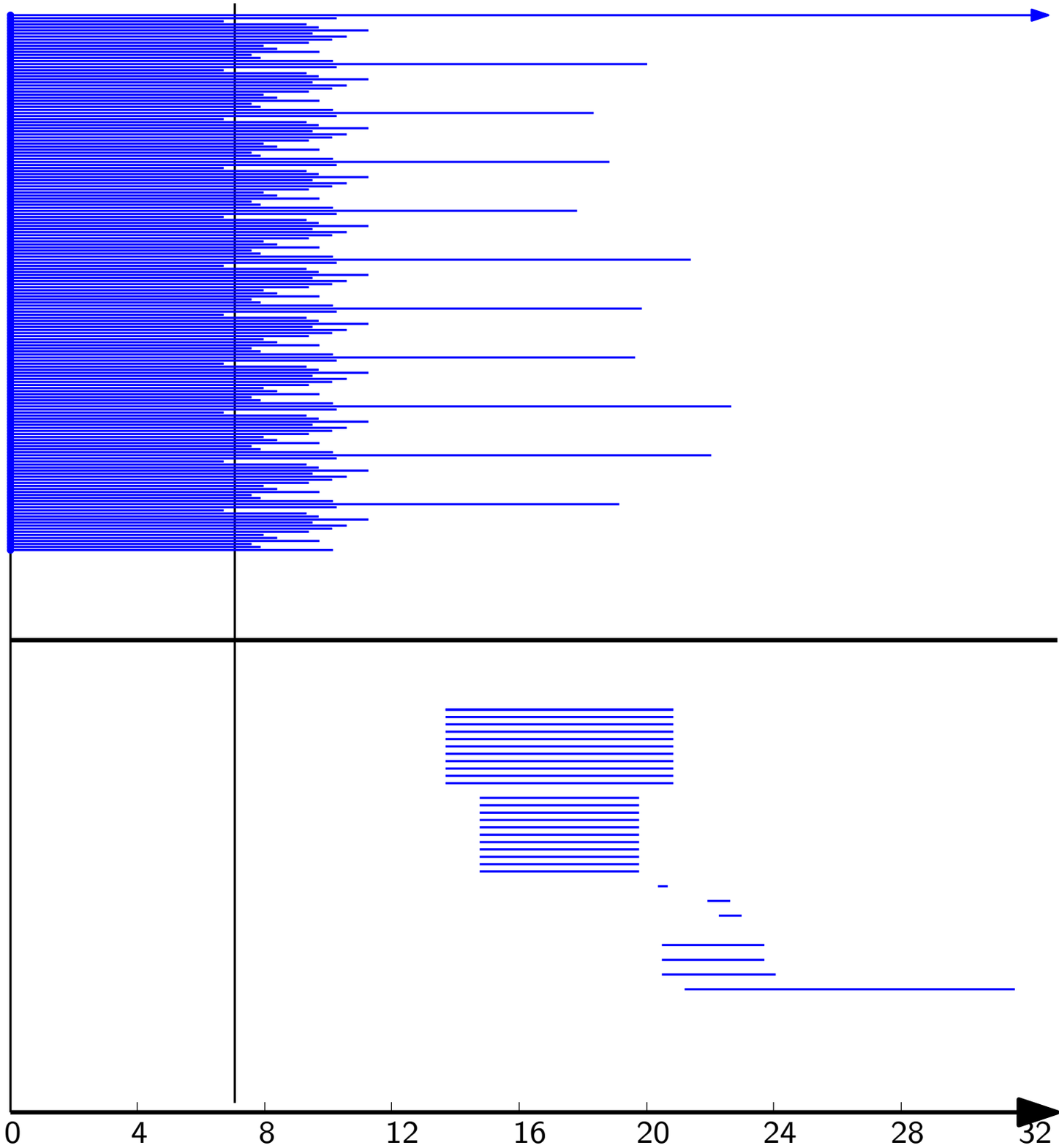

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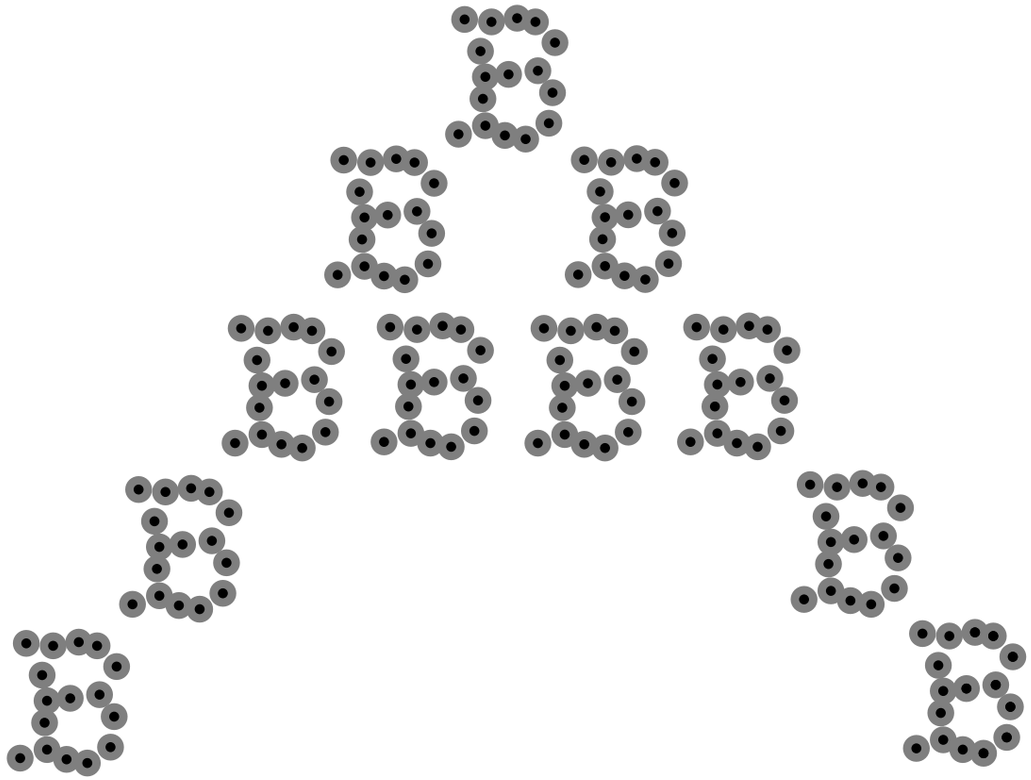

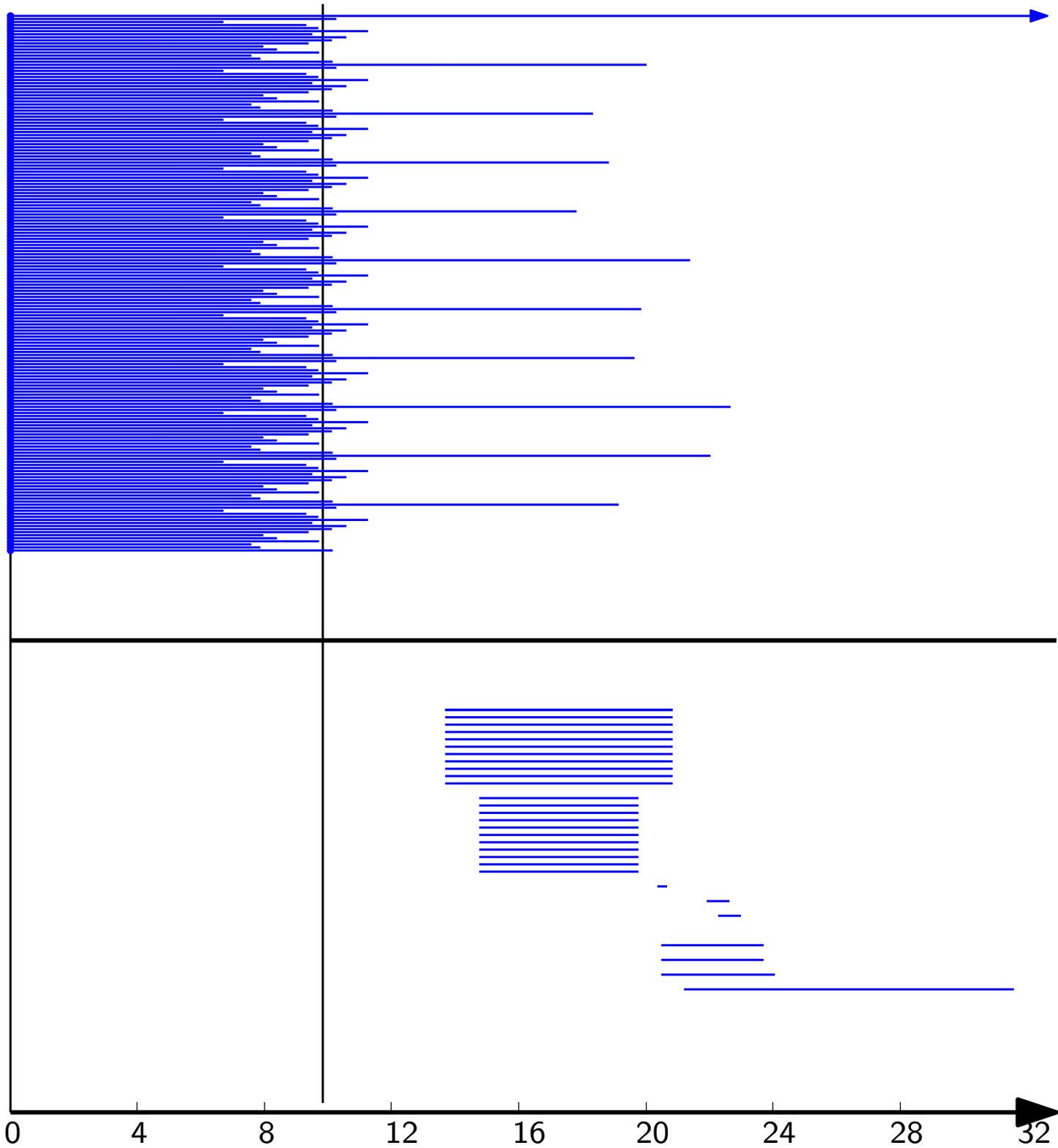

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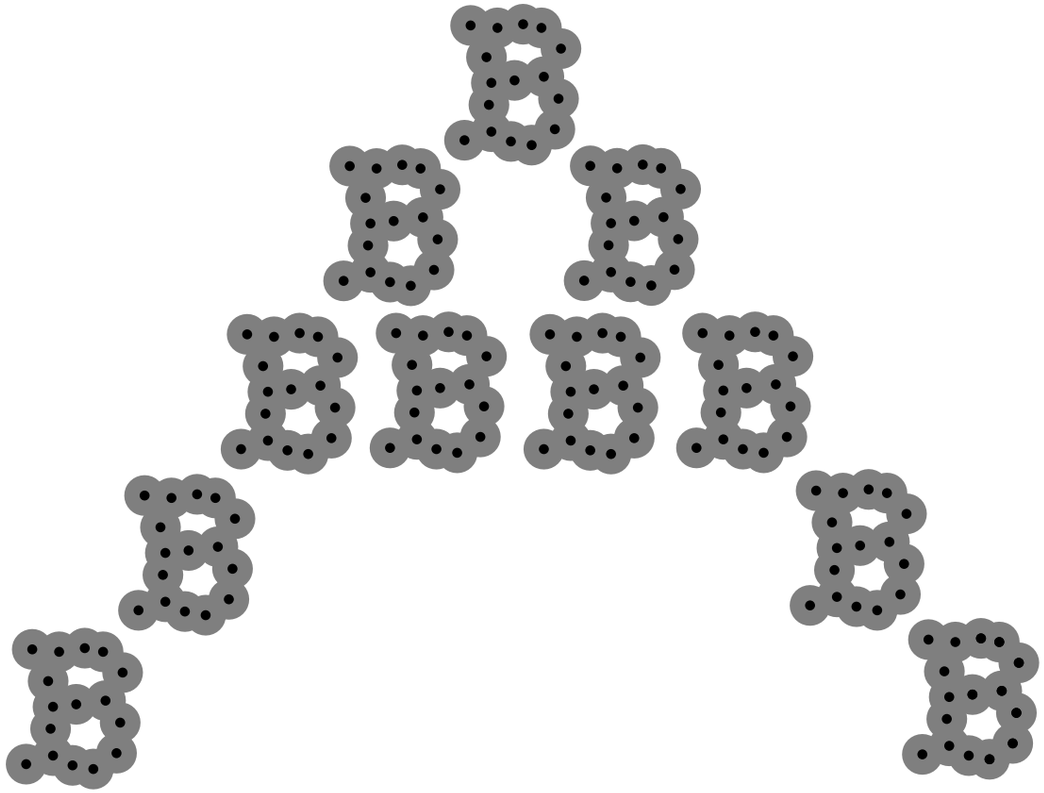

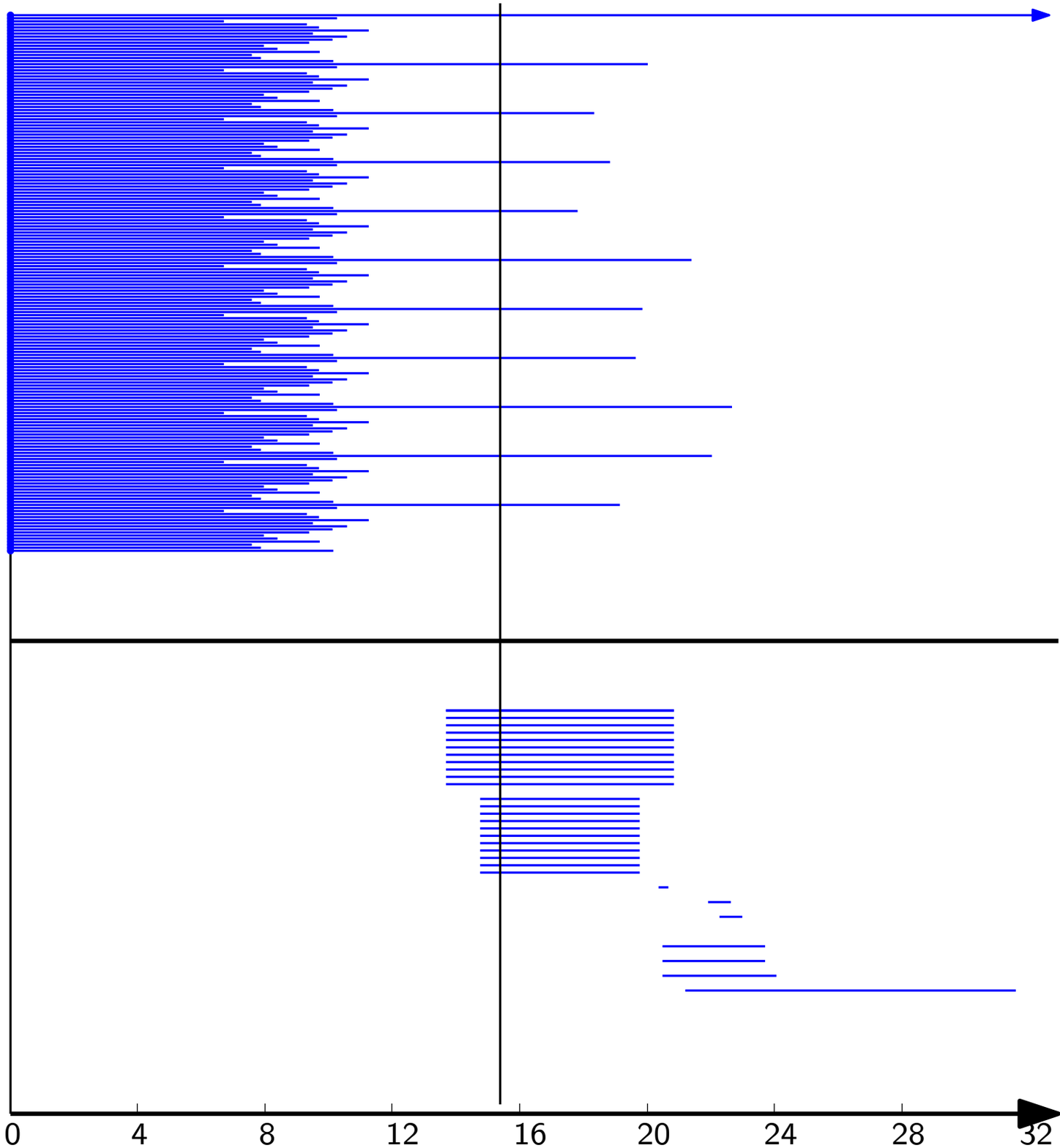

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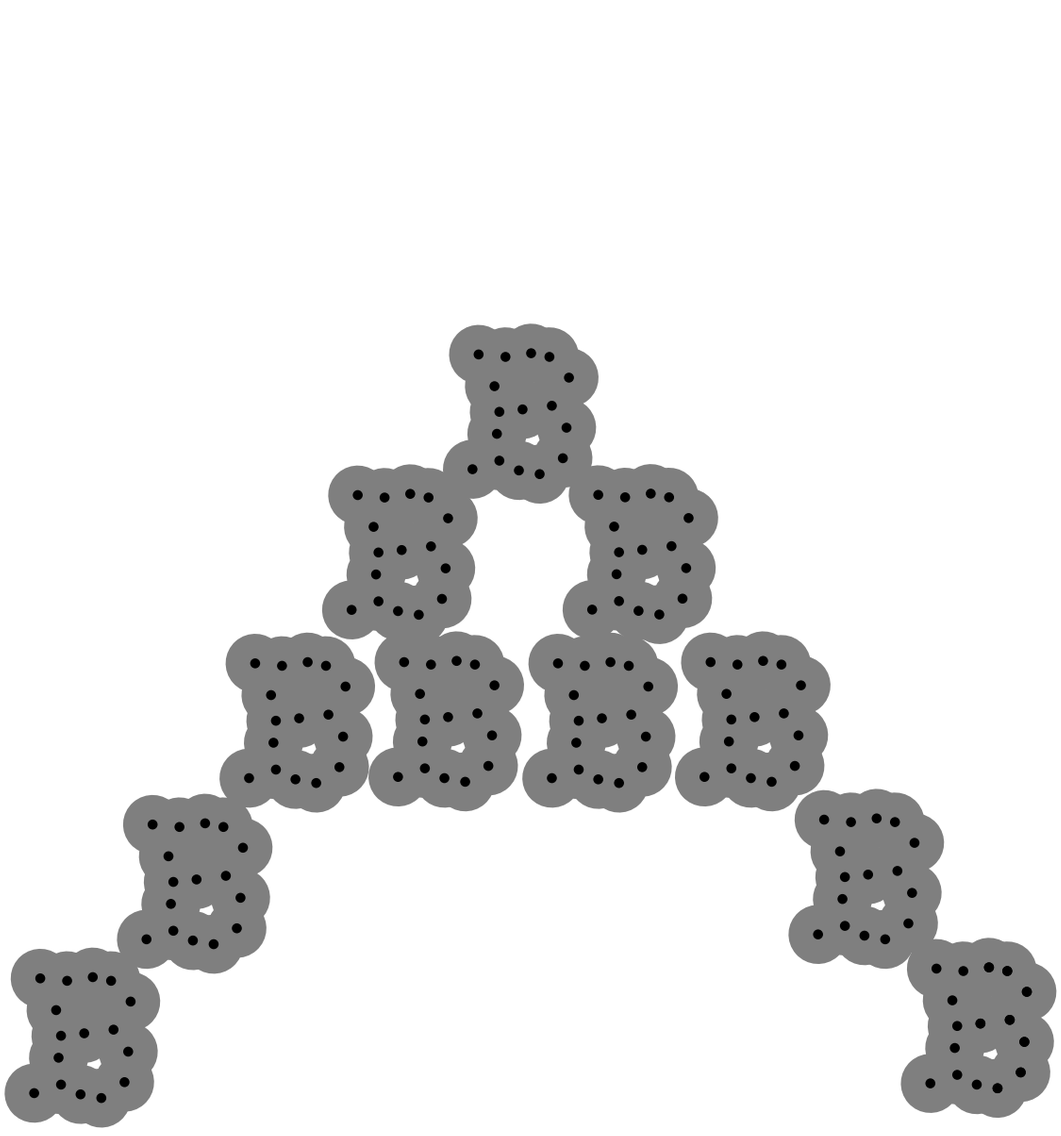

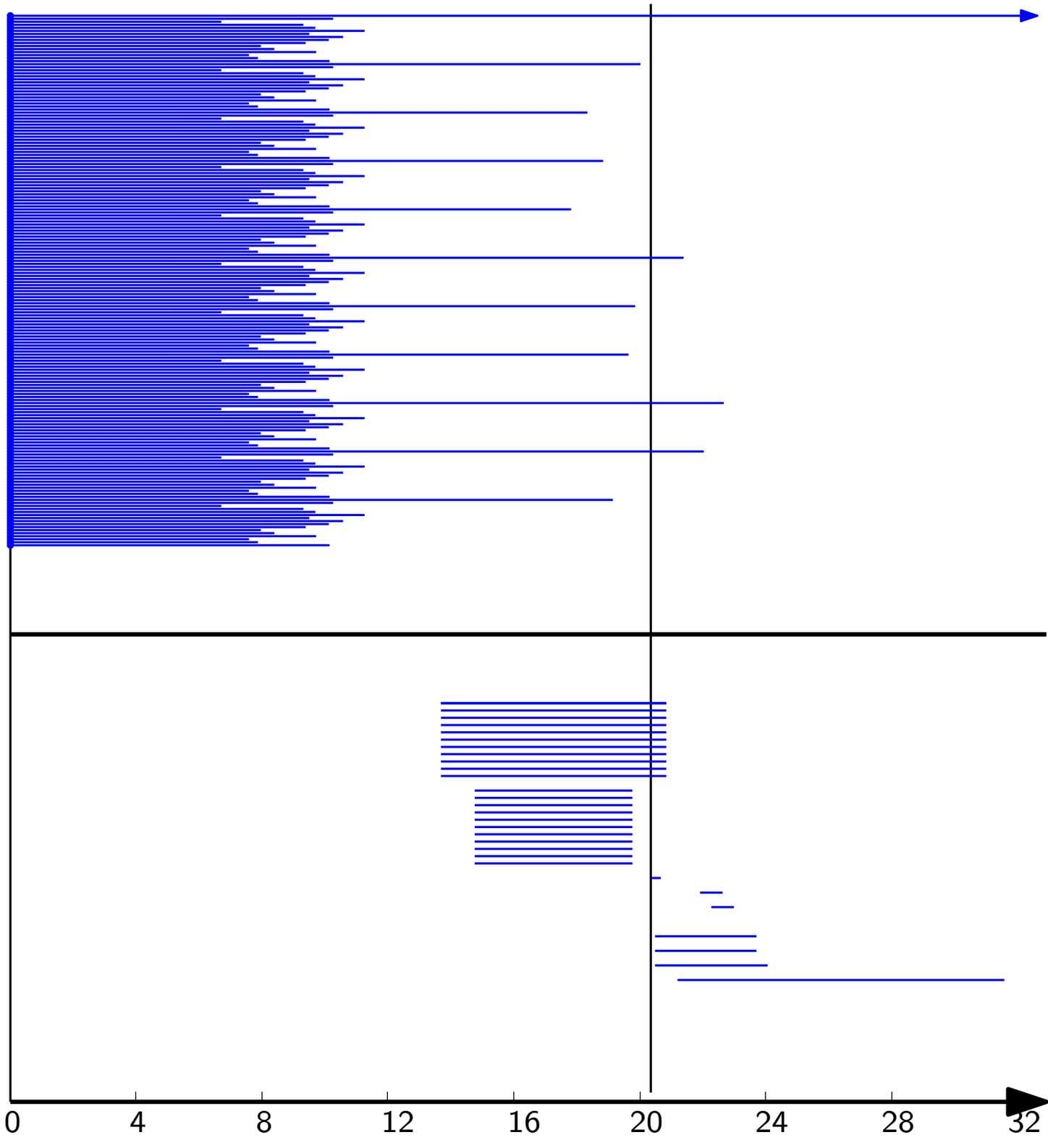

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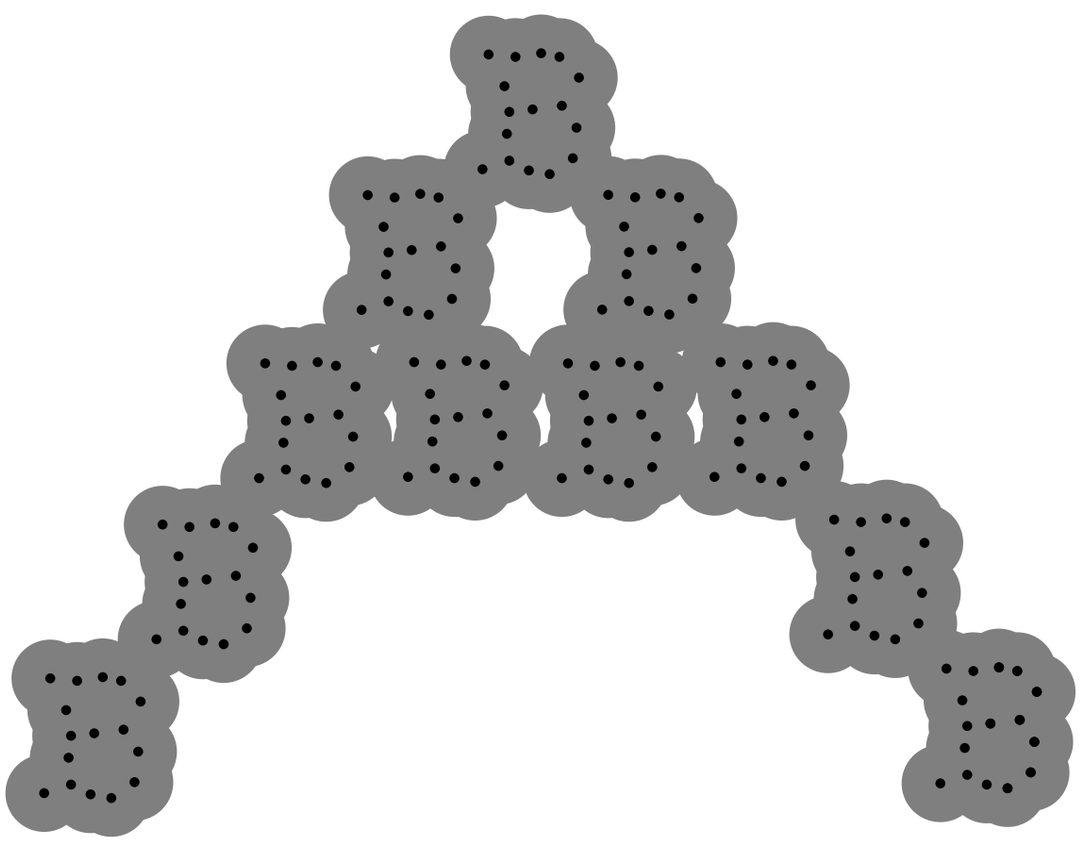

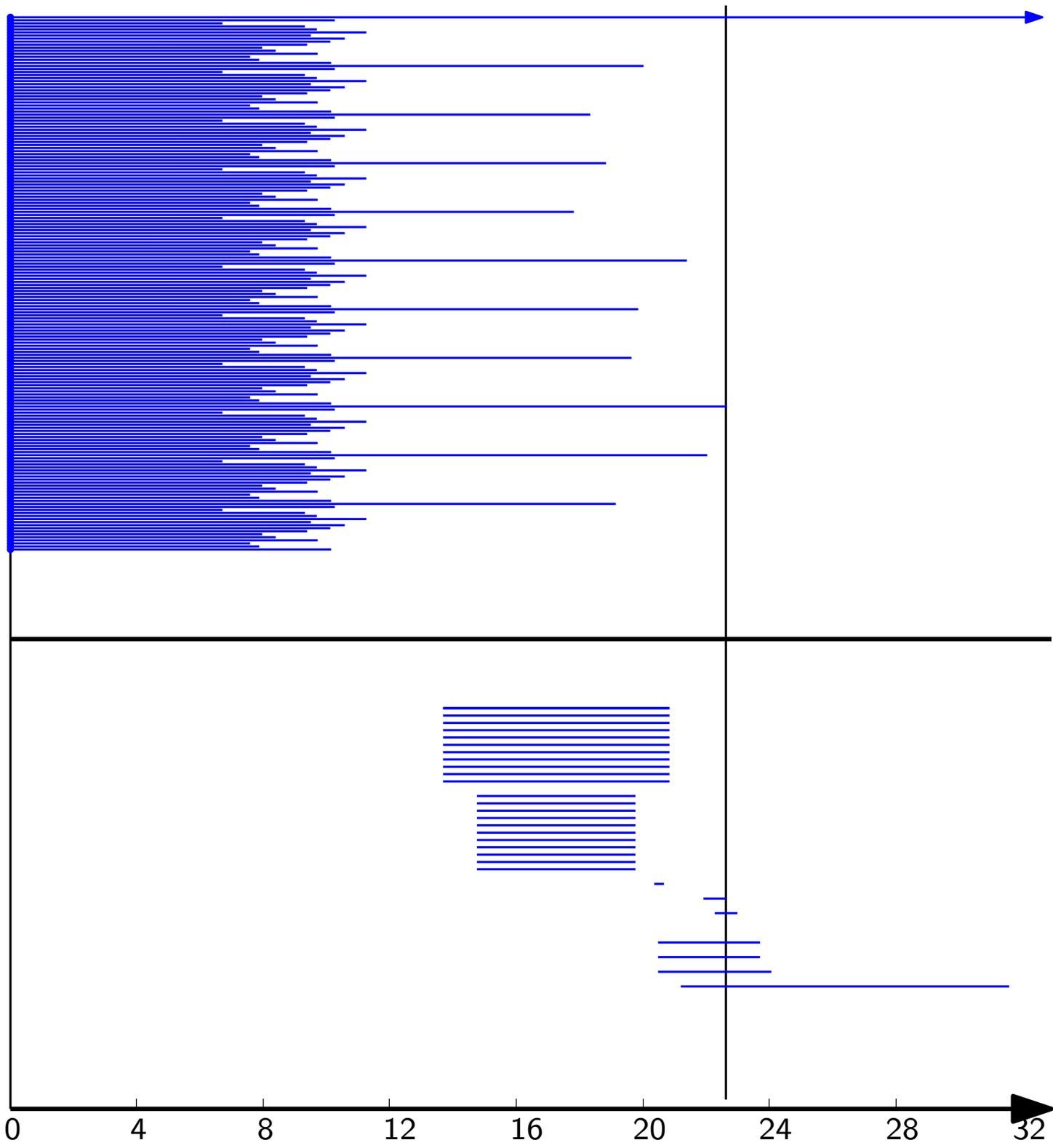

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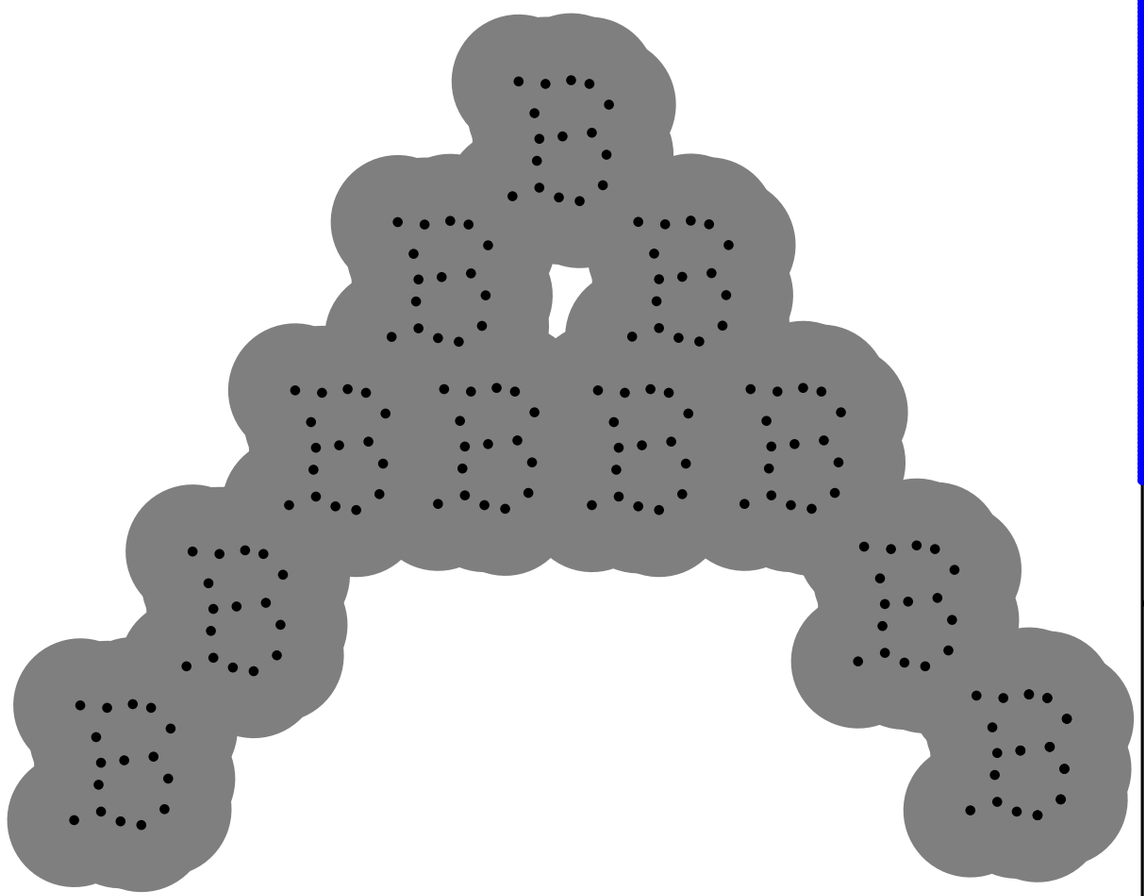

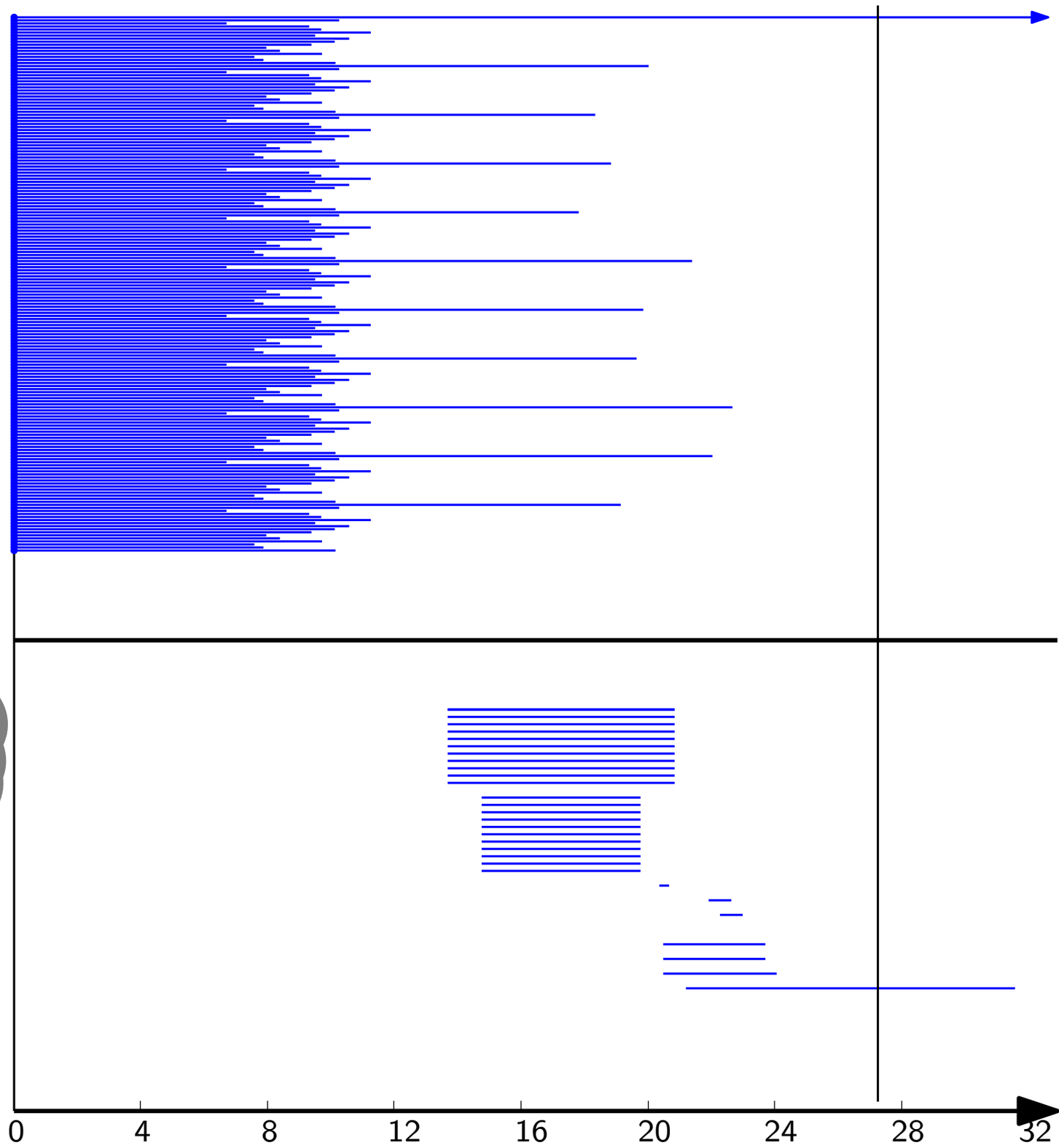

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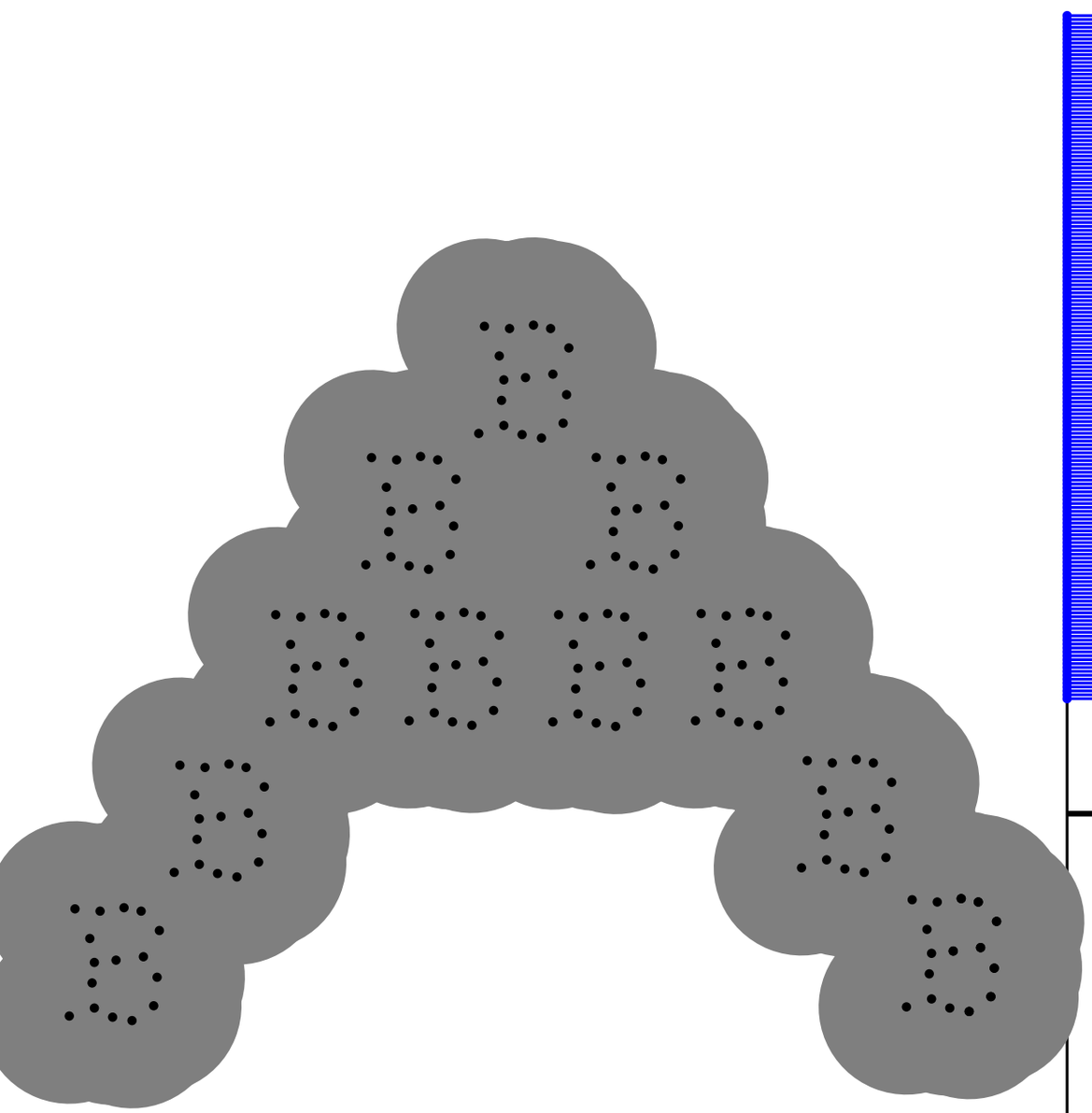

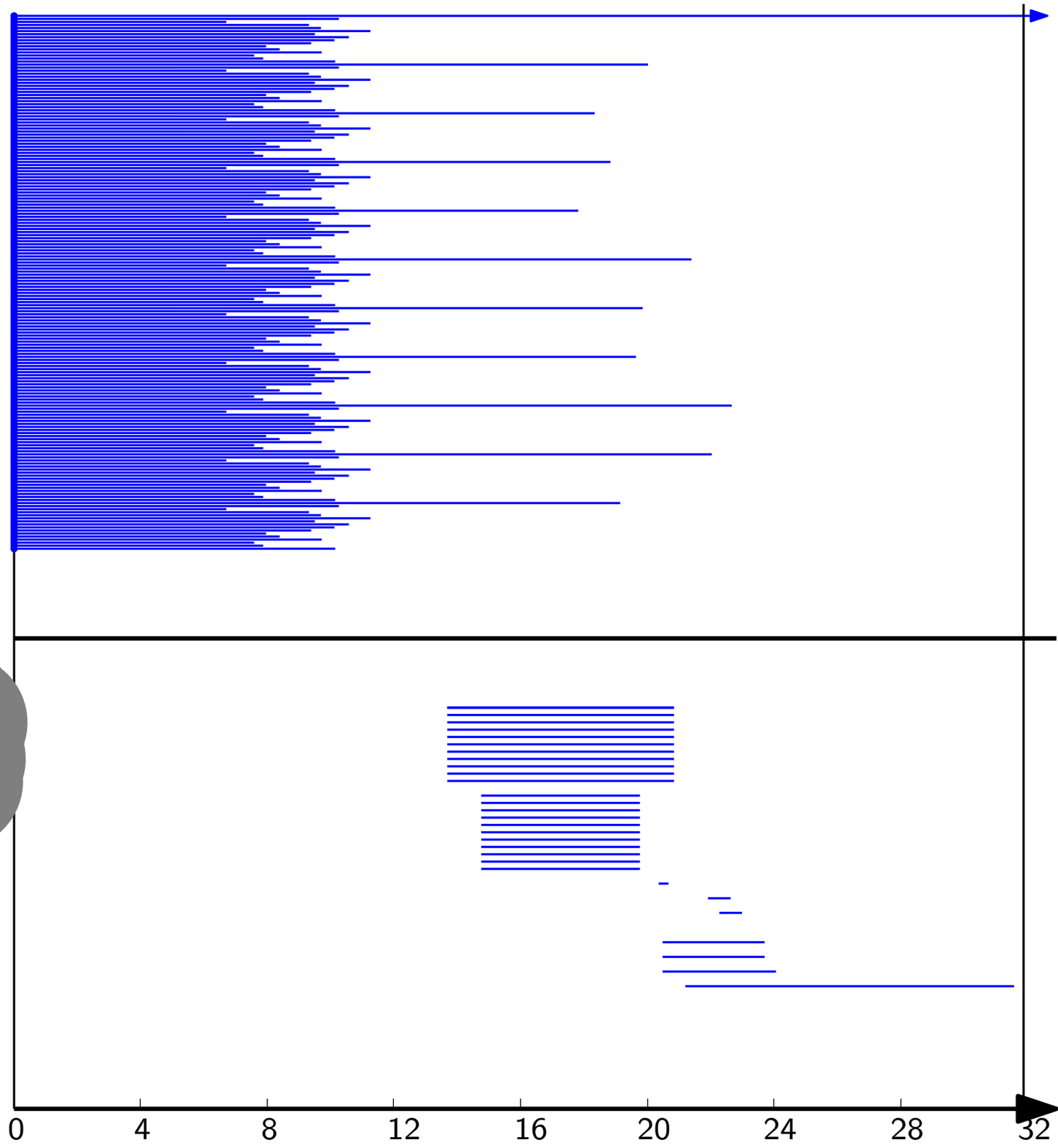

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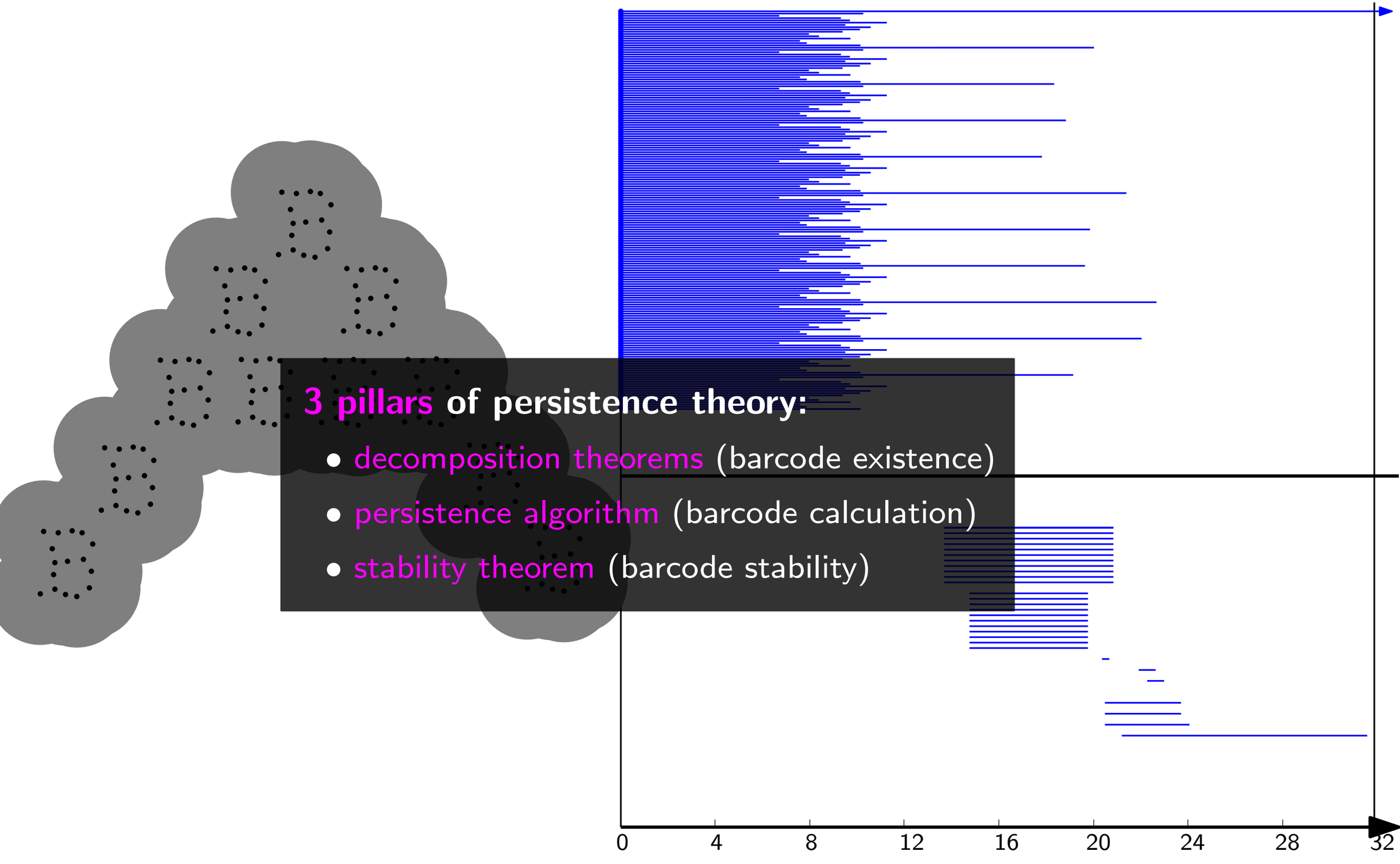
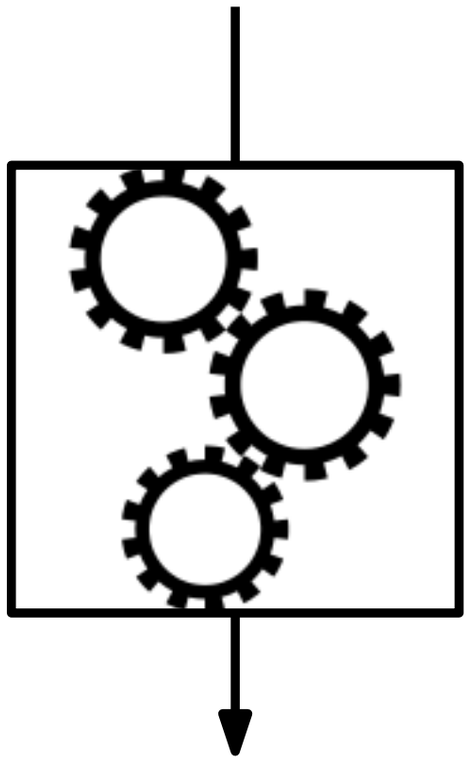


3 pillars of persistence theory:

- decomposition theorems (barcode existence)
- persistence algorithm (barcode calculation)
- stability theorem (barcode stability)

Mathematical foundations

Filtration: $F_1 \subseteq F_2 \subseteq F_3 \subseteq F_4 \subseteq F_5 \cdots$



(homology functor)

topological level

algebraic level

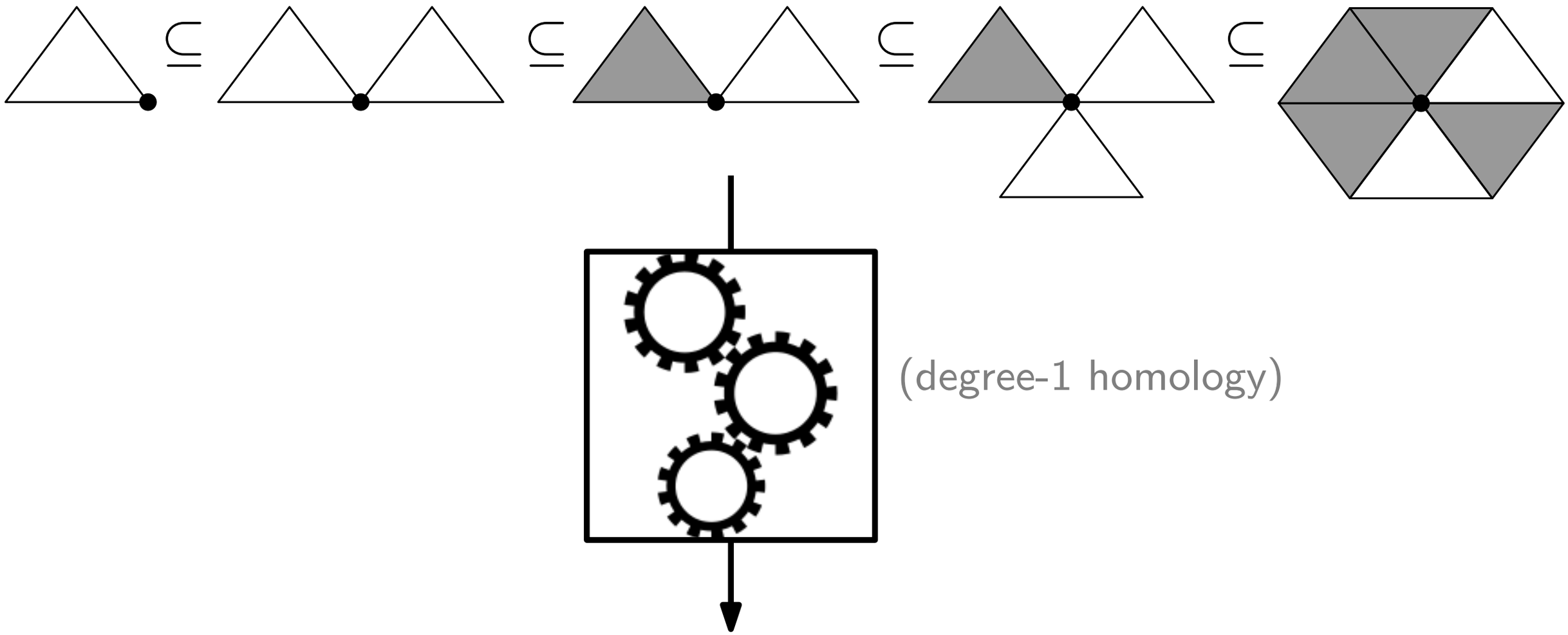
$$H_*(F_1) \to H_*(F_2) \to H_*(F_3) \to H_*(F_4) \to H_*(F_5) \to \cdots$$

Def: A *persistence module* is a sequence of vector spaces connected with linear maps:

$$H_*(F_1) \to H_*(F_2) \to H_*(F_3) \to H_*(F_4) \to \cdots$$

Mathematical foundations

Example:



(degree-1 homology)

$$\boldsymbol{k} \xrightarrow{\binom{1}{0}} \boldsymbol{k}^2 \xrightarrow{(0\ 1)} \boldsymbol{k}$$

Mathematical foundations

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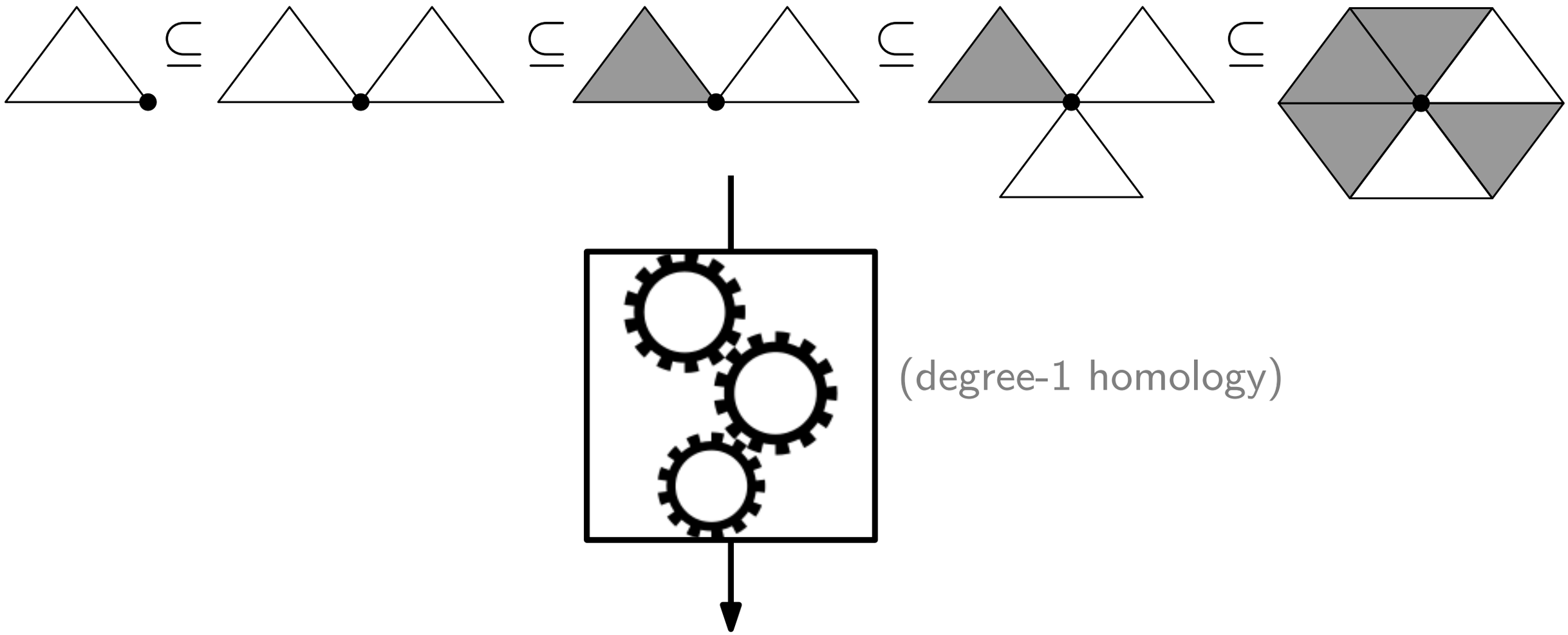

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Mathematical foundations

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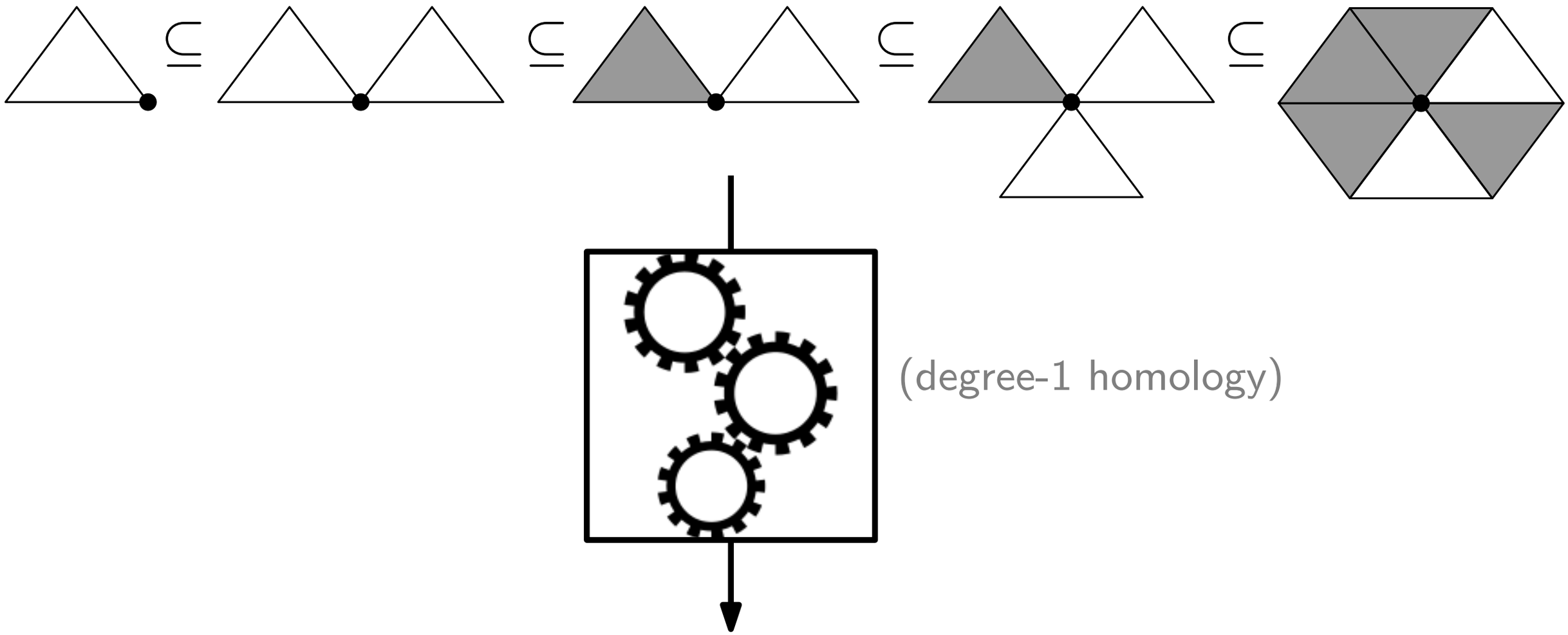

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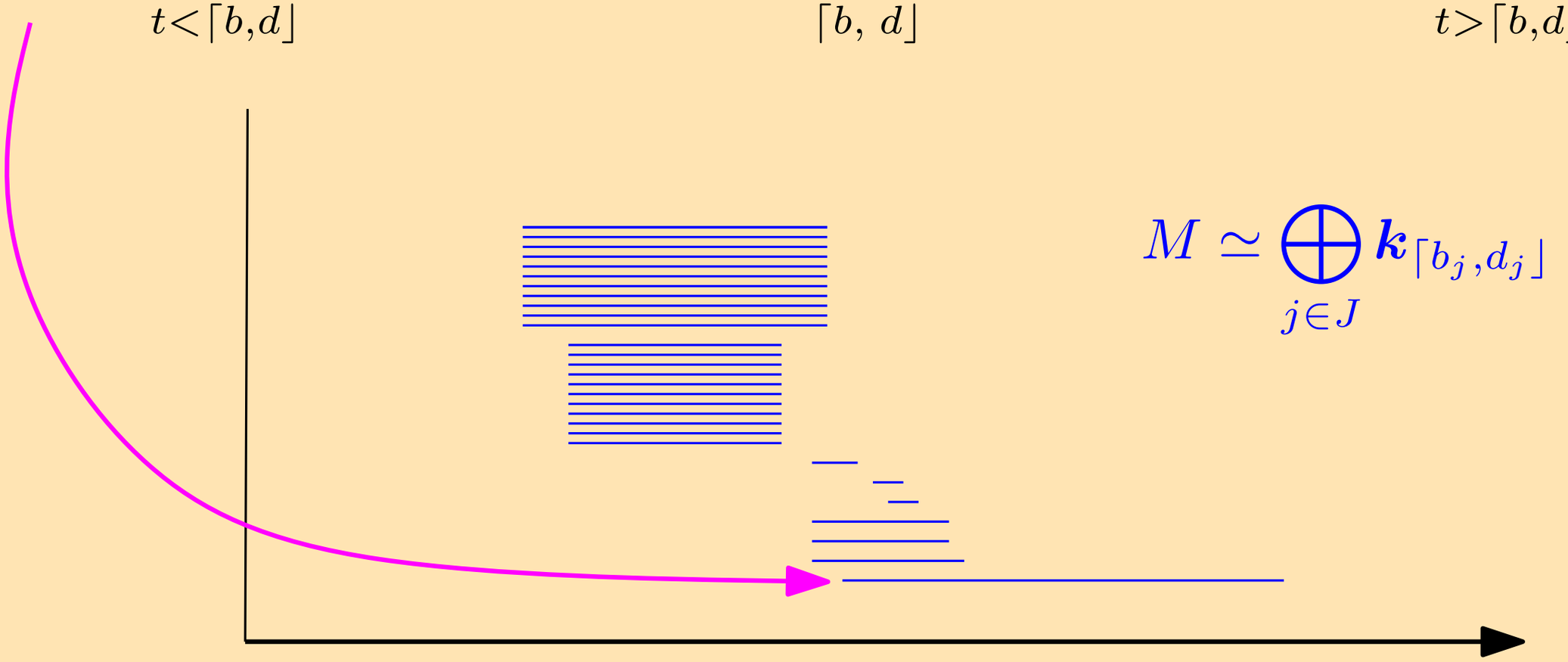
Mathematical foundations

[*The structure and stability of persistence modules*, Chazal, de Silva, Glisse, Oudot, Springer, 2016].

Thm: Let M be a persistence module over an index set $T \subseteq \mathbb{R}$. Then, M decomposes as a direct sum of *interval modules* $\boldsymbol{k}_{\lceil b,d \rfloor}$:

$$\underbrace{0 \xrightarrow{0} \cdots \xrightarrow{0} 0}_{t<\lceil b,d \rfloor} \xrightarrow{0} \underbrace{\boldsymbol{k} \xrightarrow{\mathbb{1}} \cdots \xrightarrow{\mathbb{1}} \boldsymbol{k}}_{\lceil b,\, d \rfloor} \xrightarrow{0} \underbrace{0 \xrightarrow{0} \cdots \xrightarrow{0} 0}_{t>\lceil b,d \rfloor}$$



(the barcode is a complete descriptor of the algebraic structure of M)

Mathematical foundations

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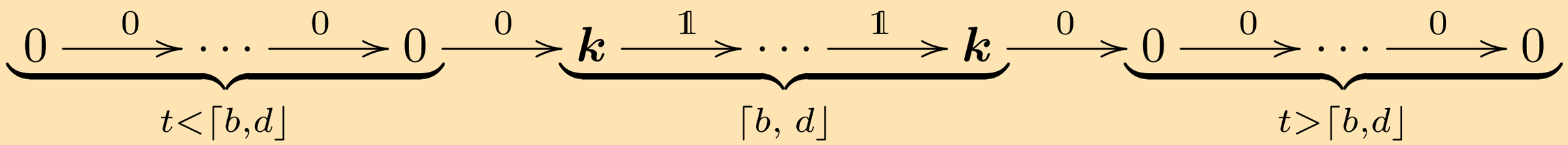


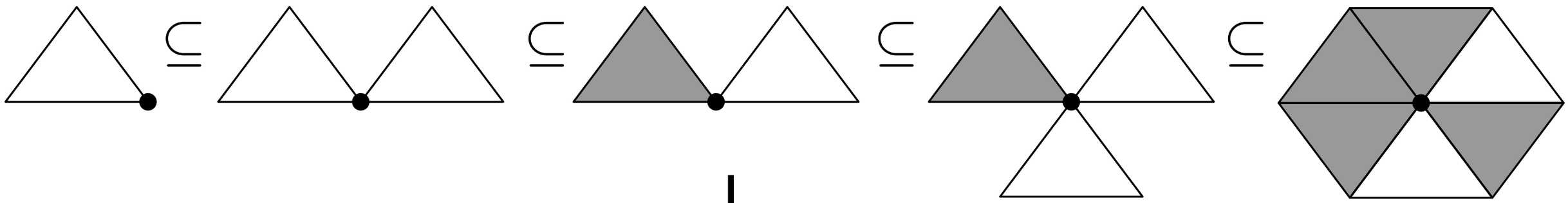
in the following cases:

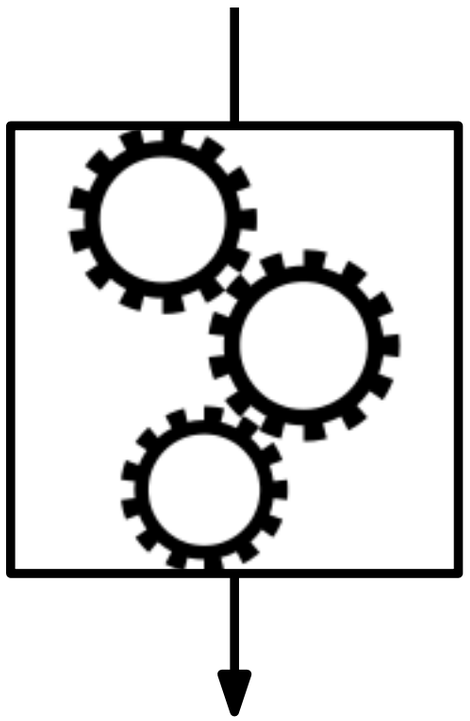
- T is finite,
- M is *pointwise finite-dimensional* (pfd), i.e., every space M_t has finite dimension.

Moreover, when it exists, the decomposition is **unique** up to isomorphism and permutation of the terms [Azumaya 1950].

Mathematical foundations

Example:

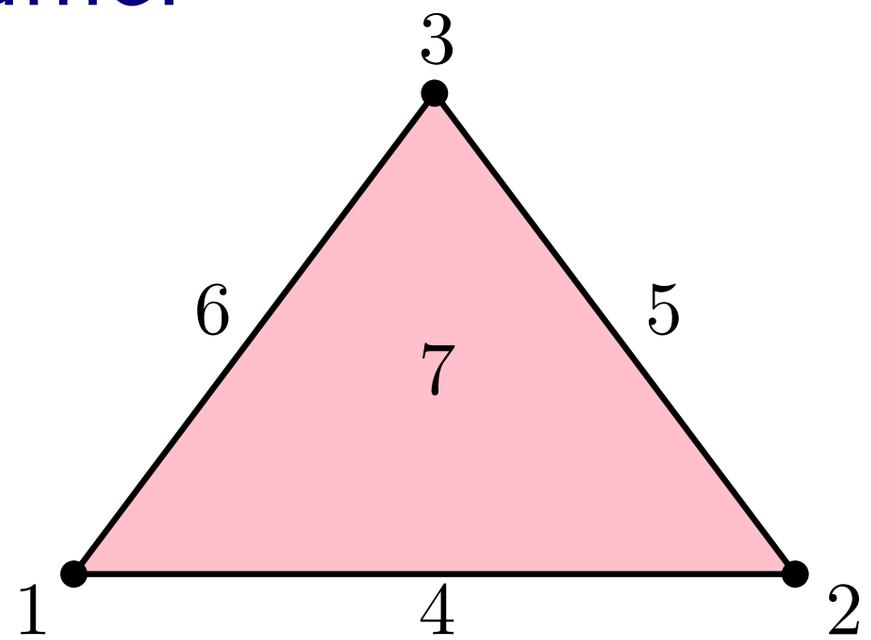




(degree-1 homology)

$$\boldsymbol{k} \xrightarrow{\binom{1}{0}} \boldsymbol{k}^2 \xrightarrow{(0\ 1)} \boldsymbol{k} \qquad \xrightarrow{\binom{0}{1}} \boldsymbol{k}^2 \xrightarrow{\binom{1\ 0}{0\ 1}} \boldsymbol{k}^2 \ \cdots$$

Good news: the algorithm is the same!



Input: simplicial filtration

Output: boundary matrix
reduced to column-echelon form

◯ simplex pairs give finite intervals:
$[2,4)$, $[3,5)$, $[6,7)$

□ unpaired simplices give infinite intervals: $[1,+\infty)$

	1	2	3	4	5	6	7
1				$*$		$*$	
2				$*$	$*$		
3					$*$	$*$	
4							$*$
5							$*$
6							$*$
7							

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1				$*$			
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3					1		
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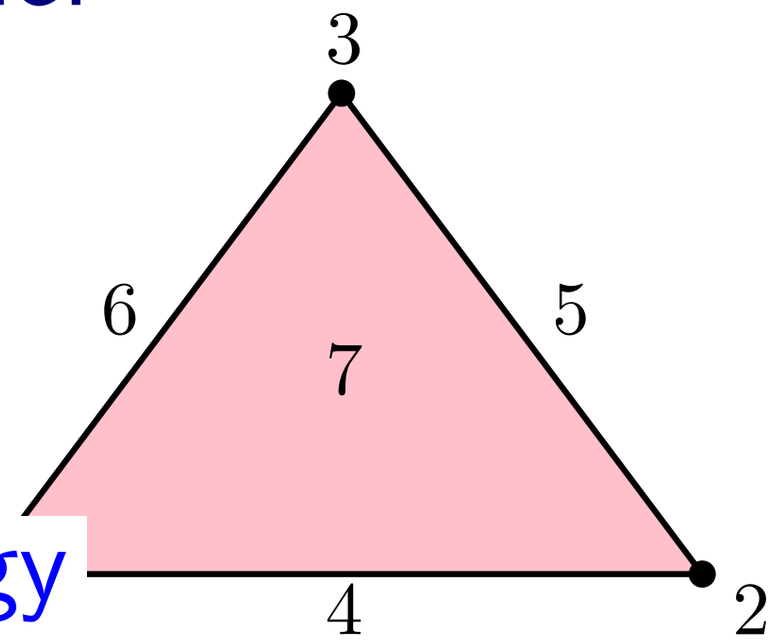

Input: simplicial filtration

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reduced to column-echelon form

◯ simplex pairs give Persistent homology
$[2,4)$, $[3,5)$, $[6,7)$

□ unpaired simplices give Regular homology

	1	2	3	4	5	6	7
1				$*$		$*$	
2				$*$	$*$		
3					$*$	$*$	
4							$*$
5							$*$
6							$*$
7							

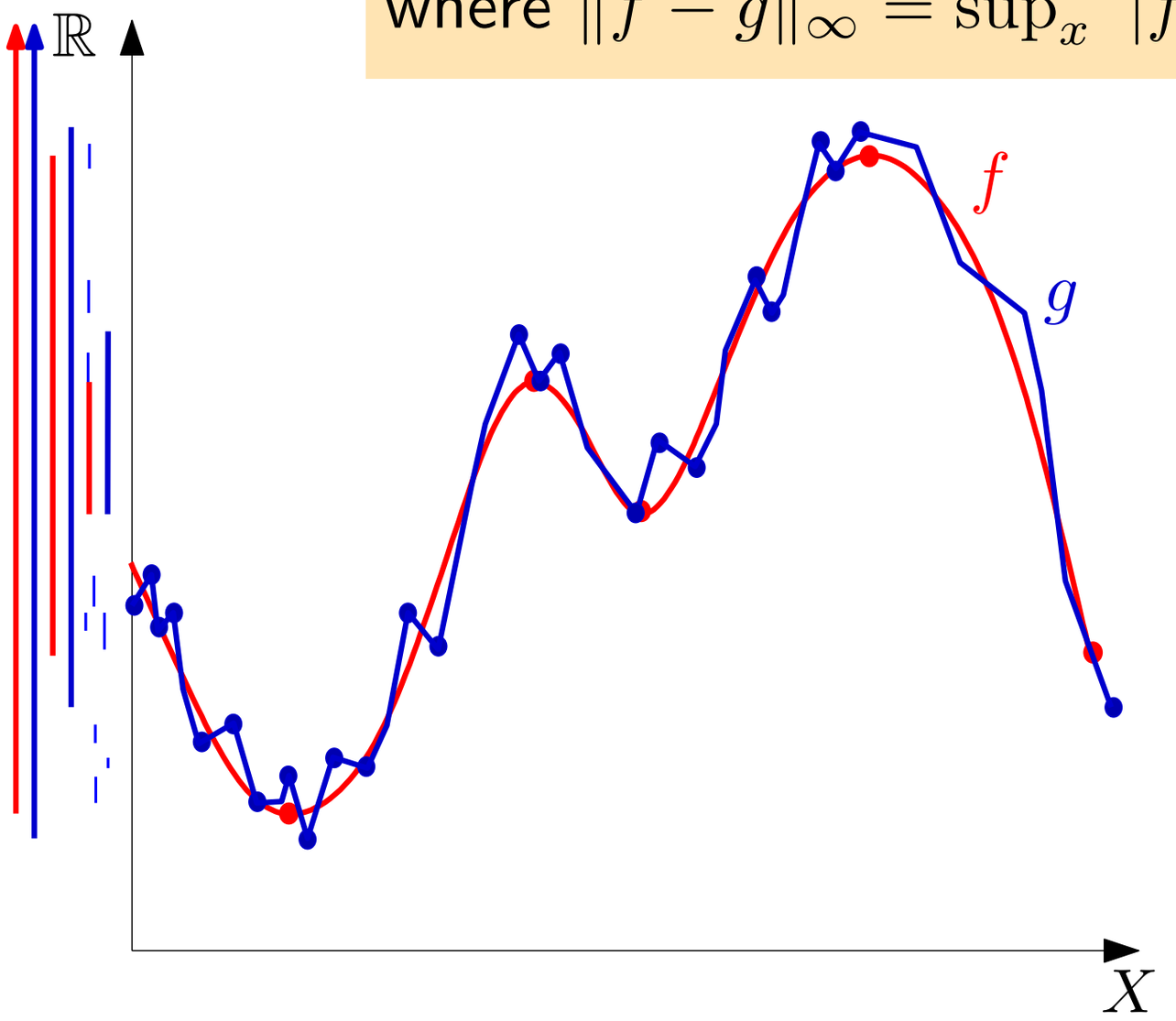
	1	2	3	4	5	6	7
1				$*$			
2				(1)	$*$		
3					(1)		
4							$*$
5							$*$
6							(1)
7							

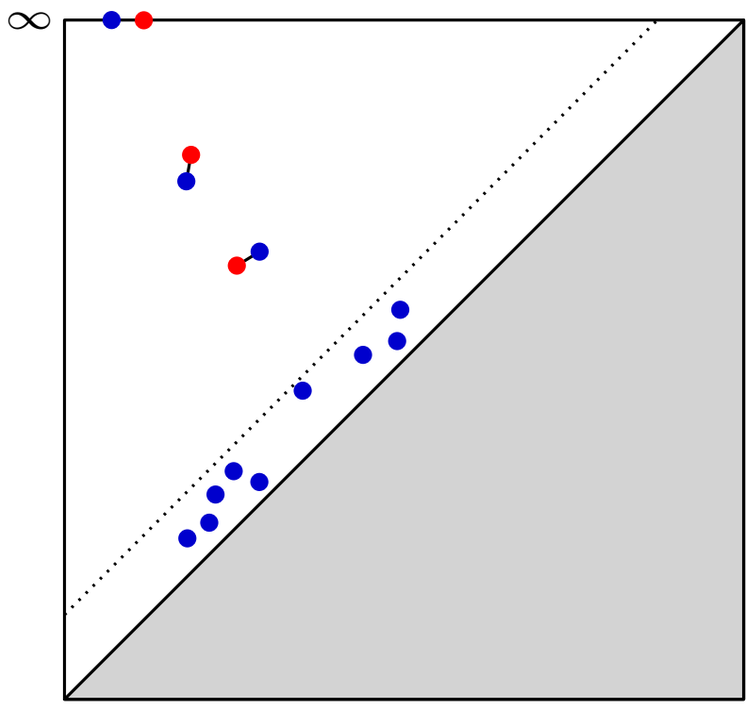
Stability properties

Thm: For any pfd functions $f, g : X \to \mathbb{R}$ and homological dimension k,

$$d_b(D_f, D_g) \leq \|f - g\|_\infty,$$

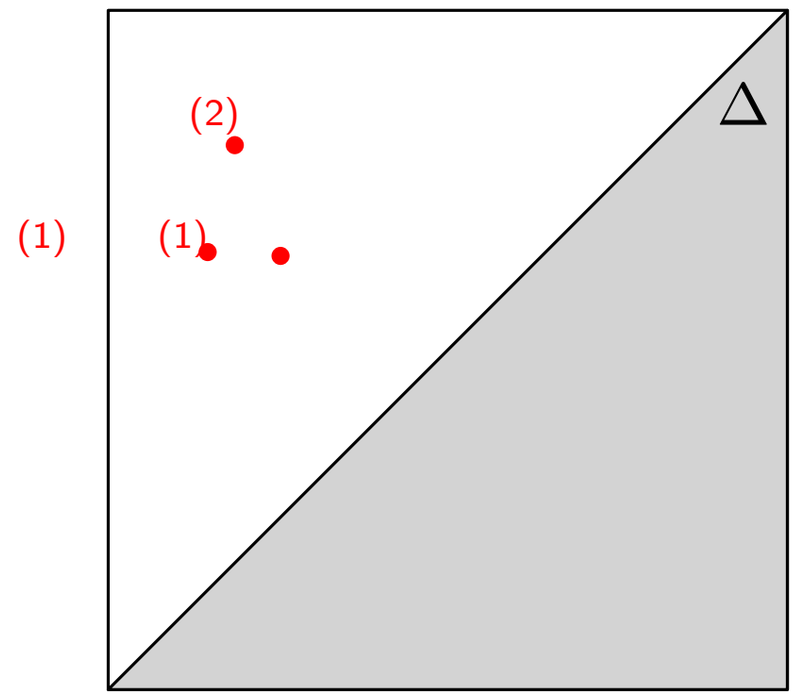
where $\|f - g\|_\infty = \sup_x \ |f(x) - g(x)|$.





Stability properties

Persistence diagram $\equiv$ **finite** multiset in the open half-plane $\Delta \times \mathbb{R}_{>0}$.



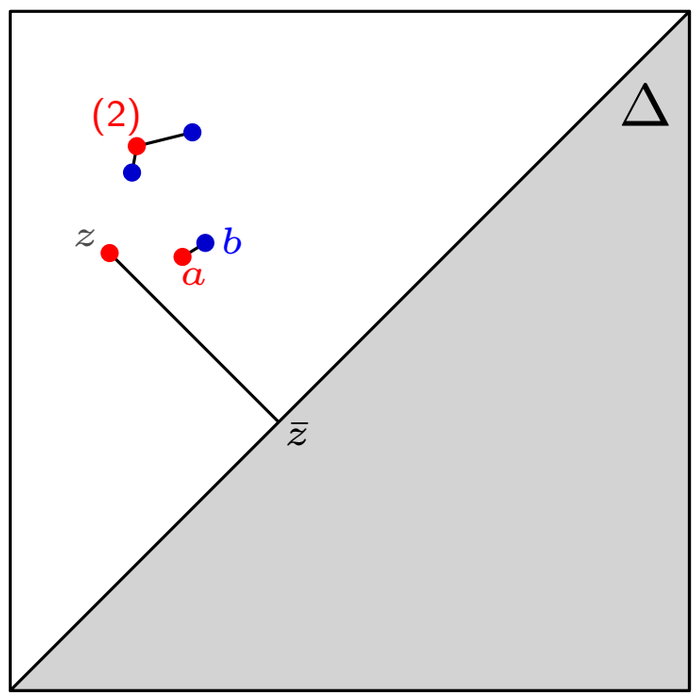
Stability properties

Persistence diagram $\equiv$ **finite** multiset in the open half-plane $\Delta \times \mathbb{R}_{>0}$.

Given a **partial matching** $M : D \leftrightarrow D'$:

- cost of a matched pair $(a, b) \in M$: $c_p(a, b) := \|a - b\|_\infty^p$,
- cost of an unmatched point $c \in D \sqcup D'$: $c_p(c) := \|c - \bar{c}\|_\infty^p$,
- **cost of** M:

$$c_p(M) := \left(\sum_{(a,\, b) \text{ matched}} c_p(a, b) \; + \sum_{c \text{ unmatched}} c_p(c) \right)^{1/p}$$



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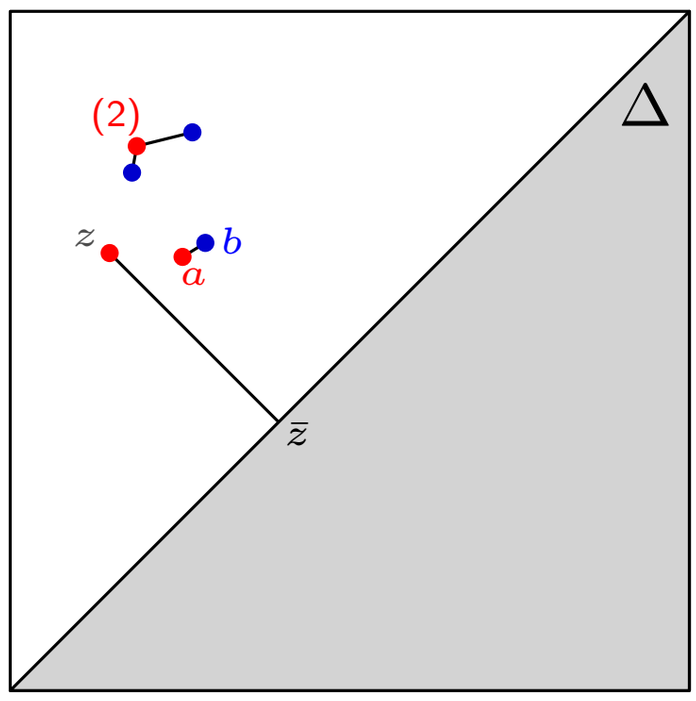


Def: p-th diagram distance (extended metric):

$$d_p(D, D') := \inf_{M : D \leftrightarrow D'} c_p(M)$$

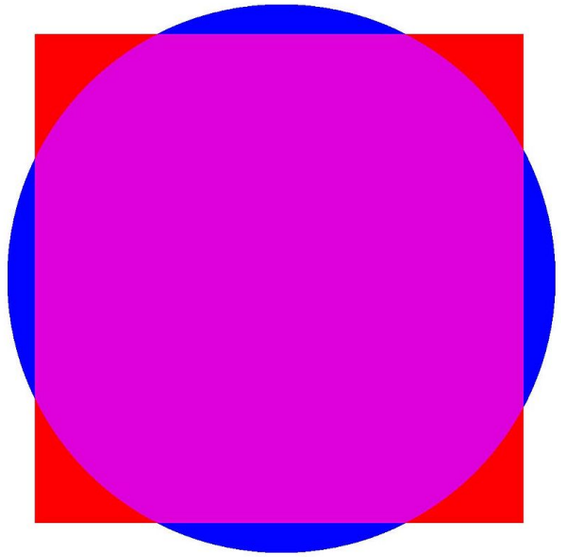
Def: bottleneck distance:

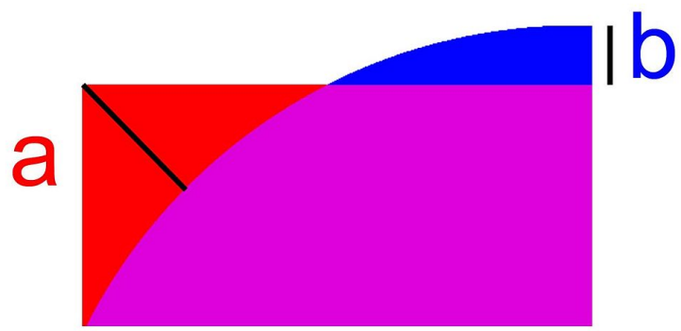
$$d_b(D, D') = d_\infty(D, D') := \lim_{p \to \infty} d_p(D, D')$$

Stability properties for point clouds

Def: The Hausdorff distance between two subspaces X, Y of a common metric space (Z, d) is:

$$d_H(X,Y) = \max\{\sup_{y\in Y} d(y,X), \sup_{x\in X} d(x,Y)\}$$
$$= \max\{\sup_{y\in Y}\inf_{x\in X} d(y,x), \sup_{x\in X}\inf_{y\in Y} d(x,y)\}$$





$$d_H(X,Y) = \max\{a,b\}$$

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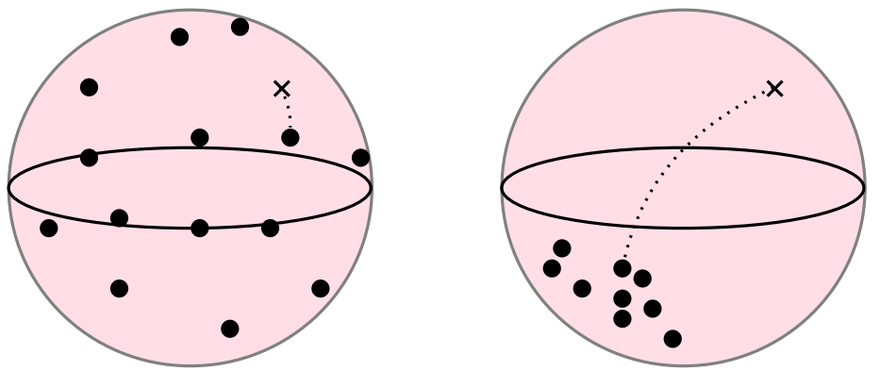
Ex: Given a sampling $\hat{X}_n \subseteq X$, $d_H(\hat{X}_n, X)$ is a measure of sampling quality.



Q: Show that $d_H(X,Y) = \inf\{\epsilon > 0 : X^\epsilon \subseteq Y \text{ and } Y^\epsilon \subseteq X\}$, where $X^\epsilon = \{z : \exists x \in X \text{ s.t. } d(x,z) \leq \epsilon\}$.

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Def: The Gromov-Hausdorff distance between metric spaces $(X, d_X), (Y, d_Y)$ is the Hausdorff distance of the best common isometric embedding:

$$d_{GH}((X,d_X),(Y,d_Y)) = \inf_\gamma d_H(\gamma(X),\gamma(Y)),$$

where $d(\gamma(x),\gamma(x')) = d_X(x,x')$ and $d(\gamma(y),\gamma(y')) = d_X(y,y')$.

Stability properties for point clouds

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Def: The Gromov-Hausdorff distance between metric spaces $(X, d_X), (Y, d_Y)$ is metric distortion of the best correspondence:

$$d_{GH}((X,d_X),(Y,d_Y)) = \inf_{\mathcal{C}} \sup_{(x,y),(x',y')\in\mathcal{C}} |d_X(x,x') - d_Y(y,y')|,$$

where $\mathcal{C} \subseteq X \times Y$ s.t. $\forall x$, $\exists y_x \in Y$ s.t. $(x, y_x) \in \mathcal{C}$ (and vice-versa).

Stability properties for point clouds

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Thm: If X and Y are common subspaces of a common metric space (Z, d), then

$$d_b(D_{\text{Cech}}(X), D_{\text{Cech}}(Y)) \leq d_H(X,Y).$$

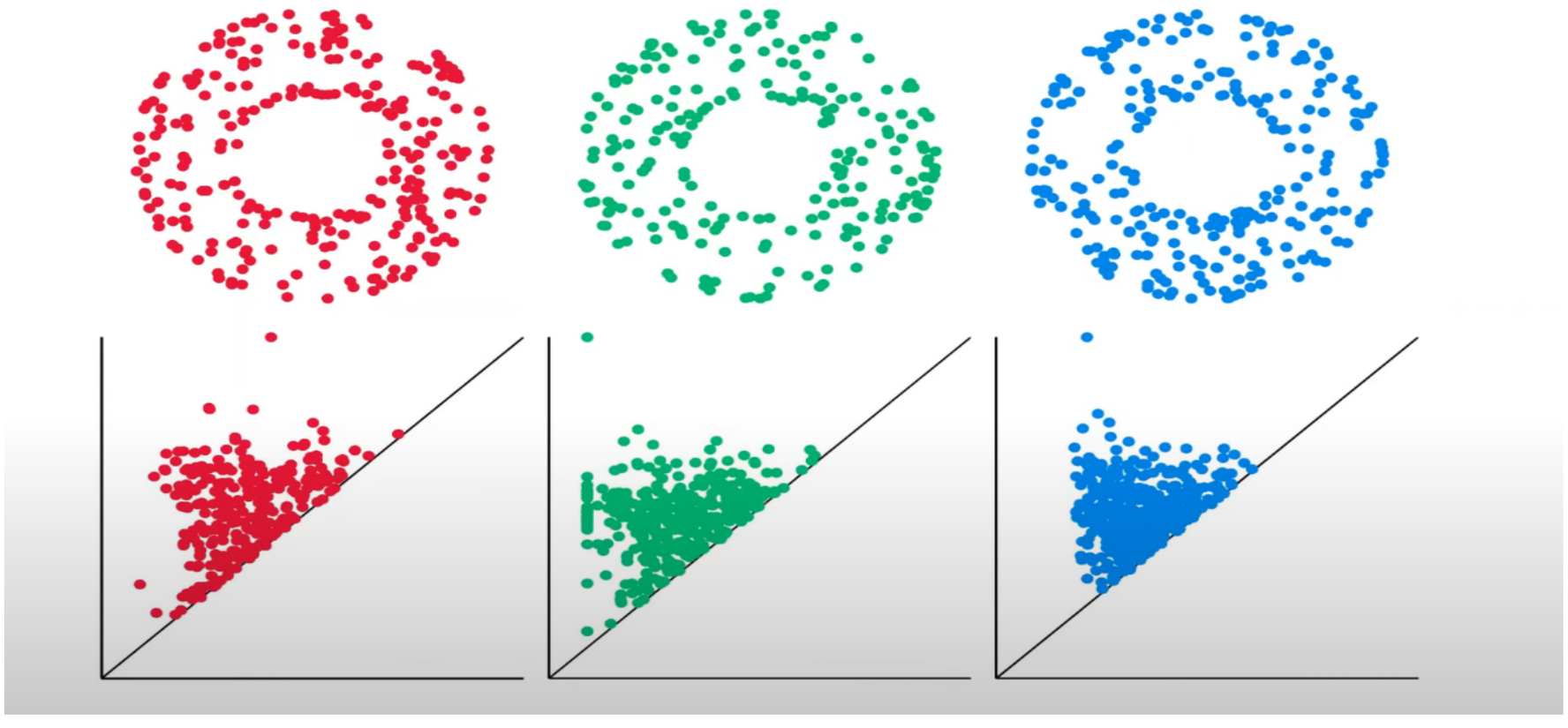
Q: Prove it.

Stability properties for point clouds

[*Persistence stability for geometric complexes*, Chazal, de Silva, Oudot, Geom. Dedicata, 2013].

Thm: If X and Y are pre-compact metric spaces, then

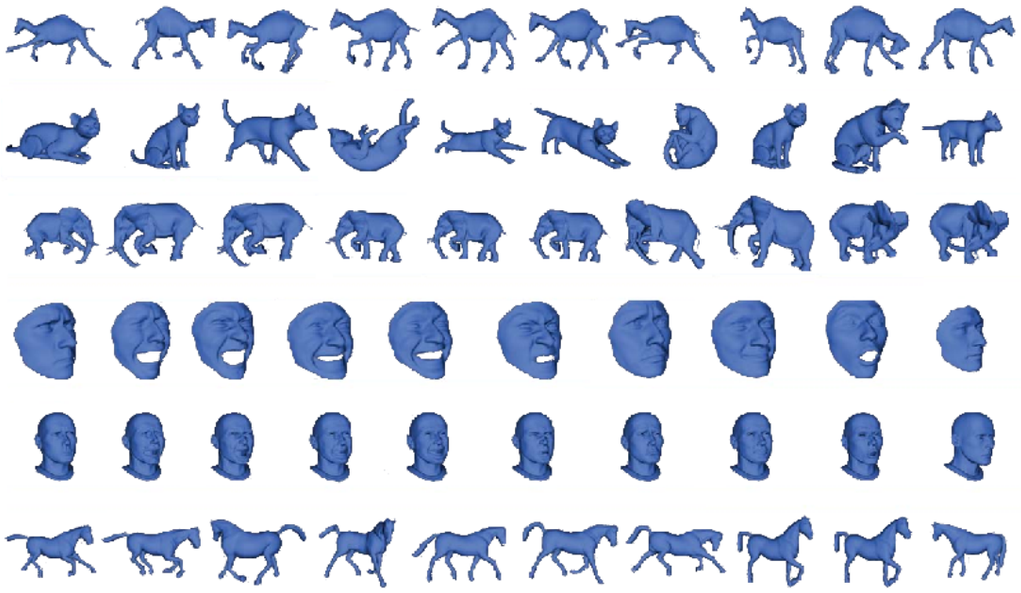
$$d_b(D_{\mathrm{Rips}}(X), D_{\mathrm{Rips}}(Y)) \leq d_{GH}(X, Y).$$

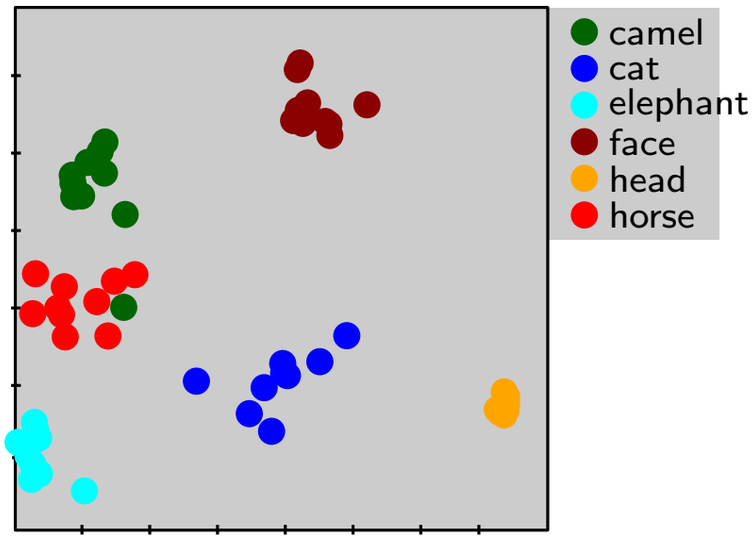


Rem: This result also holds for Čech and other families of filtrations (particular case of a more general theorem).

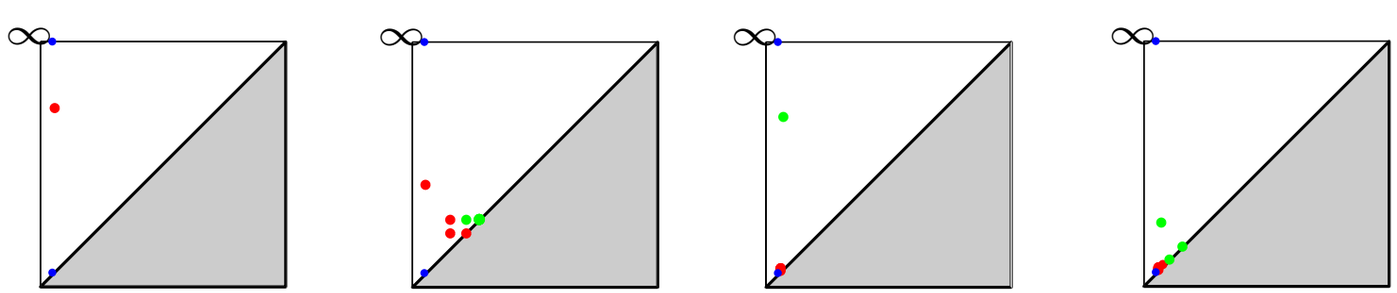
Application: non rigid shape classification

[*Gromov-Hausdorff Stable Signatures for Shapes using Persistence*, Chazal et al., Symp. Geom. Process., 2009]





MDS using bottleneck distance.



- Non rigid shapes in a same class are almost isometric, but computing Gromov-Hausdorff distance between shapes is extremely expensive.
- Compare diagrams of sampled shapes instead of shapes themselves.

Limitations

Thm: If X and Y are pre-compact metric spaces, then

$$d_b(D_{\mathrm{Rips}}(X), D_{\mathrm{Rips}}(Y)) \leq d_{GH}(X, Y).$$

$\rightarrow$ Vietoris-Rips (or Čech, witness) filtrations become quickly prohibitively large as the size of the data increases: $O(|X|^d)$, making the practical computation of persistence almost impossible.

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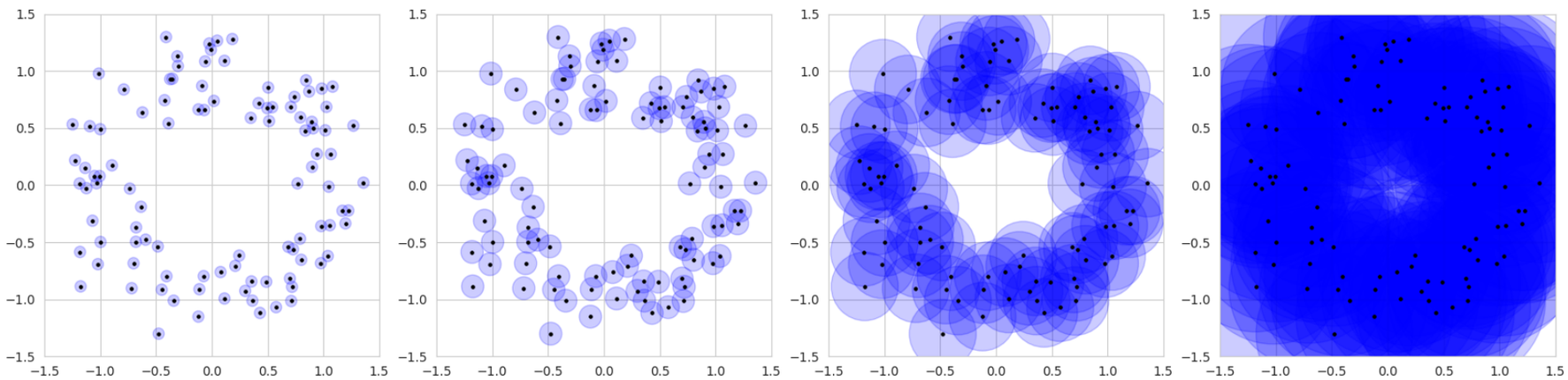
$\rightarrow$ Persistence diagrams of Vietoris-Rips (as well as Čech, witness,..) filtrations and Gromov-Hausdorff distance are very sensitive to noise and outliers.



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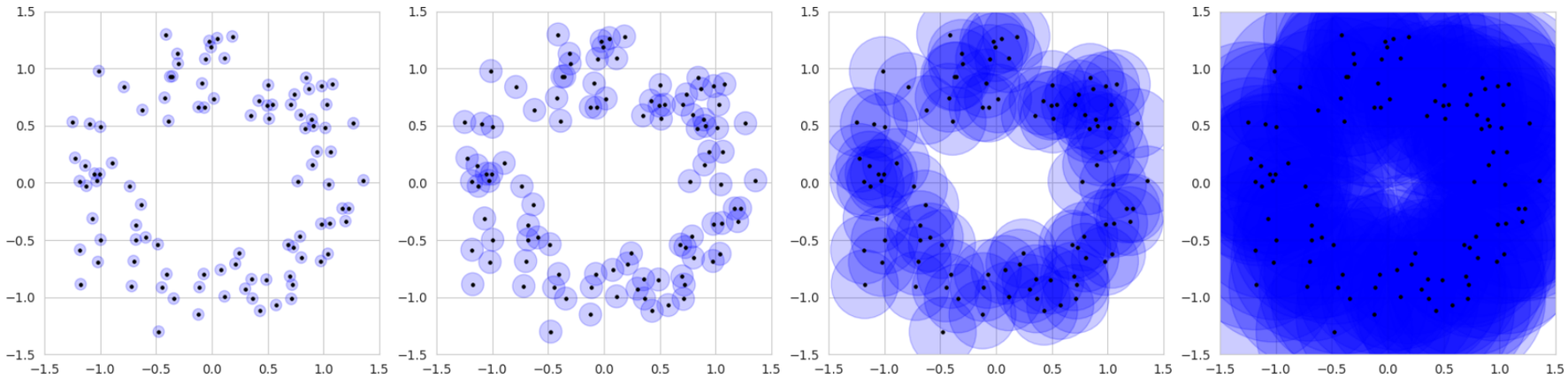

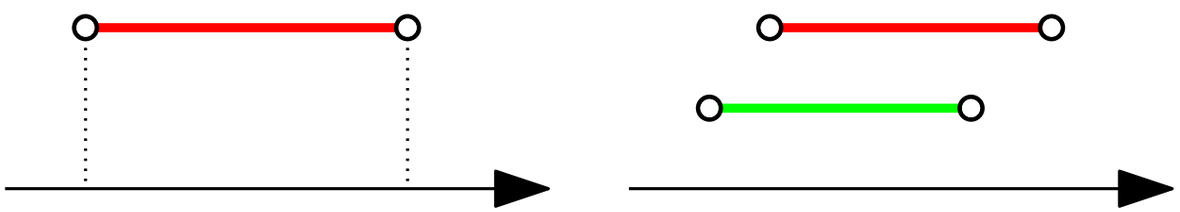

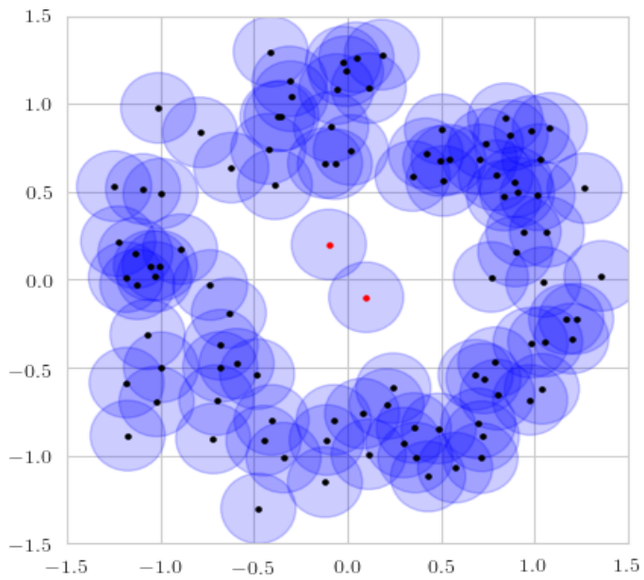

The Distance To Measure (DTM)

[*Geometric inference for probability measures*, Chazal, Cohen-Steiner, Mérigot, Found. Comput. Math., 2011]

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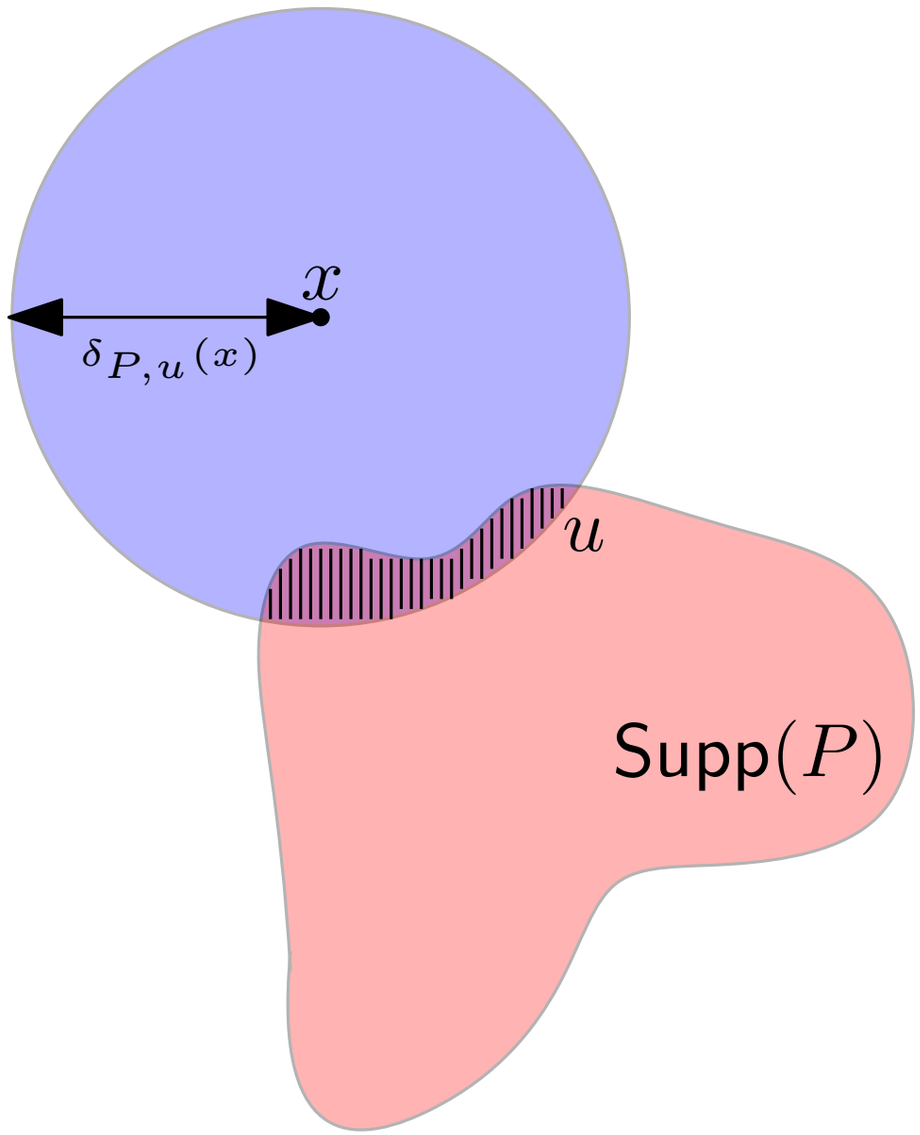
Preliminary distance function to a measure P: let $u \in]0,1[$ be a positive mass, and P a probability measure on $\mathbb{R}^d$:

$$\delta_{P,u}(x) = \inf\{r > 0 : P(B(x,r)) \geq u\}$$



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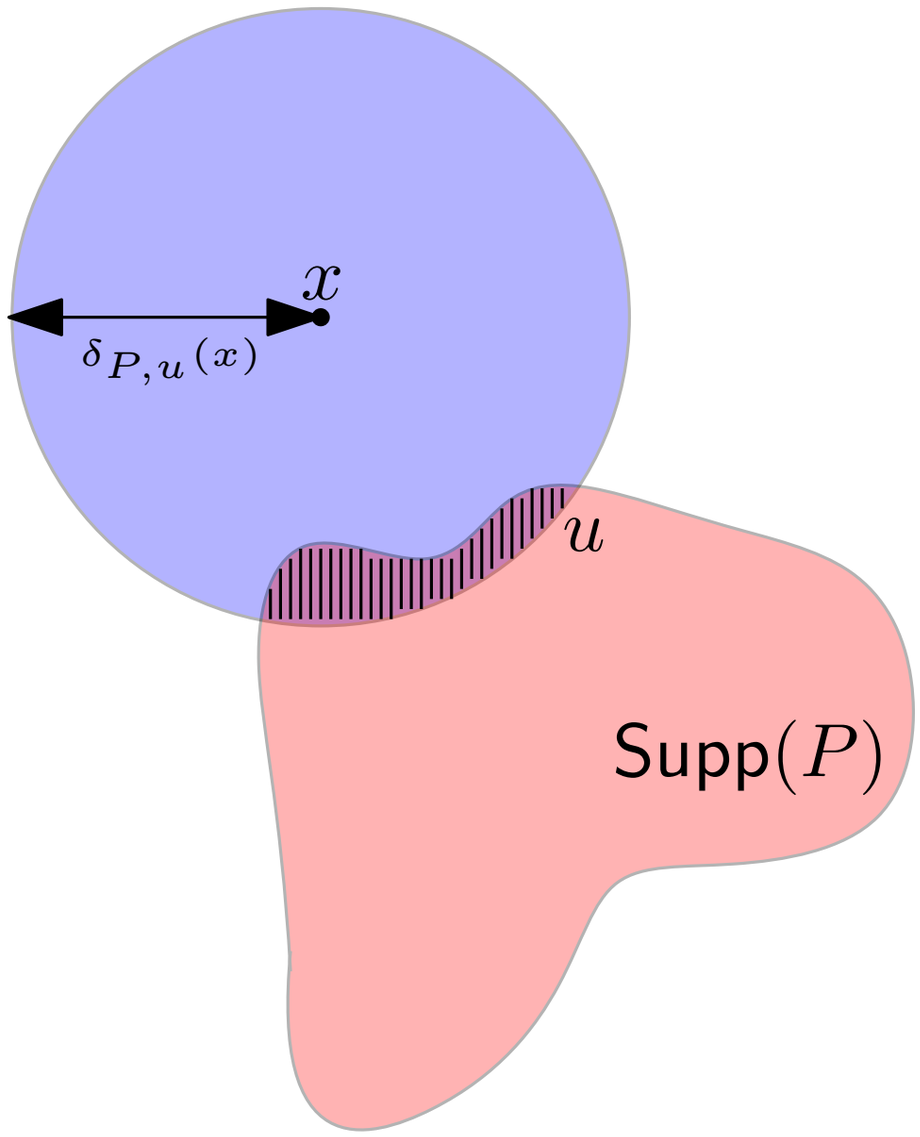

$\delta_{P,u}$ is the smallest distance needed to capture a mass of at least u.

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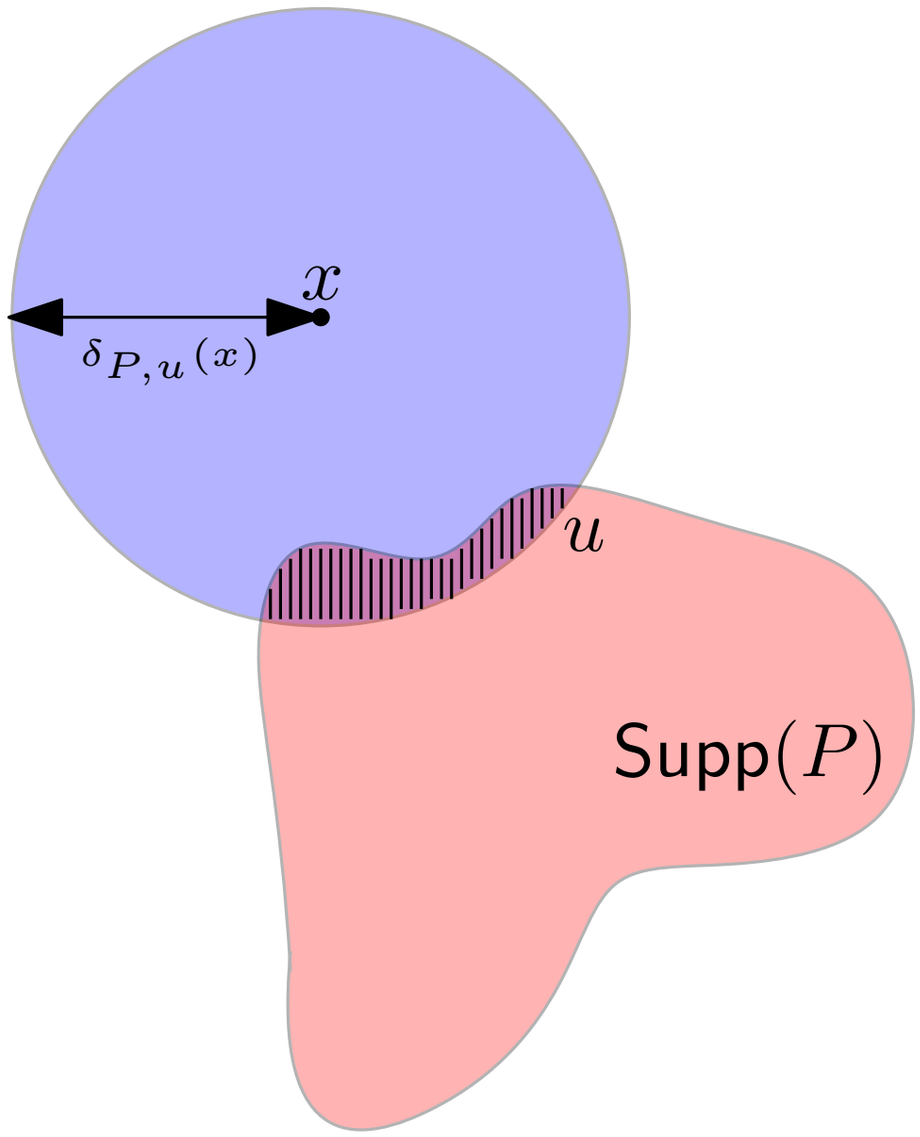

$\delta_{P,u}$ is the smallest distance needed to capture a mass of at least u.

$\delta_{P,u}$ is the quantile function at u of the r.v. $\|x - X\|$ where $X \sim P$.

The Distance To Measure (DTM)

[*Geometric inference for probability measures*, Chazal, Cohen-Steiner, Mérigot, Found. Comput. Math., 2011]

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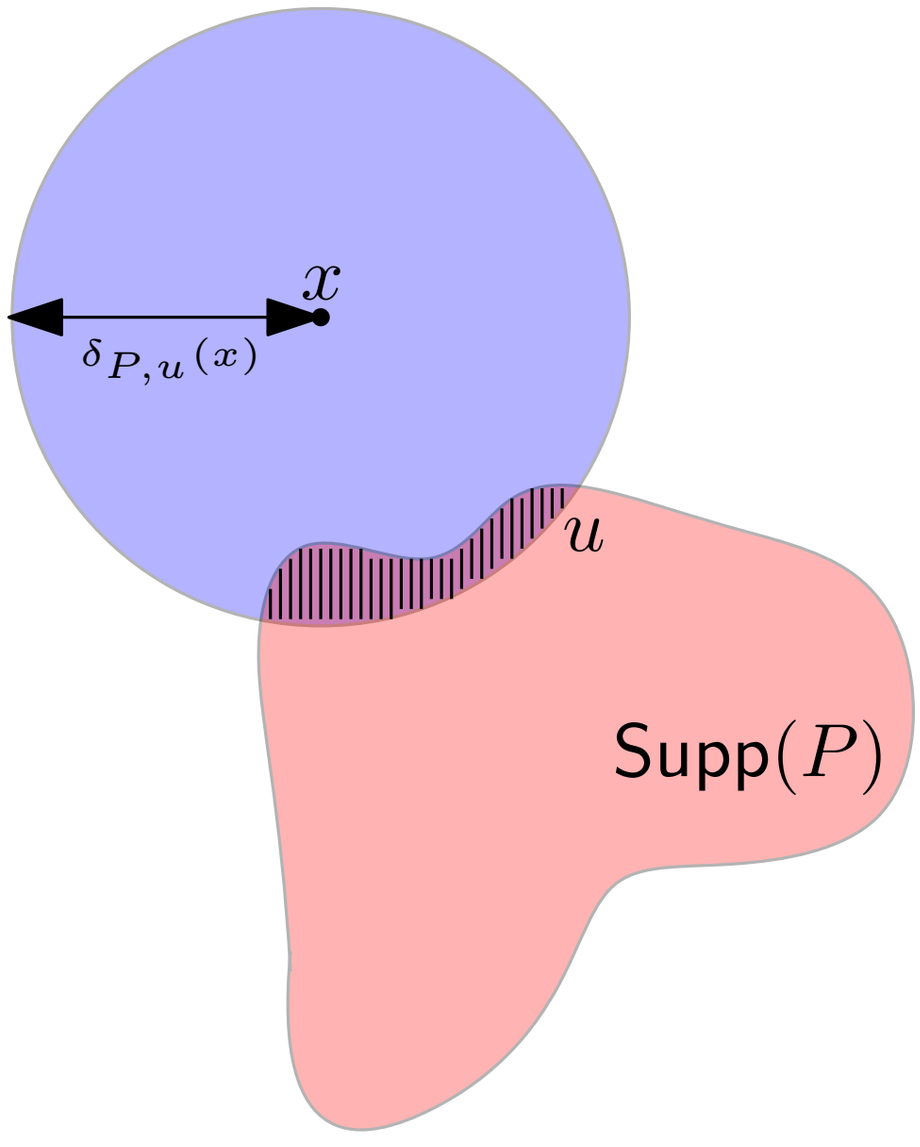

Def: Given a probability measure P on $\mathbb{R}^d$ and $m > 0$, the distance function to the measure P (DTM) is defined by

$$d_{P,m} : x \in \mathbb{R} \mapsto \left(\frac{1}{m}\int_0^m \delta_{P,u}^2(x)\mathrm{d}u\right)^{1/2}$$

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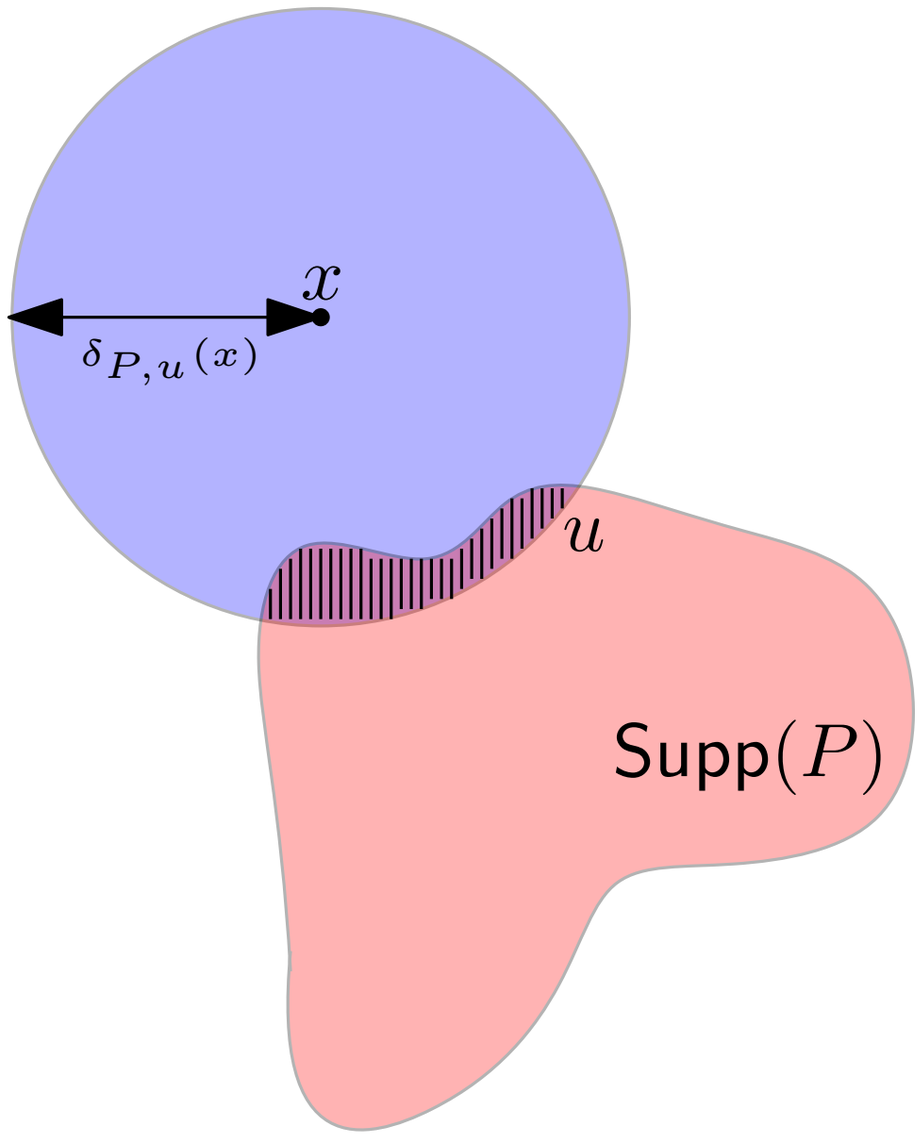

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The DTM is robust, i.e., stable under Wasserstein perturbations:

$$\|d_{P,m} - d_{Q,m}\|_\infty \leq \frac{1}{\sqrt{m}} W_2(P,Q)$$

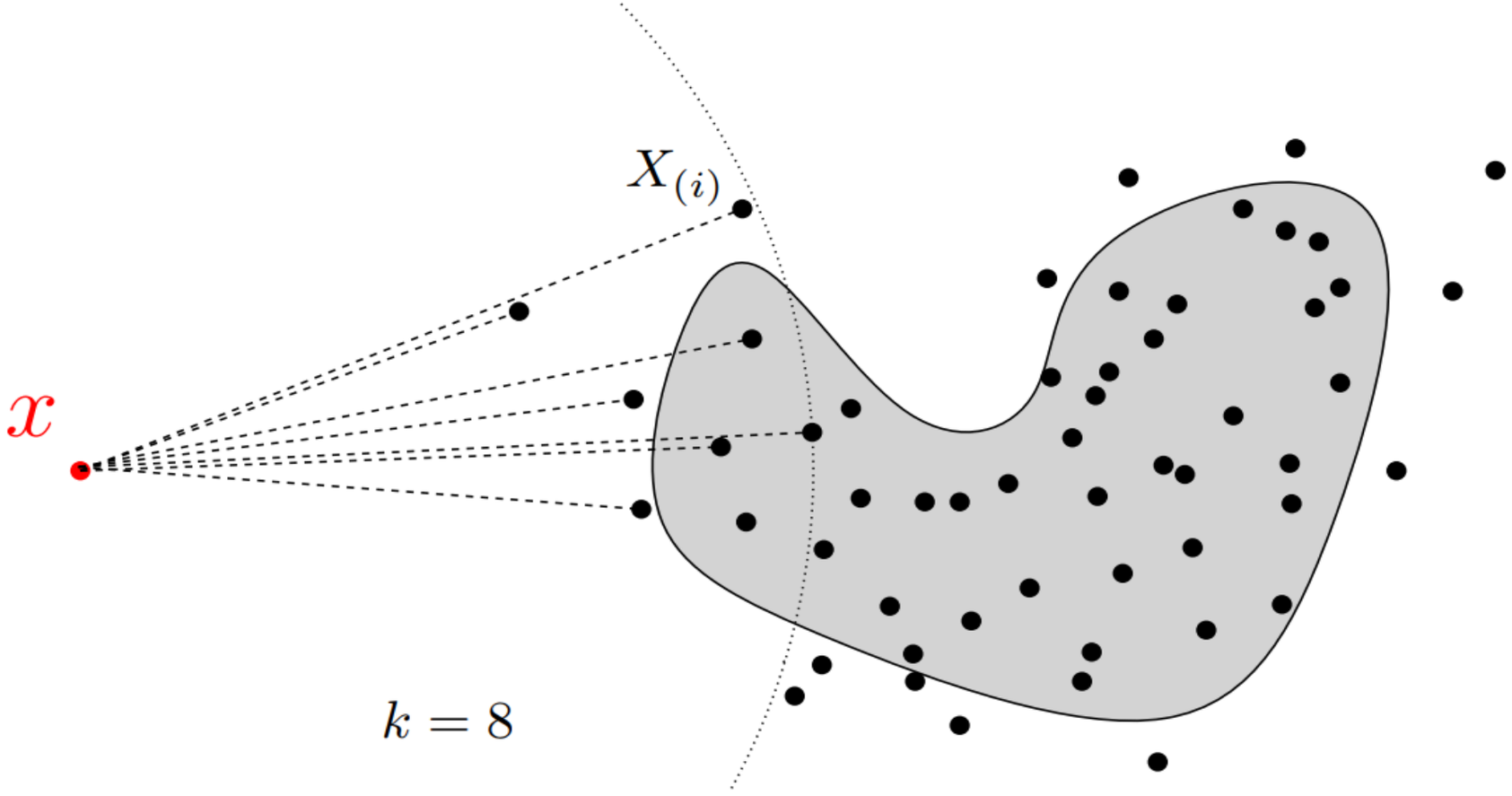
The Distance To Measure (DTM)

[*Geometric inference for probability measures*, Chazal, Cohen-Steiner, Mérigot, Found. Comput. Math., 2011]

Def: Let $X_1, \ldots, X_n$ sampled according to P and let P_n be the empirical measure. Then

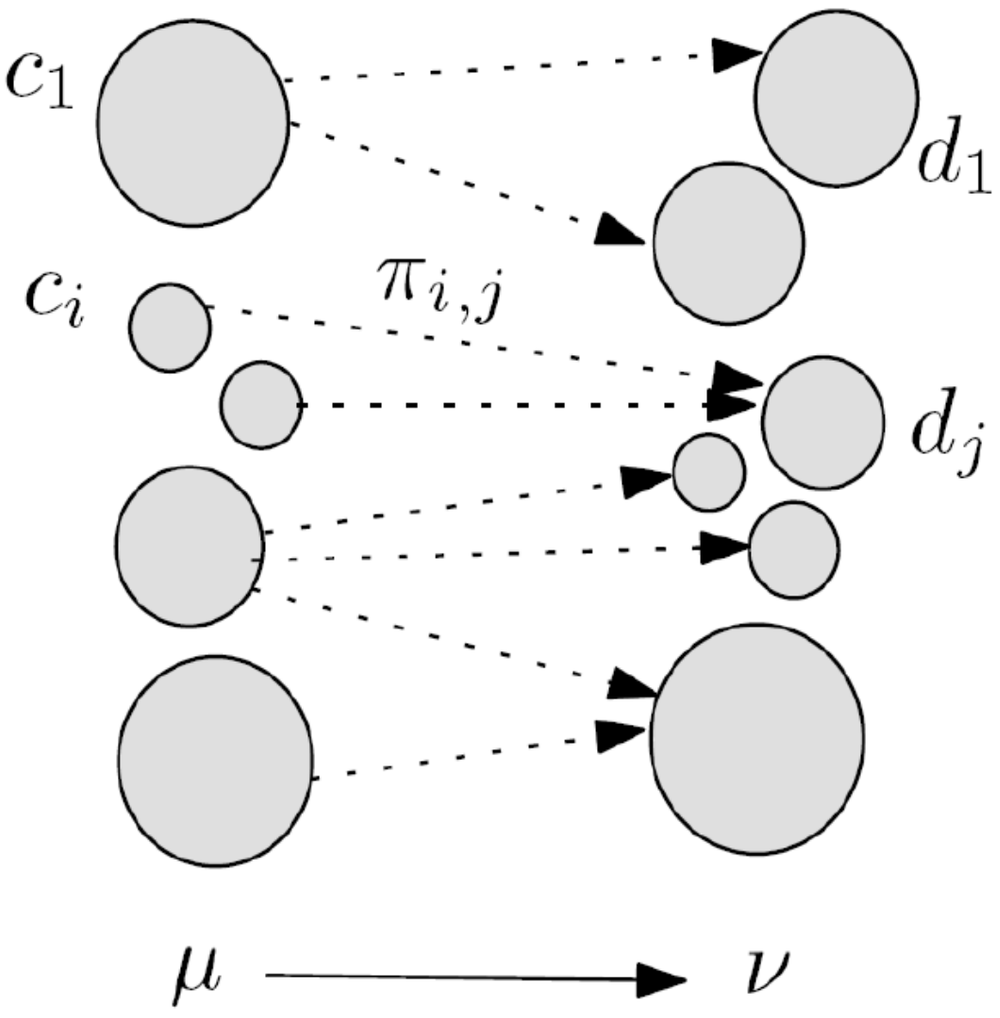
$$d_{P_n,k/n}(x) = \frac{1}{k} \sum_{i=1}^{k} \|x - X_{(i)}\|^2,$$

where $\|X_{(1)} - x\| \leq \|X_{(2)} - x\| \leq \cdots \leq \|X_{(k)} - x\| \leq \cdots \leq \|X_{(n)} - x\|$.



The Wasserstein distance

Let (X, d) be a metric space and let μ, ν be probability measures on X with finite p-moments ($p \geq 1$). The Wasserstein distance $W_p(\mu, \nu)$ quantifies the optimal cost of pushing μ onto ν, the cost of moving a small mass dx from x to y being $d(x, y)^p dx$.

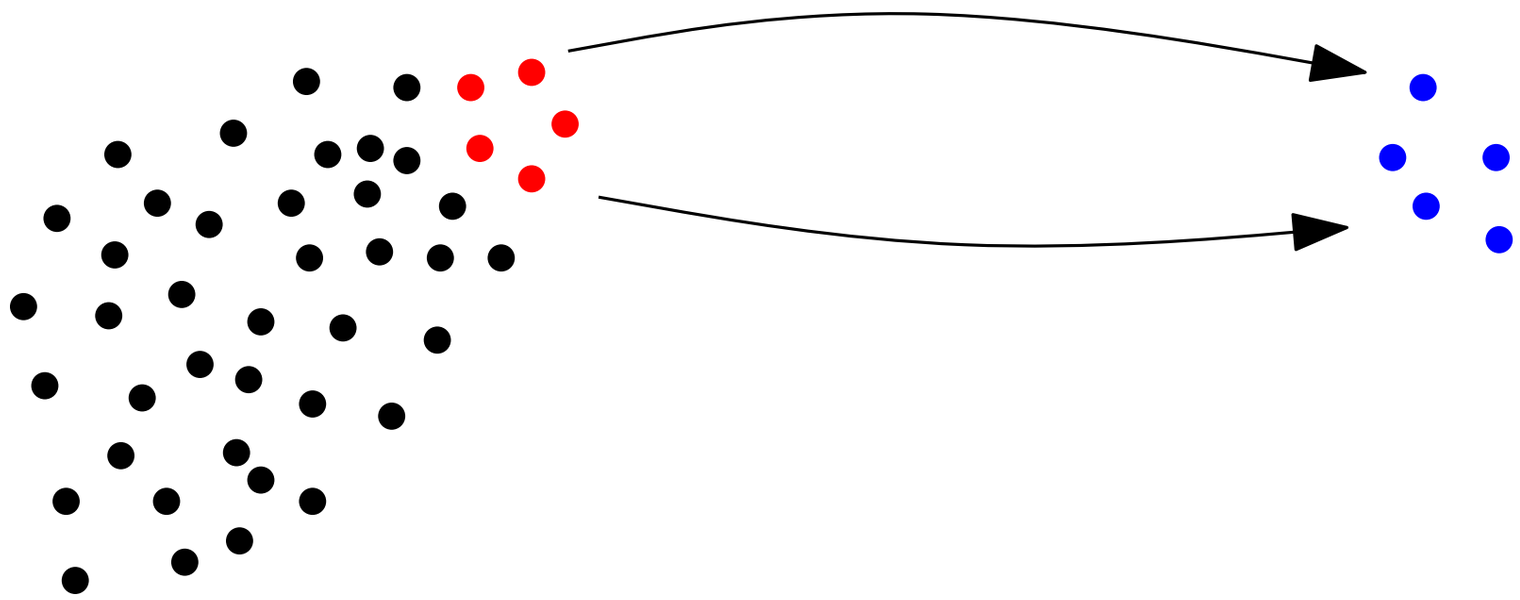


- Transport plan: Π a probability measure on $X \times X$ s.t. $\Pi(A \times \mathbb{R}^d) = \mu(A)$ and $\Pi(\mathbb{R}^d \times B) = \nu(B)$ for any borelian sets $A, B \subseteq X$.
- Cost of a transport plan:

$$C(\Pi) = \left(\int_{X \times X} d(x, y)^p d\Pi(x, y) \right)^{\frac{1}{p}}$$

- $W_p(\mu, \nu) = \inf_\Pi C(\Pi)$.

The Wasserstein distance



Ex: If $P = \{p_1, \ldots, p_n\}$ is a point cloud, and $P' = \{p_1, \ldots, p_{n-k-1}, o_1, \ldots, o_k\}$ with $d(o_i, P) = R$, then

$$d_H(P, P') \geq R \qquad \text{but} \qquad W_2(\mu_P, \mu_{P'}) \leq \sqrt{\frac{k}{n}}(R + \operatorname{diam}(P))$$

DTM-based filtrations

[*DTM-based filtrations*, Anai et al., Symp. Comp. Geom., 2019]

Def: Let V be a point cloud (in a metric space). The DTM-based complex $W(V)$ is the filtered simplicial complex indexed by $\mathbb{R}$ whose vertex set is V and whose other simplices are defined with

$$\sigma = [p_0, p_1 \ldots, p_k] \in W(V, \alpha) \iff \cap_{i=0}^{k} B(p_i, r_{p_i}(\alpha)) \neq \emptyset$$

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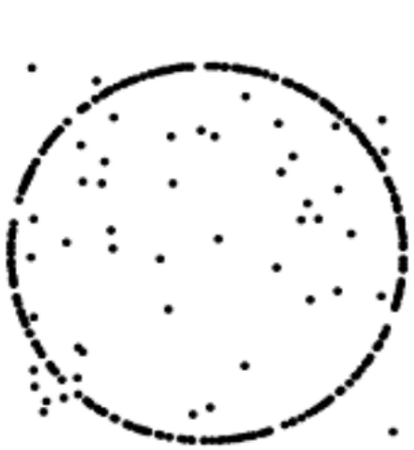

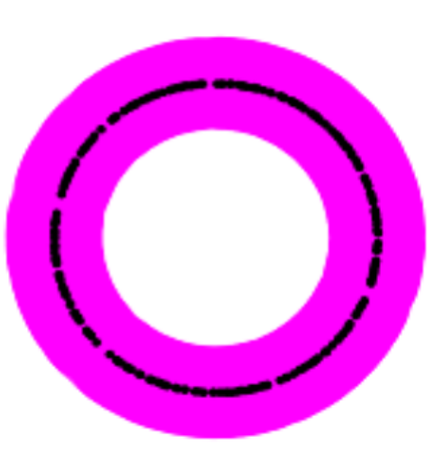

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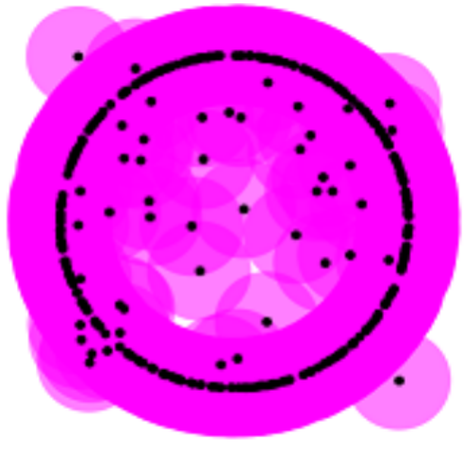

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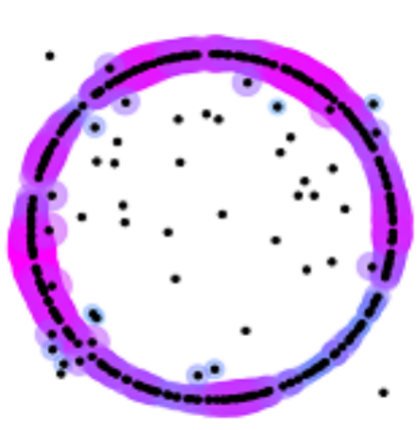
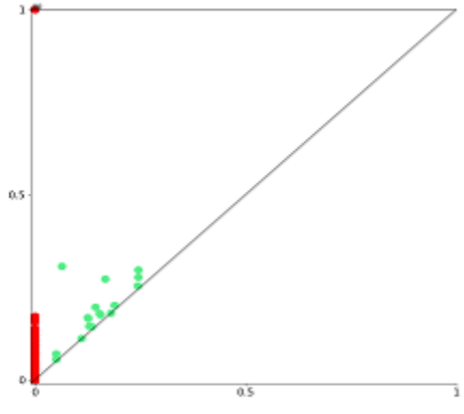
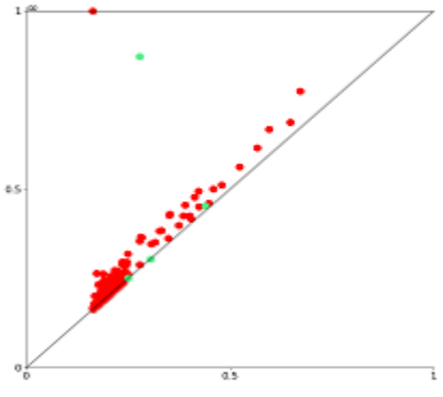


DTM-based





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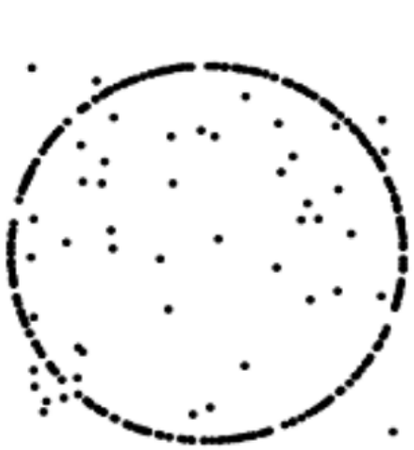

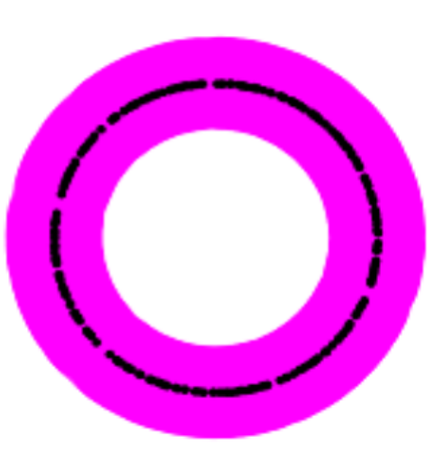

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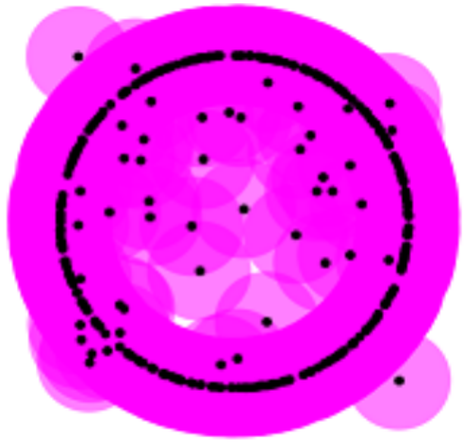

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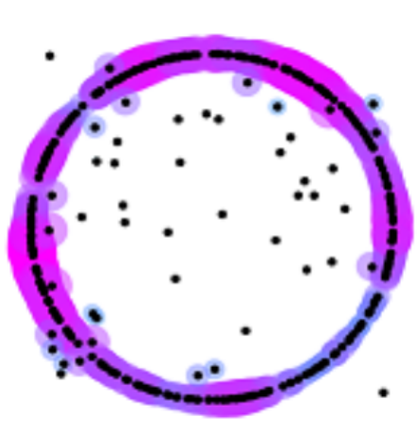
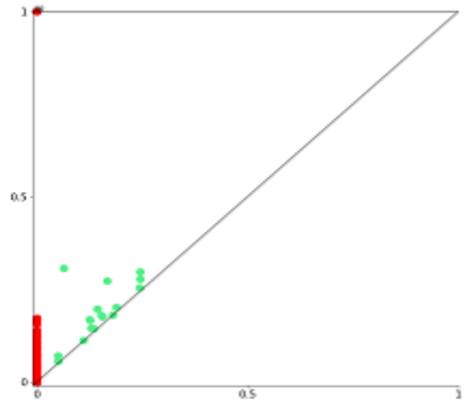
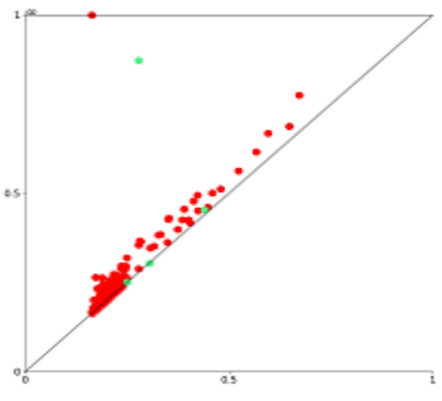


DTM-based

Thm: $d_b(D_W(X), D_W(Y)) \leq \sqrt{\frac{n}{k}} W_2(X, Y) + 2^{1/q} d_H(X, Y)$.

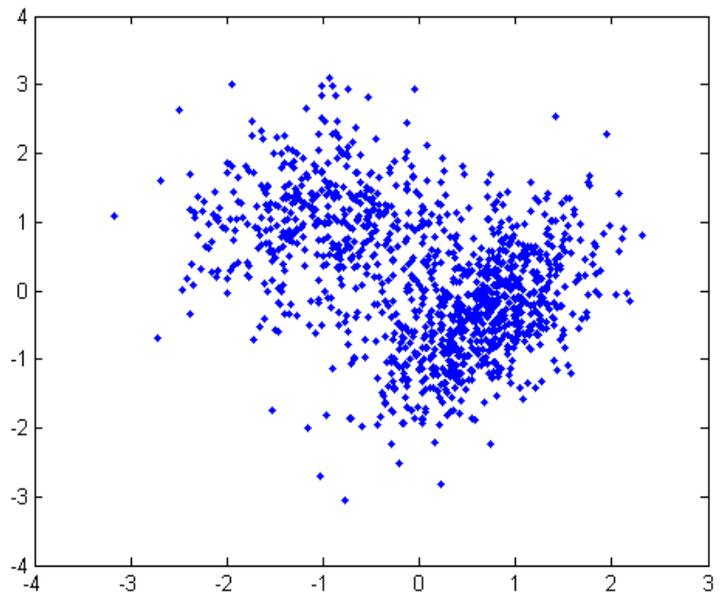


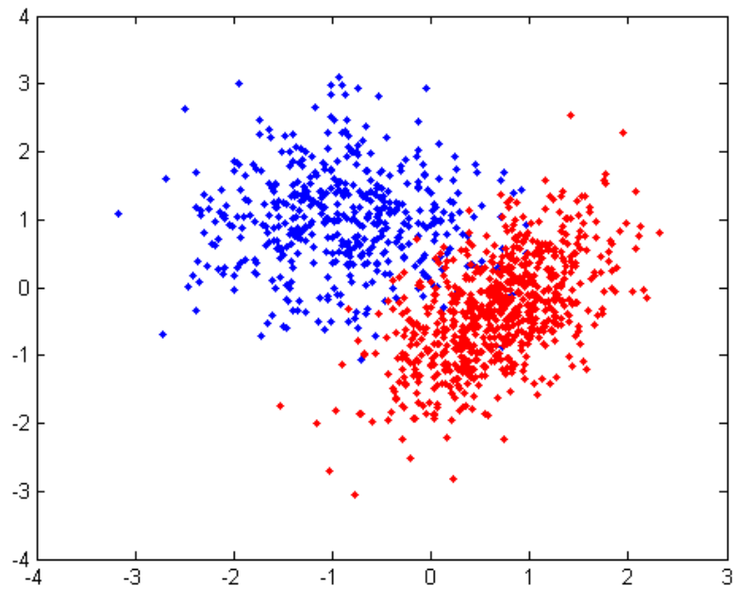


Clustering and 0-dimensional Persistent Homology

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).

Clustering and 0-dimensional Persistent Homology

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.

Not a single/universal notion of cluster.

A wealth of approaches:

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

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- Variational
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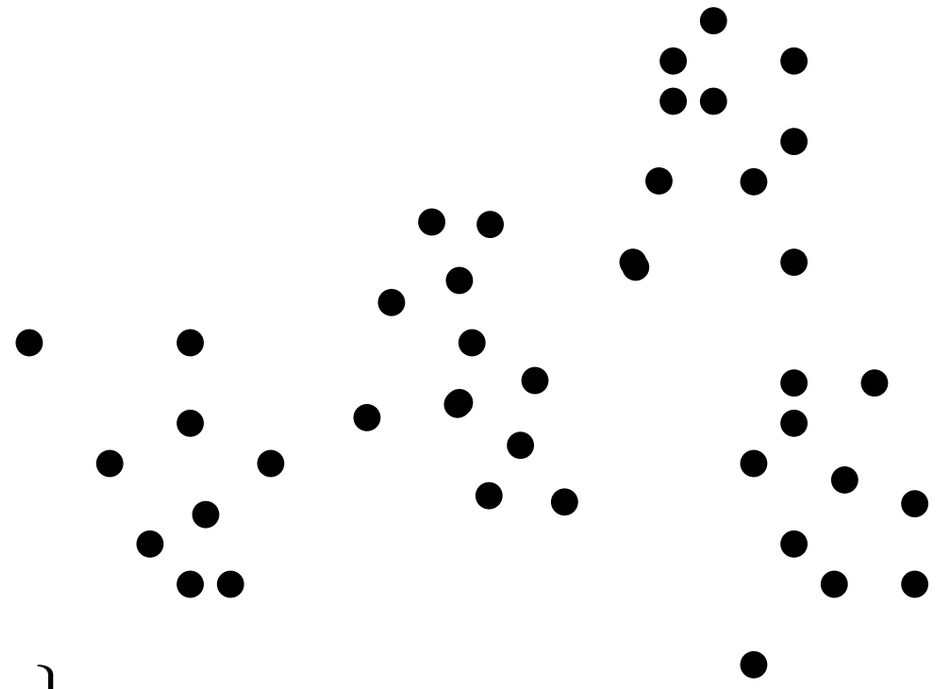
In this lecture:

- 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 $L = \{y_1, \ldots, y_k\}$ that minimizes

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

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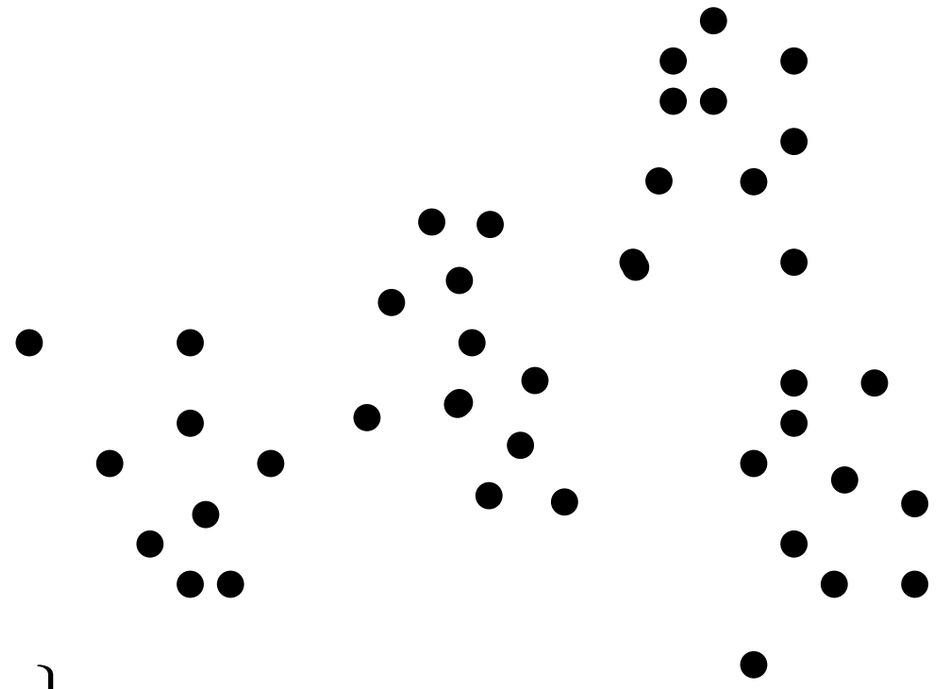

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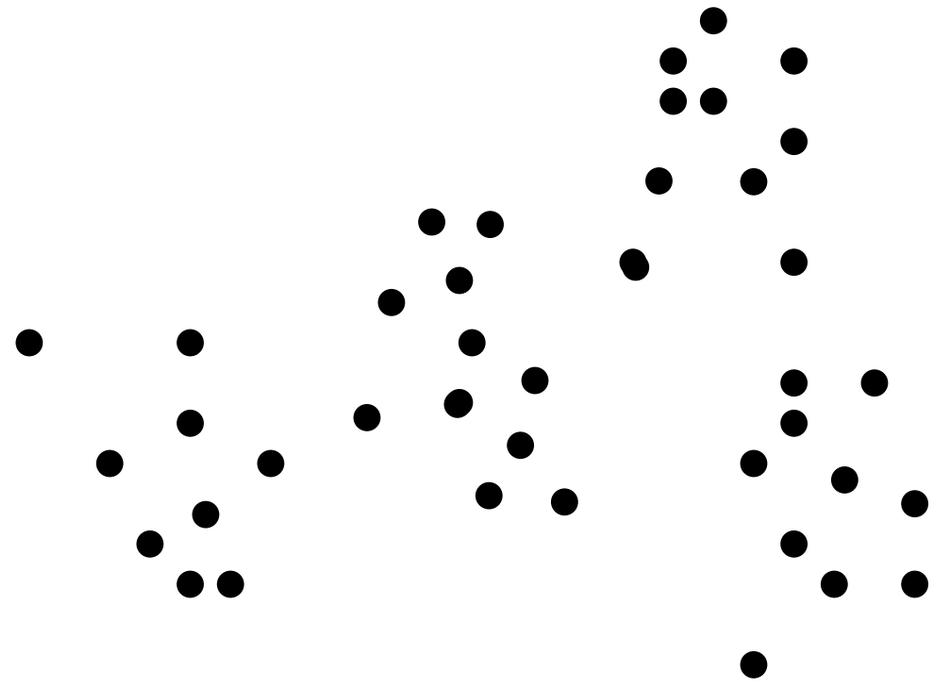
This is a NP hard problem!

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

The k-means algorithm



Lloyd's algorithm

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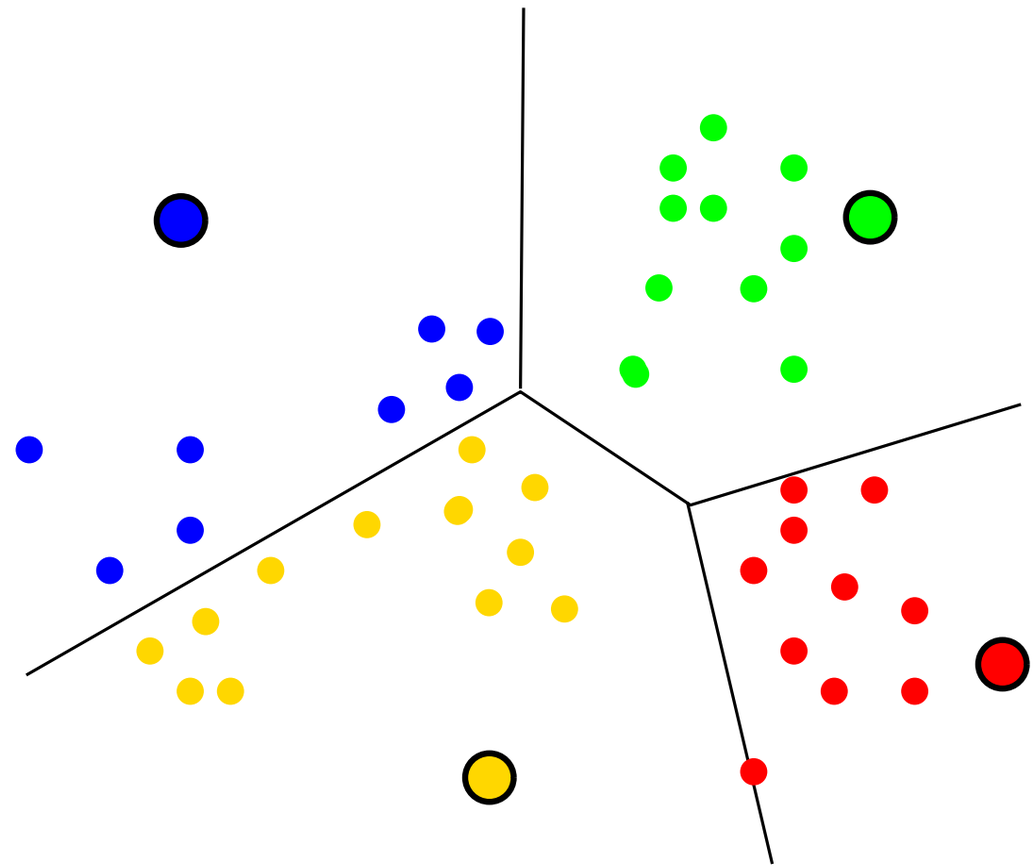

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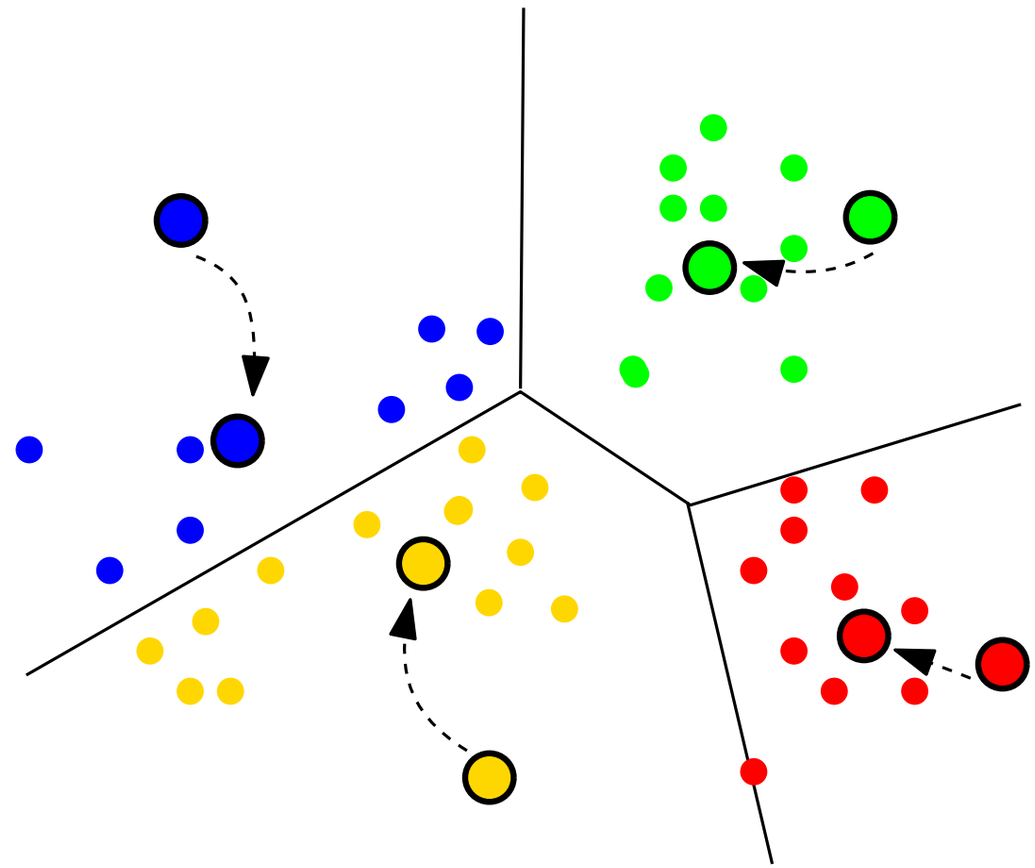

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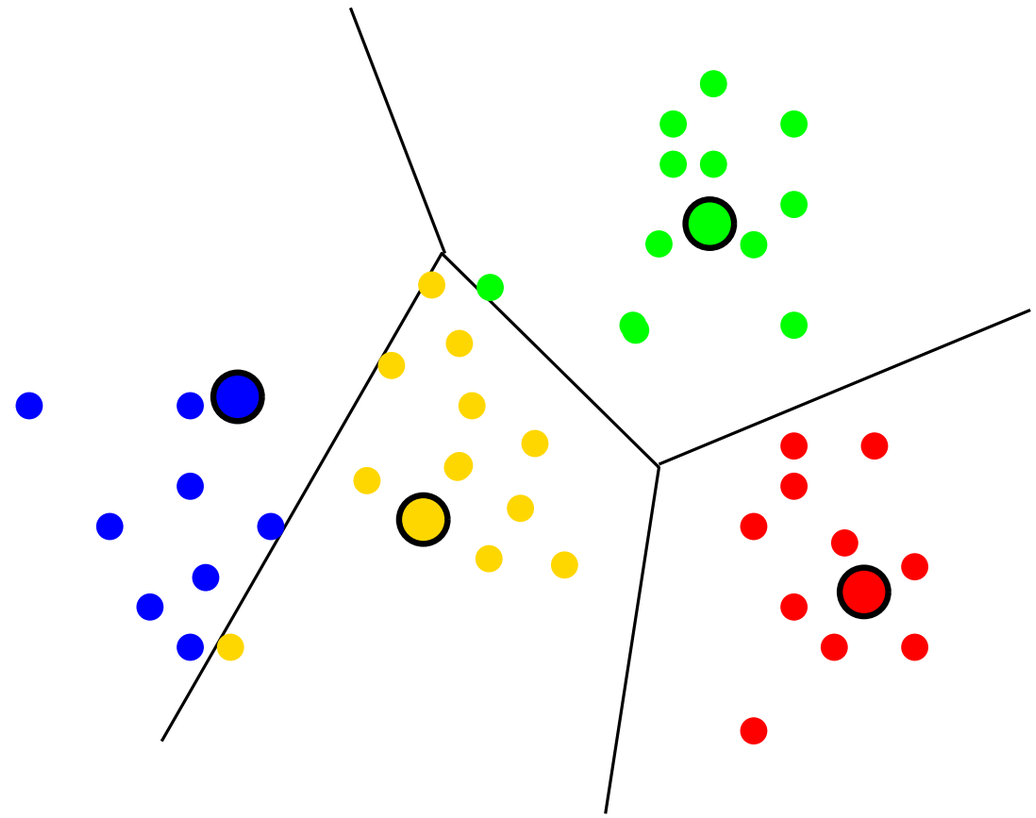

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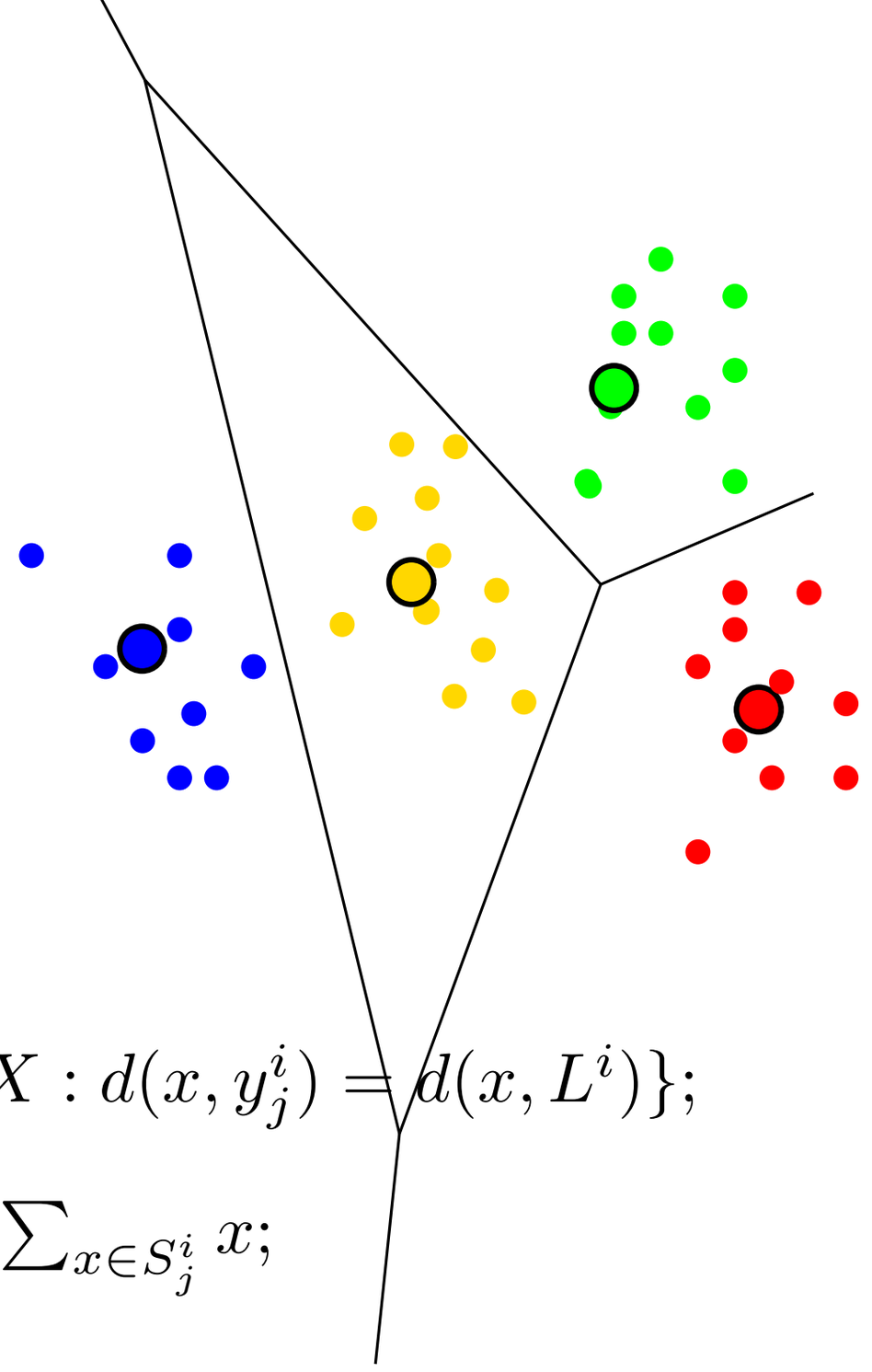

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Particular instance of the EM algorithm with (hard instead of soft) Gaussian mixture model with fixed bandwidths.

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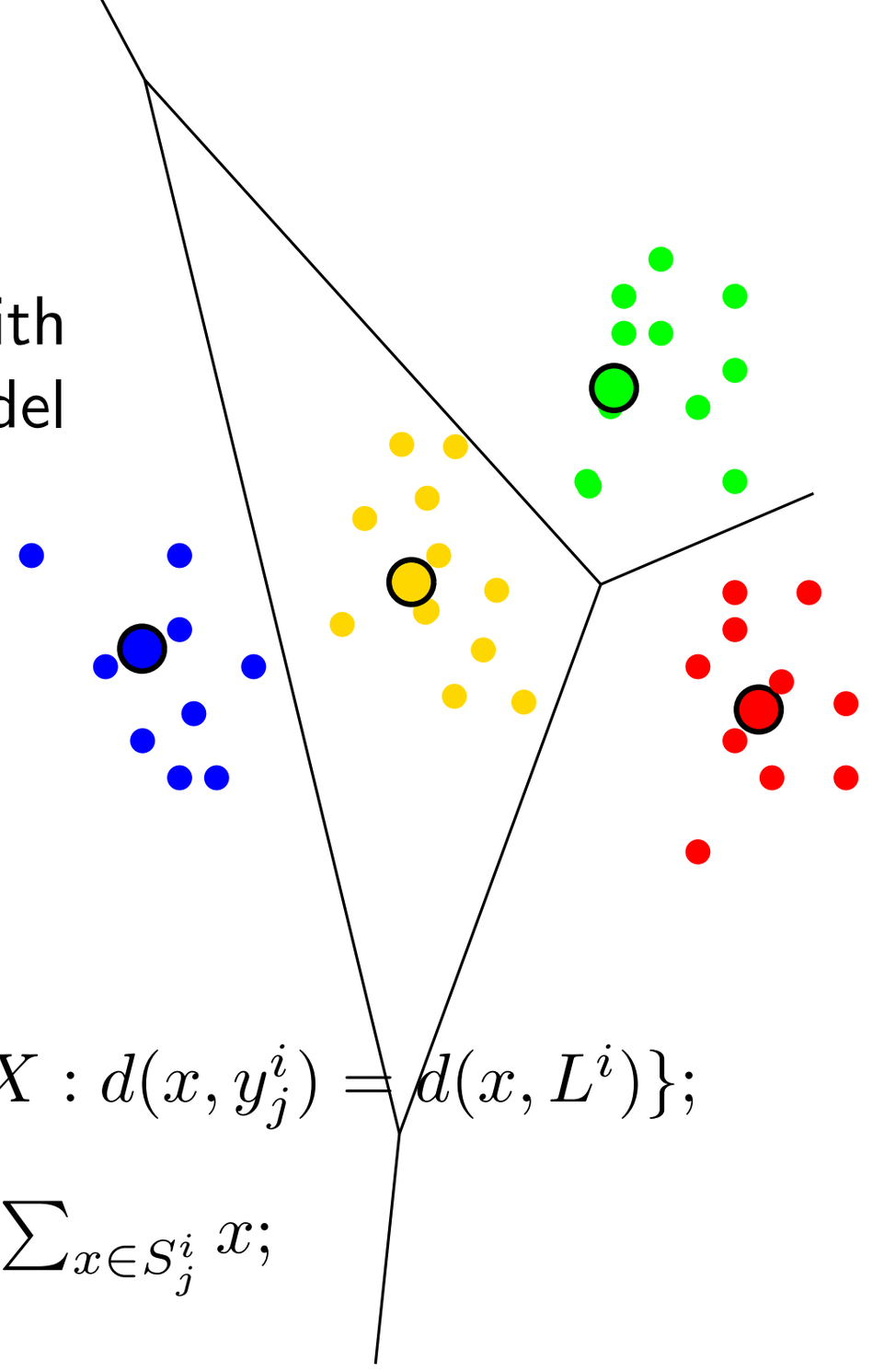

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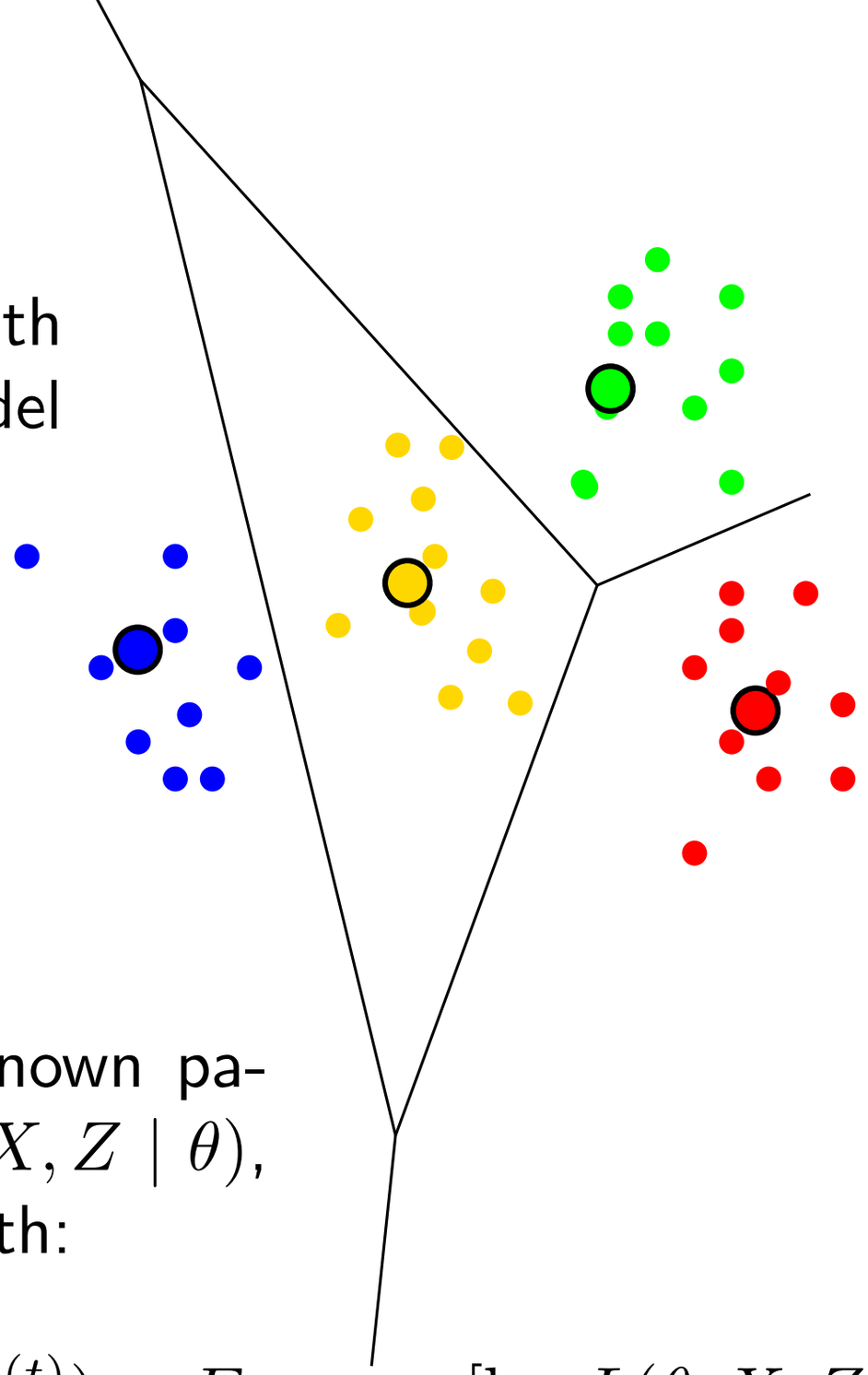

Given data set X, latent variables Z, unknown parameters θ, and likelihood $L(\theta; X, Z) = p(X, Z \mid \theta)$, the EM algorithm seeks to find the MLE with:

Expectation step (E step): compute $Q(\theta \mid \theta^{(t)}) = E_{Z|X,\theta^{(t)}} [\log L(\theta; X, Z)]$

Maximization step (M step): Find $\theta^{(t+1)} = \arg\max_{\theta} Q(\theta \mid \theta^{(t)})$

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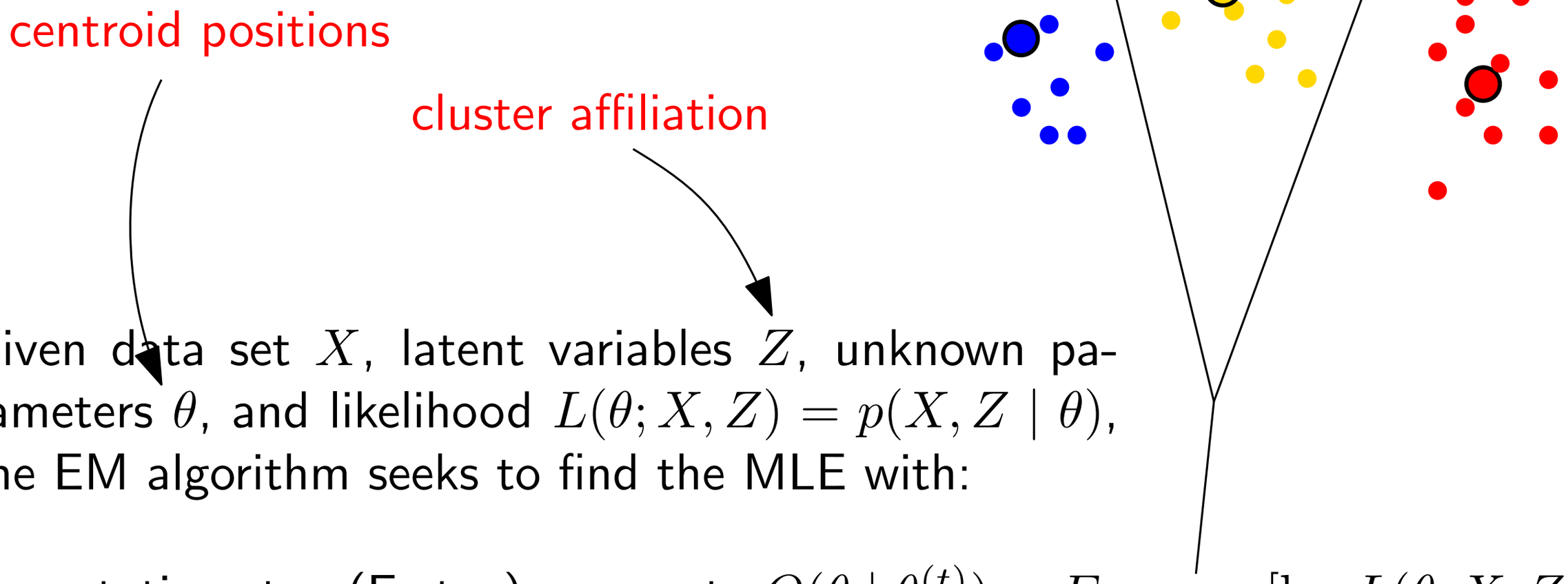


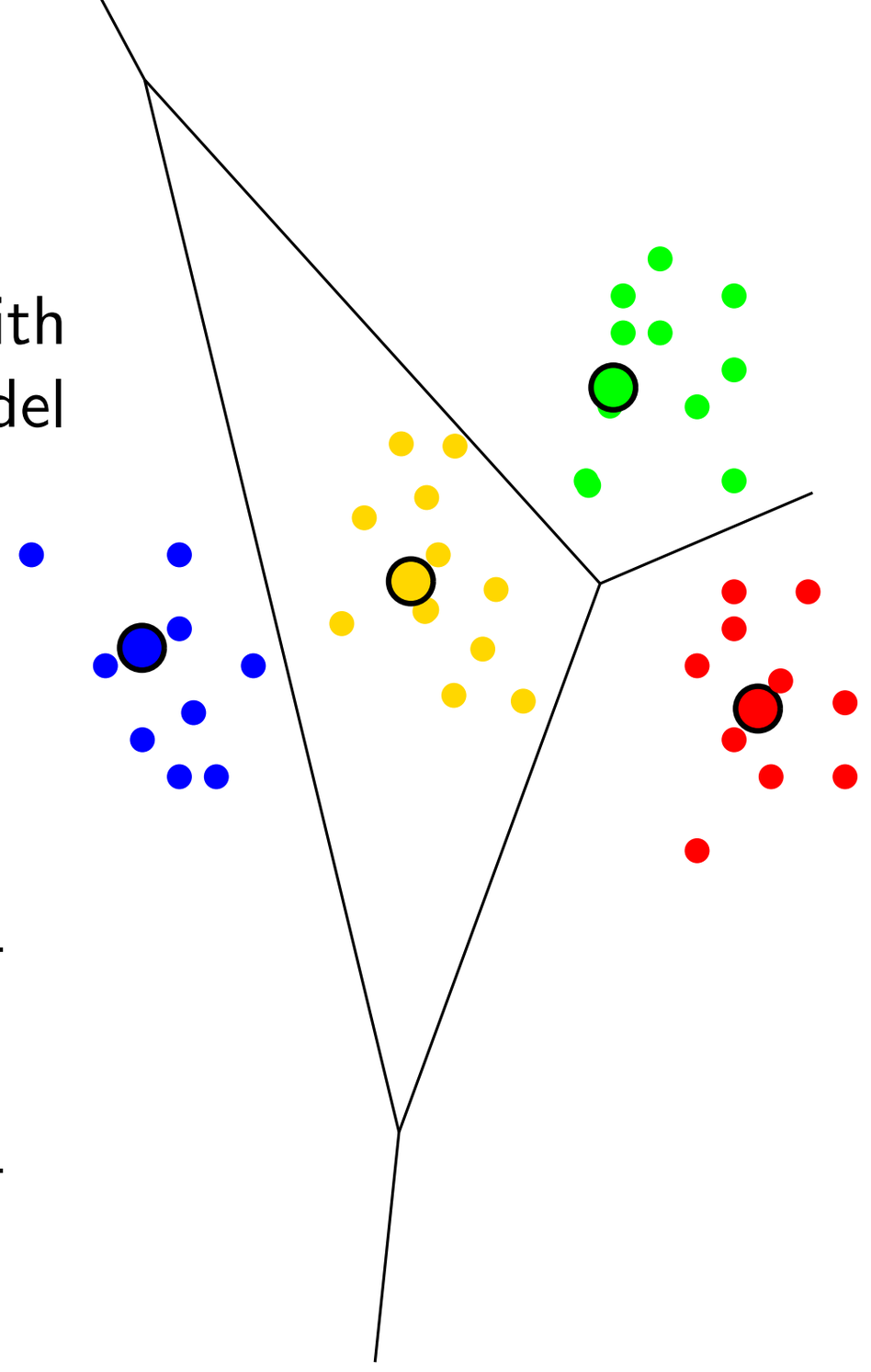
Given data set X, latent variables Z, unknown parameters θ, and likelihood $L(\theta; X, Z) = p(X, Z \mid \theta)$, the EM algorithm seeks to find the MLE with:

Expectation step (E step): compute $Q(\theta \mid \theta^{(t)}) = E_{Z|X,\theta^{(t)}} [\log L(\theta; X, Z)]$

Maximization step (M step): Find $\theta^{(t+1)} = \arg\max_{\theta} Q(\theta \mid \theta^{(t)})$

The k-means algorithm

Particular instance of the EM algorithm with (hard instead of soft) Gaussian mixture model with fixed bandwidths.



Warning:

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

Hierarchical clustering algorithms

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

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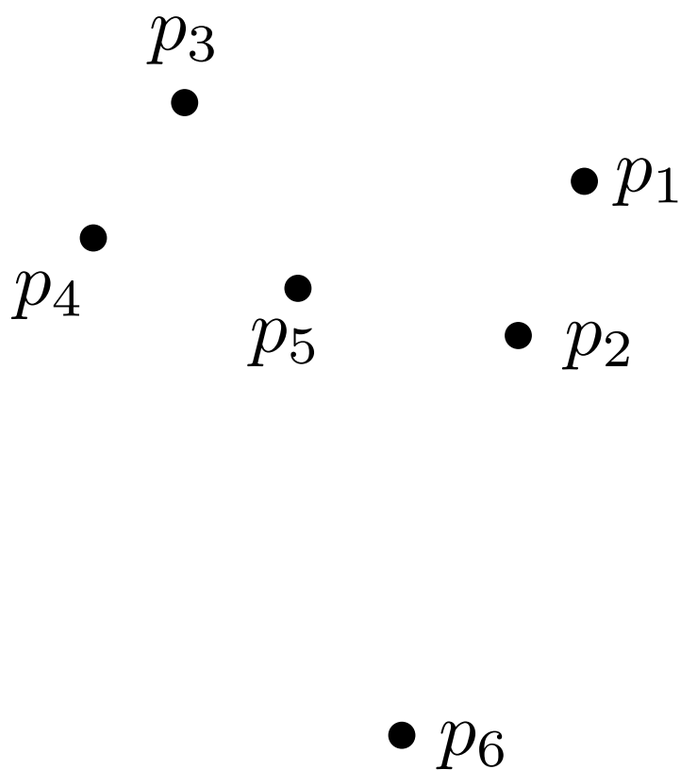
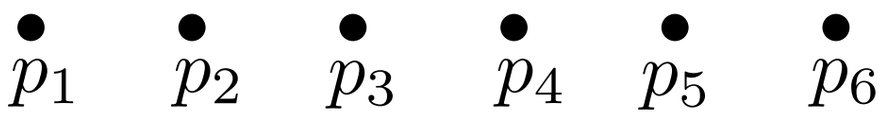
Agglomerative (bottom-up)

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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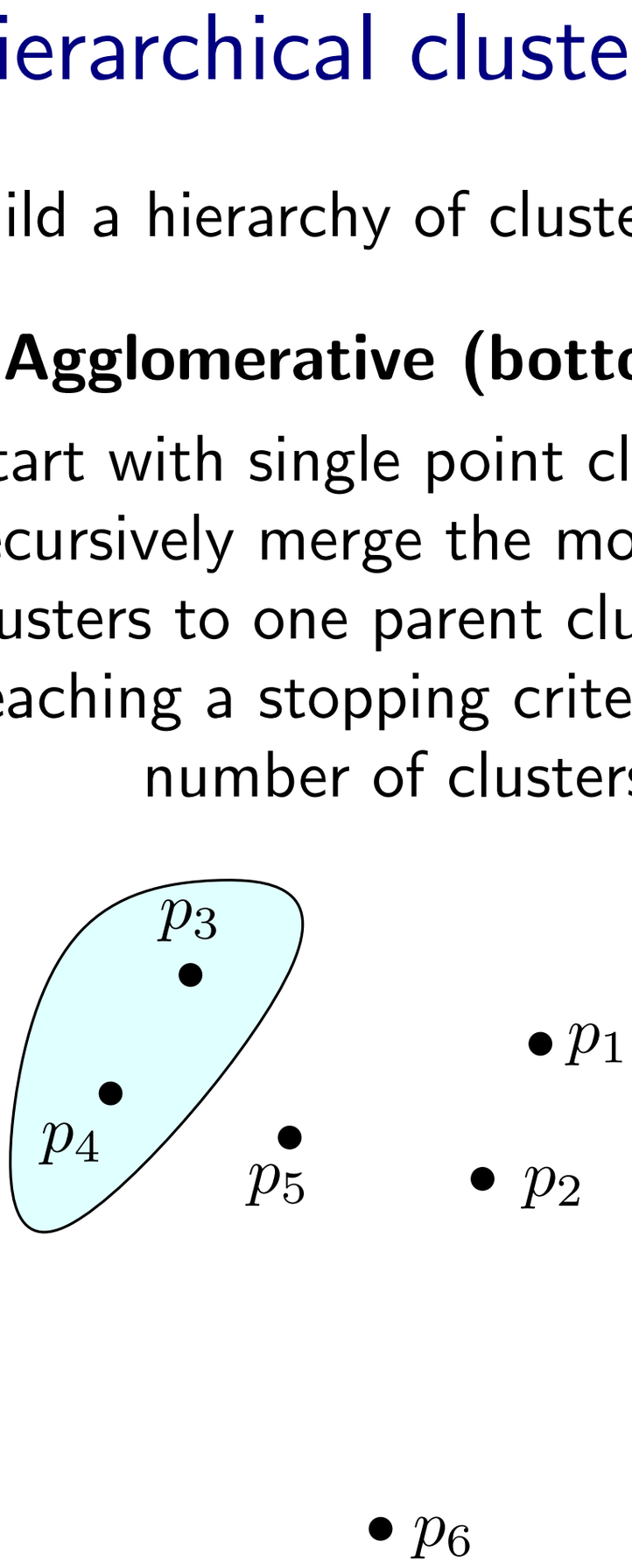

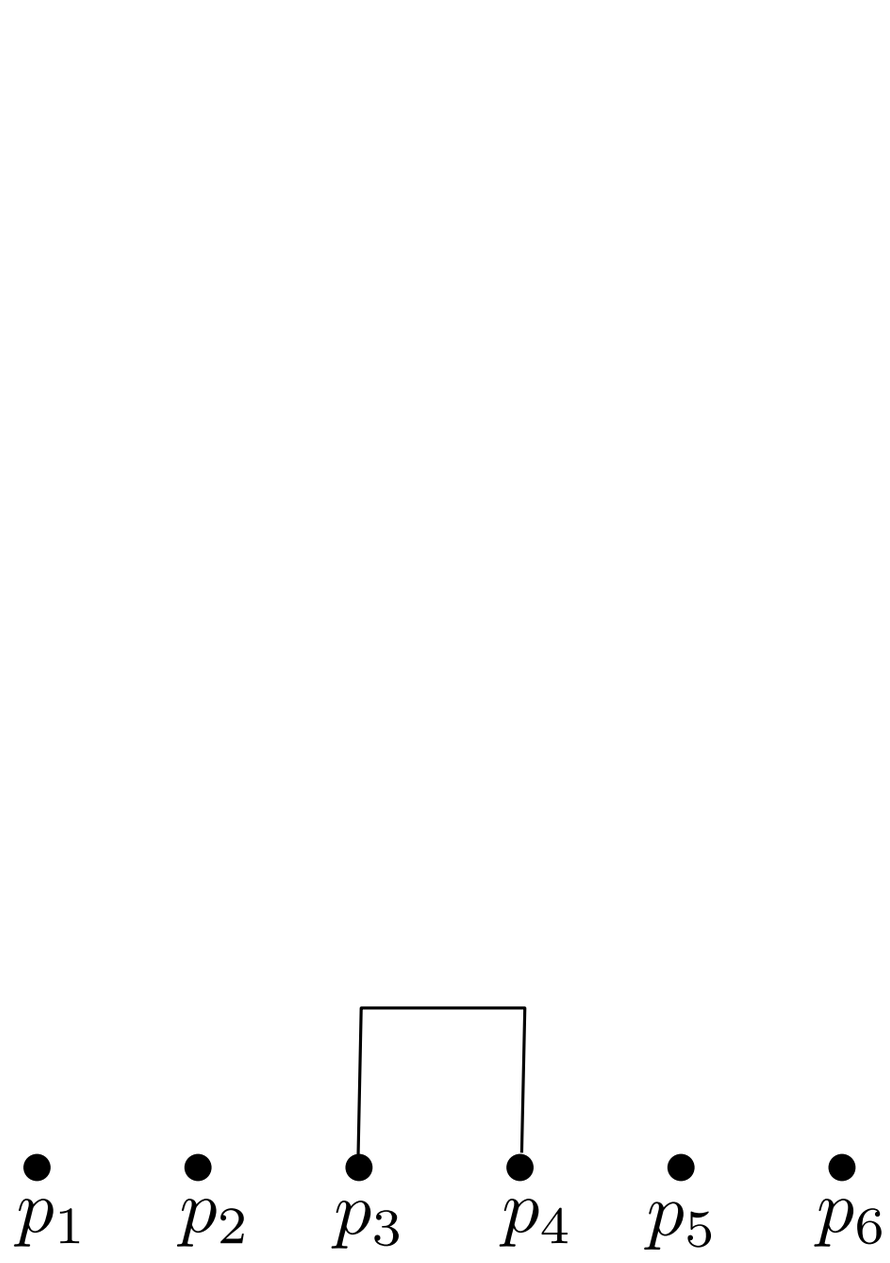

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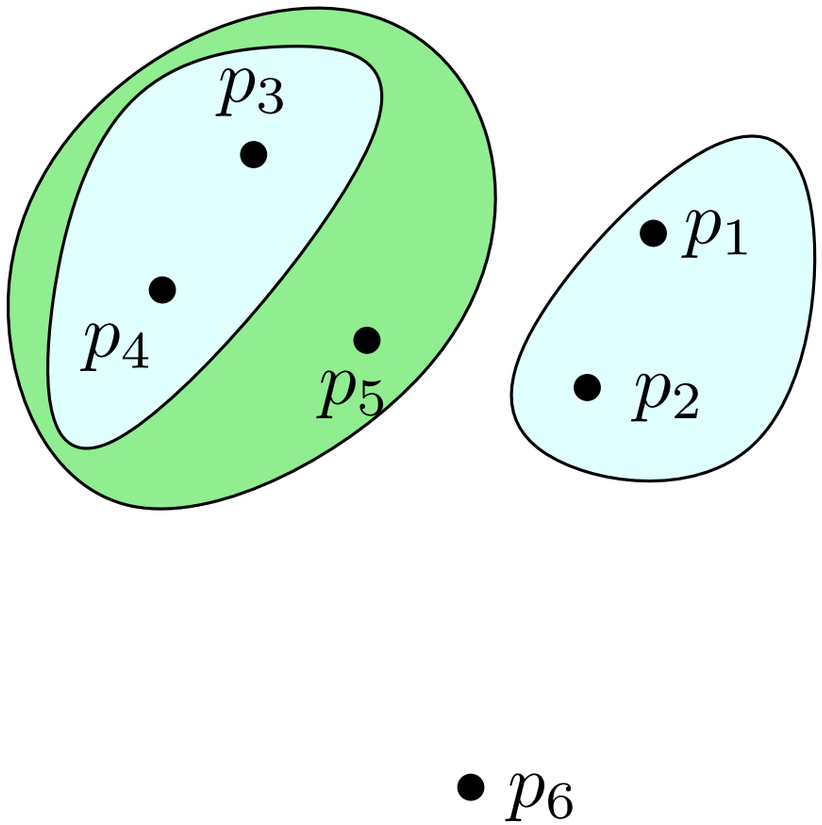

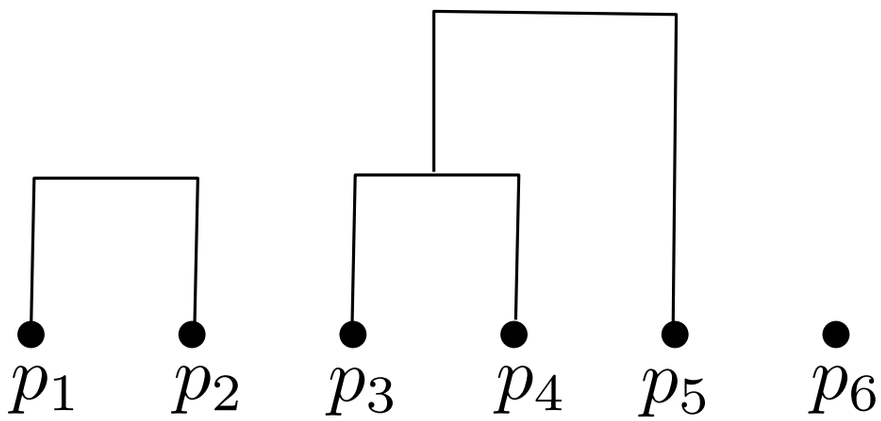

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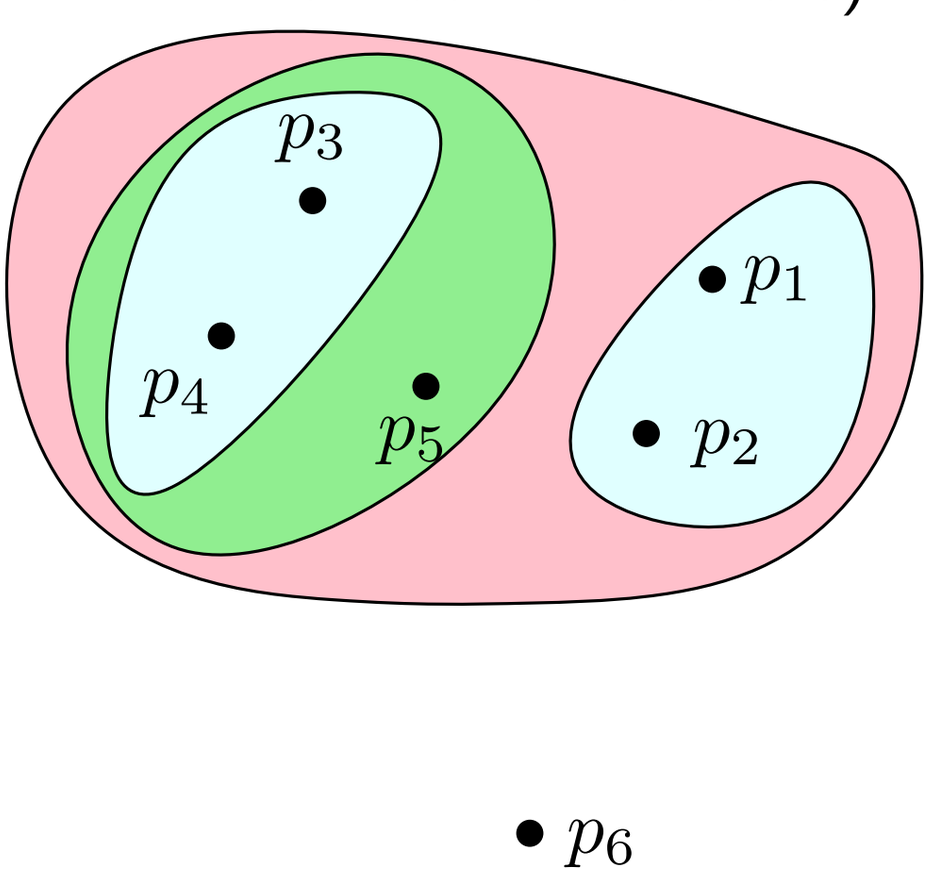

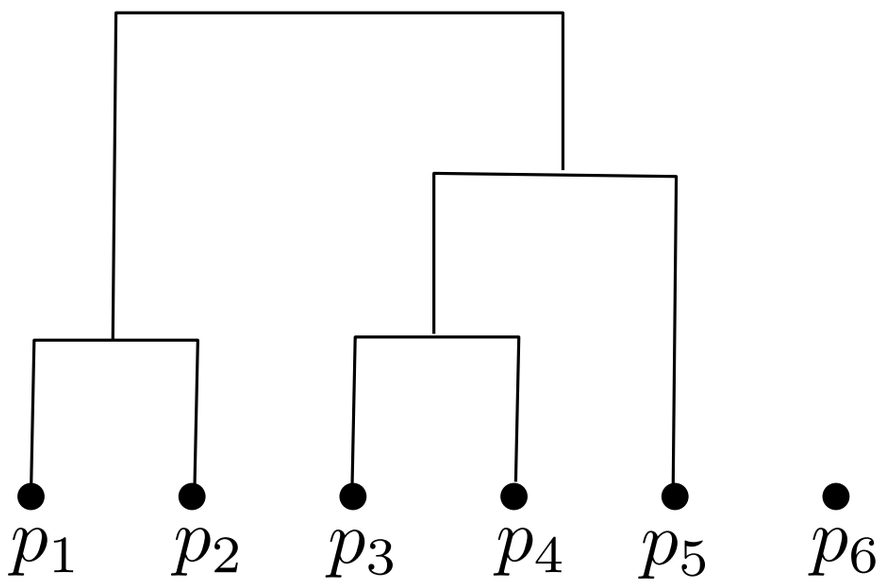

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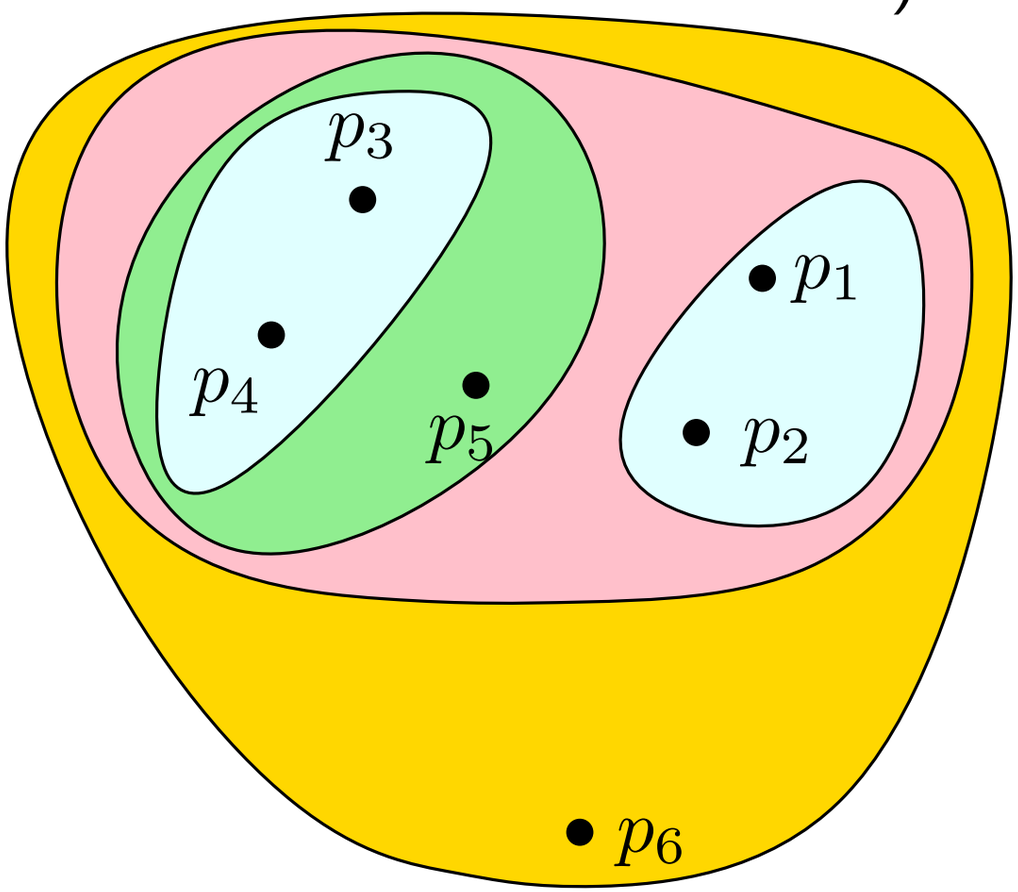

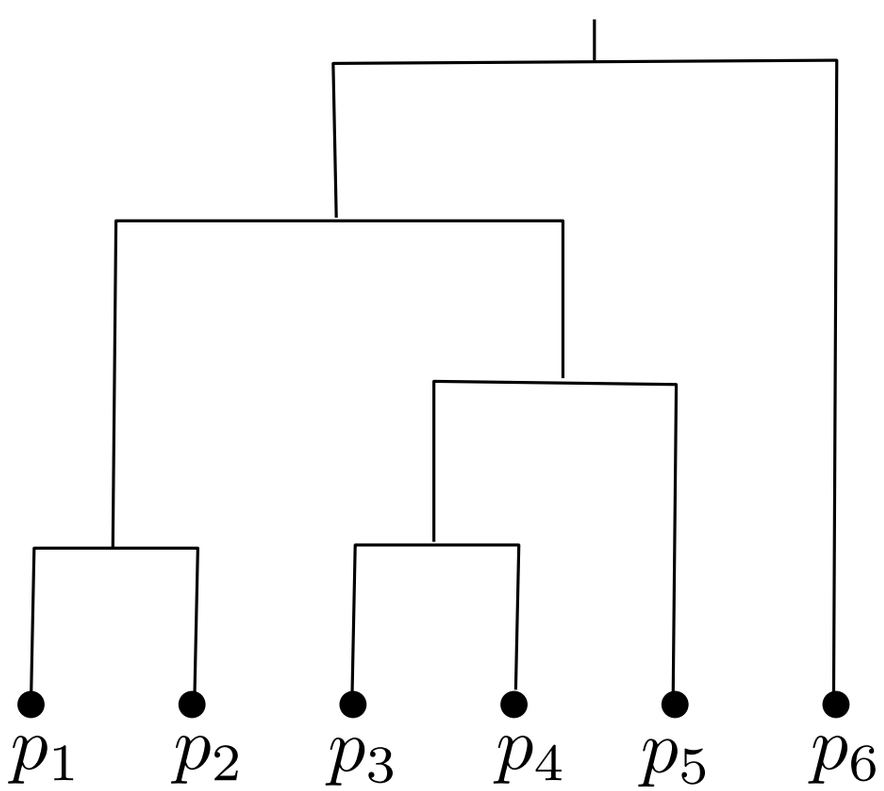

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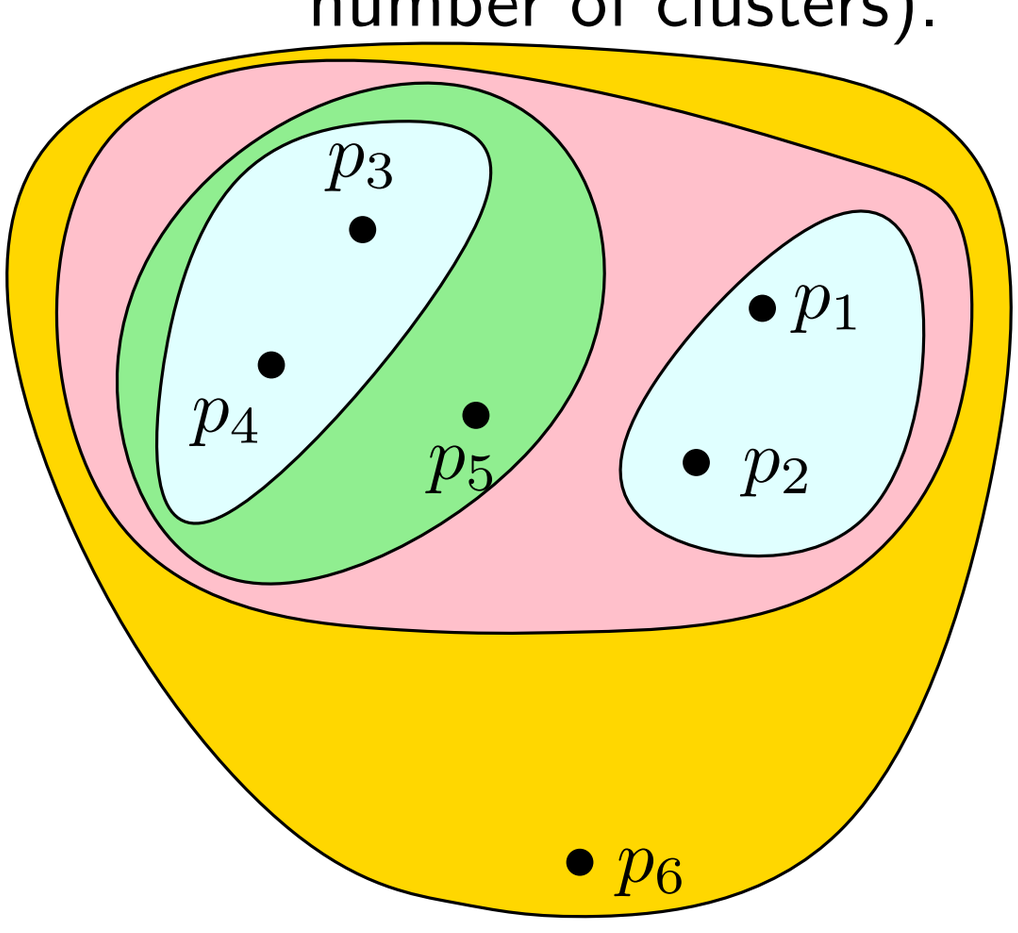
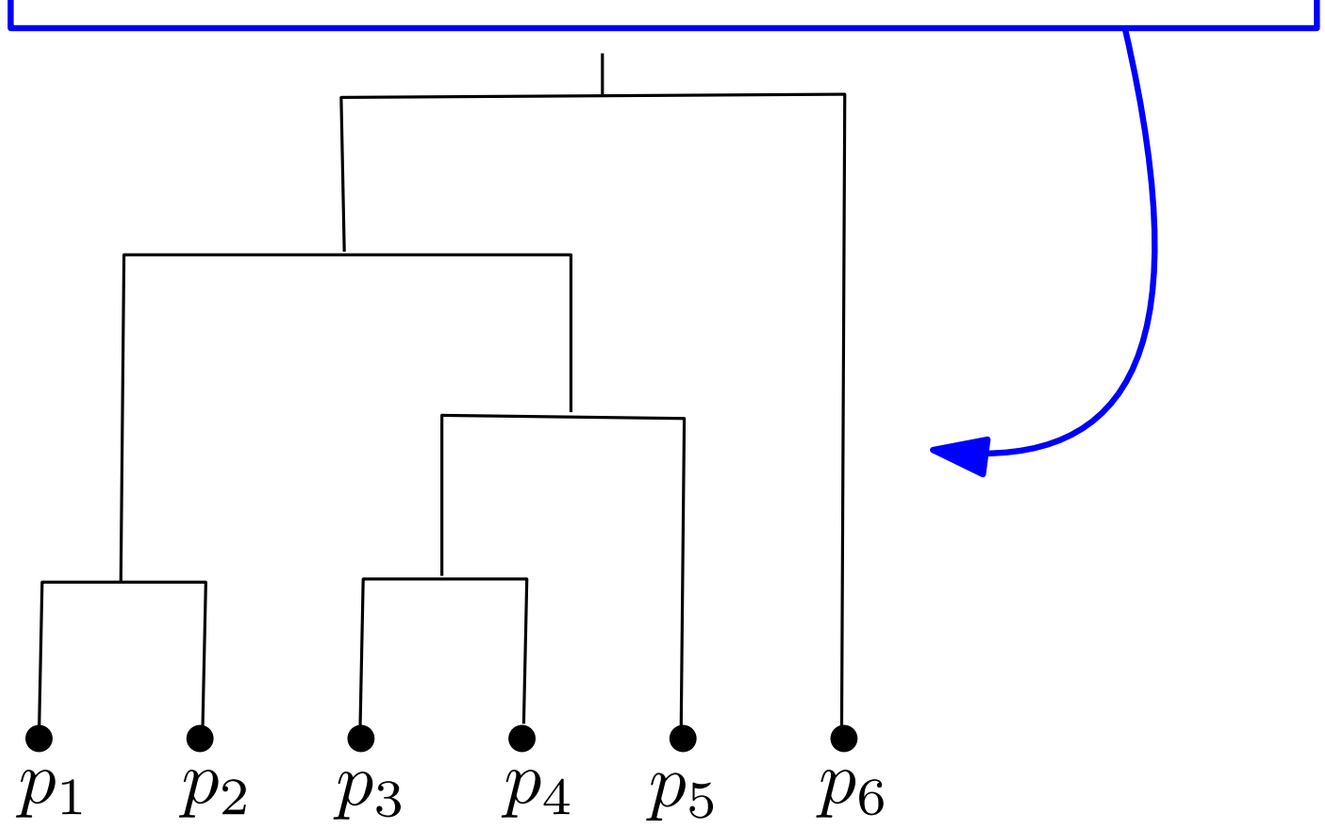


Dendogram, i;e. a tree such that:
- each leaf node is a singleton,
- each node represent a cluster,
- the root node contains the whole data,
- each internal node has two daughters, corresponding to the clusters that were merged to obtain it.



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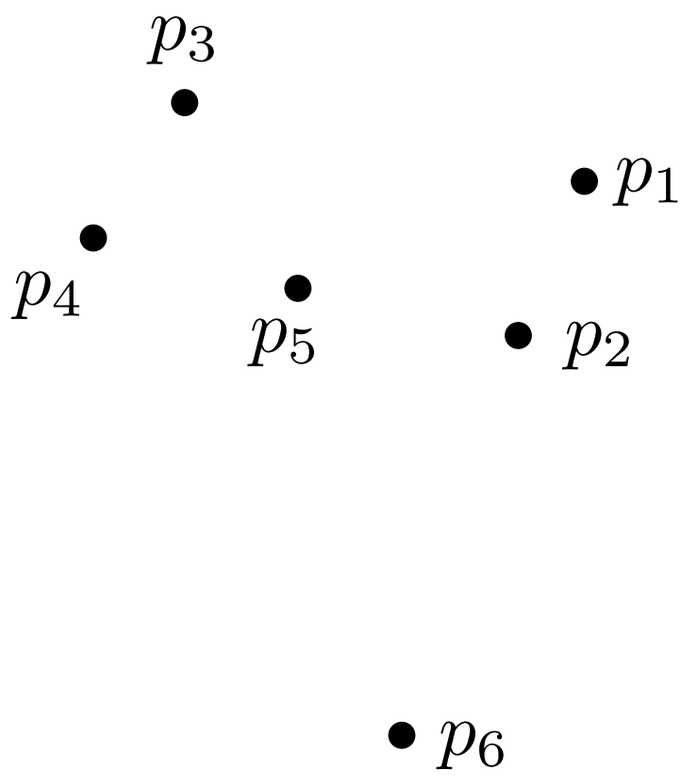
Start with single point cluster and recursively merge the most similar clusters to one parent cluster until reaching a stopping criterion (e.g. number of clusters).

Dividing (top-down)

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



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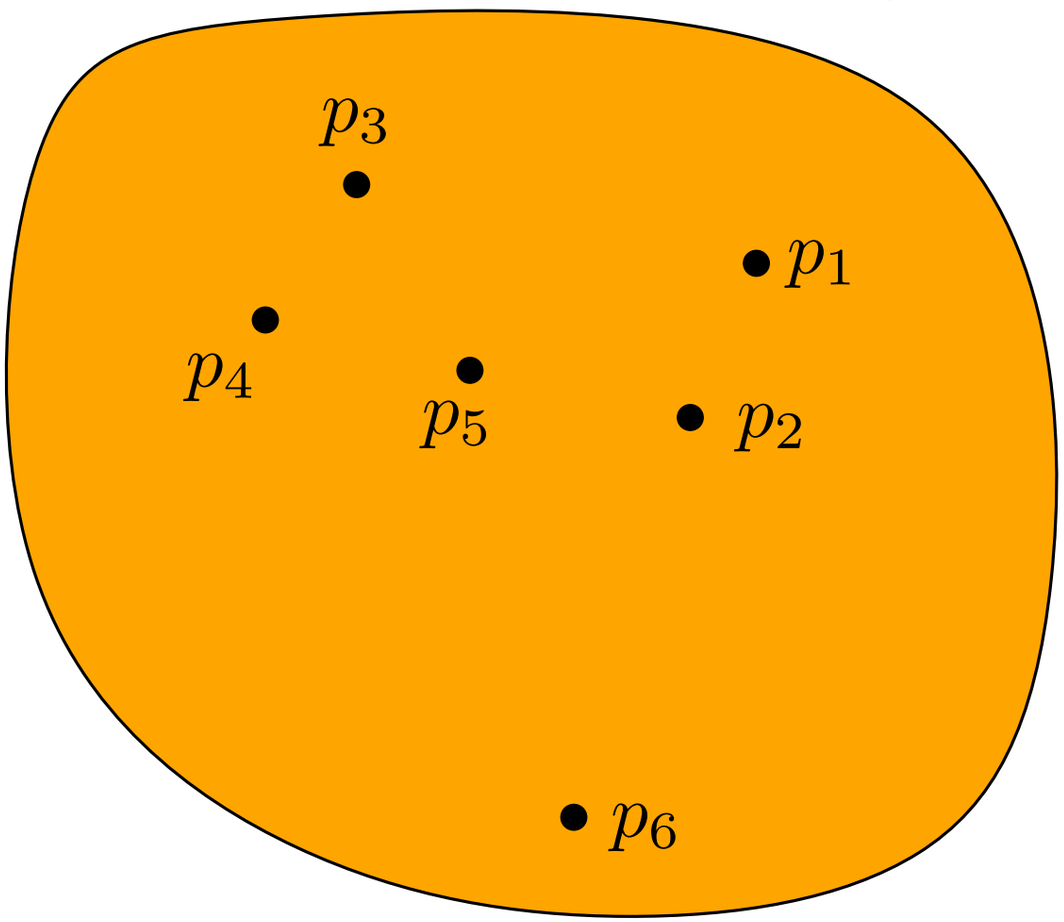

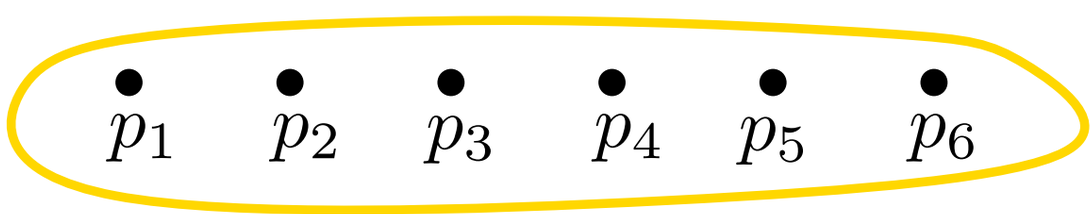

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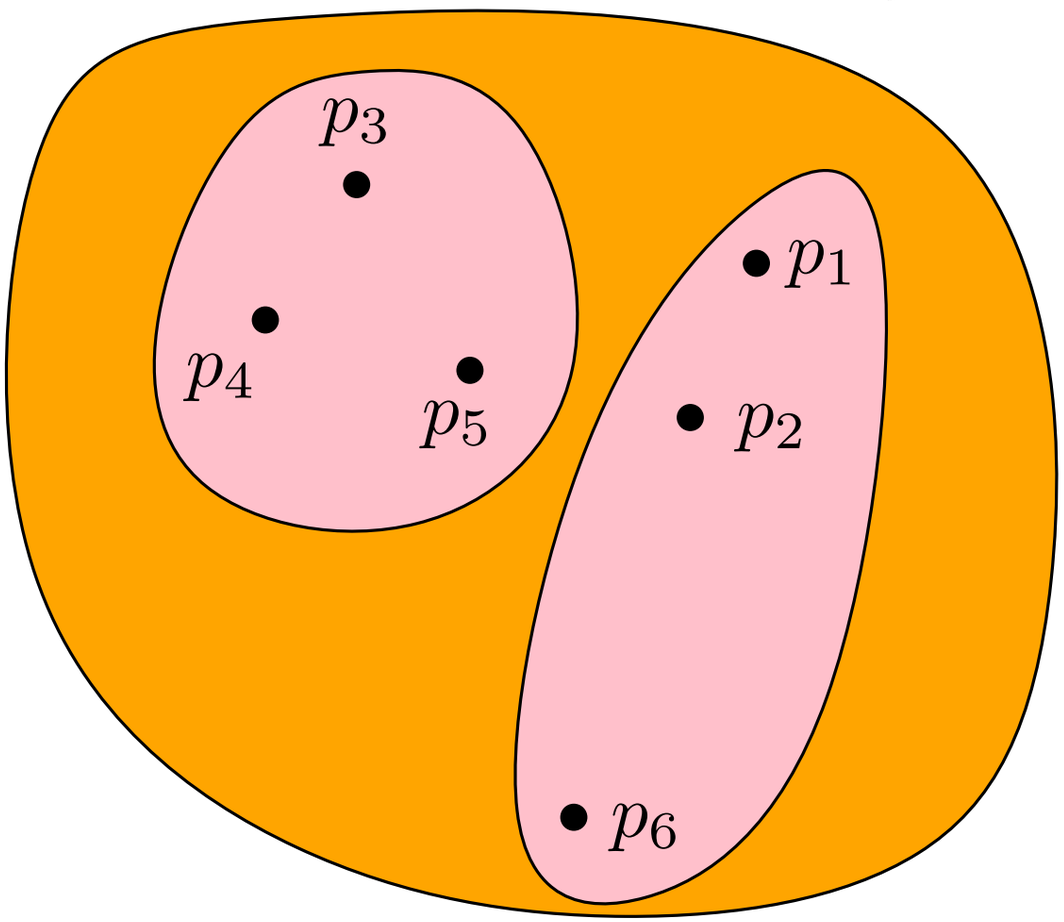

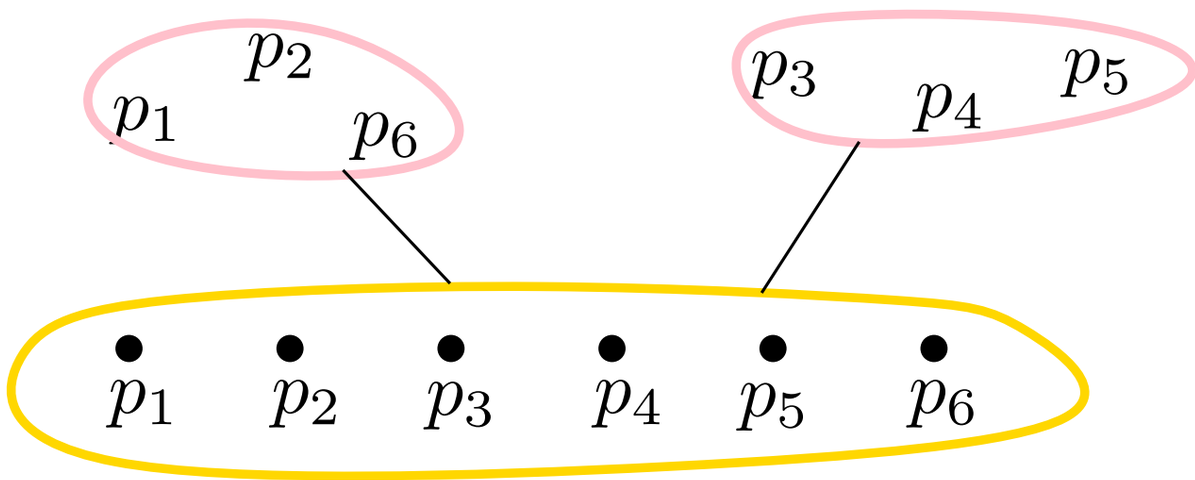

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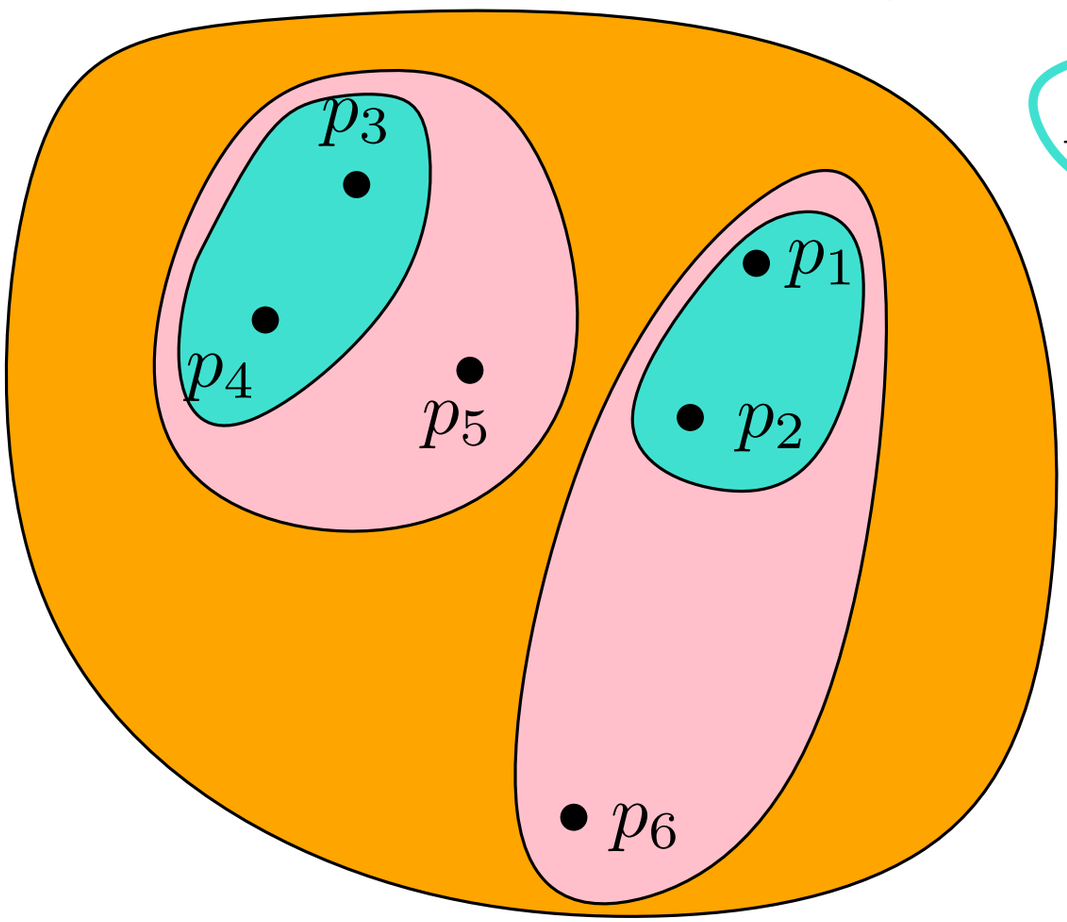

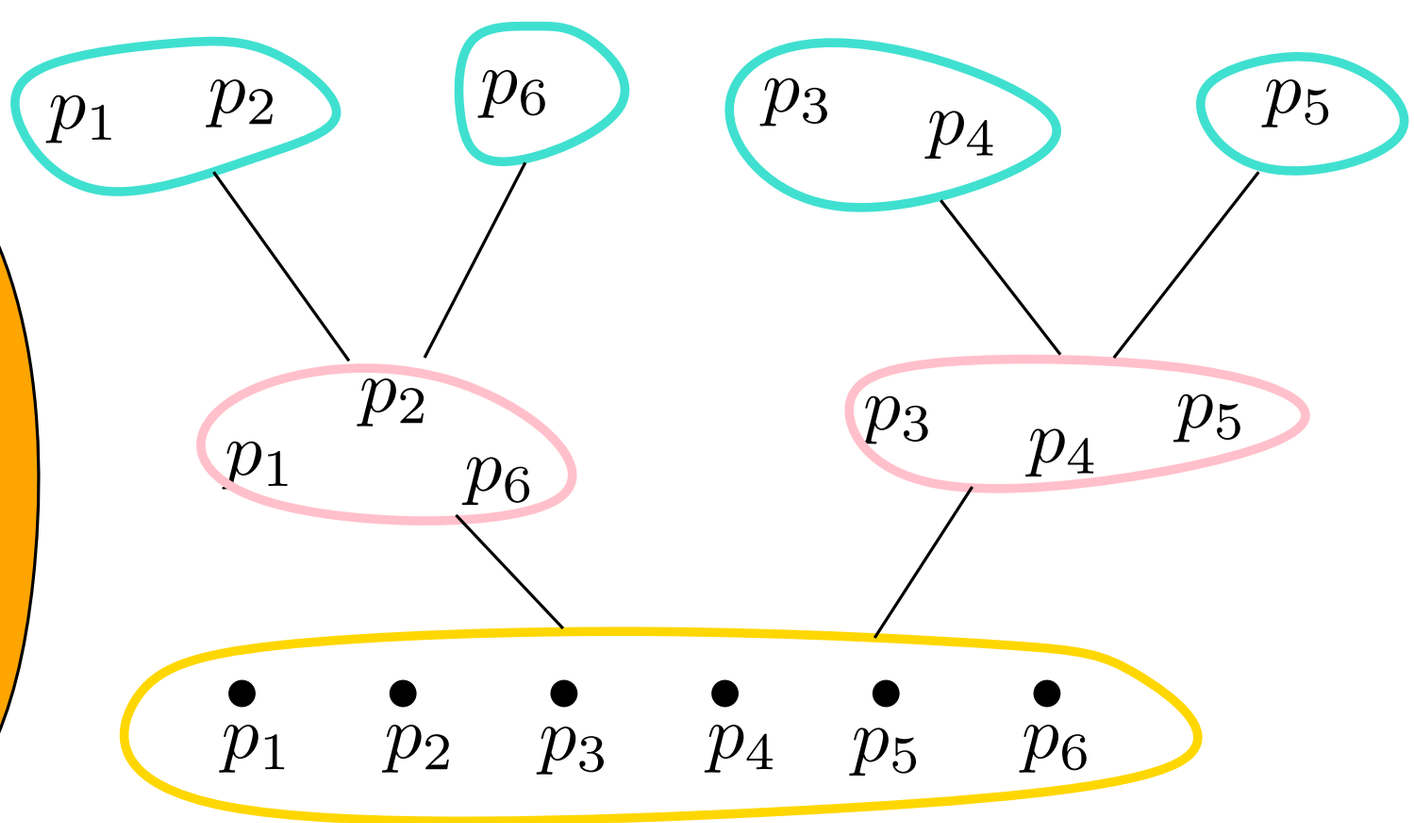

Single linkage clustering

Input: A set $X_n = \{x_1, \ldots, x_n\}$ 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.

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Output: the resulting dendogram

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sup: complete linkage

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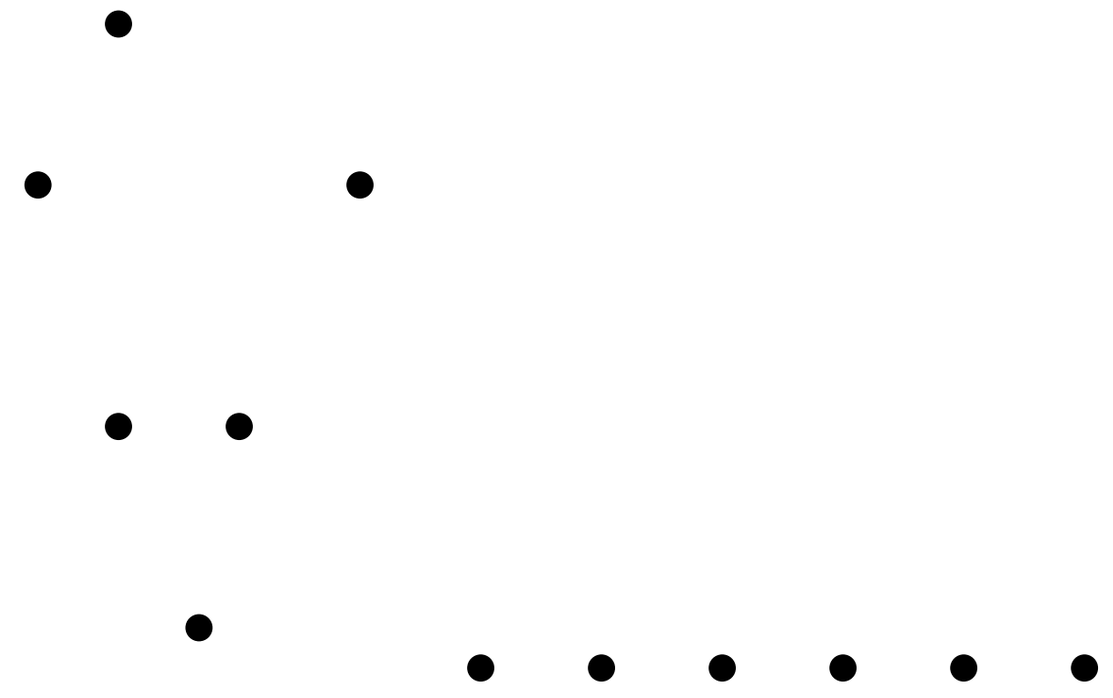

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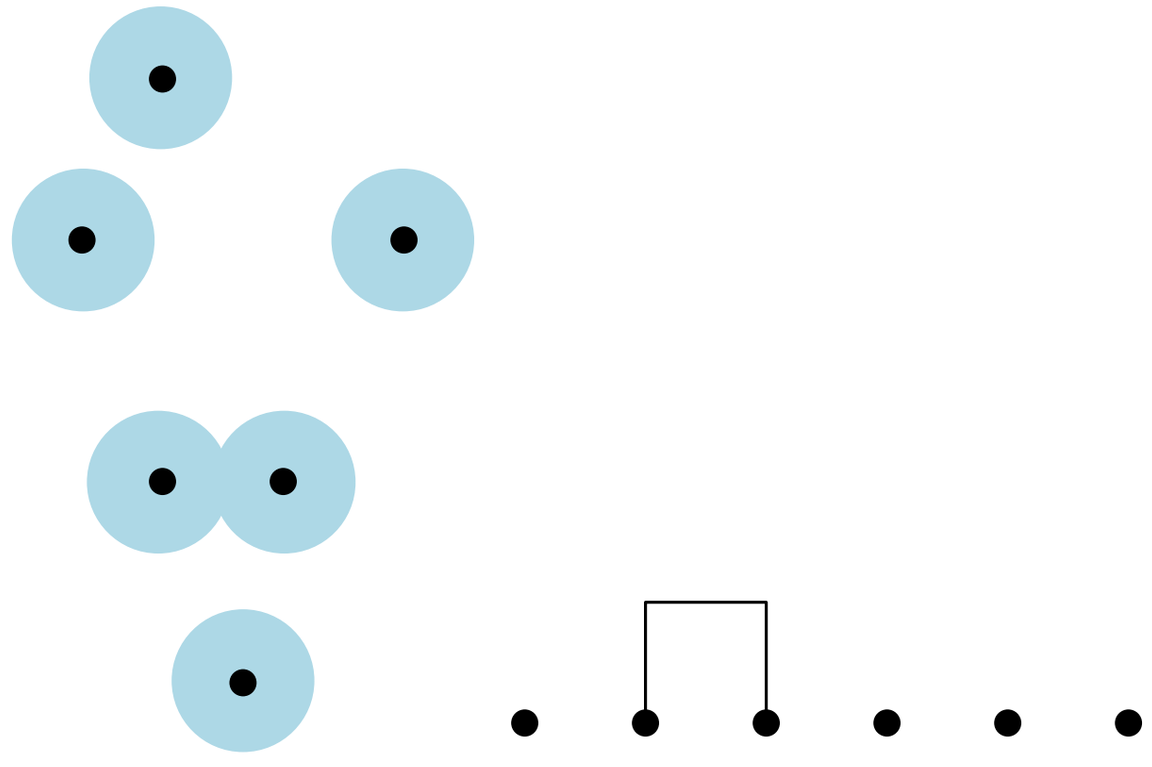

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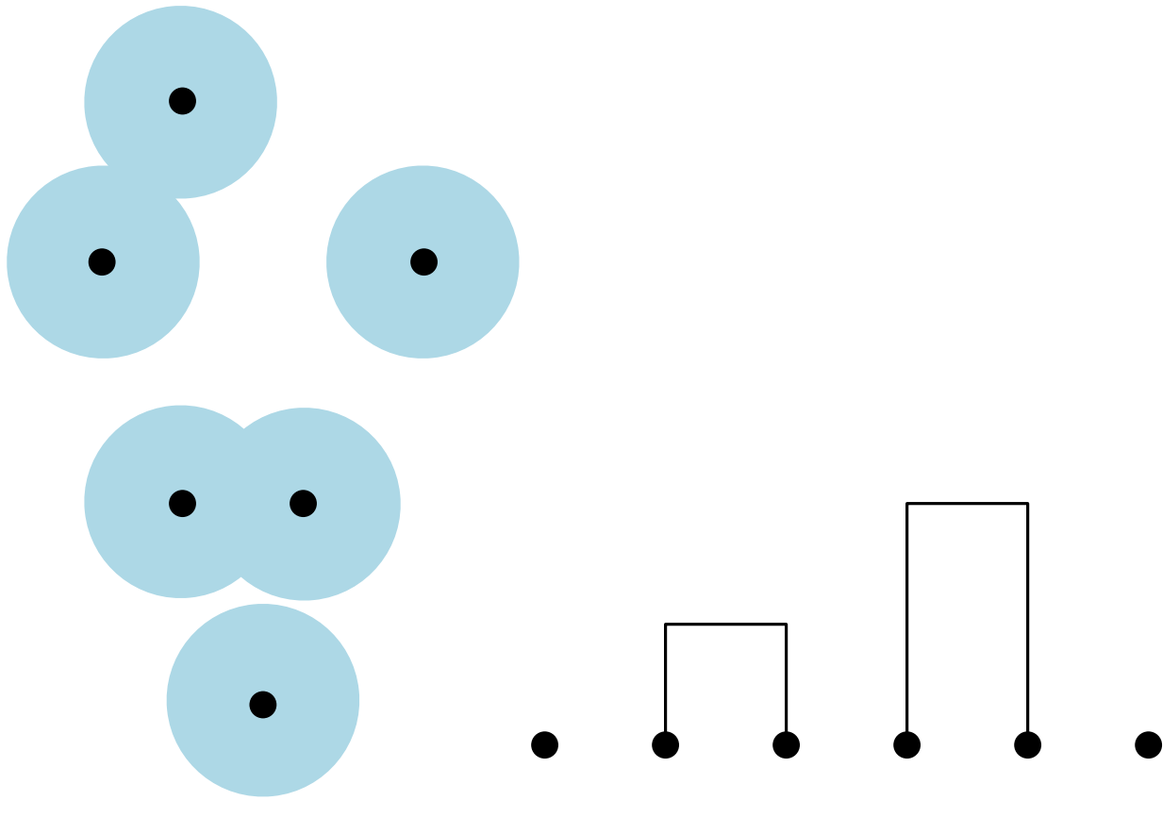

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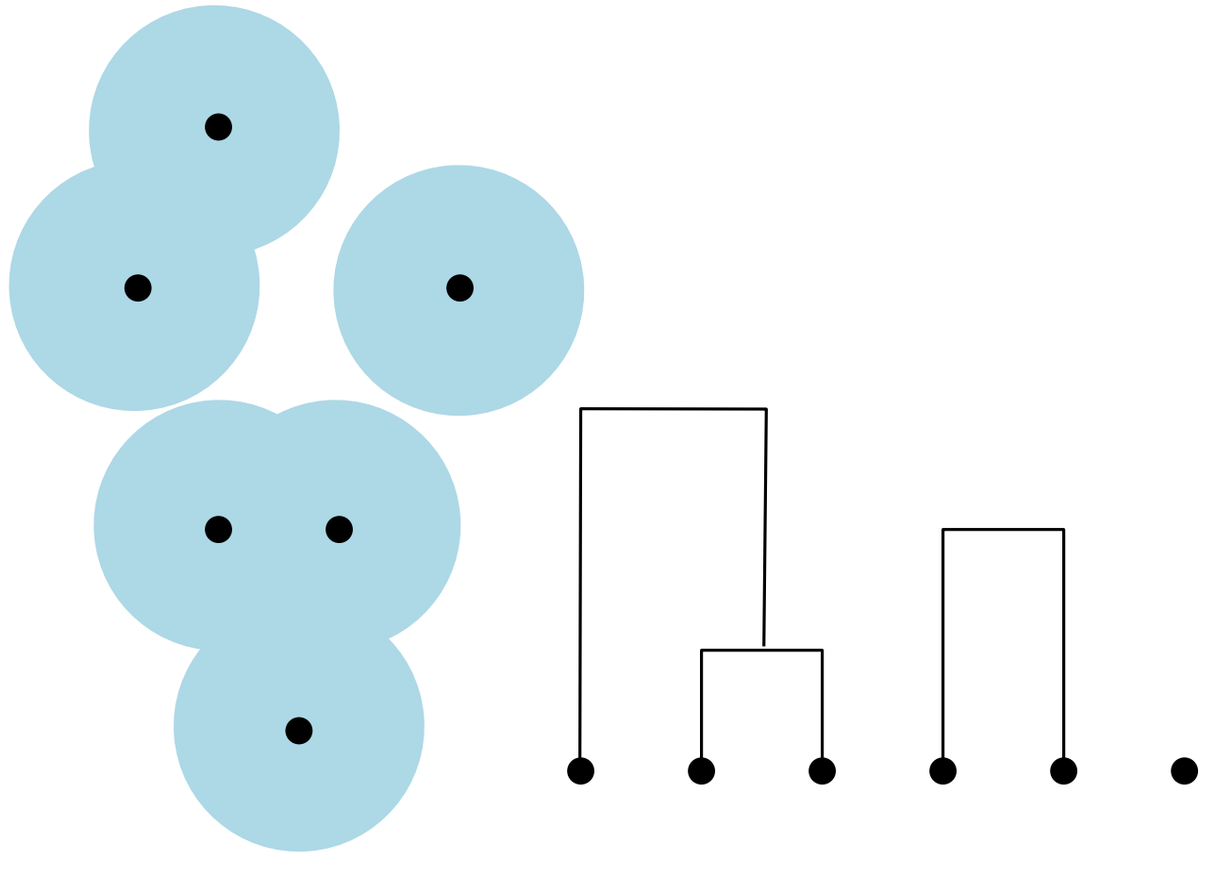

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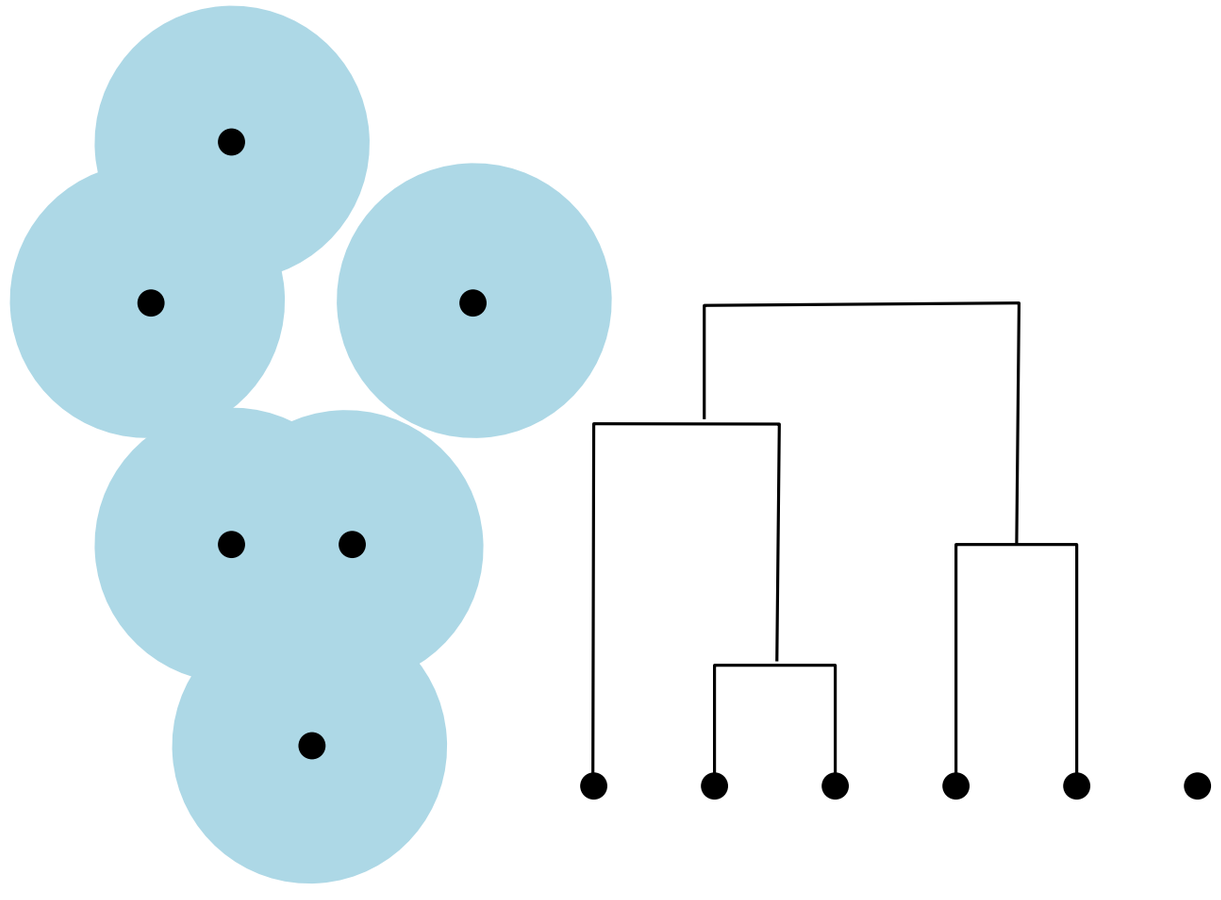

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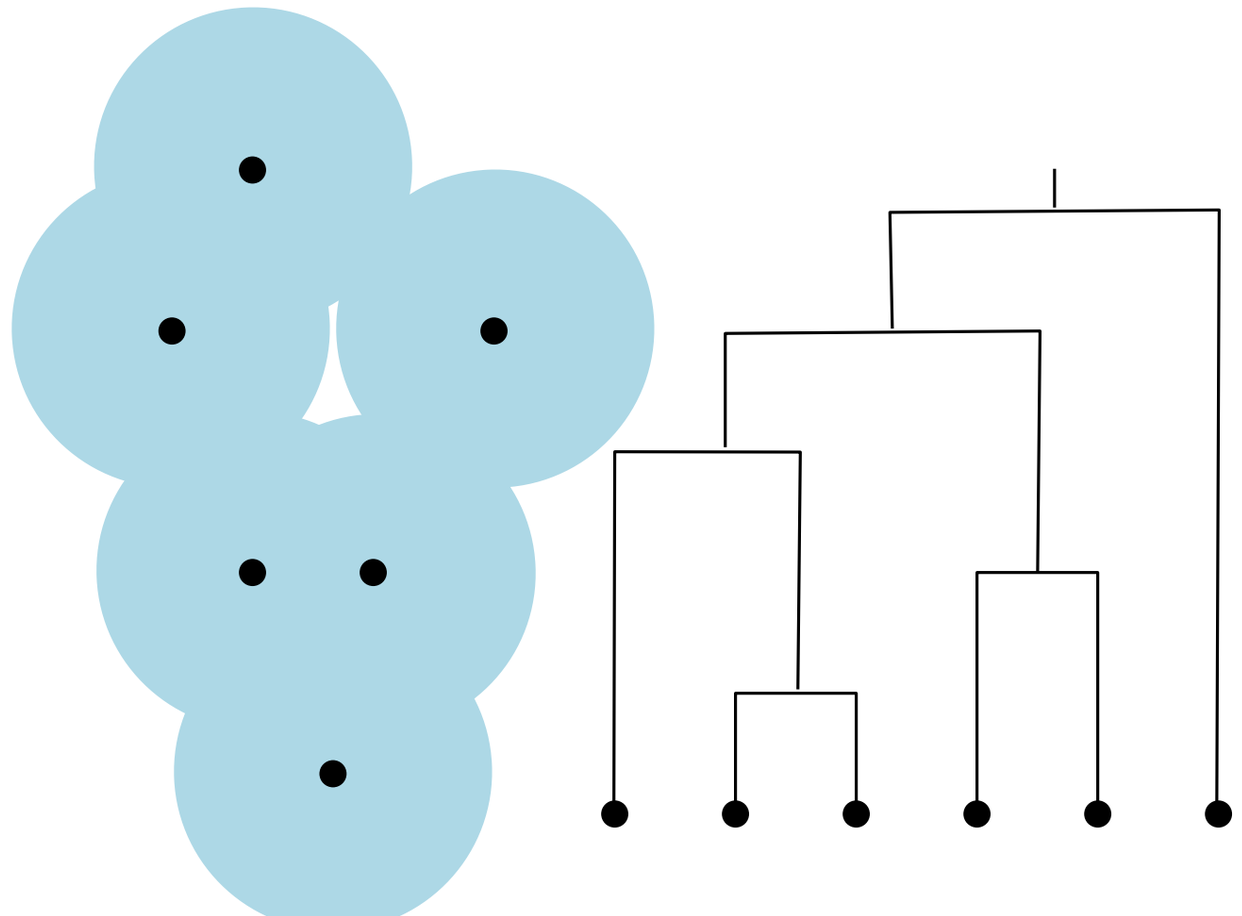

The (in)stability of dendograms

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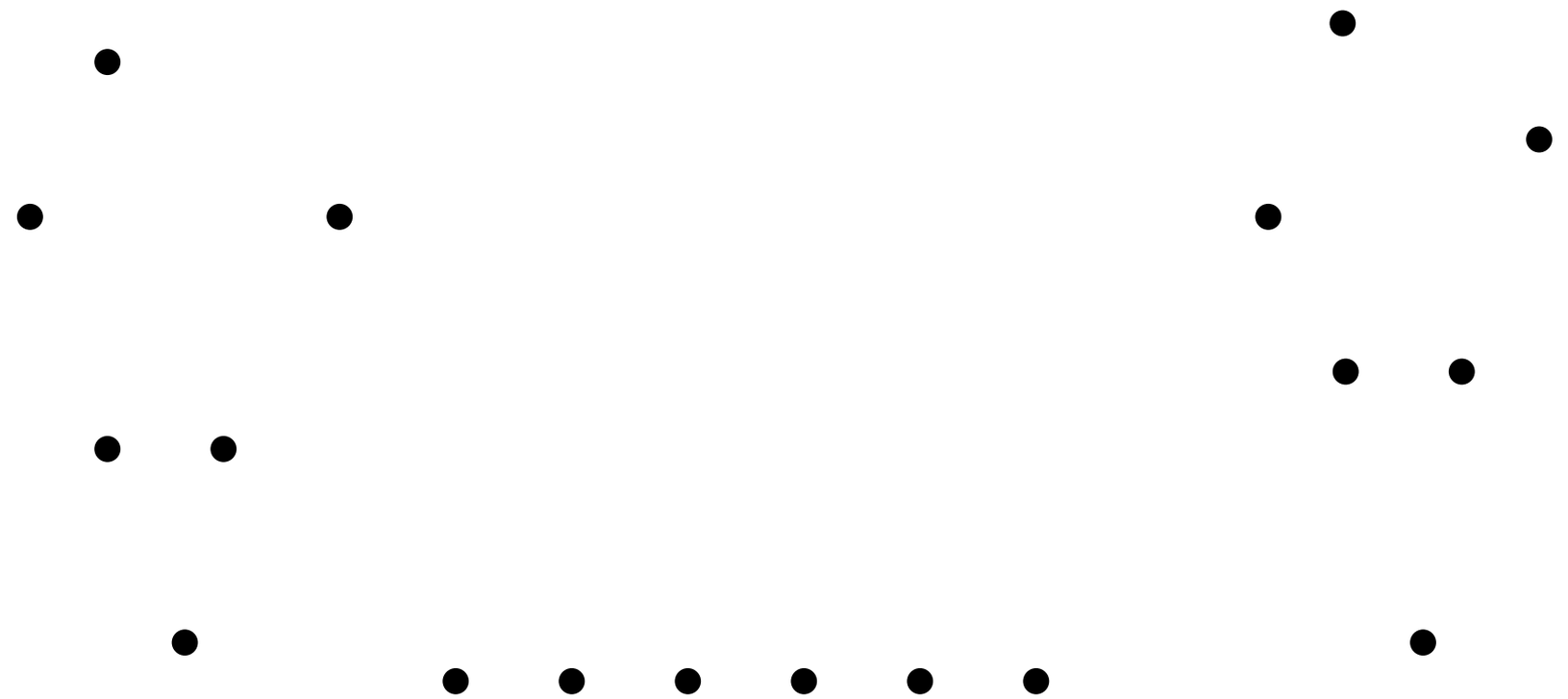

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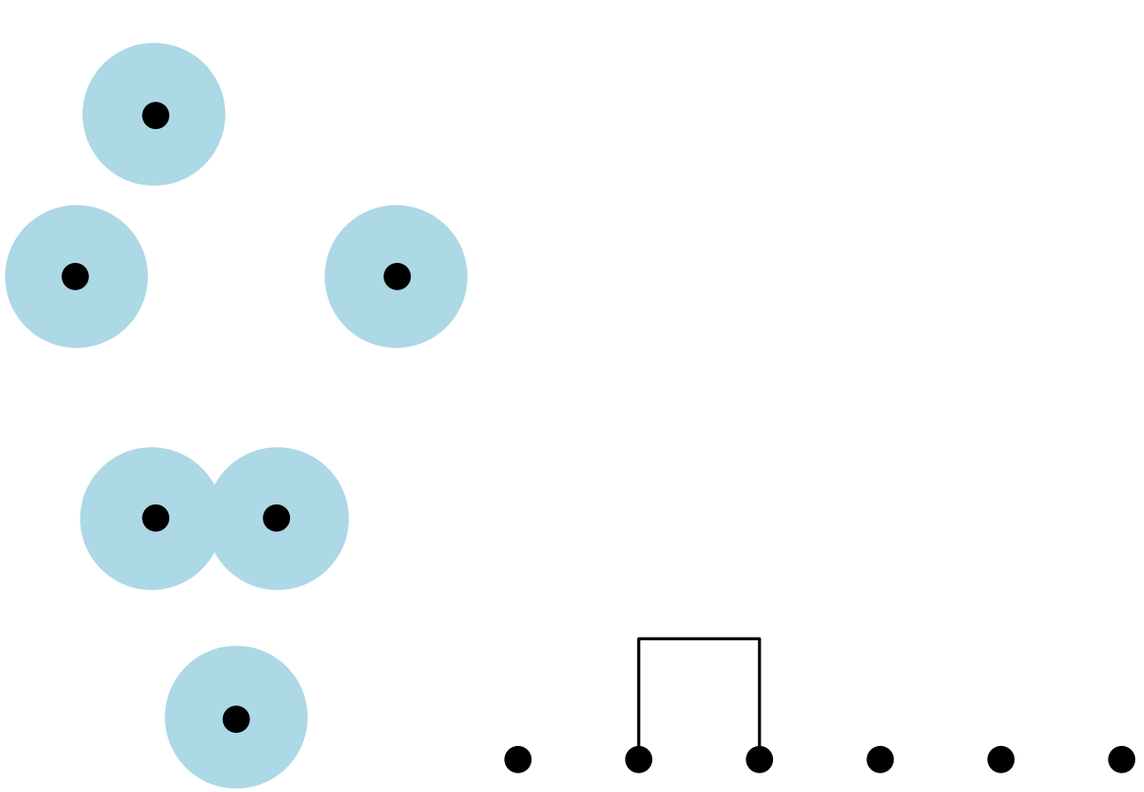

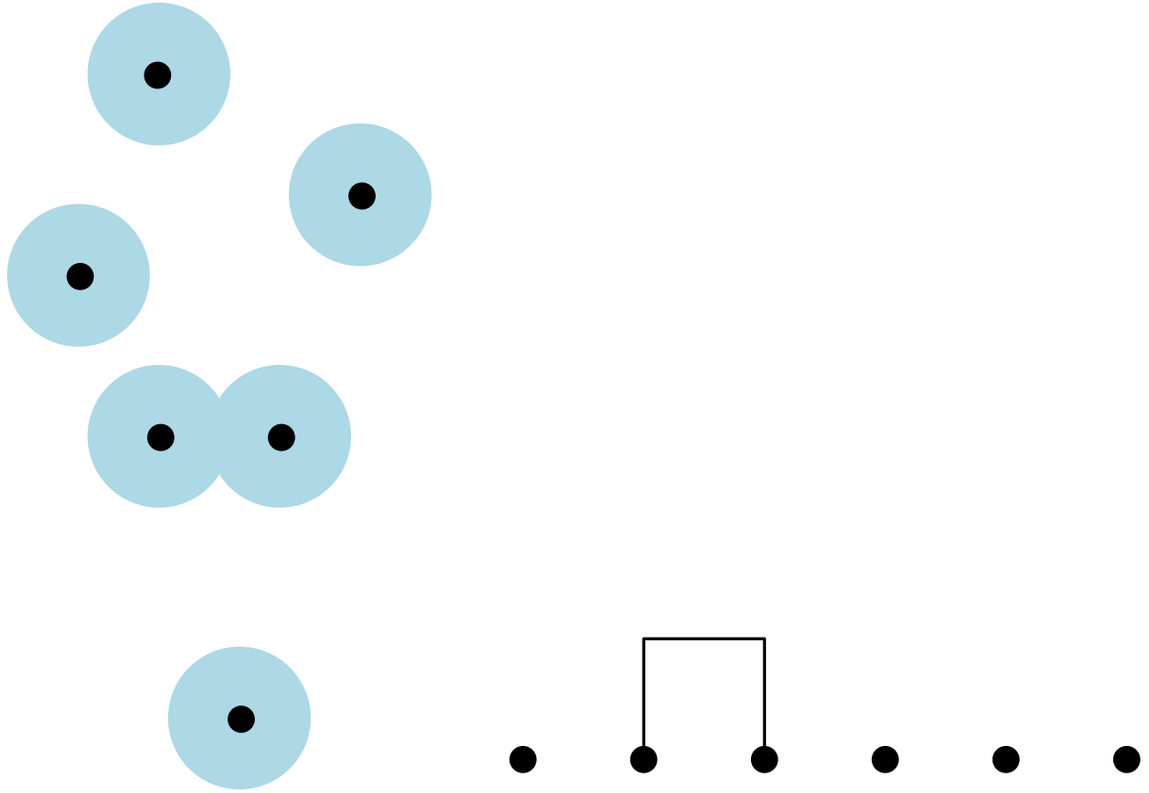

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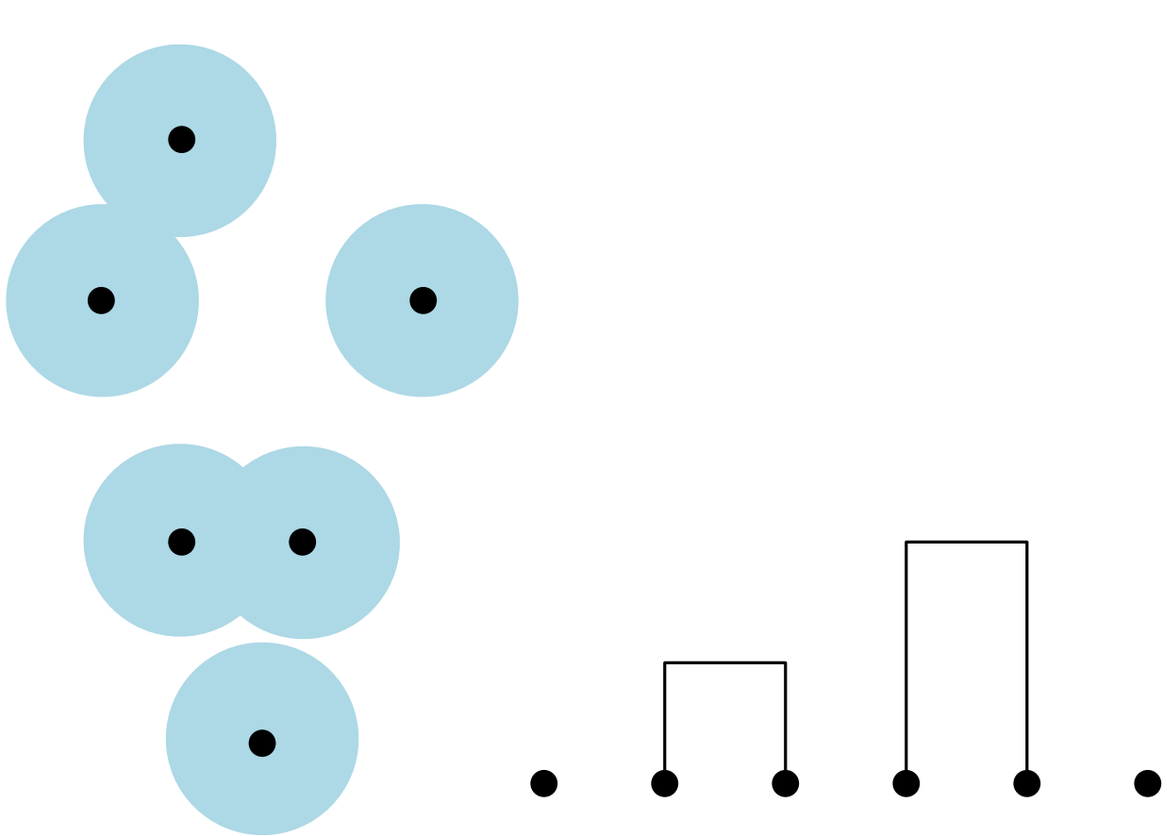

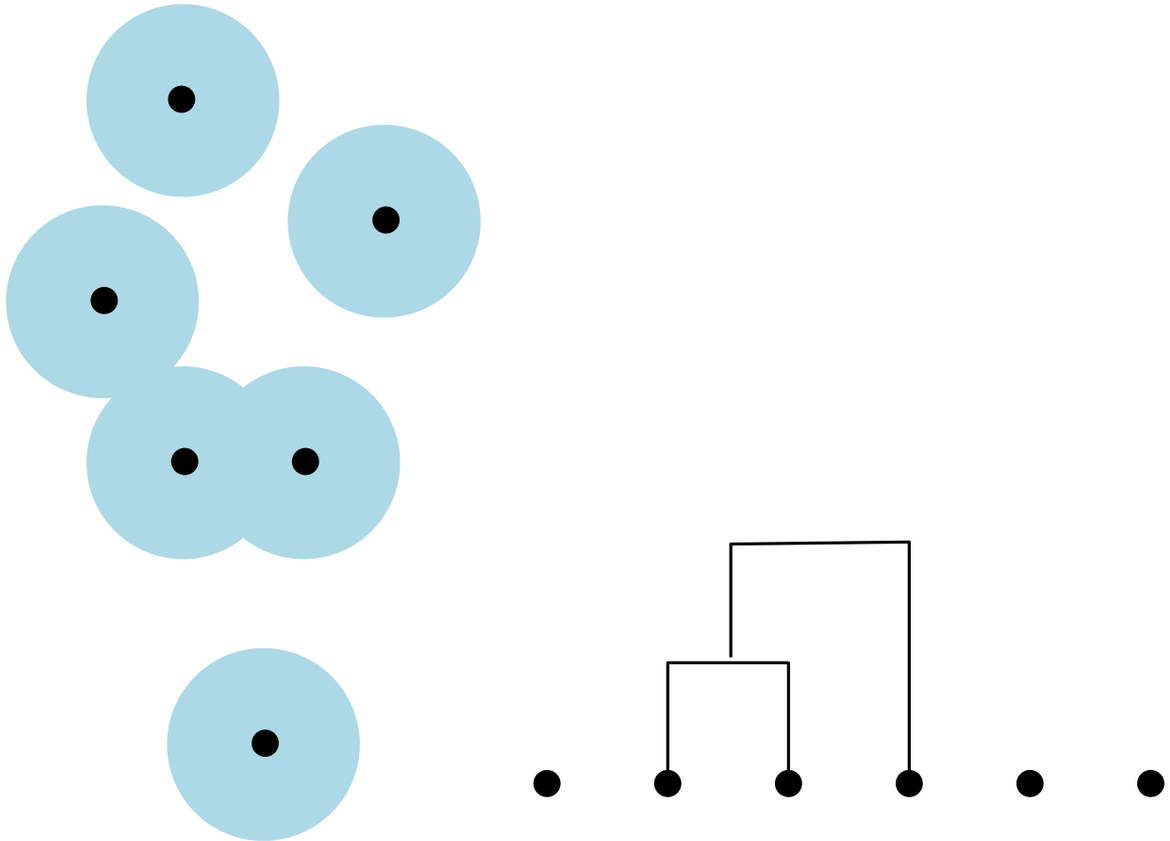

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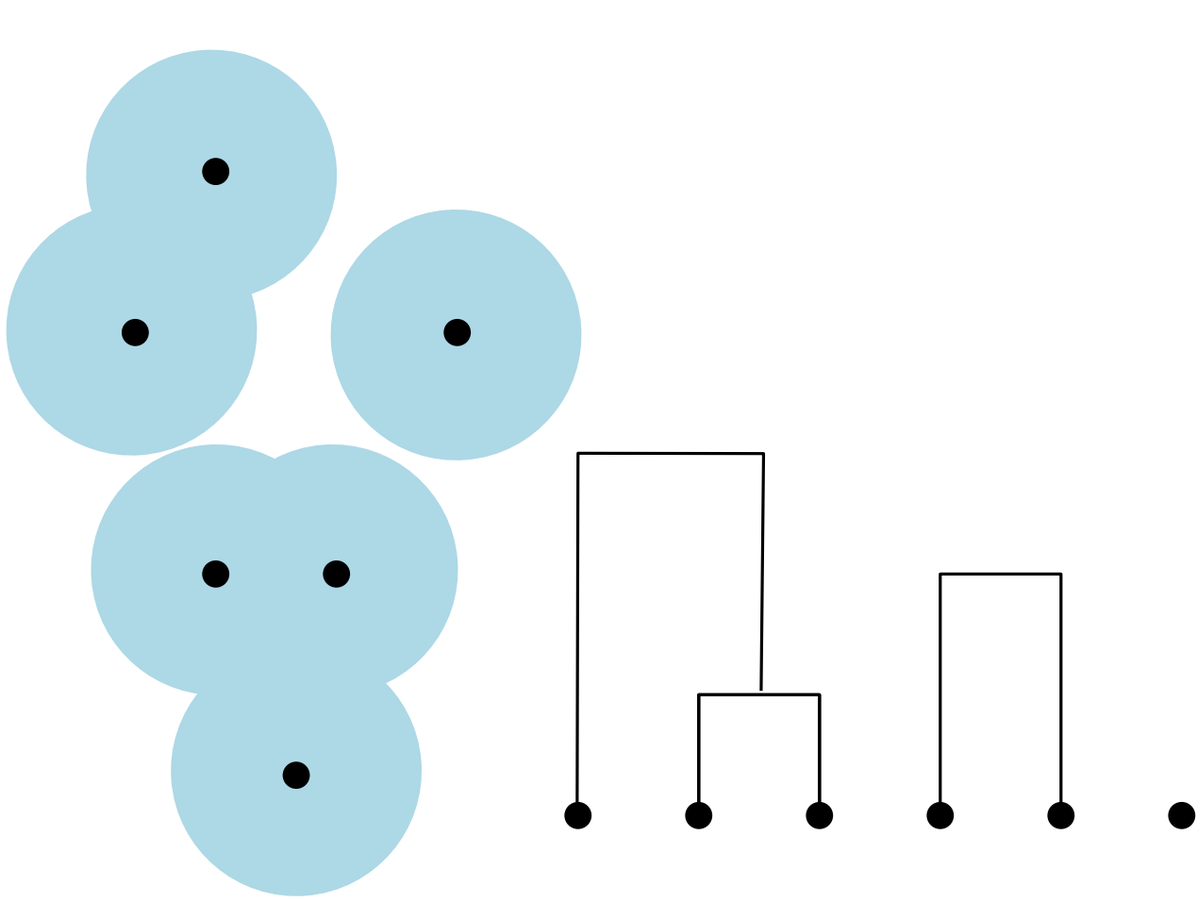

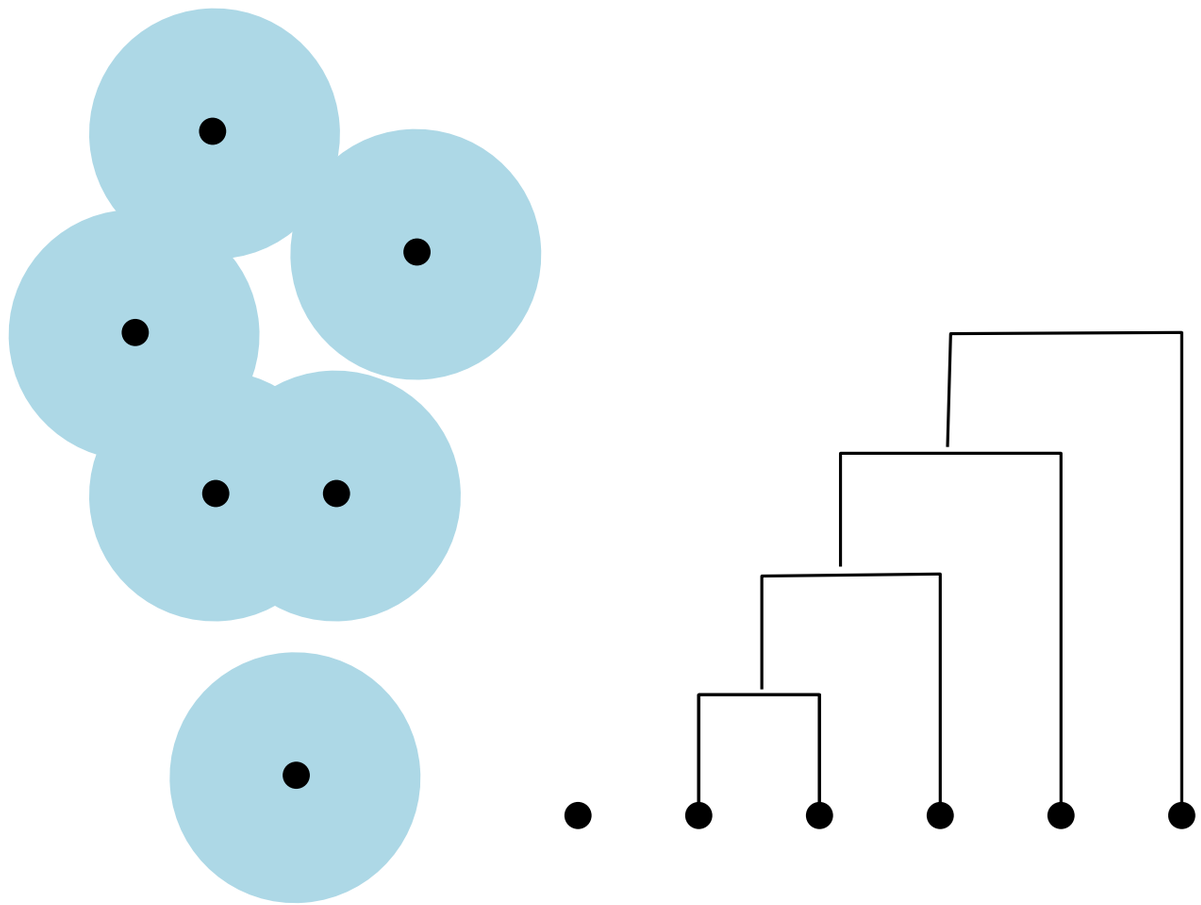

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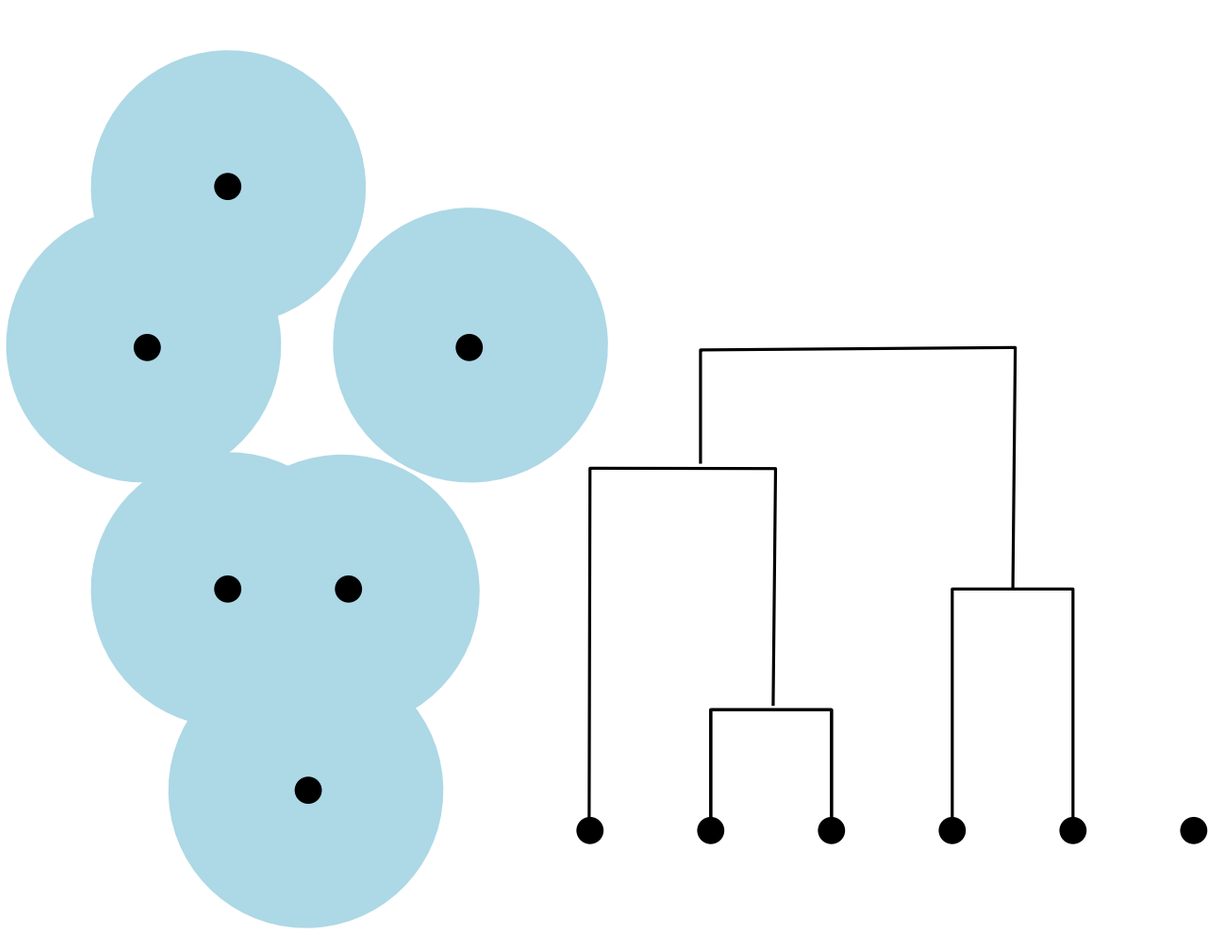

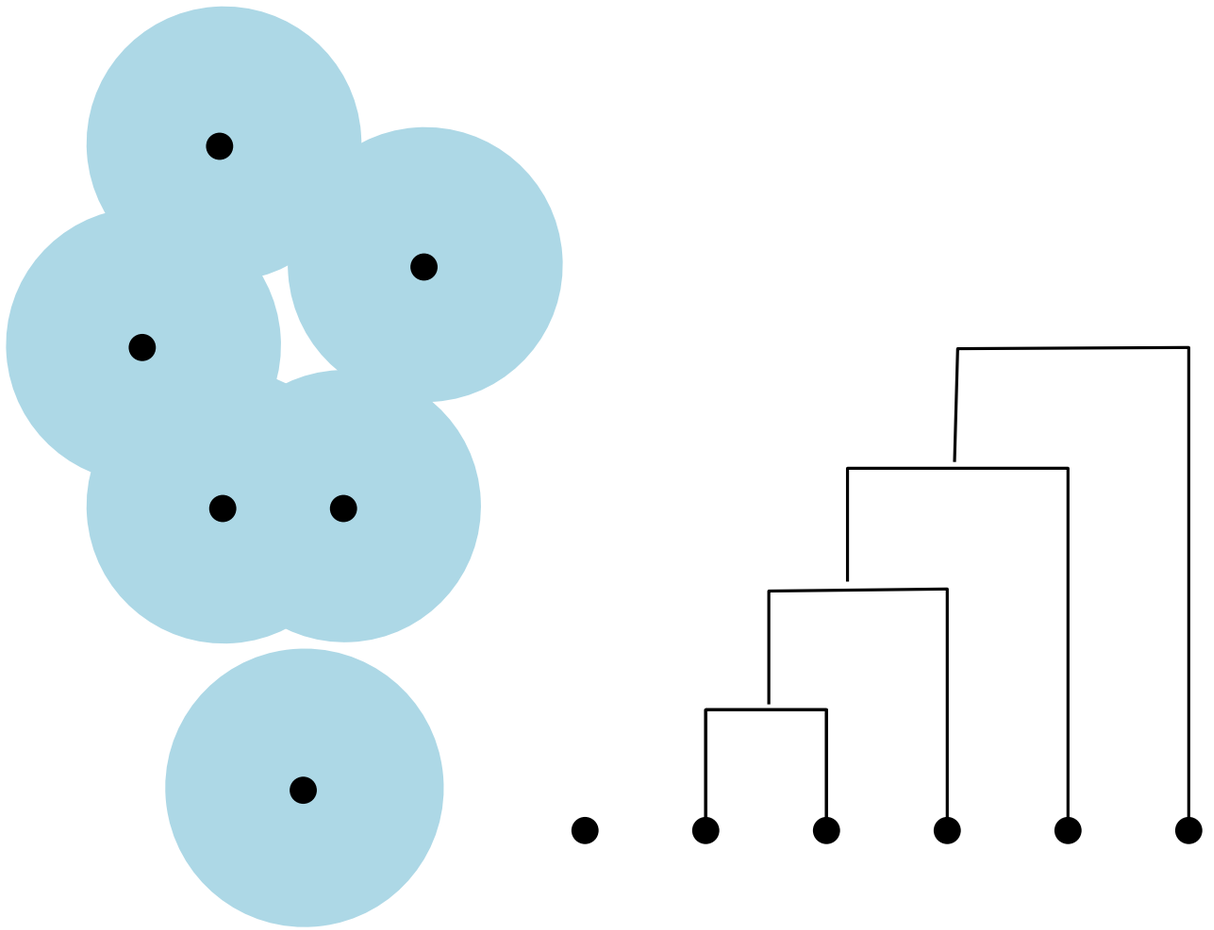

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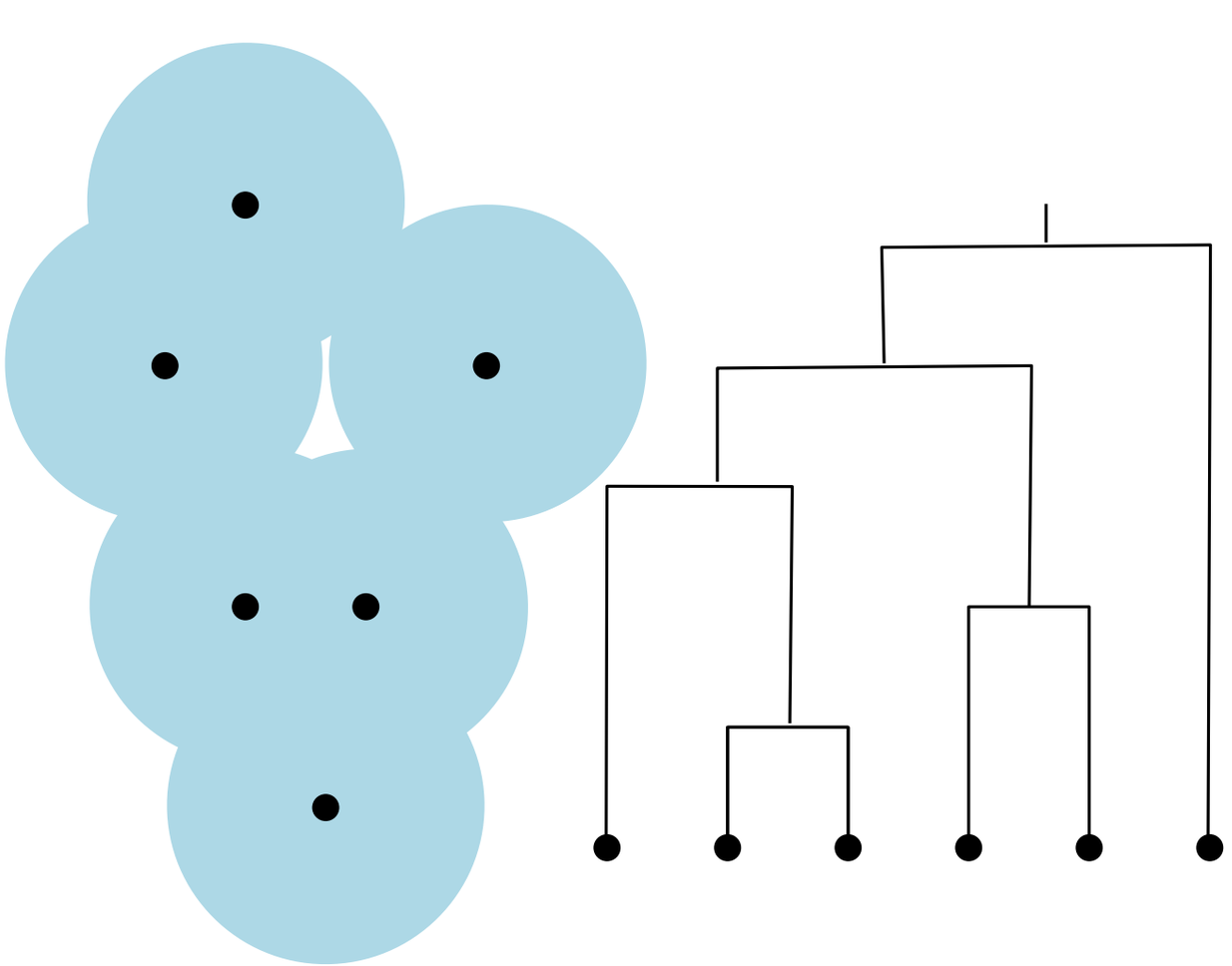

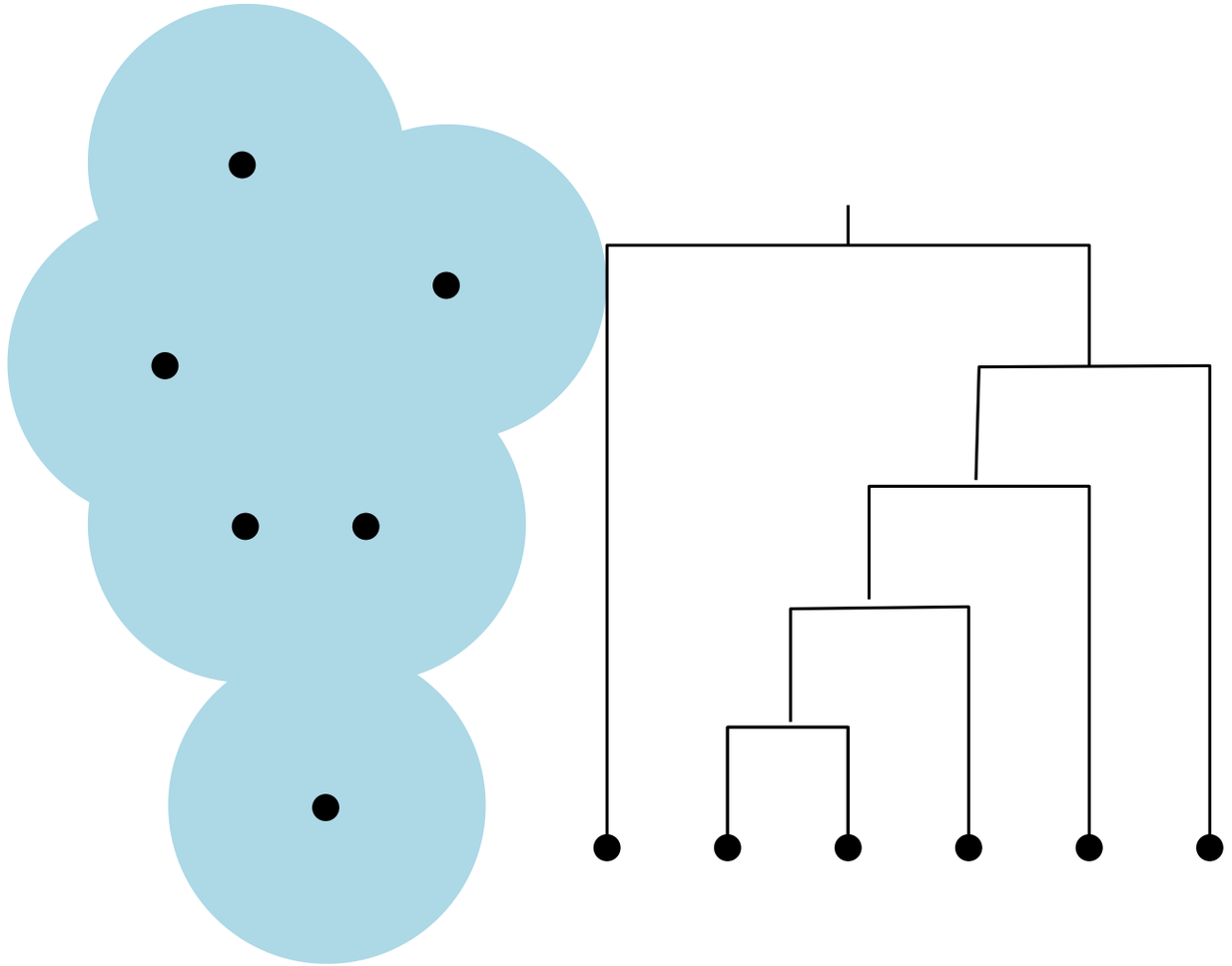

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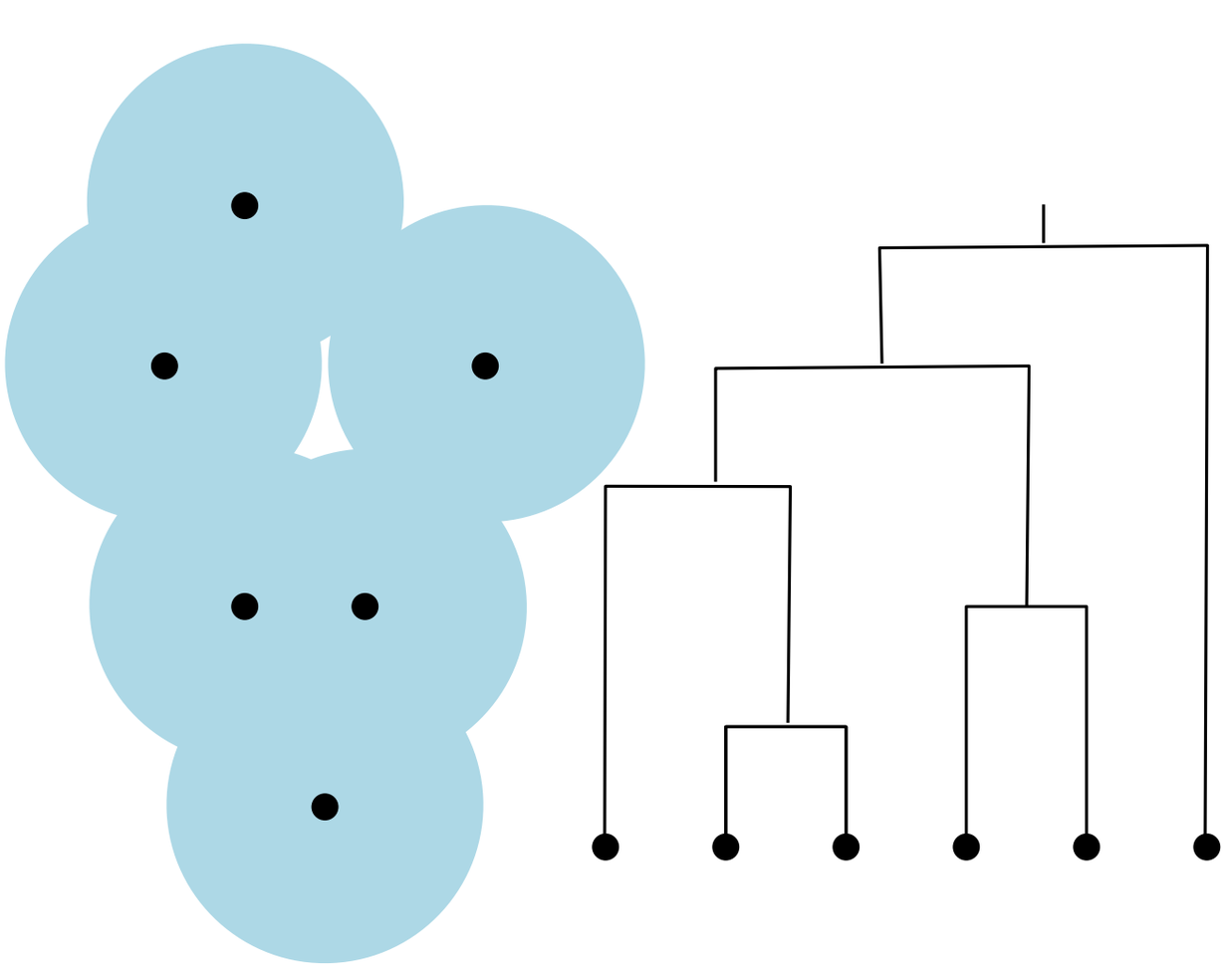
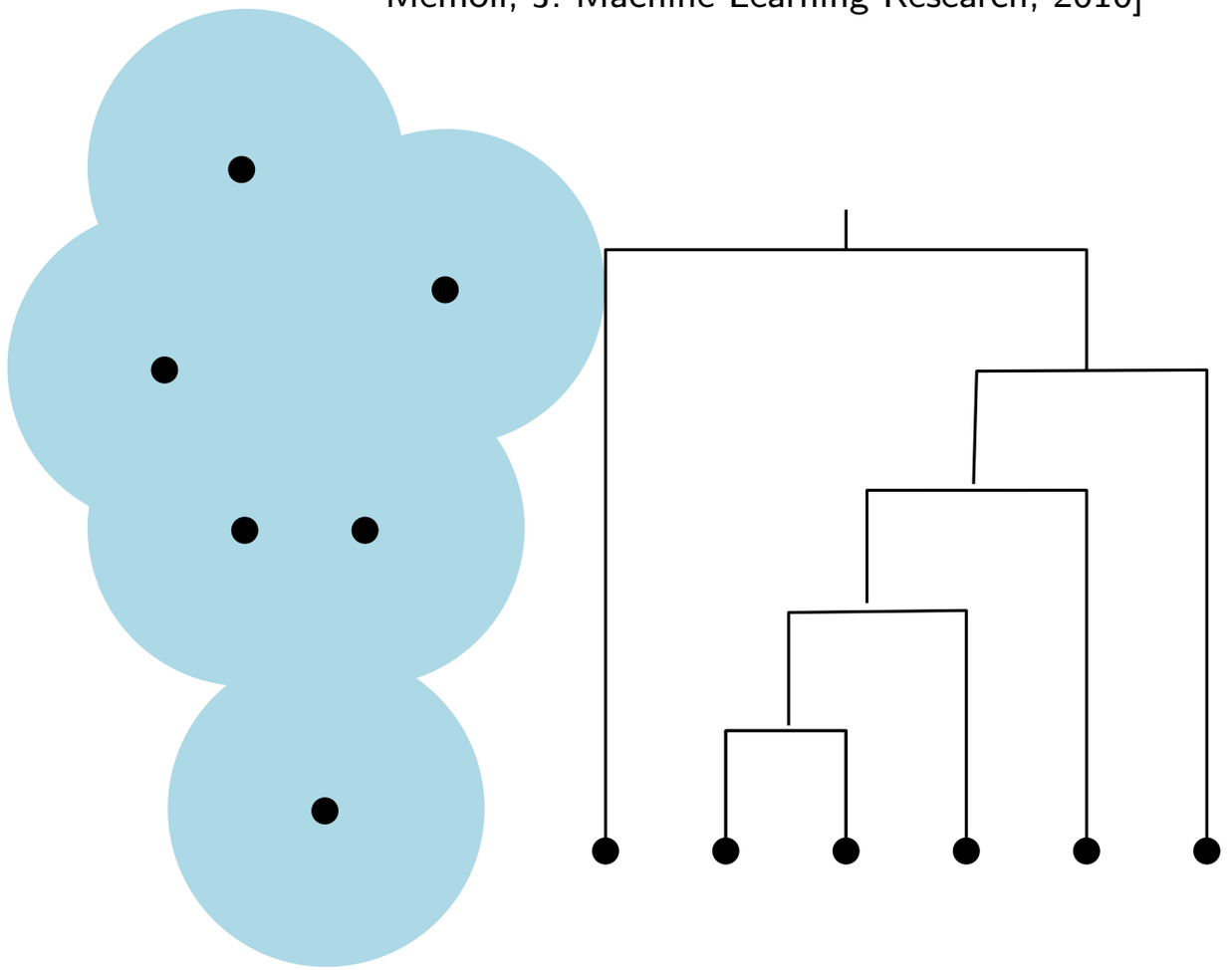
[*Characterization, Stability and Convergence of Hierarchical Clustering Methods*, Carlsson, Mémoli, J. Machine Learning Research, 2010]





Let $d_{\mathcal{D}}(x, y) =$ height of lowest common ancestor of x, y in dendrogram $\mathcal{D}$.

ultrametric!

Thm: $d_{GH}((X, d_{\mathcal{D}}), ((Y, d_{\mathcal{D}})) \leq d_{GH}((X, d_X), (Y, d_Y))$.

The (in)stability of dendograms

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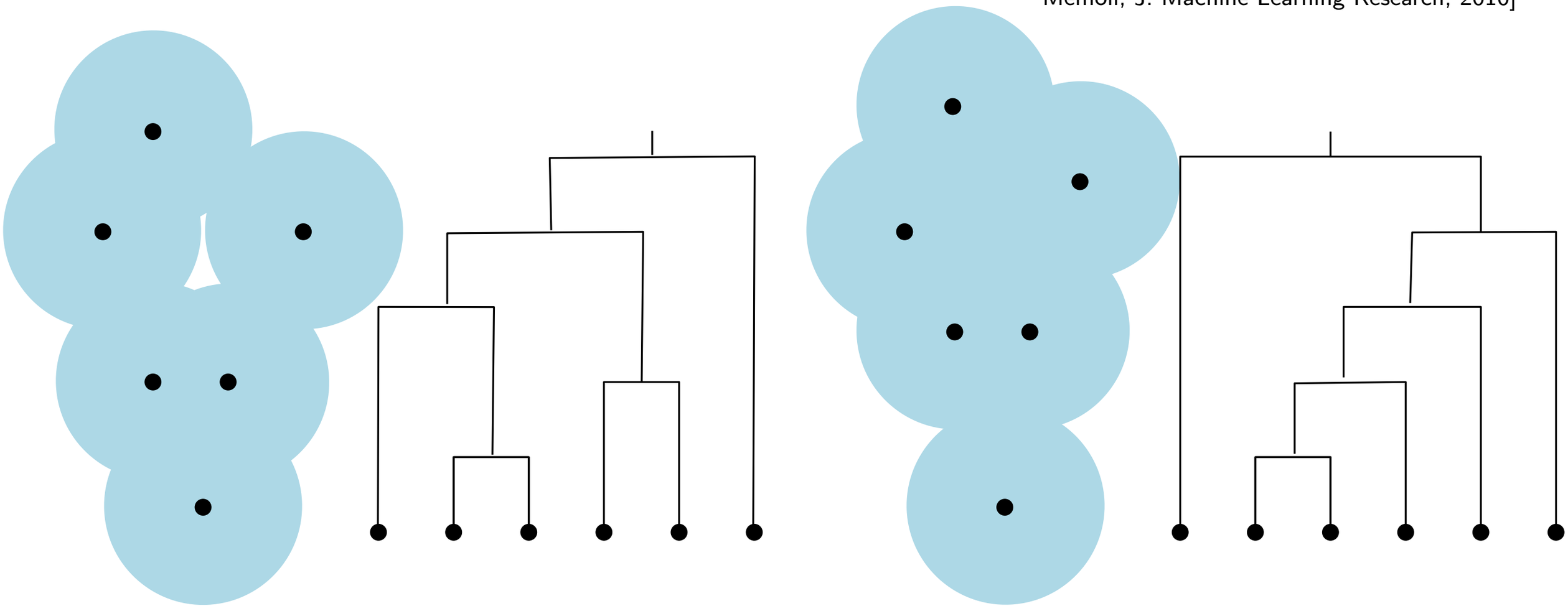

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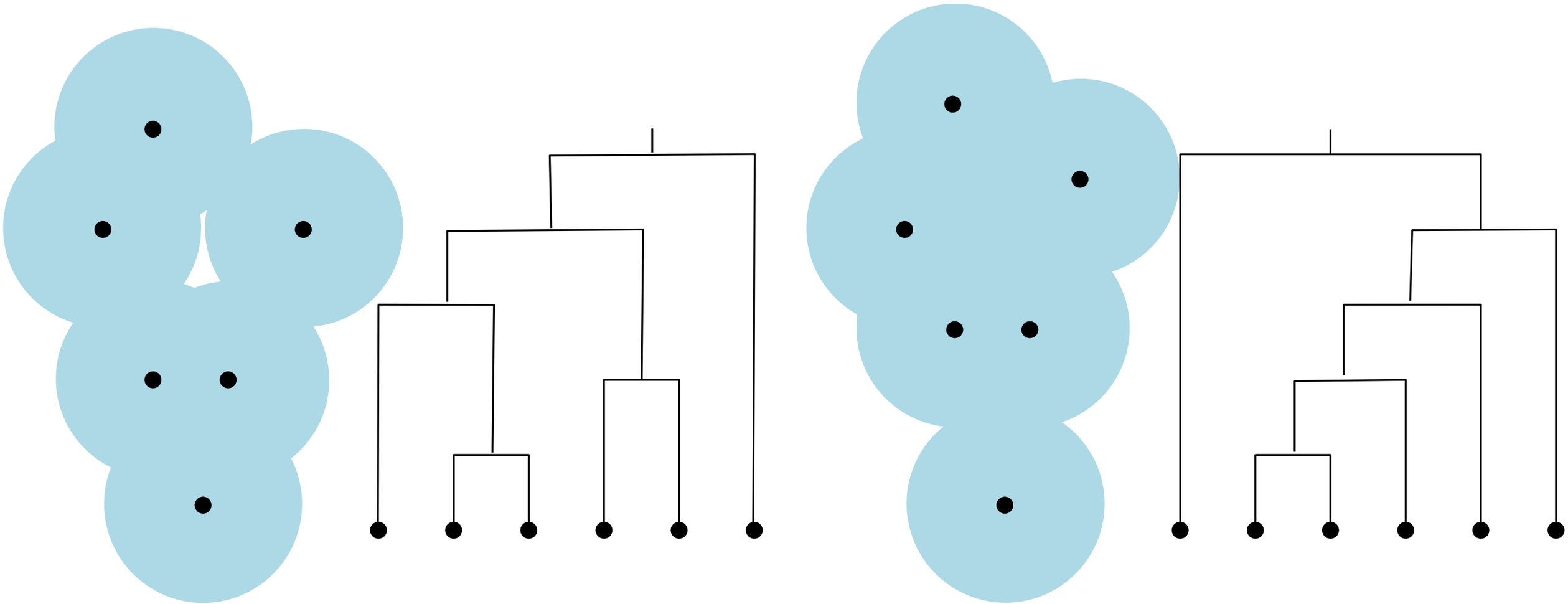
This is actually not true for complete and average clustering!

The (in)stability of dendograms



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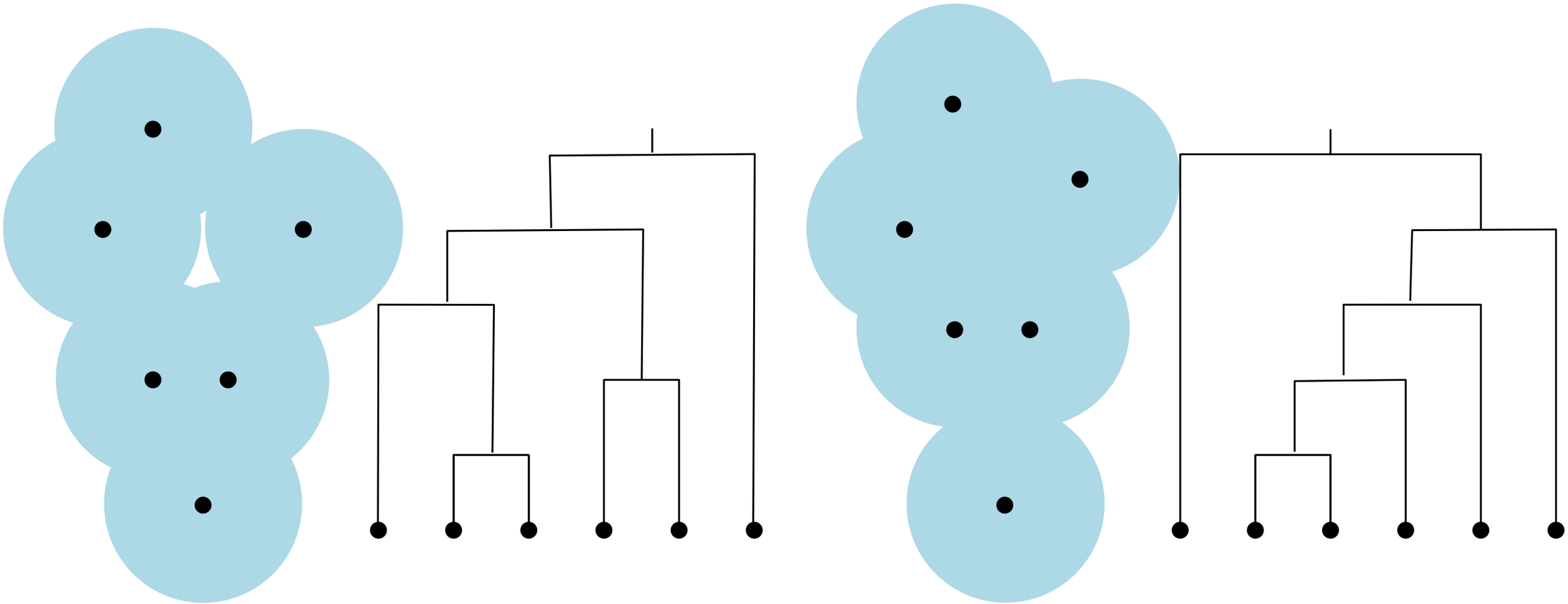

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(For Euclidean data), single linkage clustering keeps track of the evolution of the connected components of the distance function to the data.

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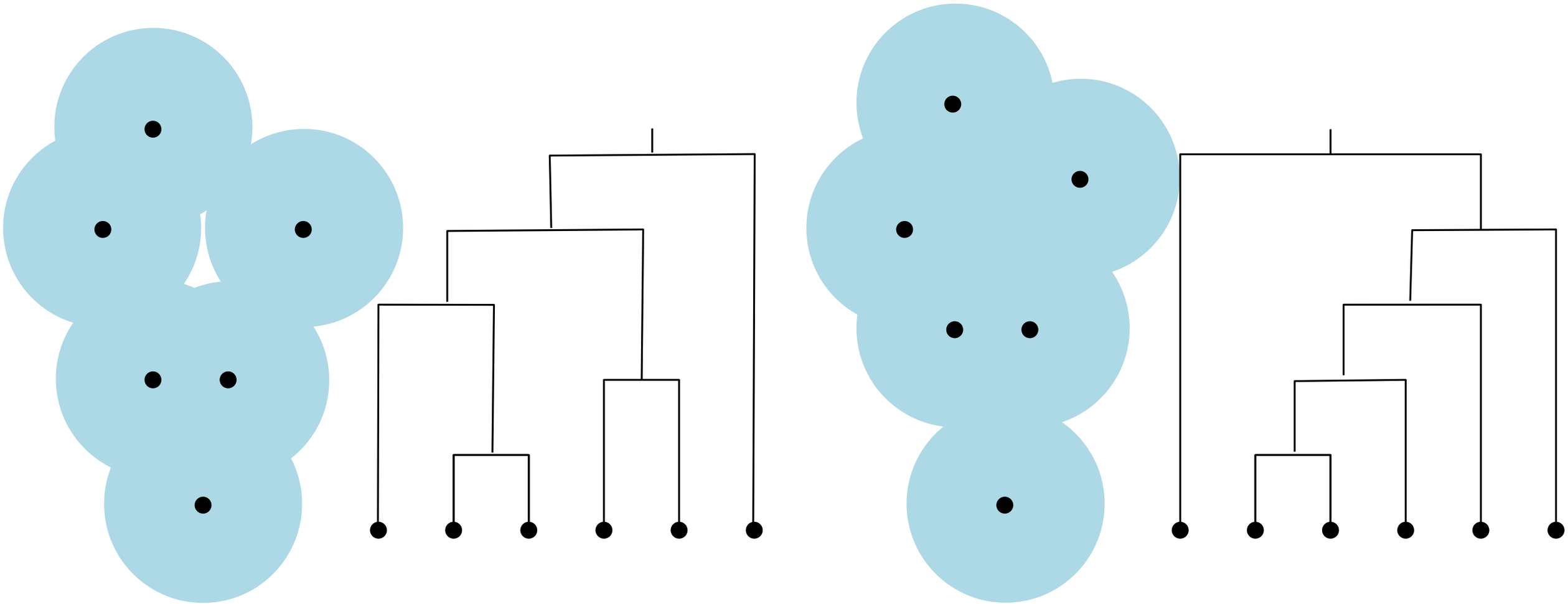

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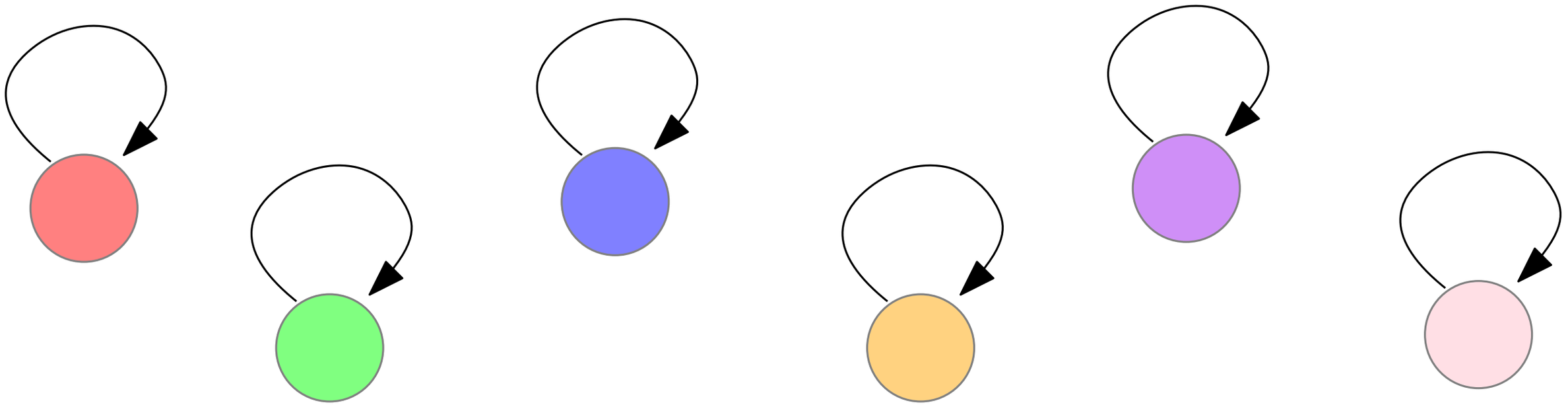

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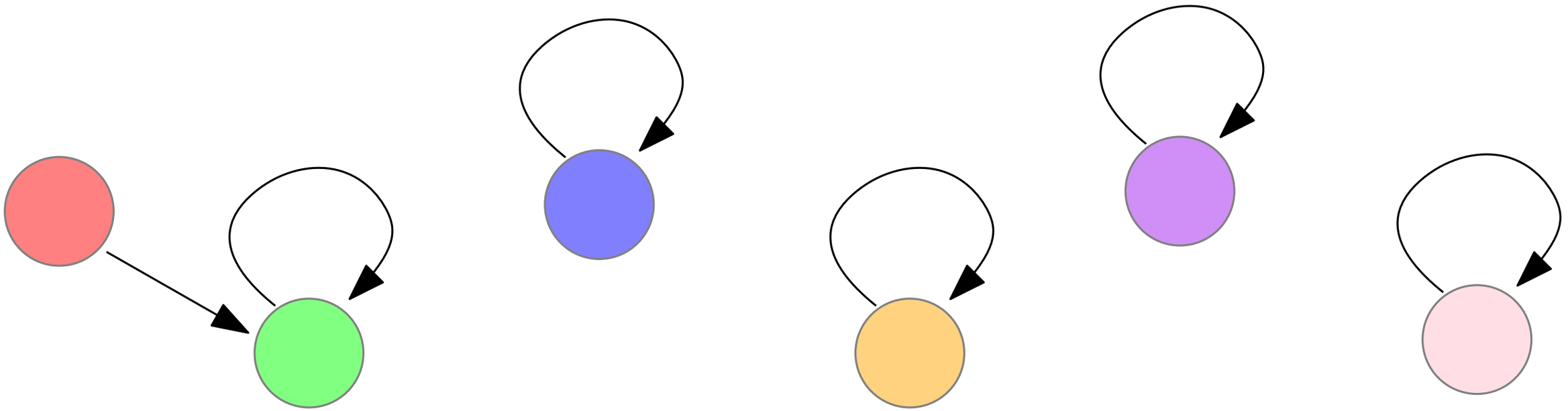

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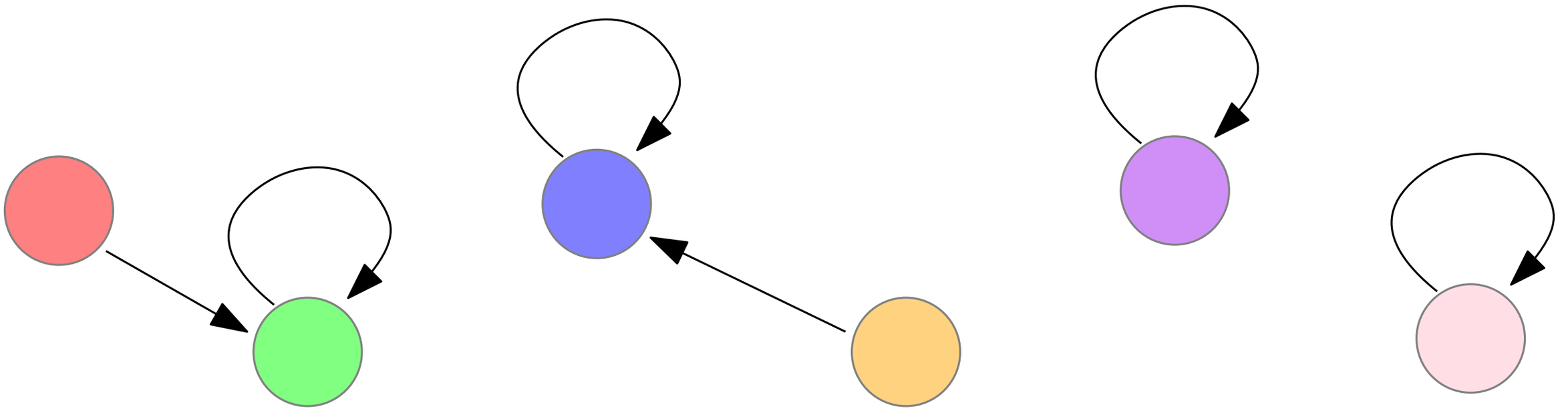

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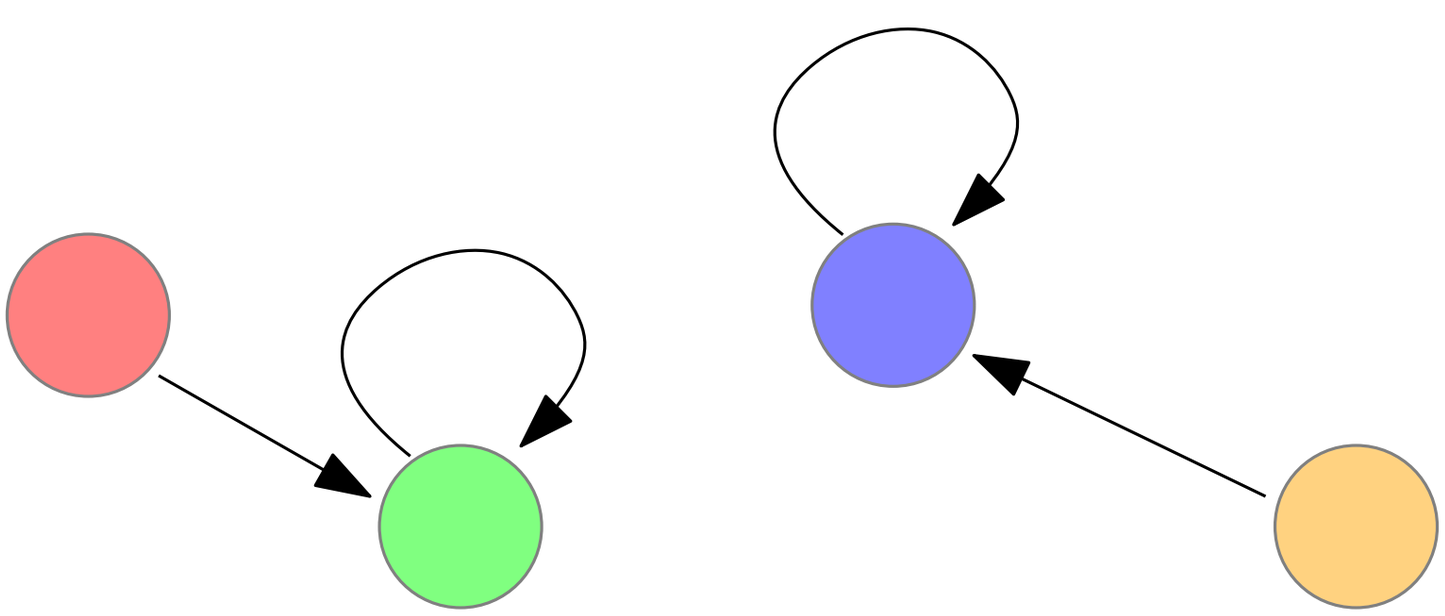

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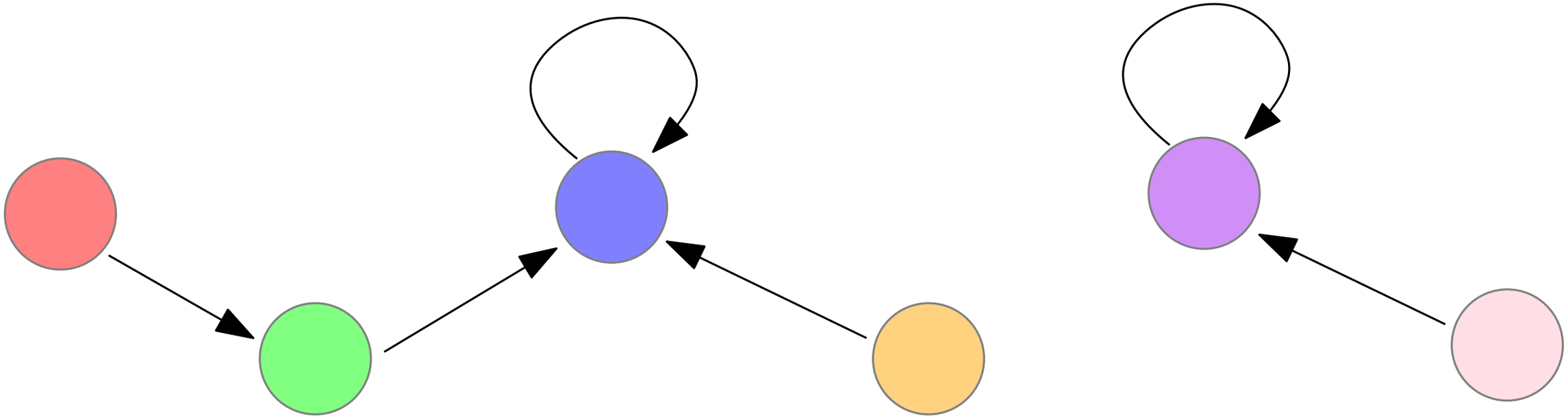

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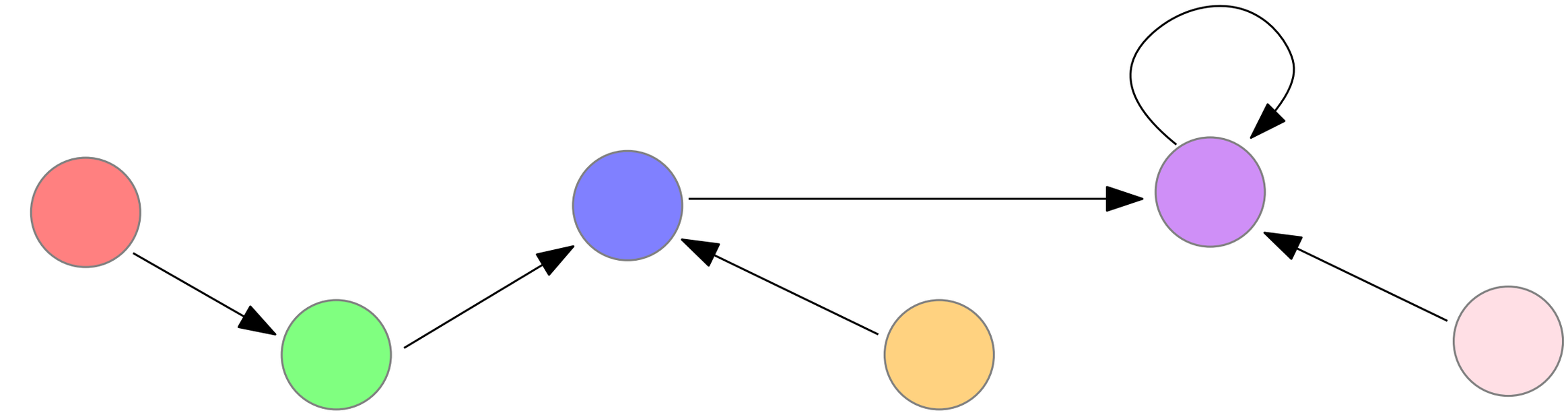

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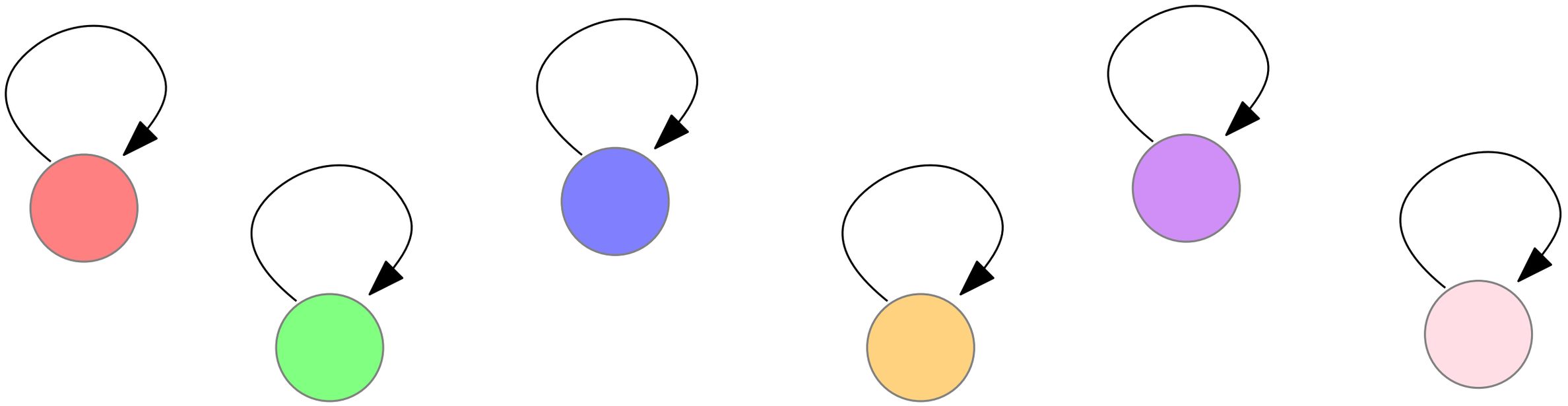

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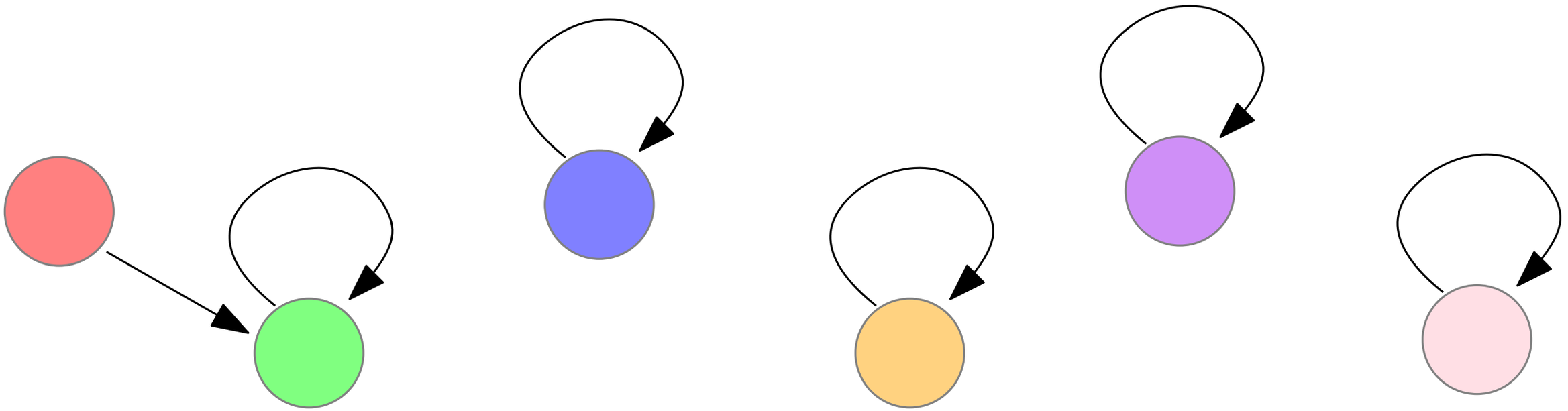

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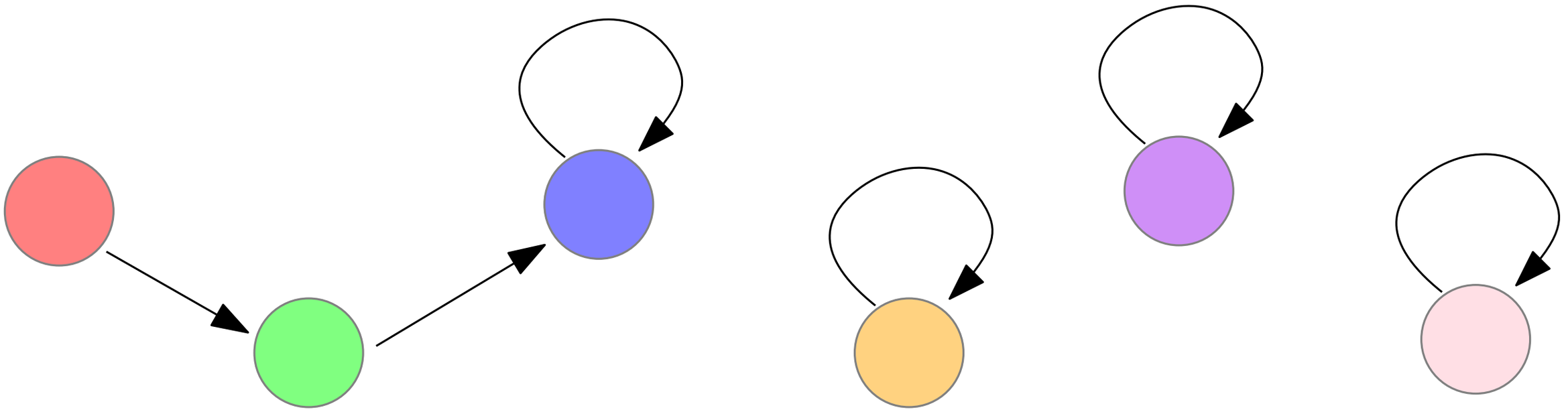

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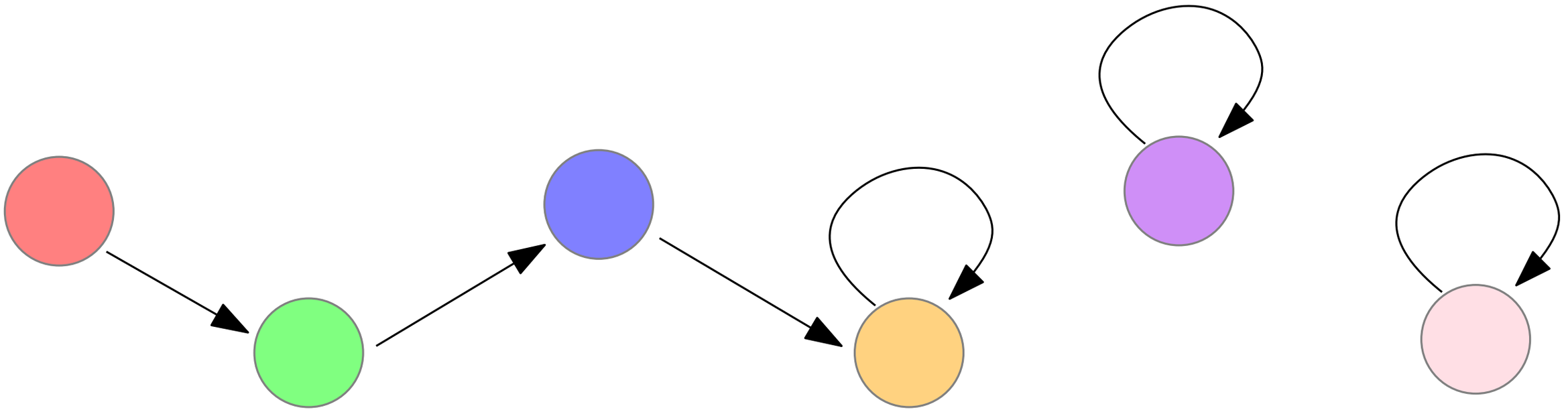

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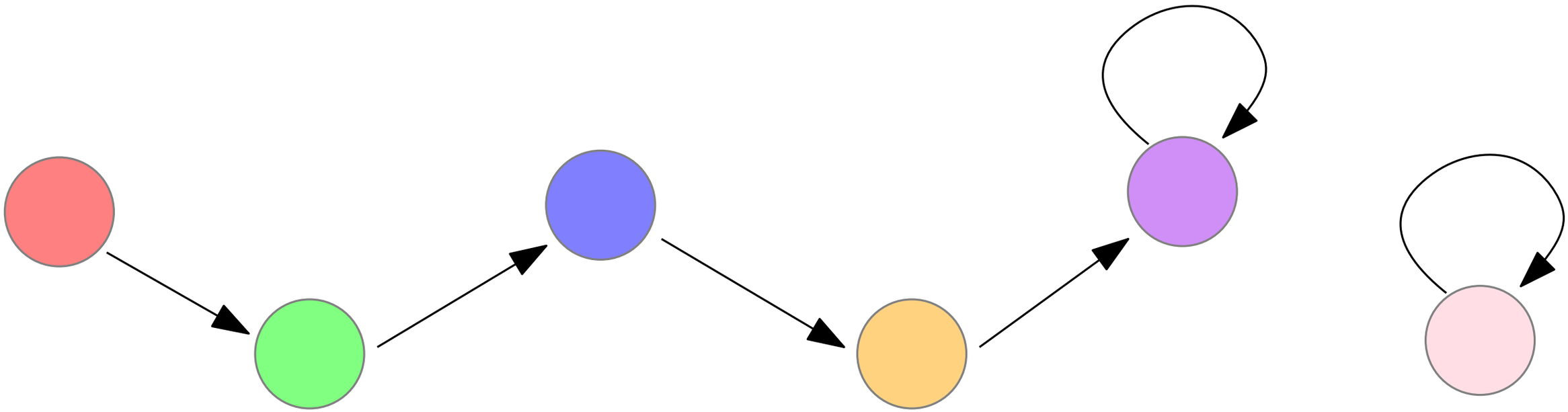

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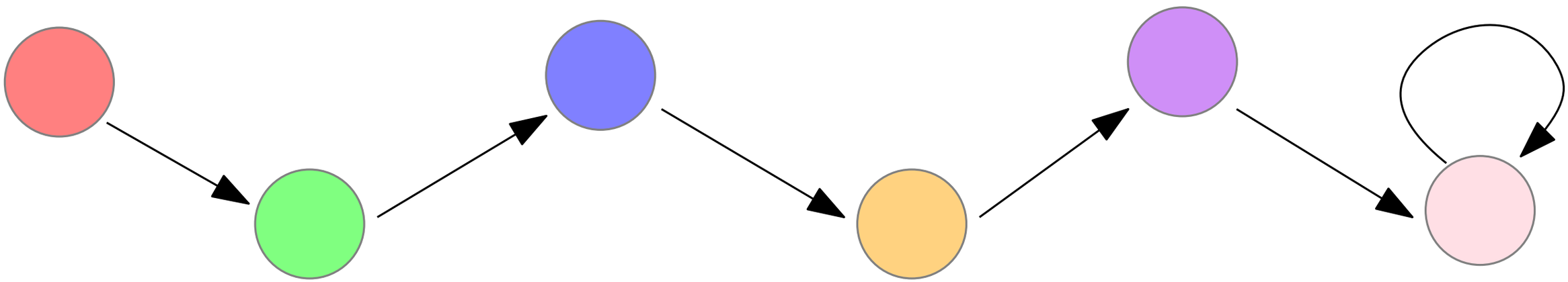

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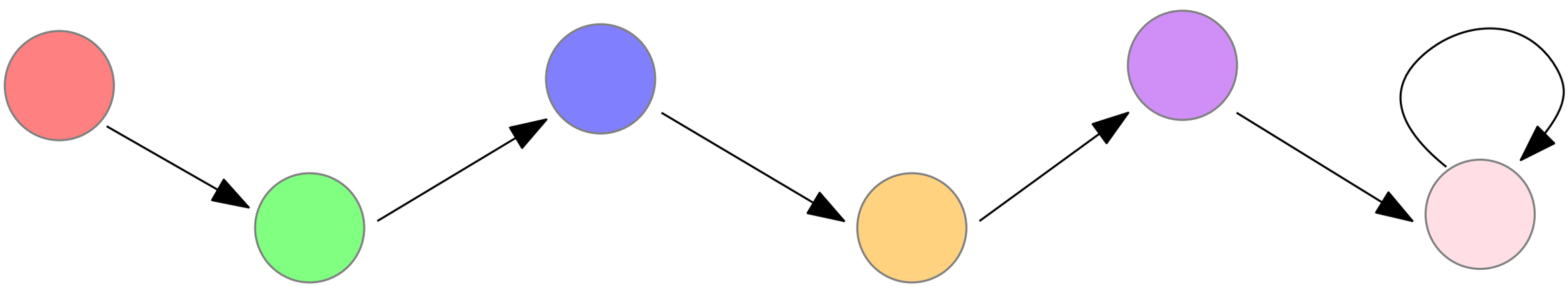

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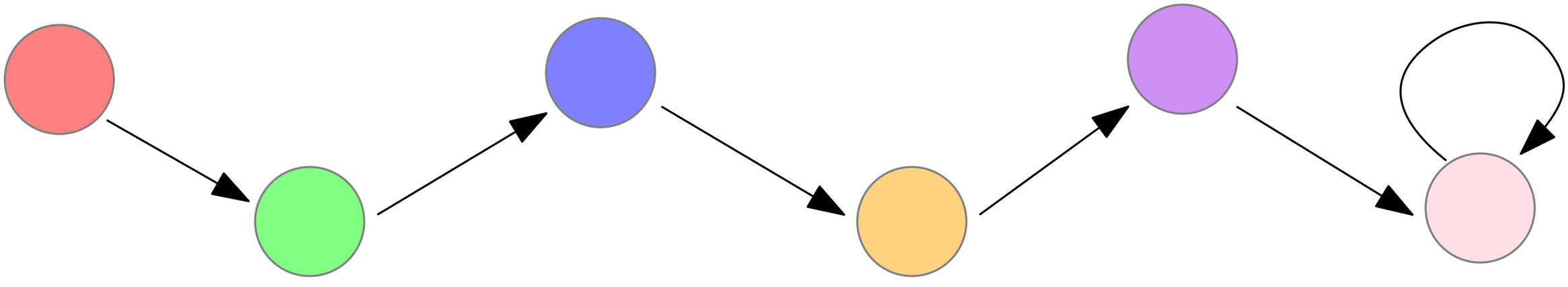

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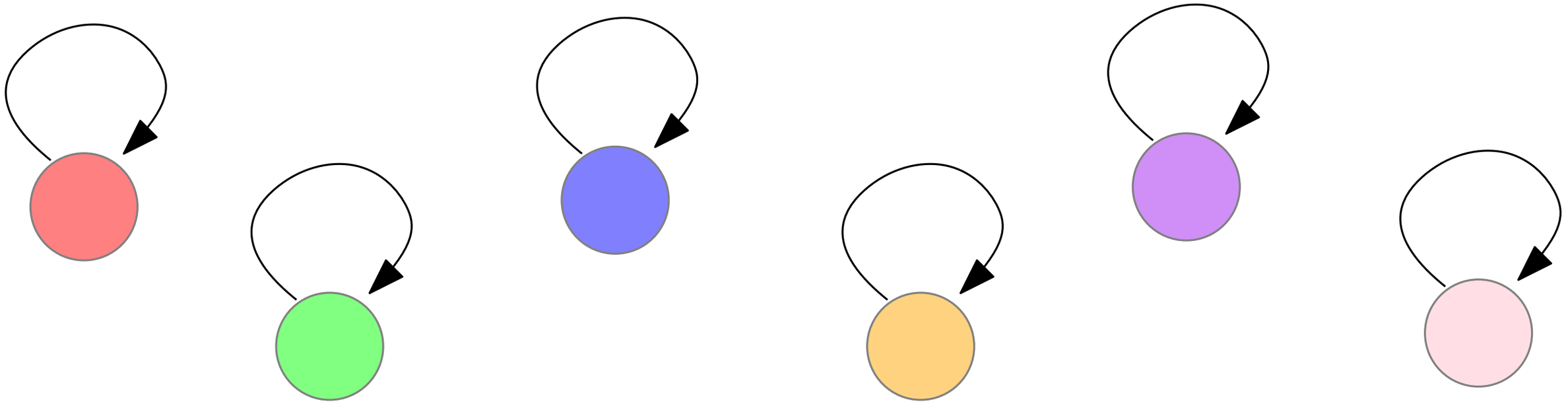

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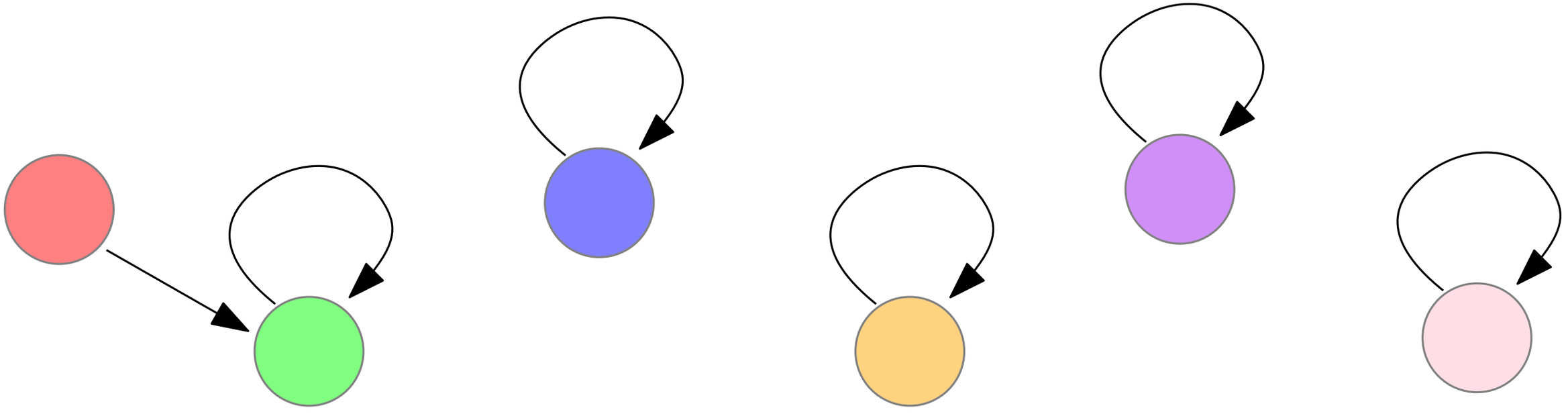

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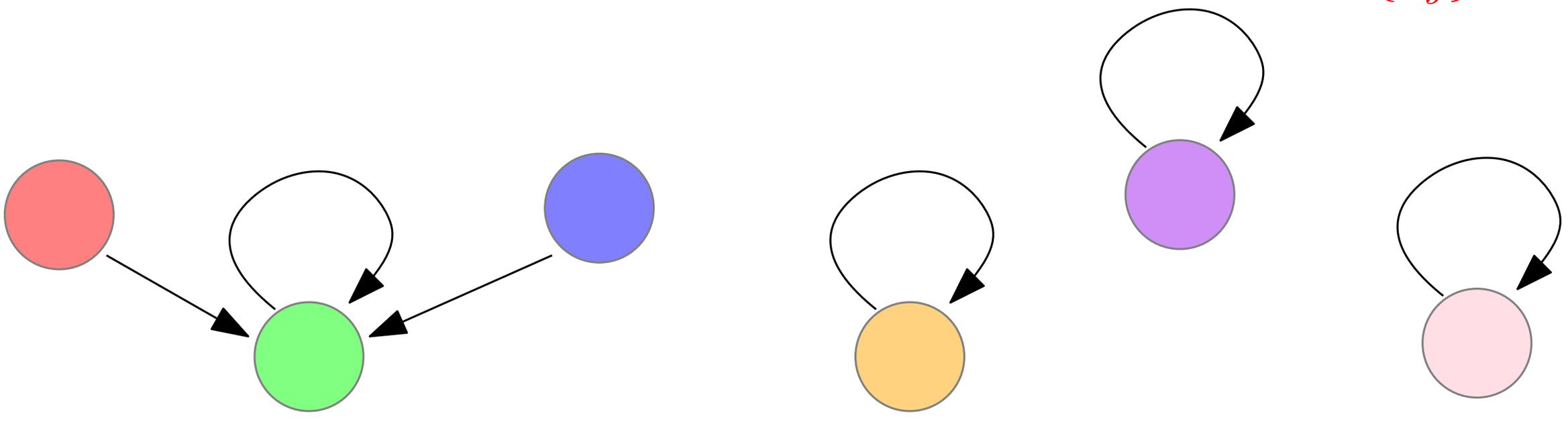

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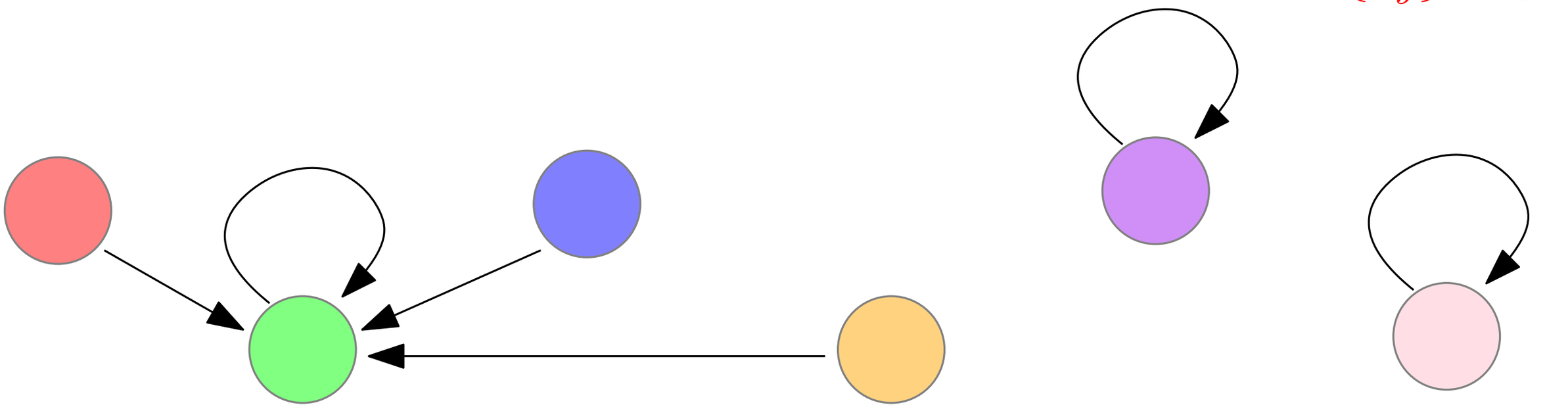

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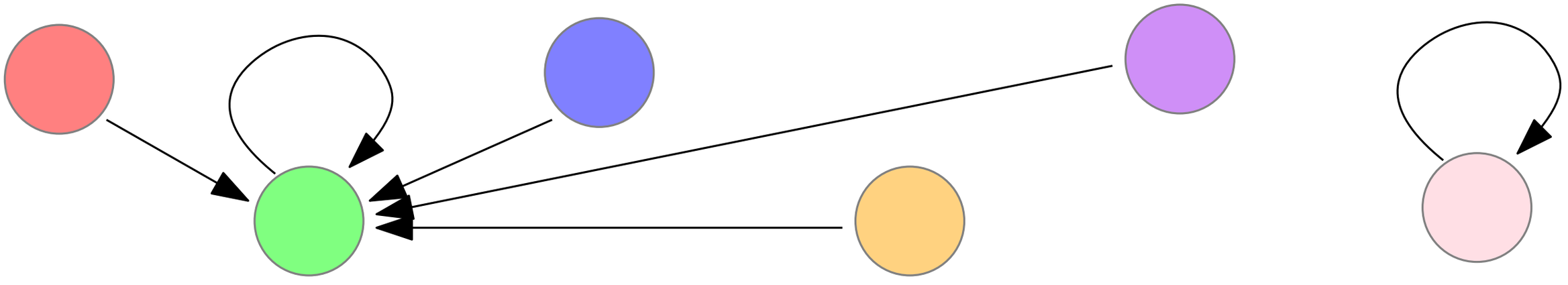

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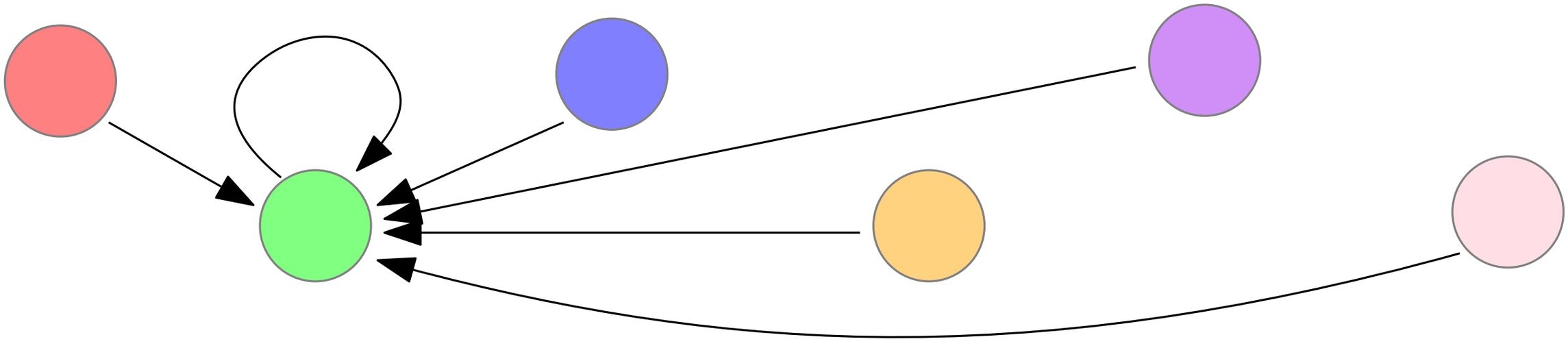

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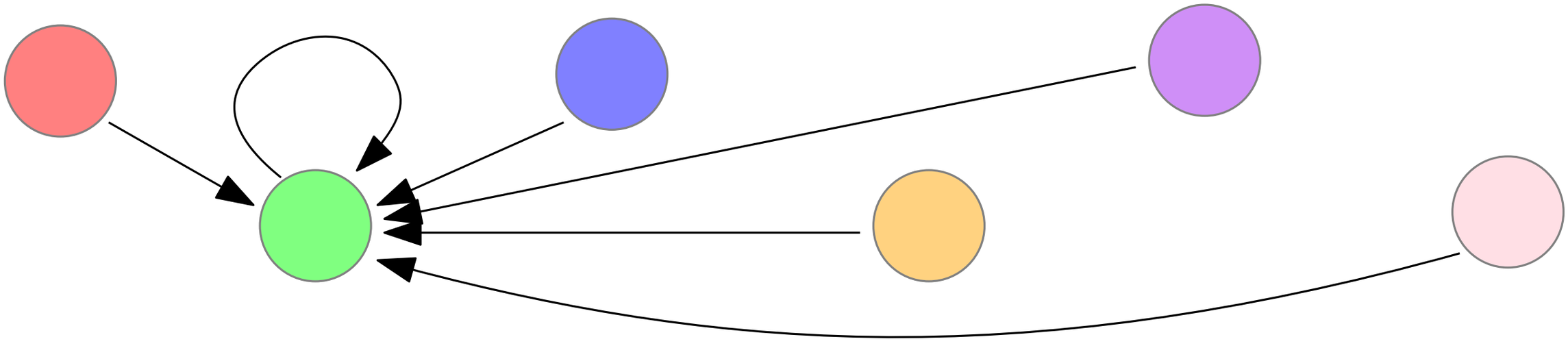
Find takes logarithmic time!



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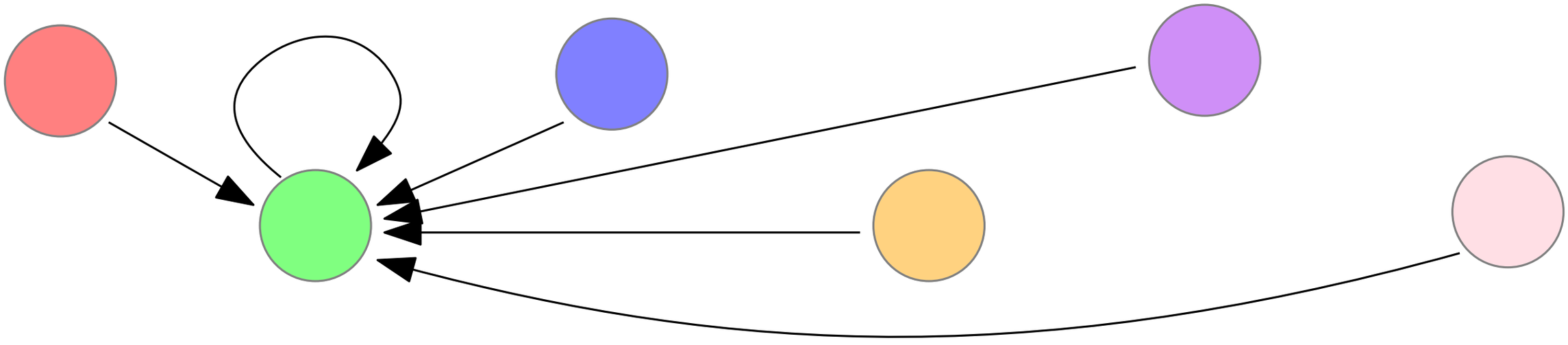
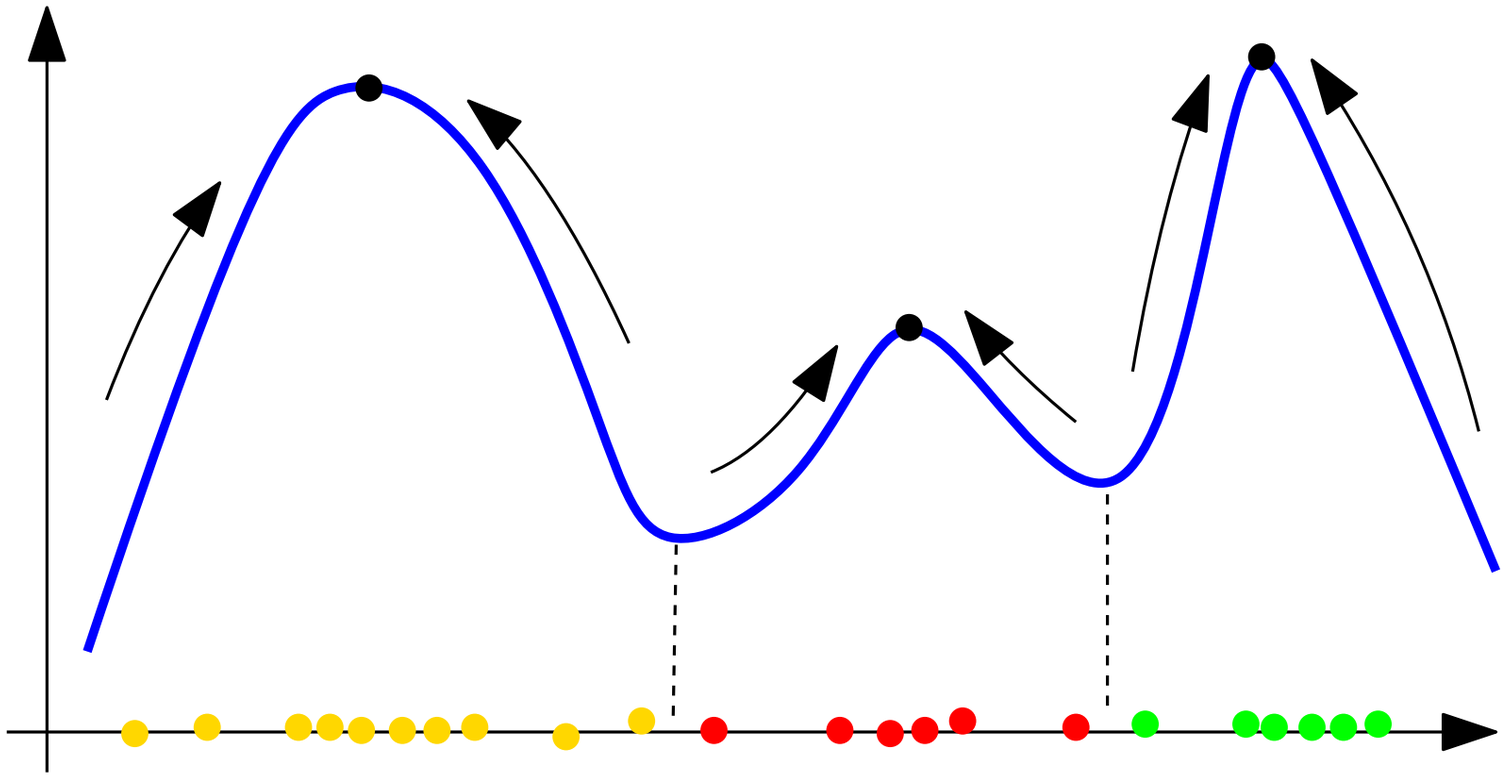
$+$ path compression: Find takes $O(\alpha(n))$ time!

i.e., attach all nodes directly to their parents $\alpha =$ inverse of Ackermann function



Mode seeking clustering



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

Two approaches:

- **Iterative**, such as, e.g., Mean Shift. [*Mean shift: a robust approach toward feature space analysis*, Comaniciu et al., IEEE Trans. on Pattern Analysis and Machine Intelligence, 2002]
- **Graph-based**, such as, e.g., [*A Graph-Theoretic Approach to Nonparametric Cluster Analysis*, Koontz et al., IEEE Trans. on Computers, 1976].

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where $N(x)$ is a neighborhood of x, and K is a kernel, e.g., Gaussian kernel $K(x,y) = \exp\left(-\frac{\|x-y\|_2^2}{2\sigma^2}\right)$.

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Do that for many random guesses, postprocess and merge similar centroids, and use final centroid distances to assess clusters.

Mean Shift

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where M n kernel $K(x, y)$

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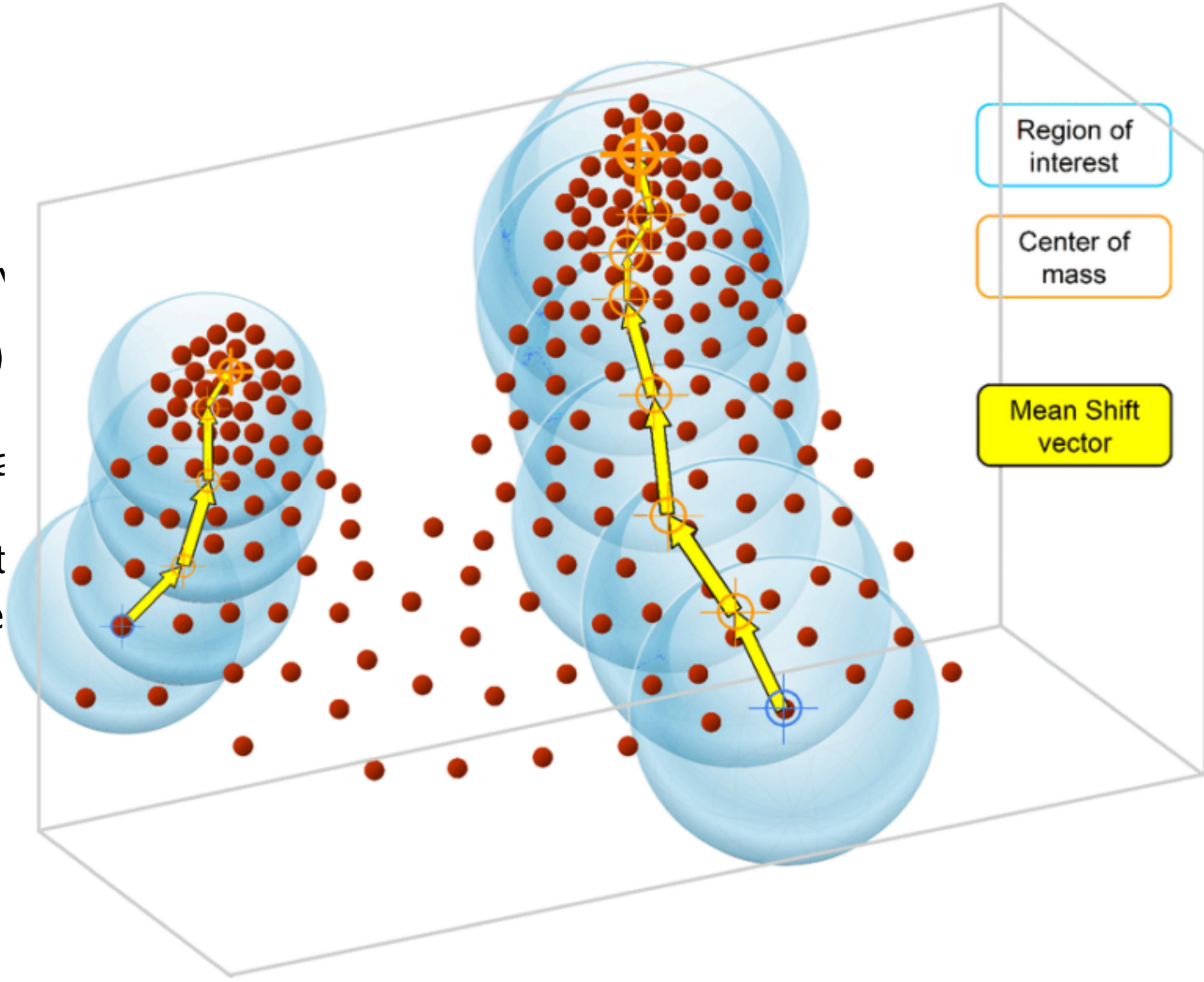

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cluster affiliation

centroid positions + bandwidths

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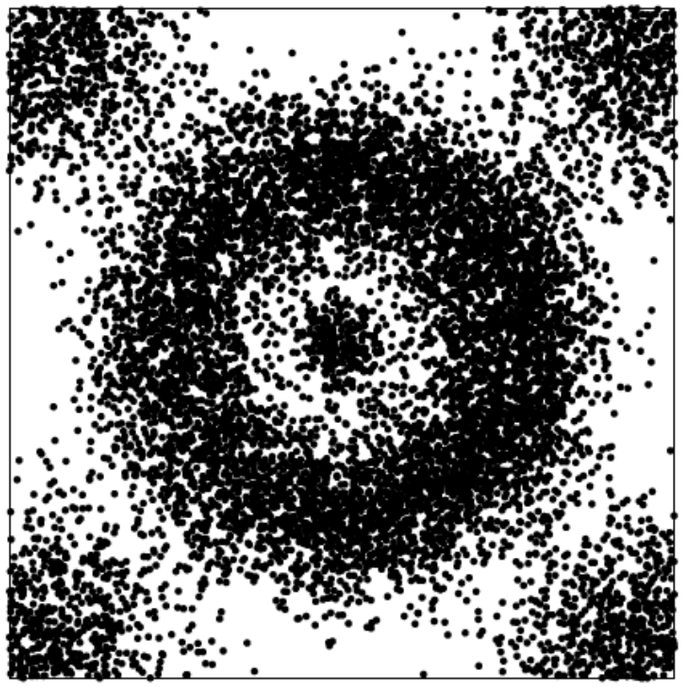
The Koonz, Narendra and Fukunaga algorithm (1976)



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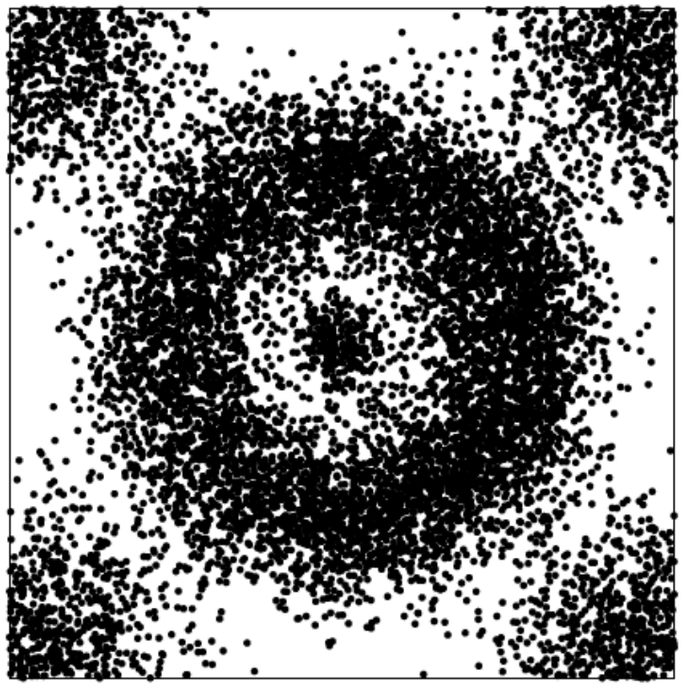
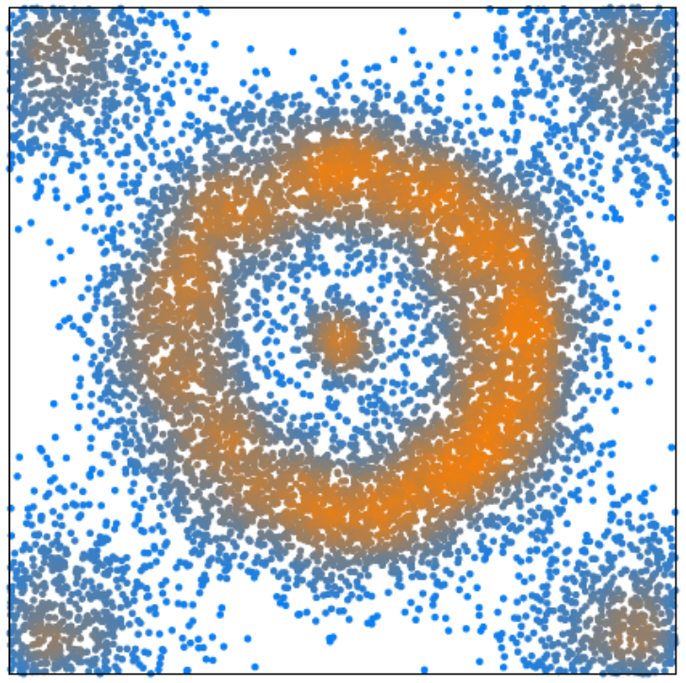


Density estimation



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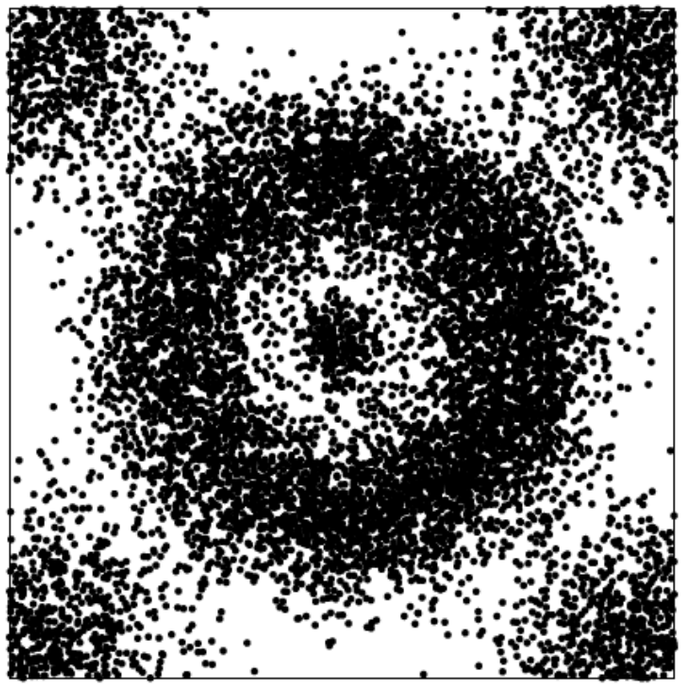

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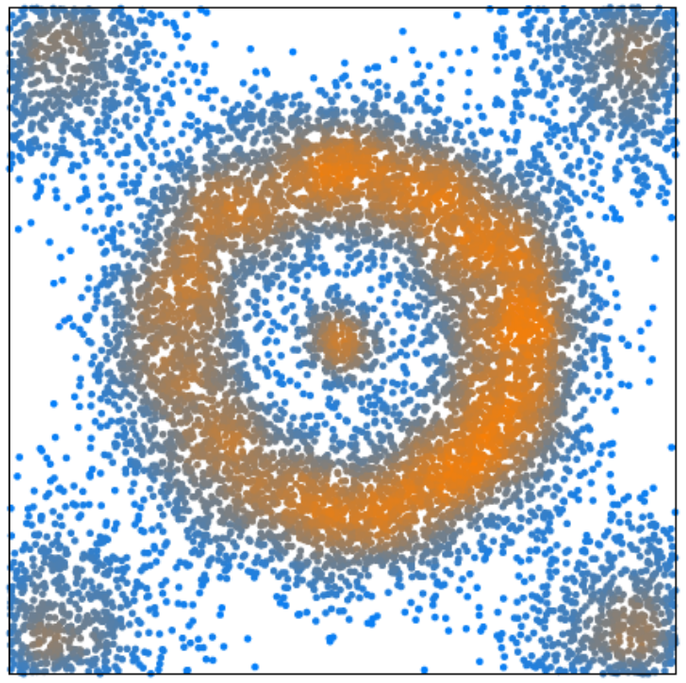
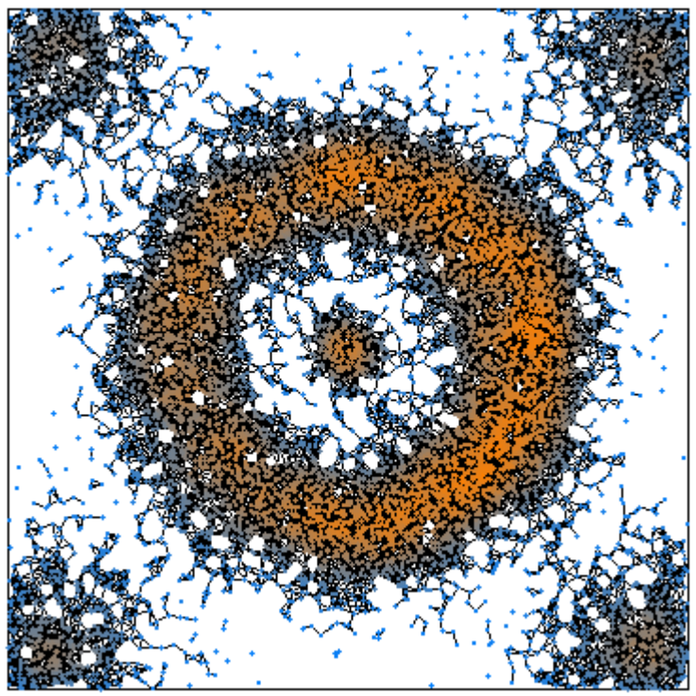


Neighborhood graph



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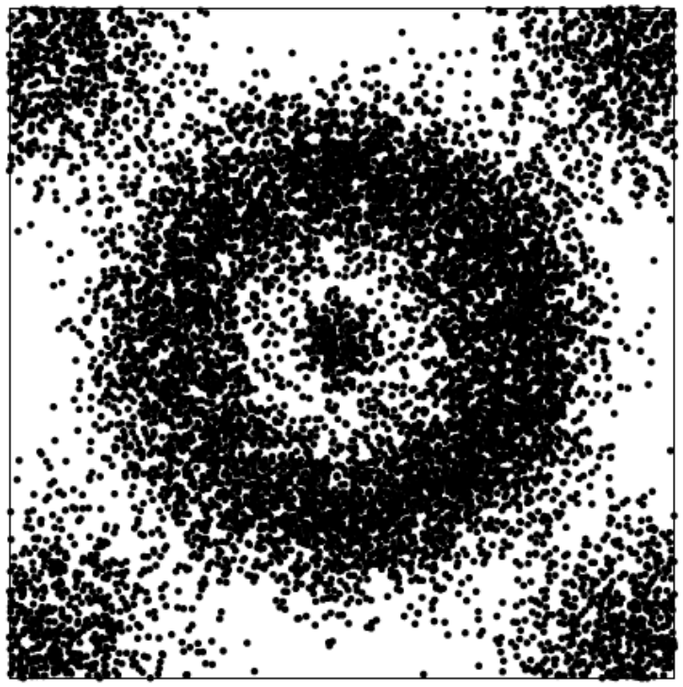

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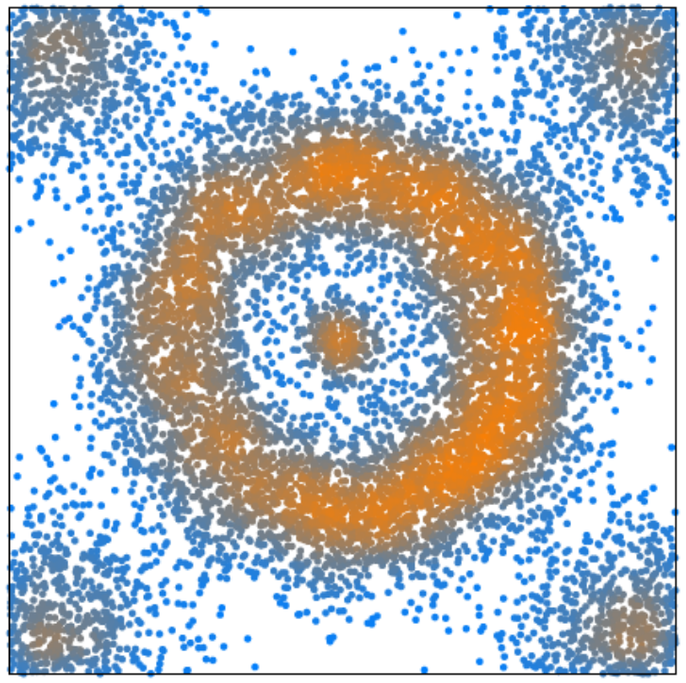

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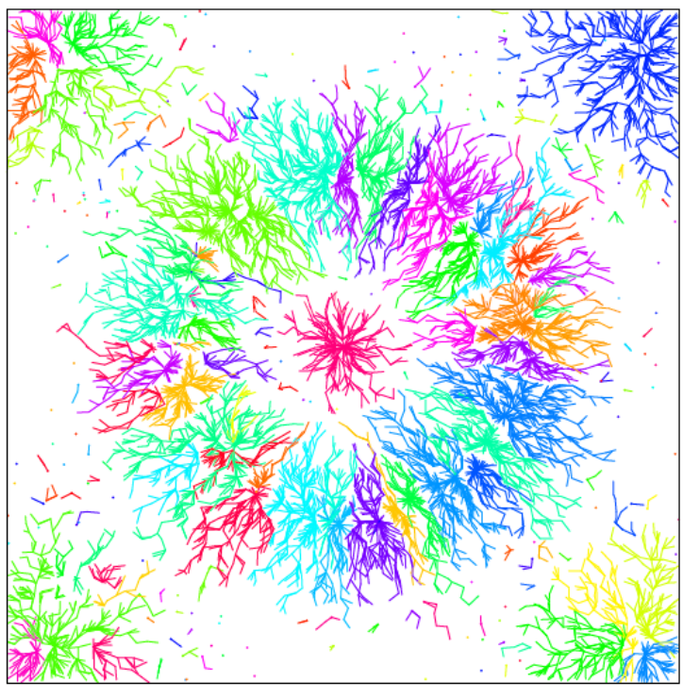
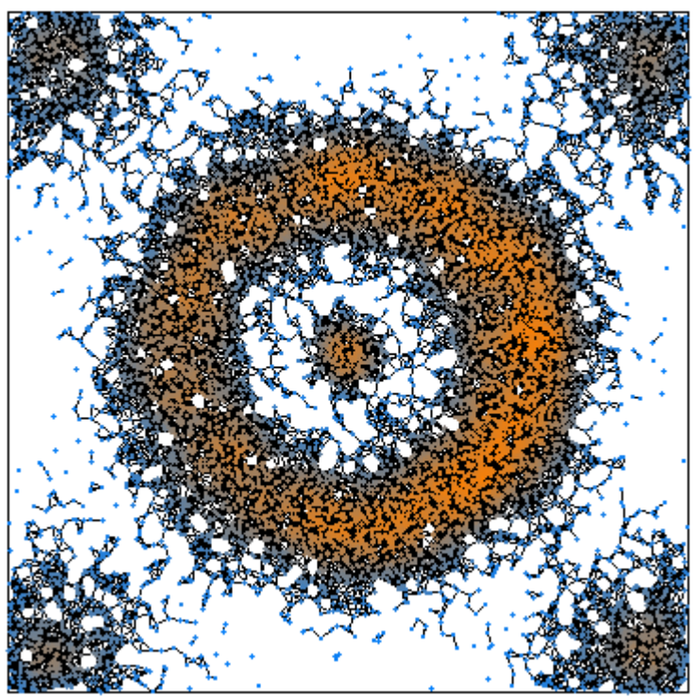


Discrete approximation of the gradient; for each vertex v, a gradient edge is selected among the edges adjacent to v.



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)

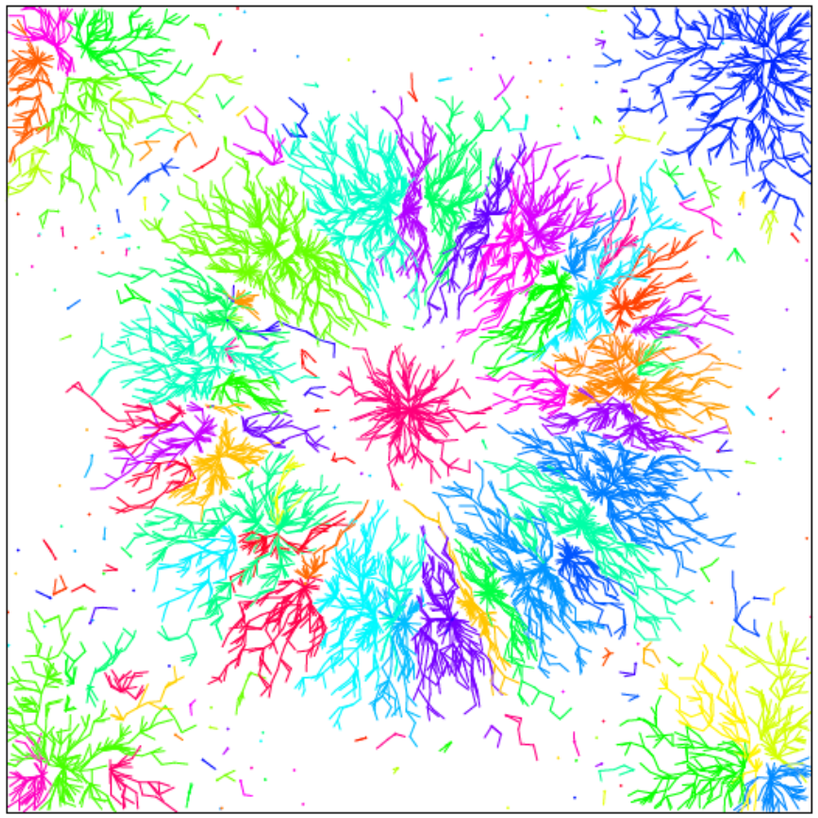
Sort the vertex indices $\{1, 2, \ldots, n\}$ in decreasing order: $\hat{f}(1) \geq \hat{f}(2) \geq \cdots \geq \hat{f}(n)$;
Initialize a union-find data structure (disjoint-set forest) $\mathcal{U}$ and two vectors g, r of size n;

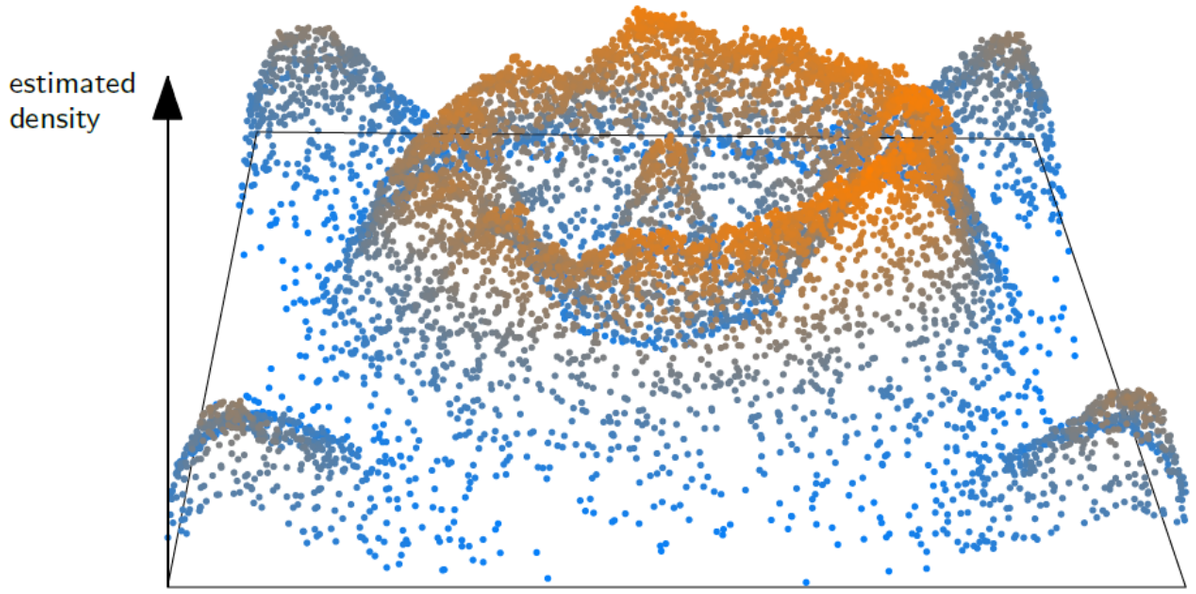
for $i = 1$ to n **do**
    Let N be the set of neighbors of i in G that have indices higher than i;
    if $N = \emptyset$
        Create a new entry e in $\mathcal{U}$ and attach vertex i to it: $\mathcal{U}$.`MakeSet`(i);
        $r(e) \leftarrow i$ *// $r(e)$ stores the root vertex associated with 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*
        $e_i \leftarrow \mathcal{U}$.`Find`$(g(i))$;
        Attach vertex i to the entry e_i: $\mathcal{U}$.`Union`(i, e_i);

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

The Koonz, Narendra and Fukunaga algorithm (1976)

Drawbacks:





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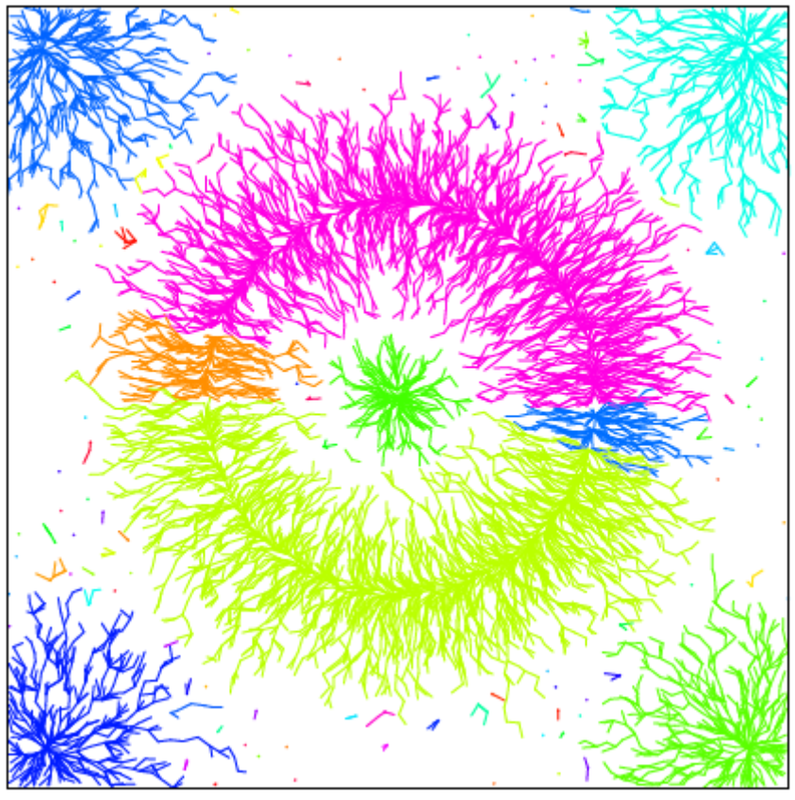

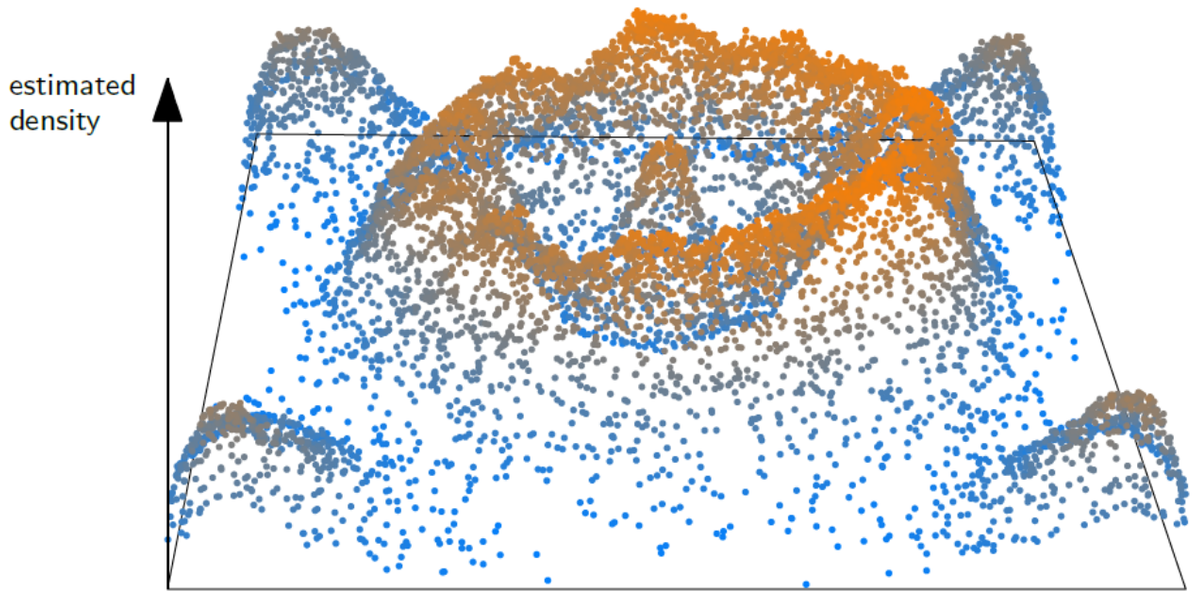

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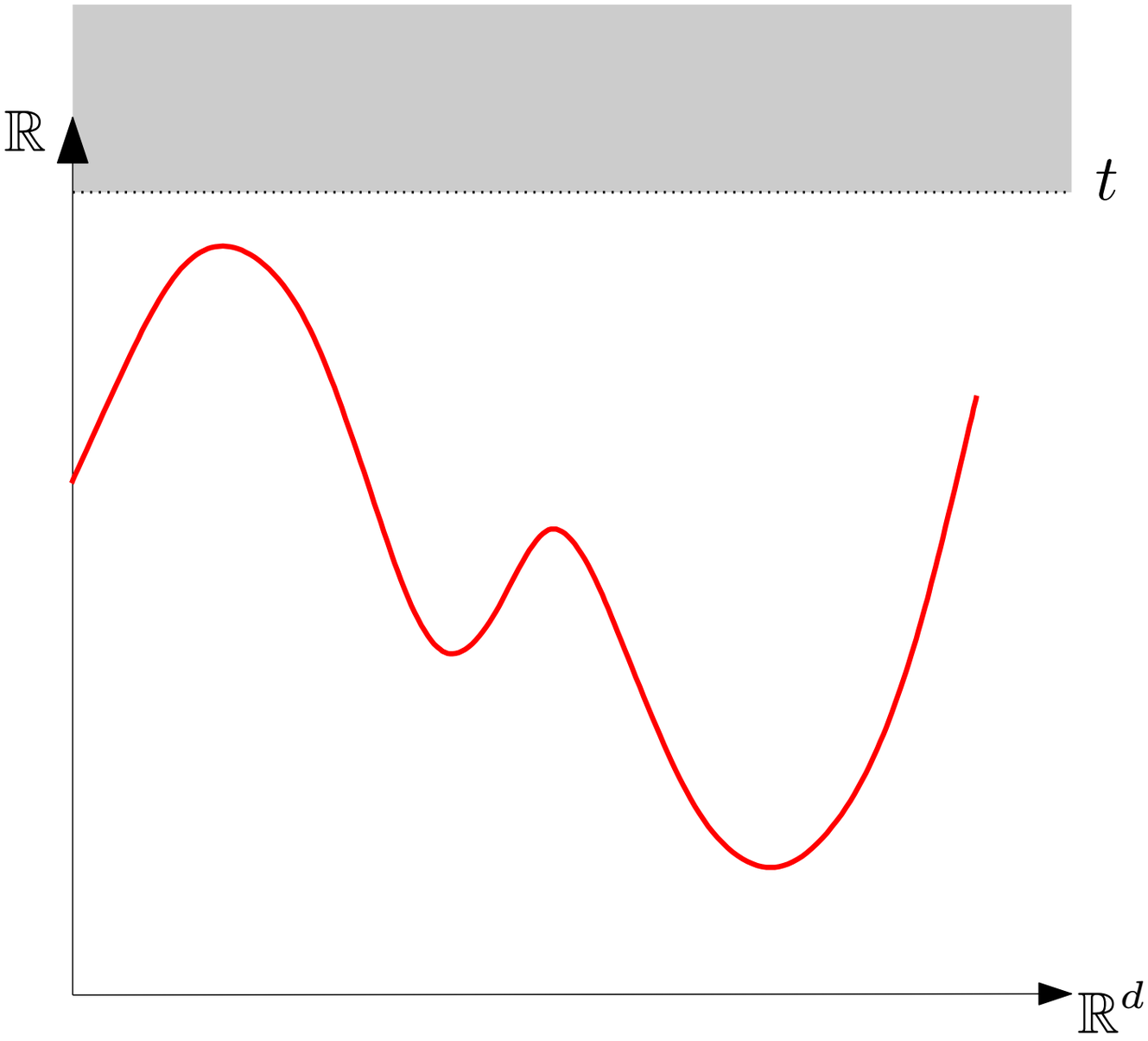
Approaches to overcome these issues:

- Smooth out the density estimate (e.g. mean-shift)... But how to choose the smoothing parameter?
- Merge clusters with 0-dimensional persistent homology!

0-dimensional PH of density

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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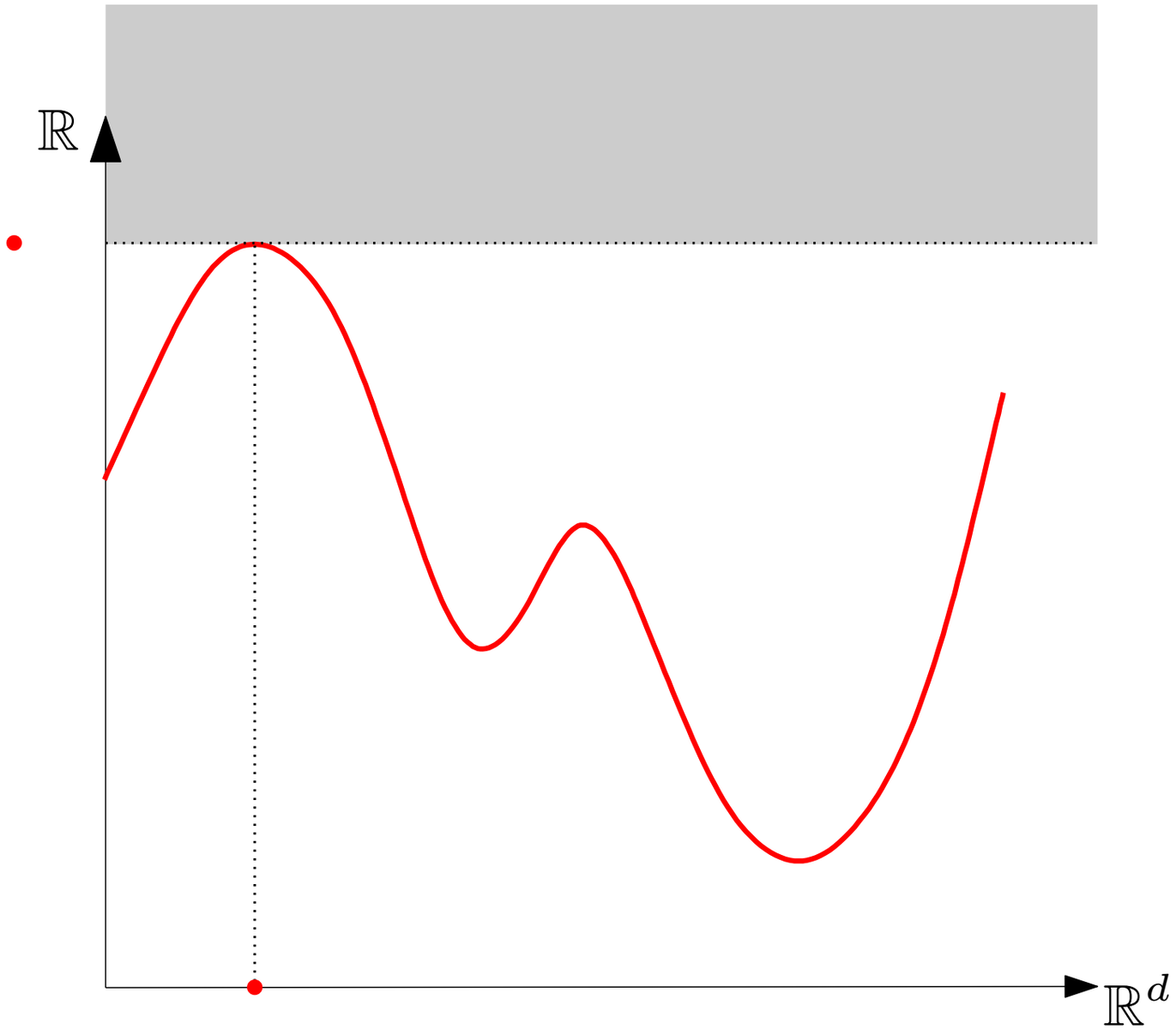

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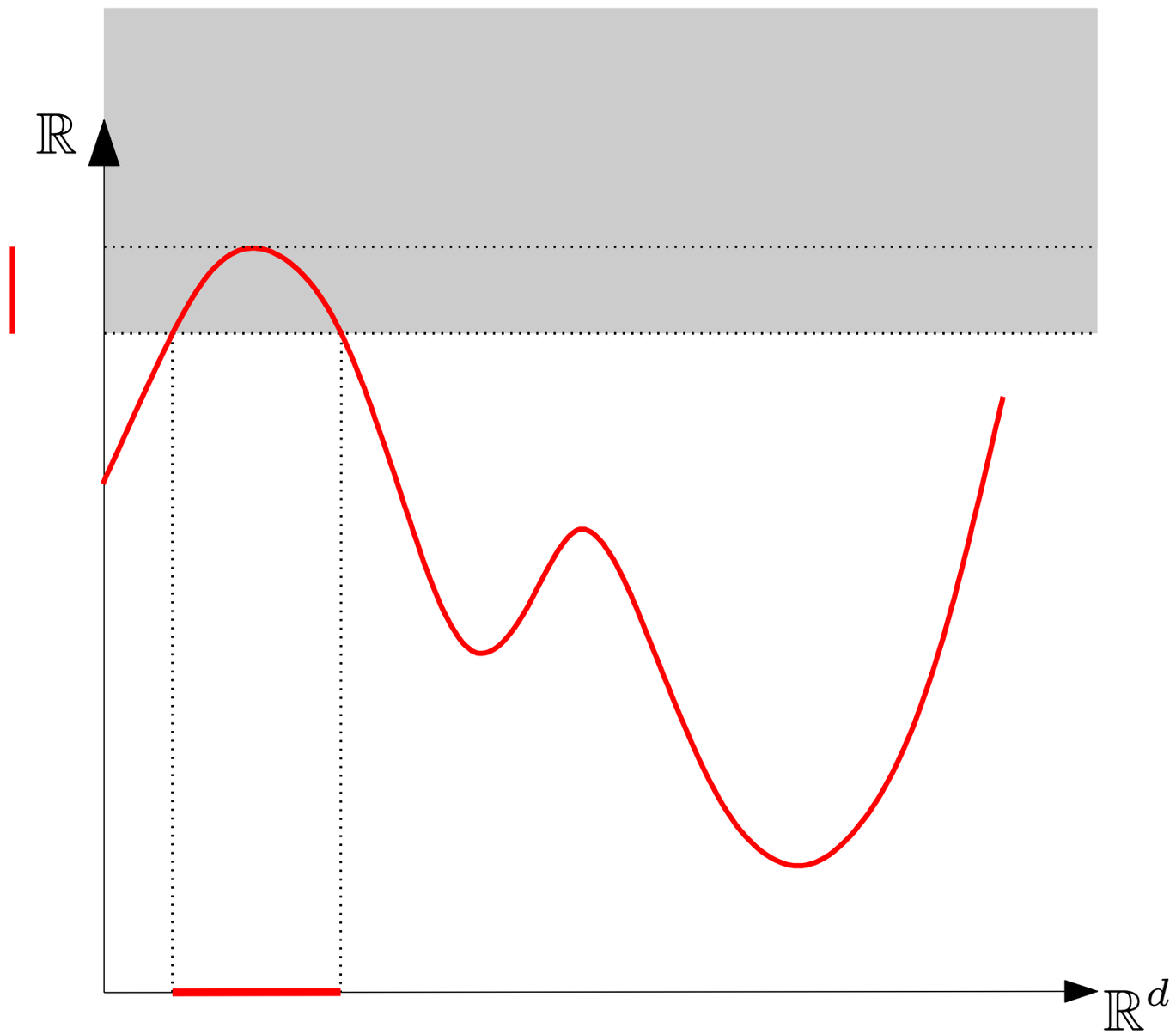

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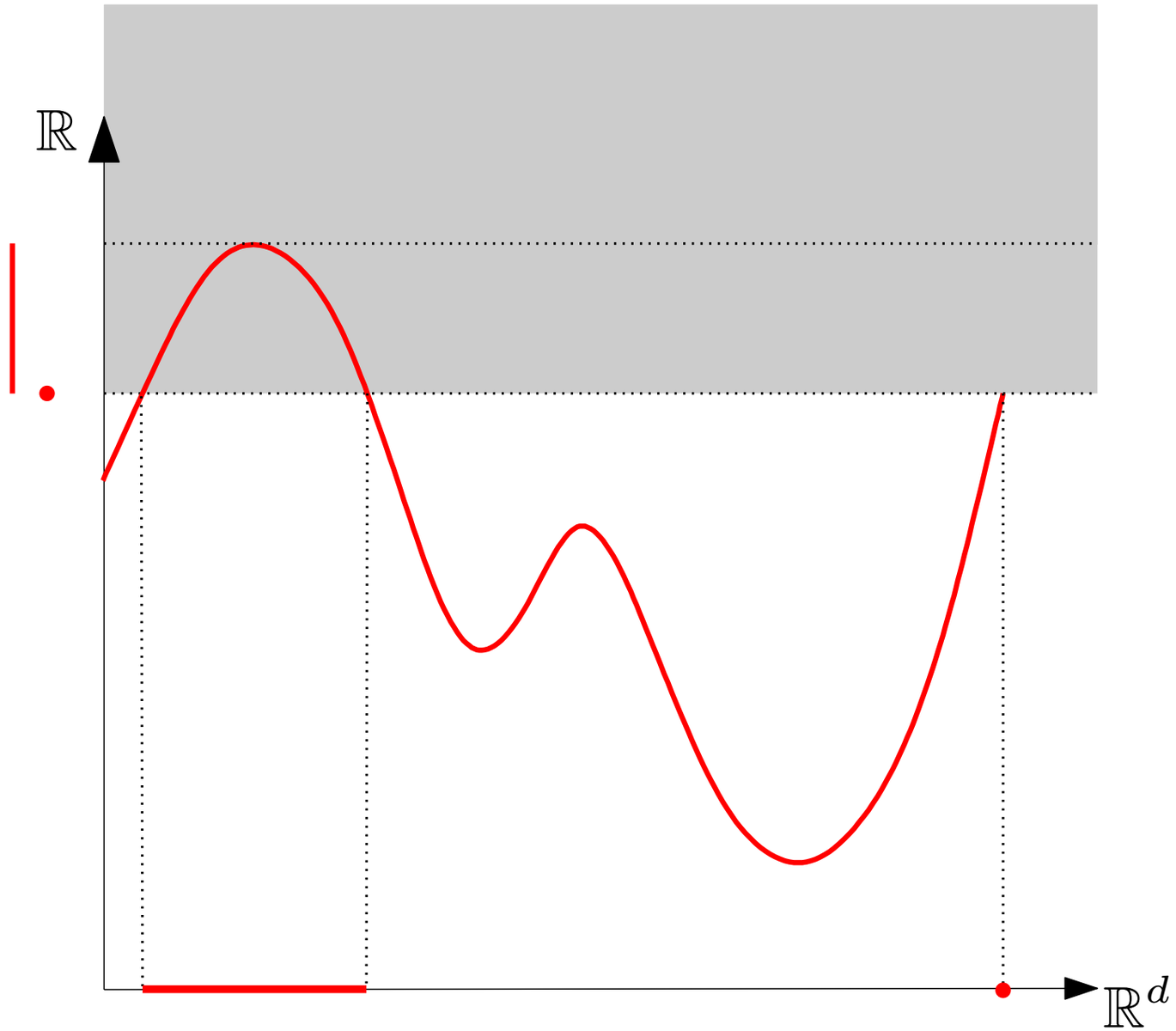

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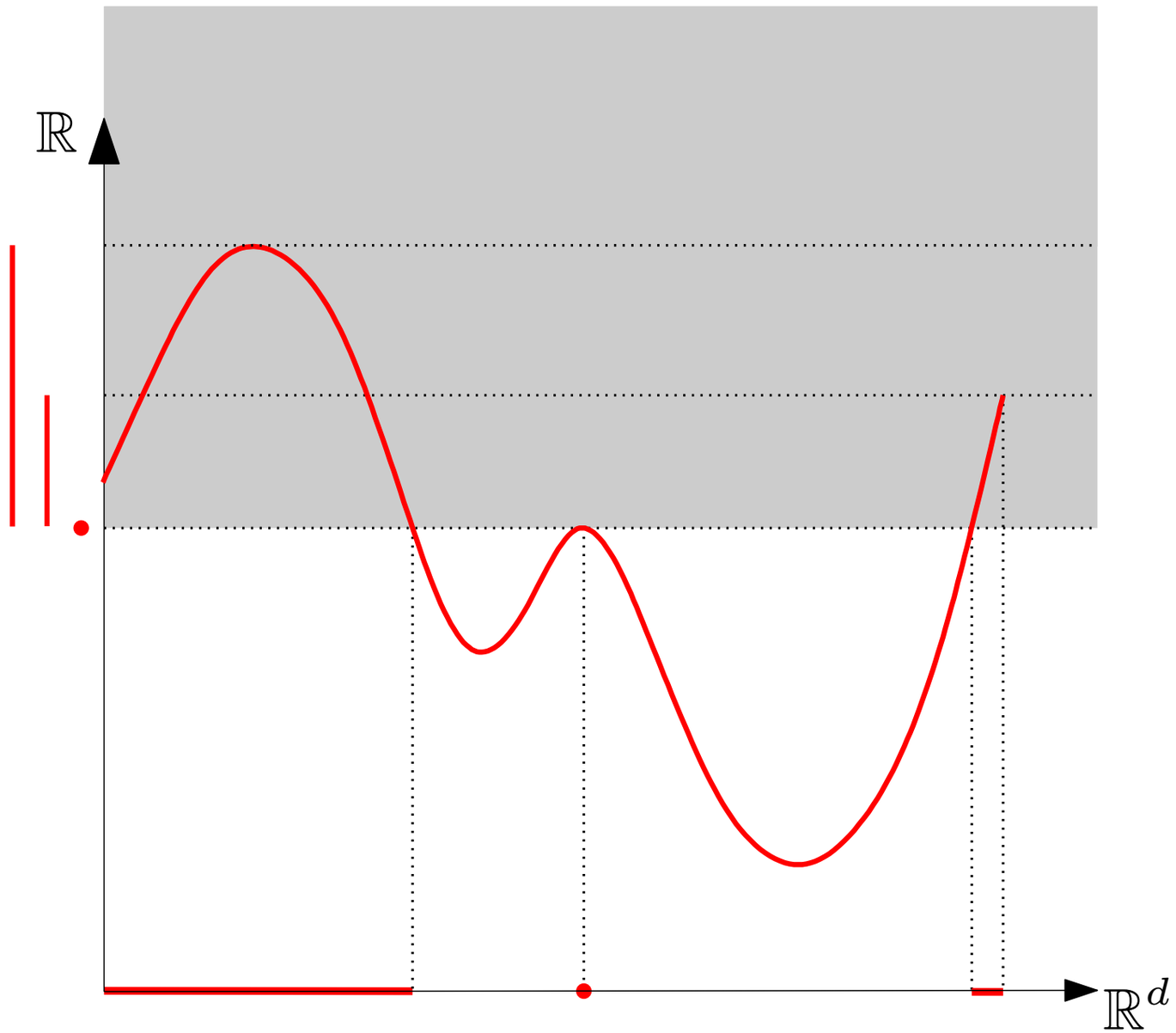

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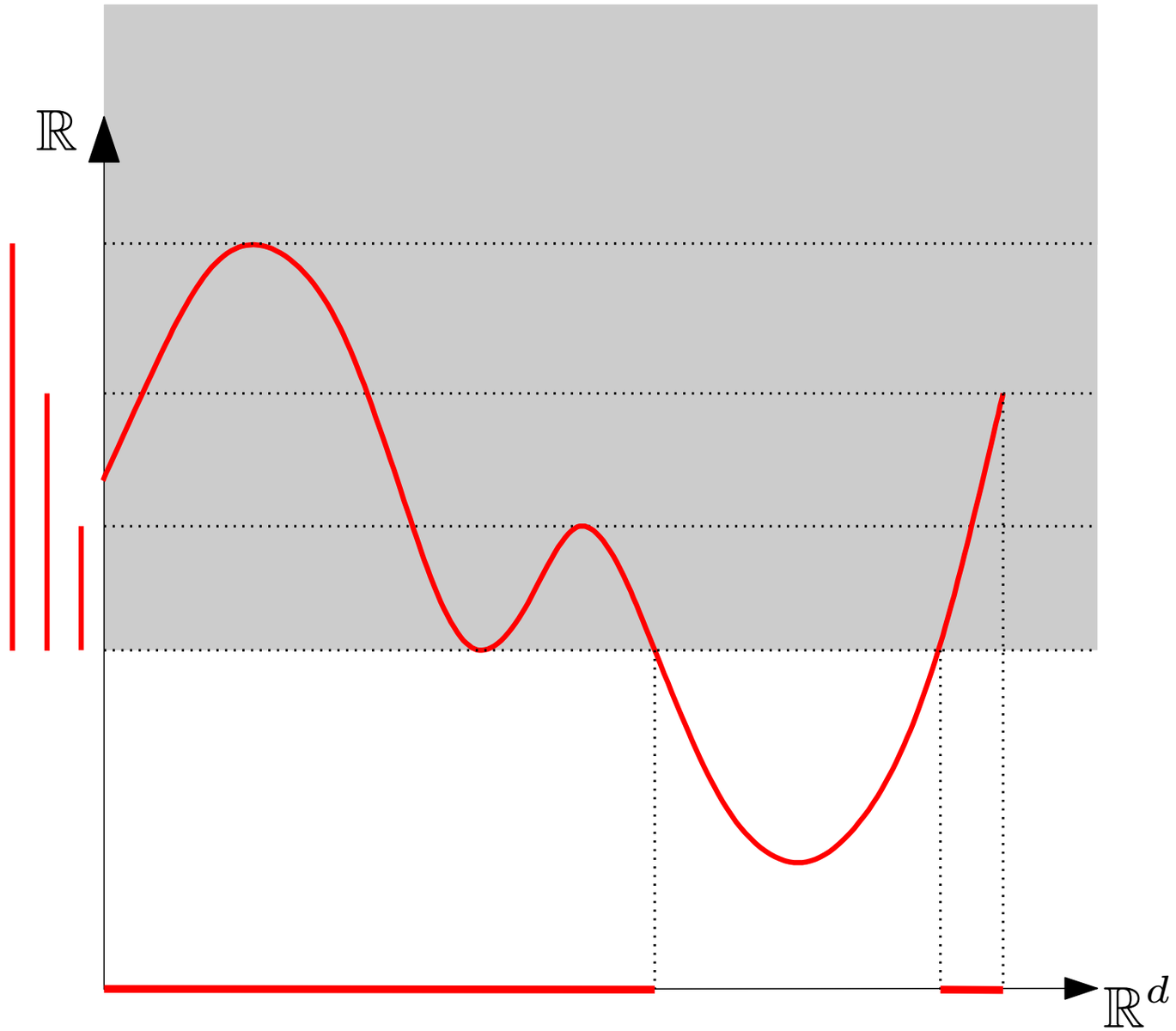

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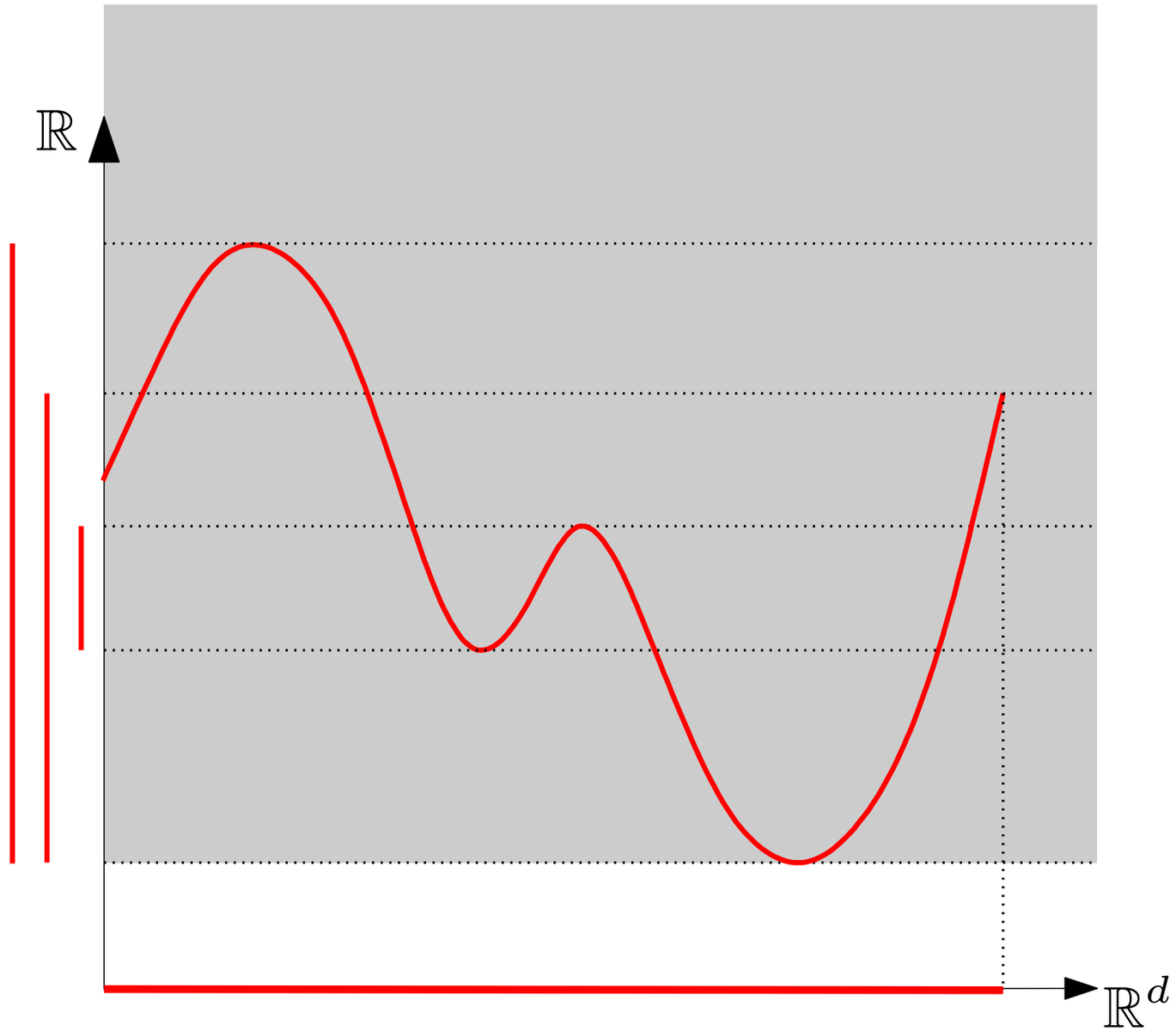

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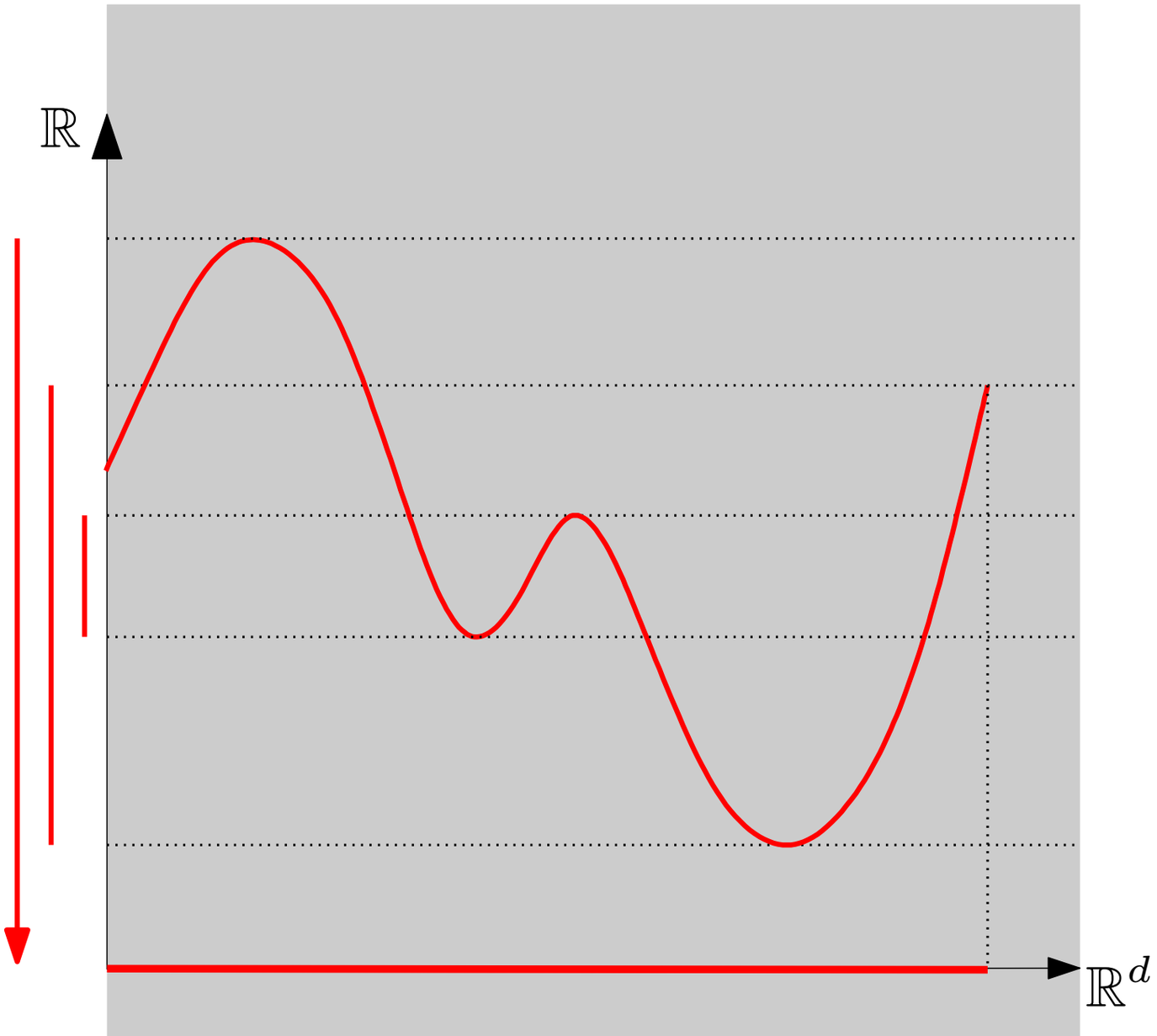

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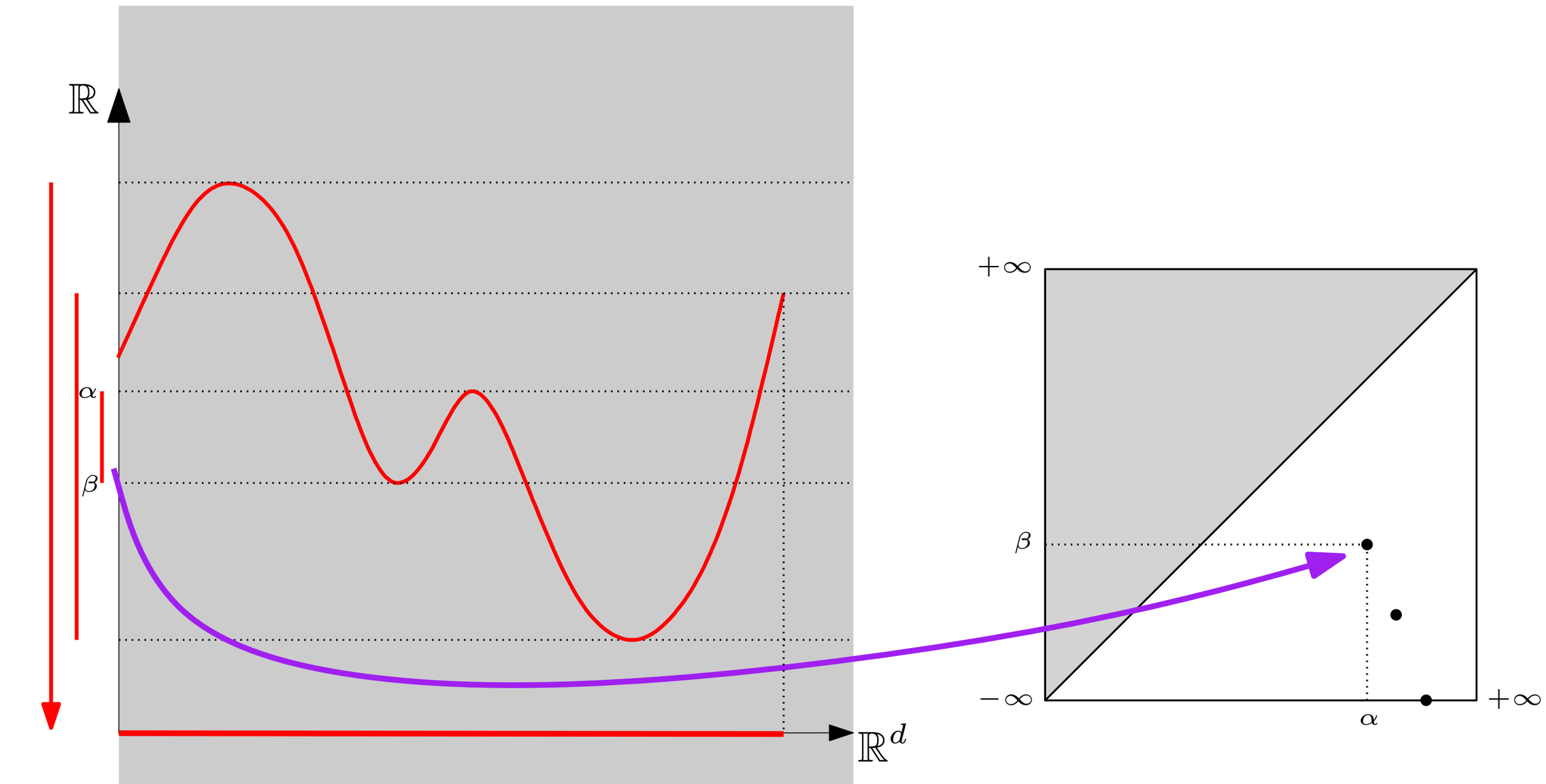

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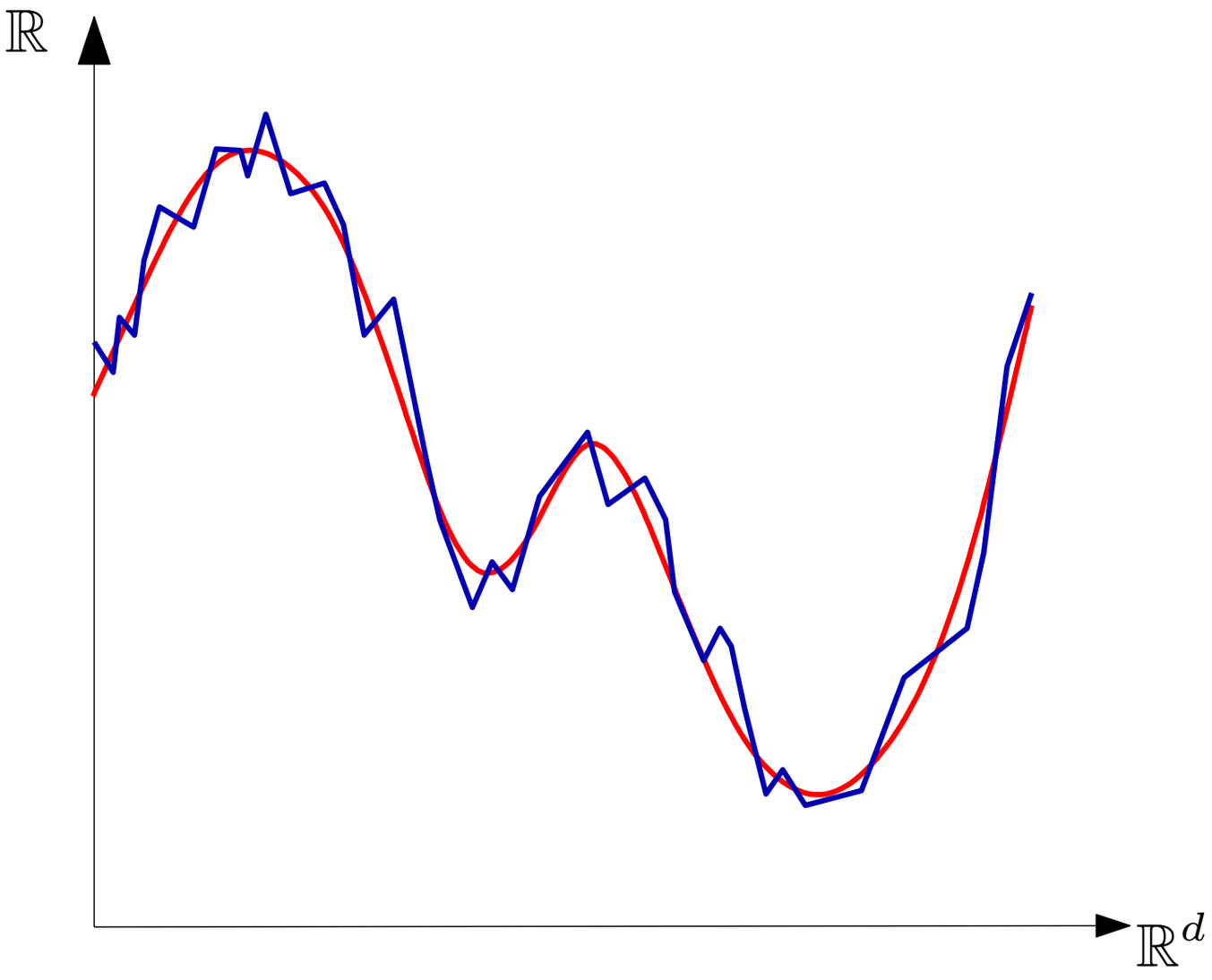
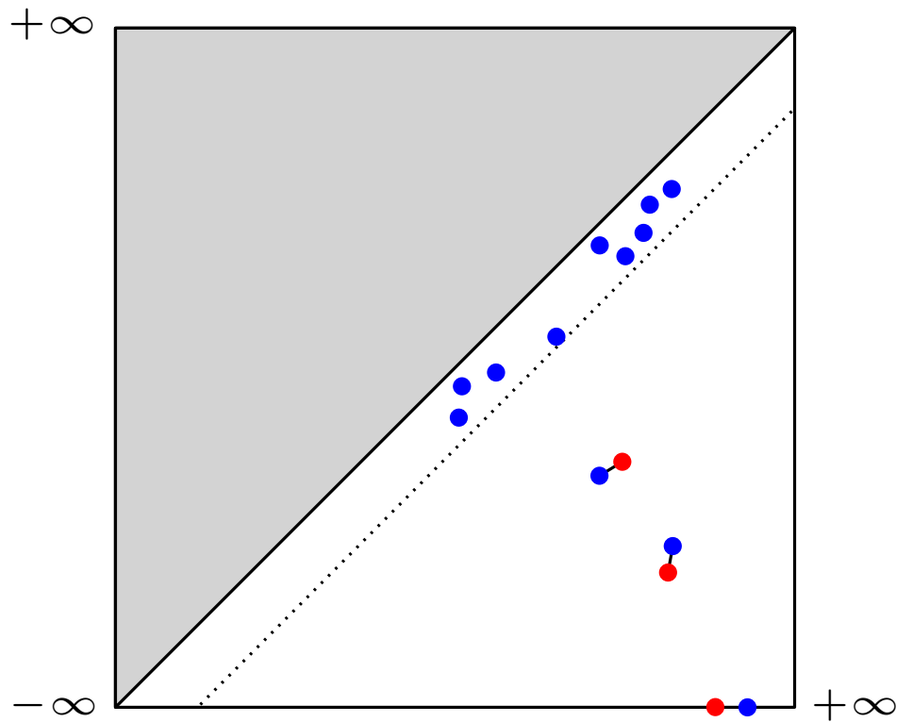
Given an estimator $\hat{f}$:

Stability theorem $\Rightarrow d_b(D_f, D_{\hat{f}}) \leq \|f - \hat{f}\|_\infty$.





Persistence-based clustering

[*Persistence-Based Clustering in Riemannian Manifolds*, Chazal, Oudot, Skraba, Guibas, J. ACM, 2013]

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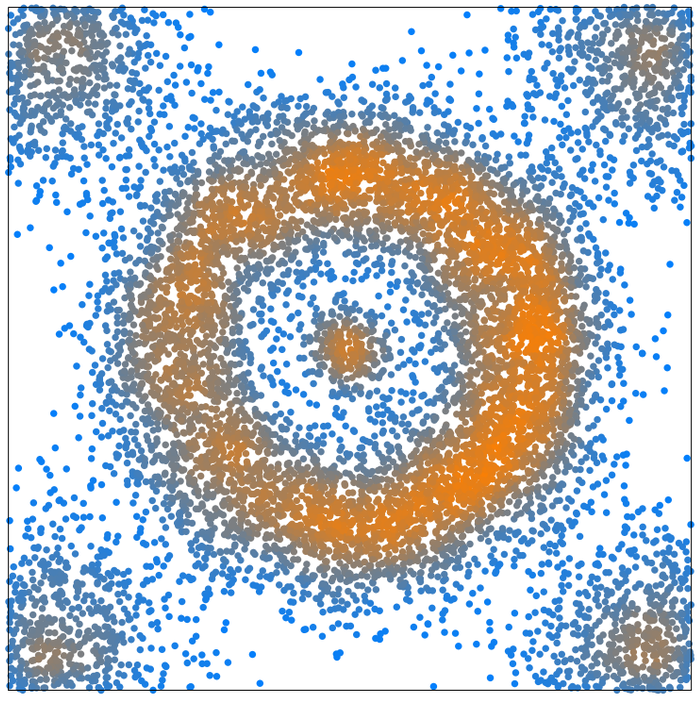

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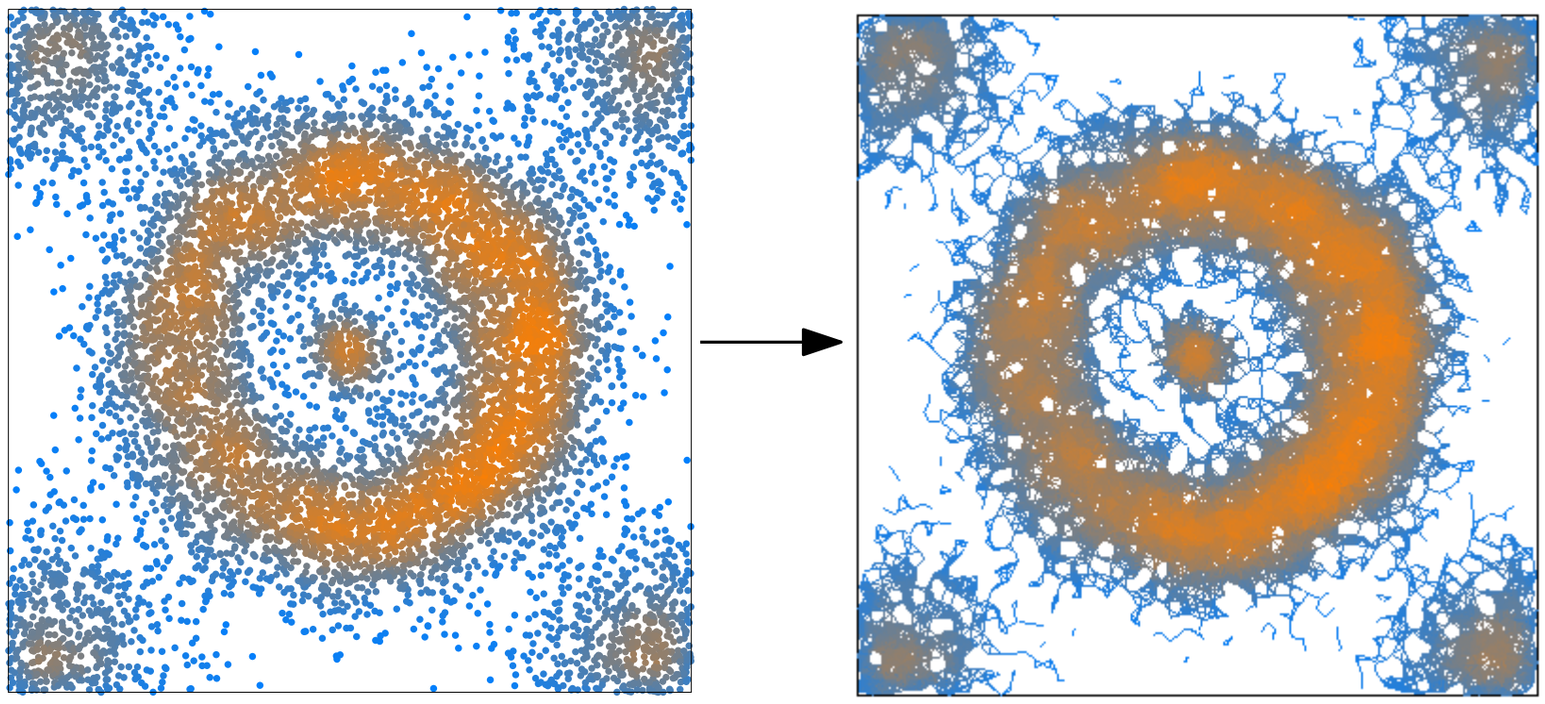

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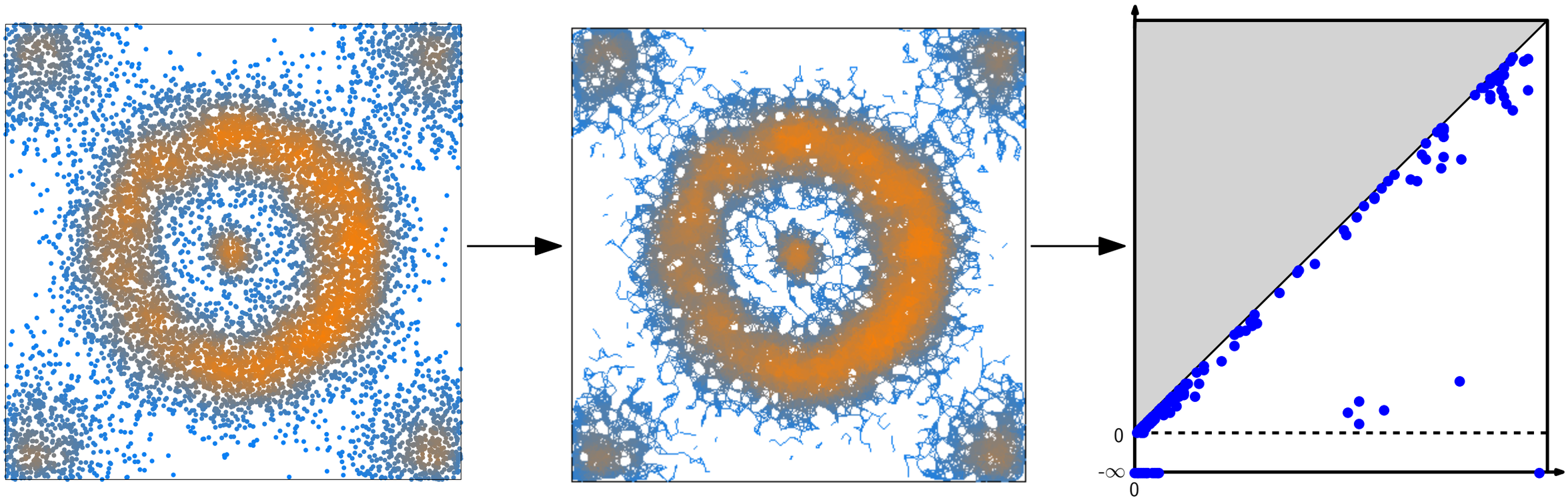

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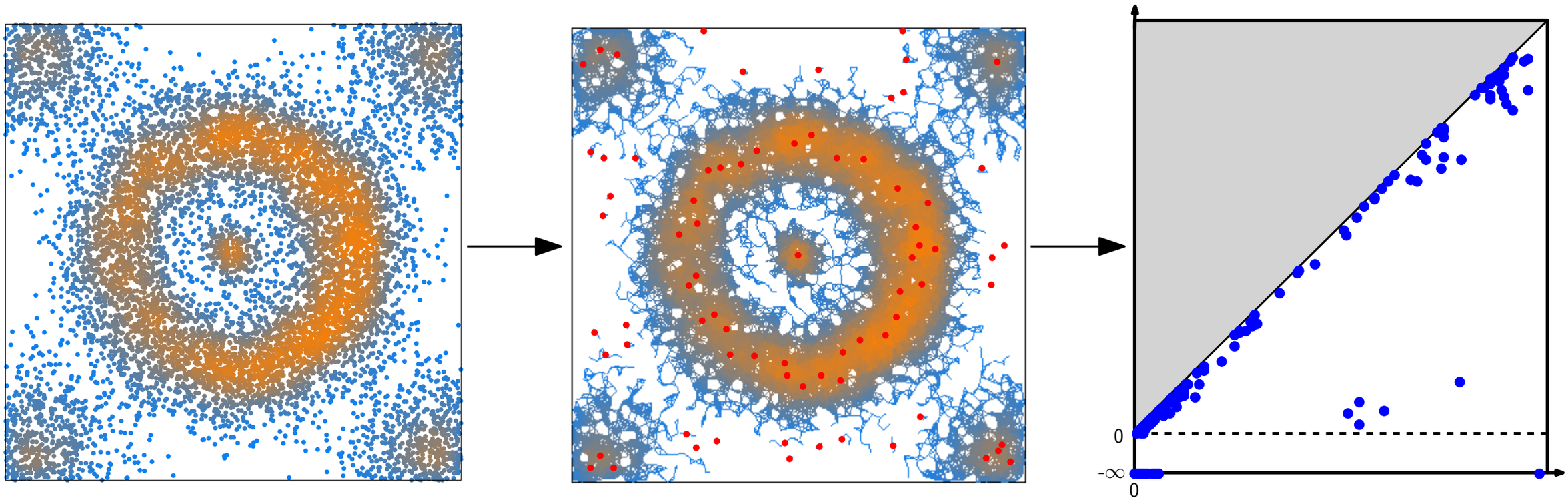

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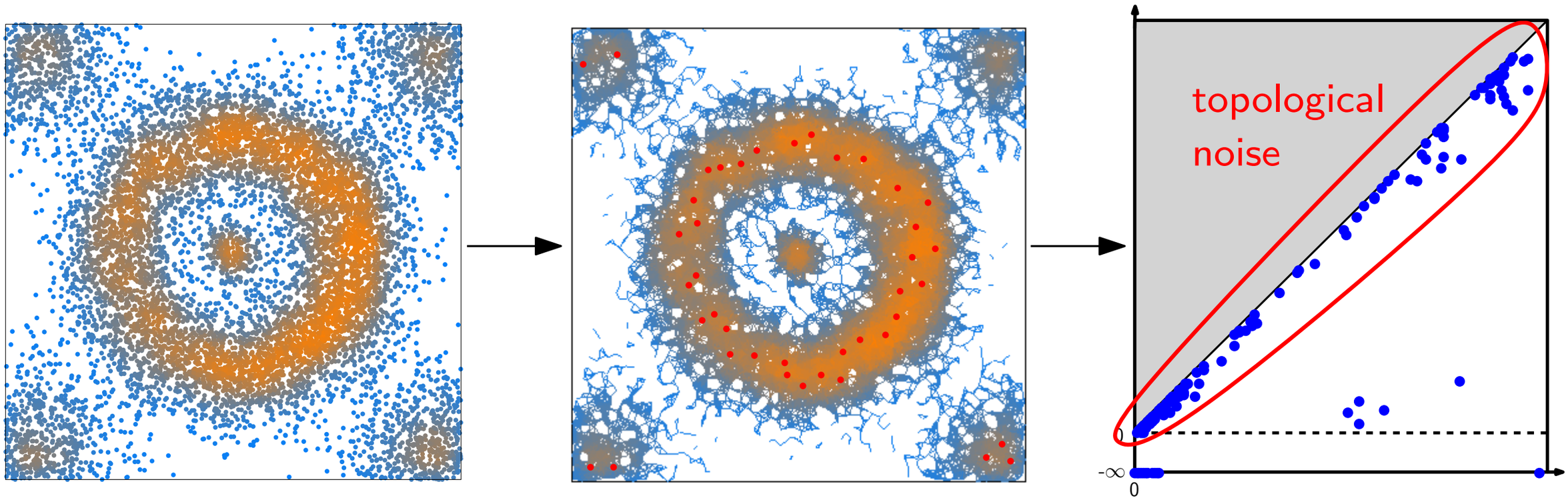
  (apply 0-dimensional persistence algorithm $\rightarrow$ union-find data structure)



Estimating the correct number of clusters

- Density estimator $\hat{f}$ defines an order on the point cloud

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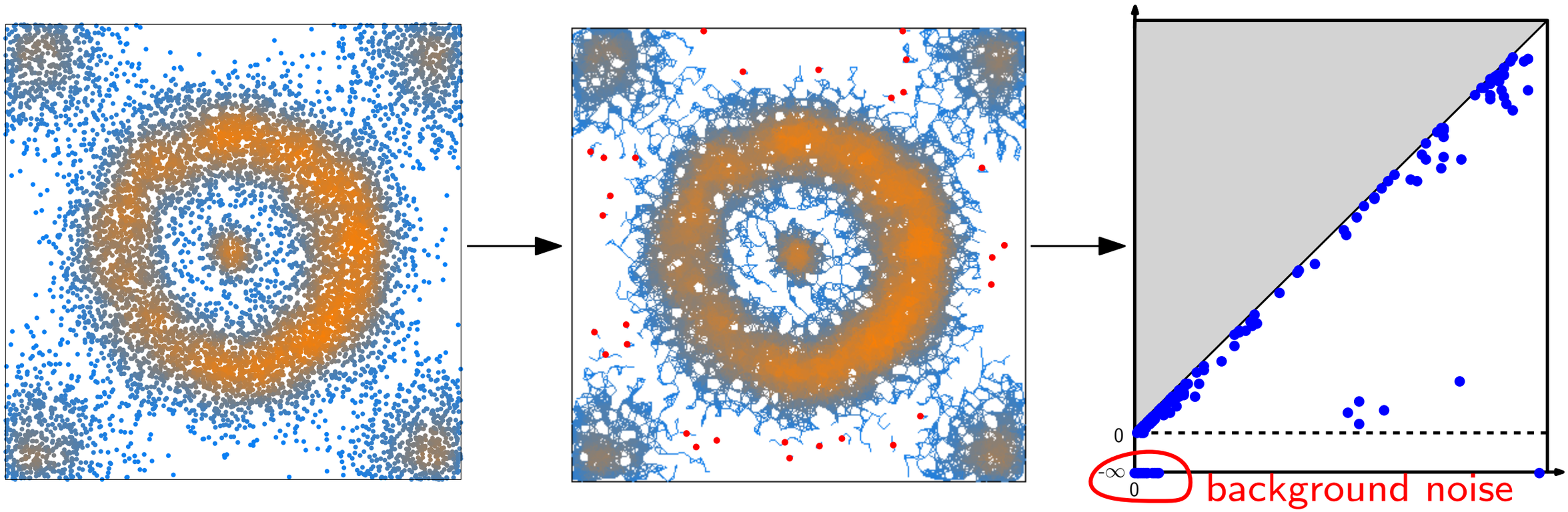

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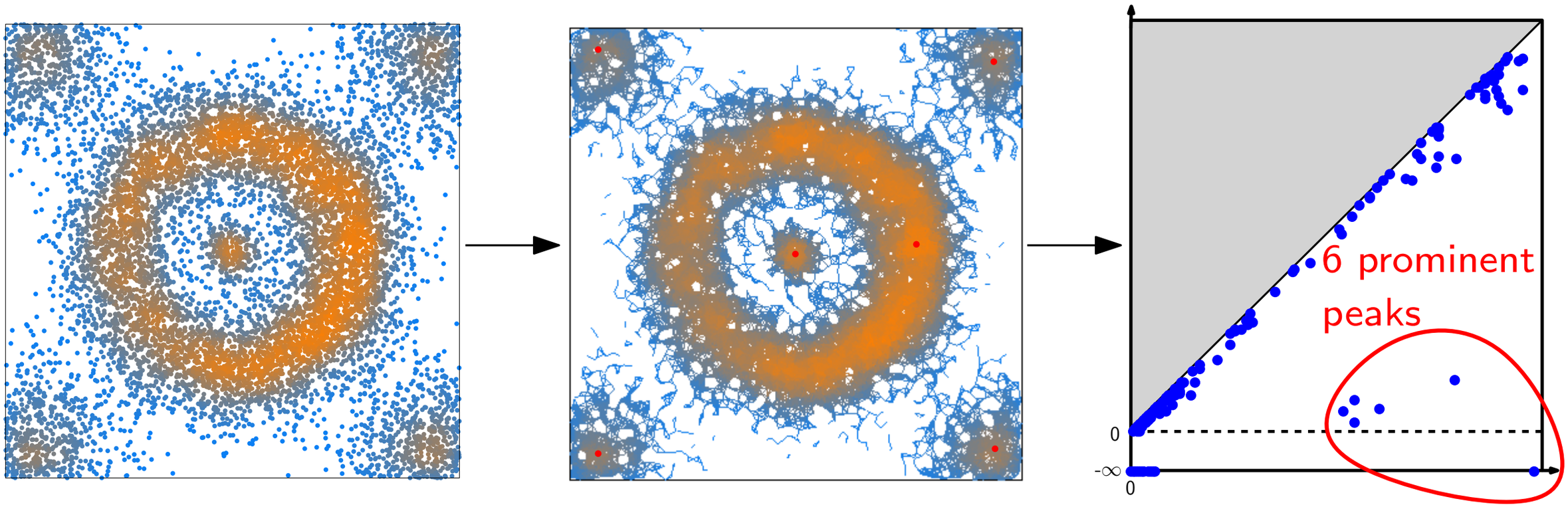

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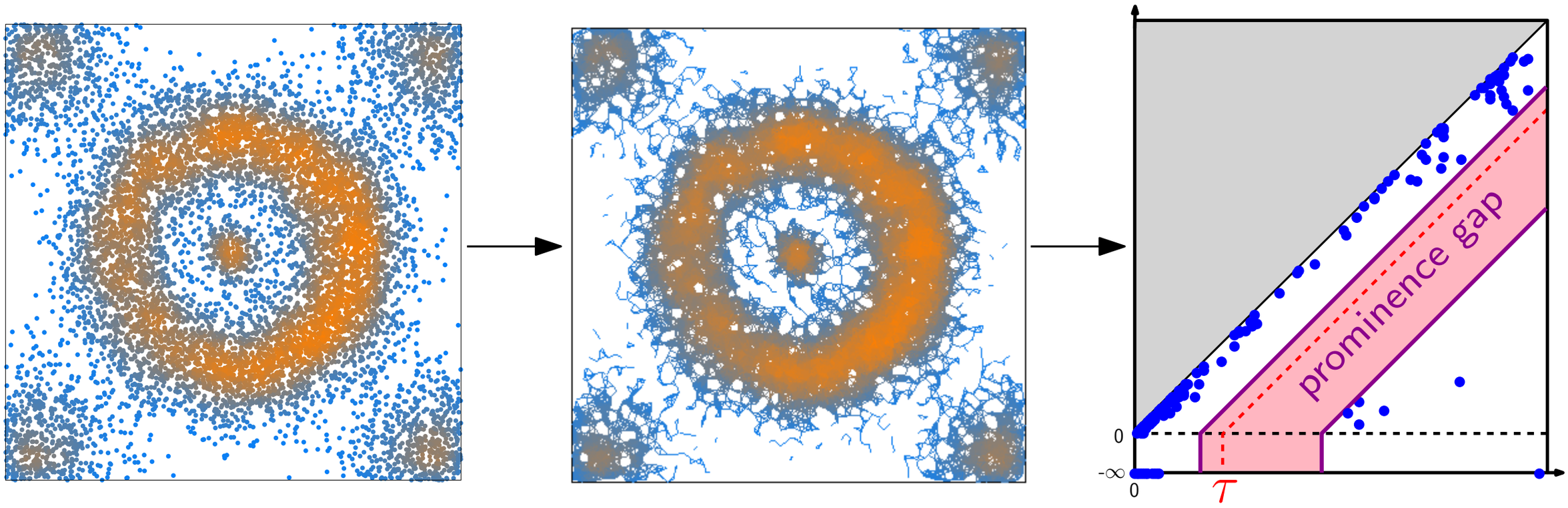

Estimating the correct number of clusters

Hypotheses:

- $f : \mathbb{R}^d \to \mathbb{R}$ a c-Lipschitz probability density function,
- $P \subset \mathbb{R}^d$ a finite set of n points 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 $1 - e^{-\Omega(n)}$.

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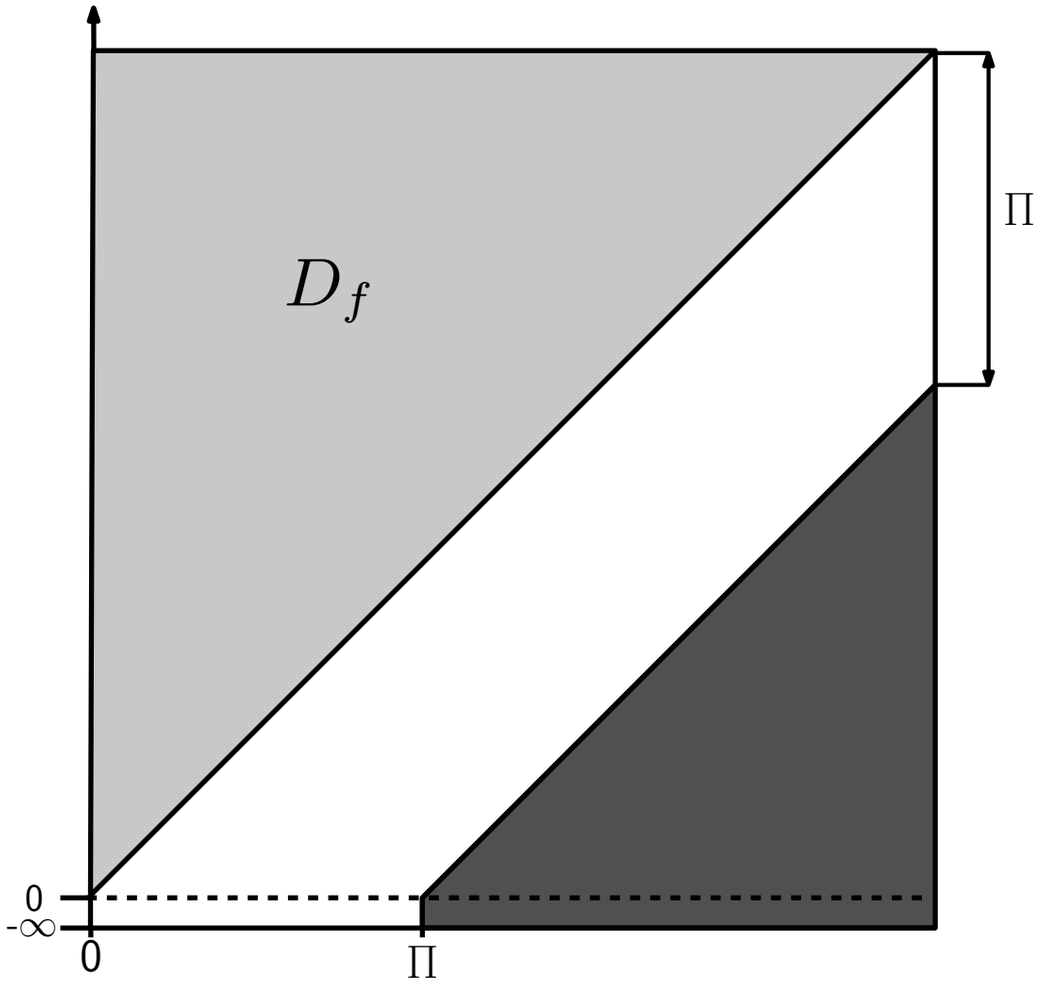

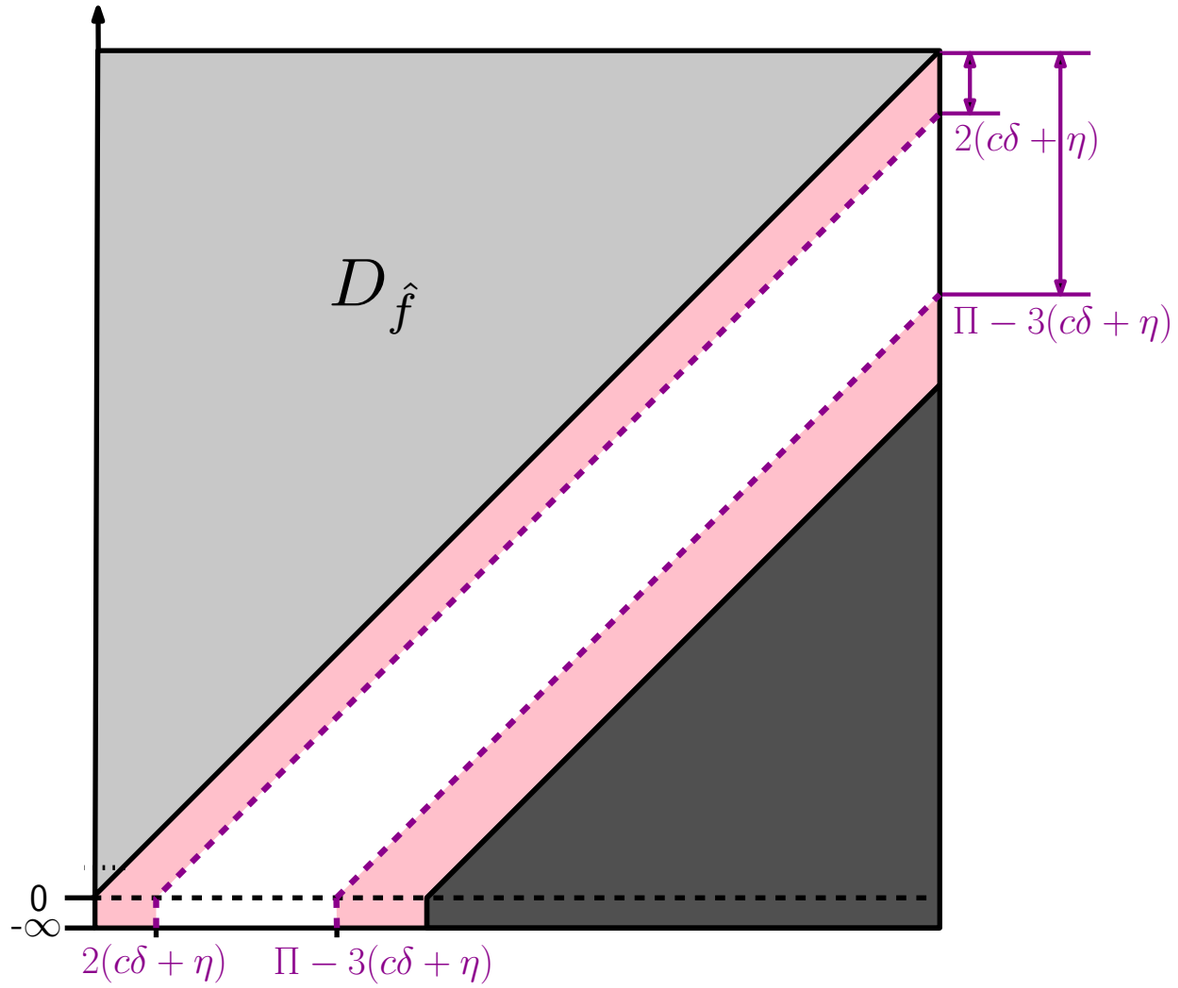

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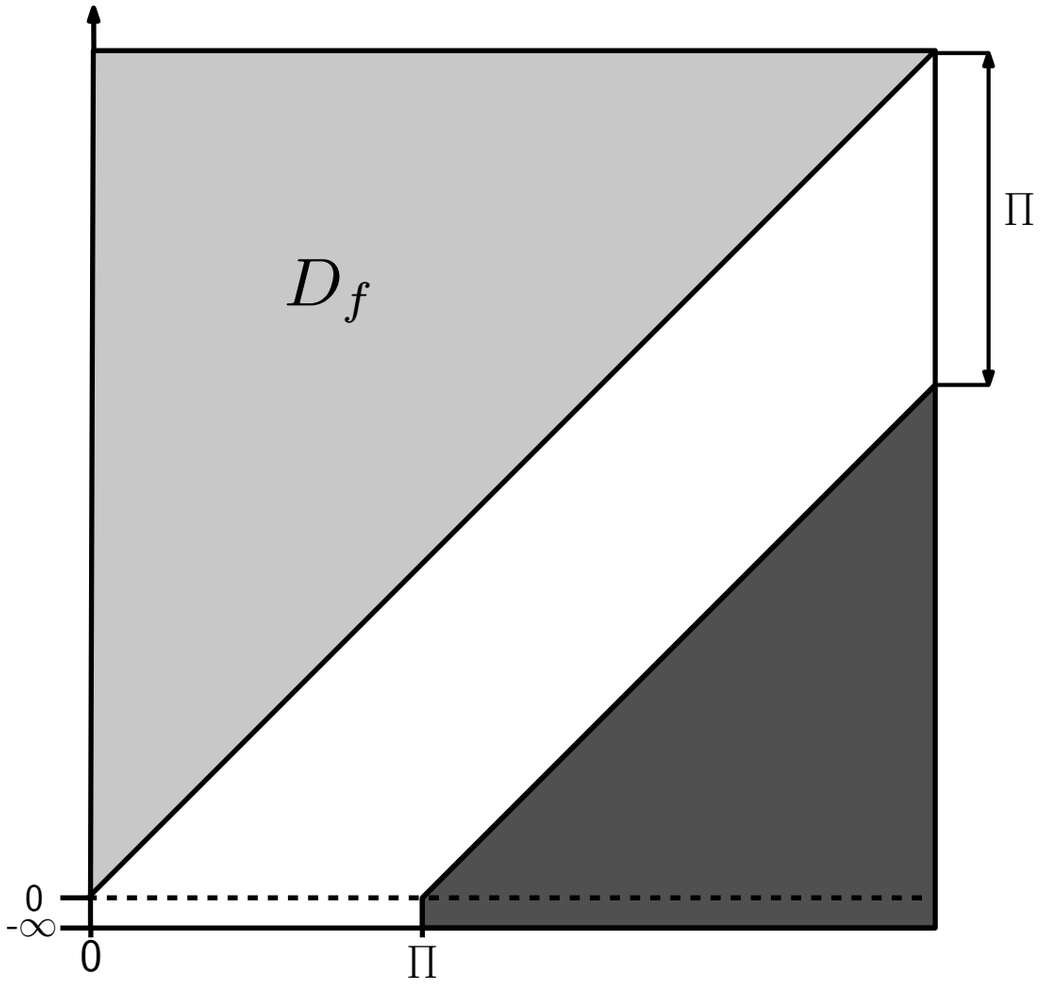
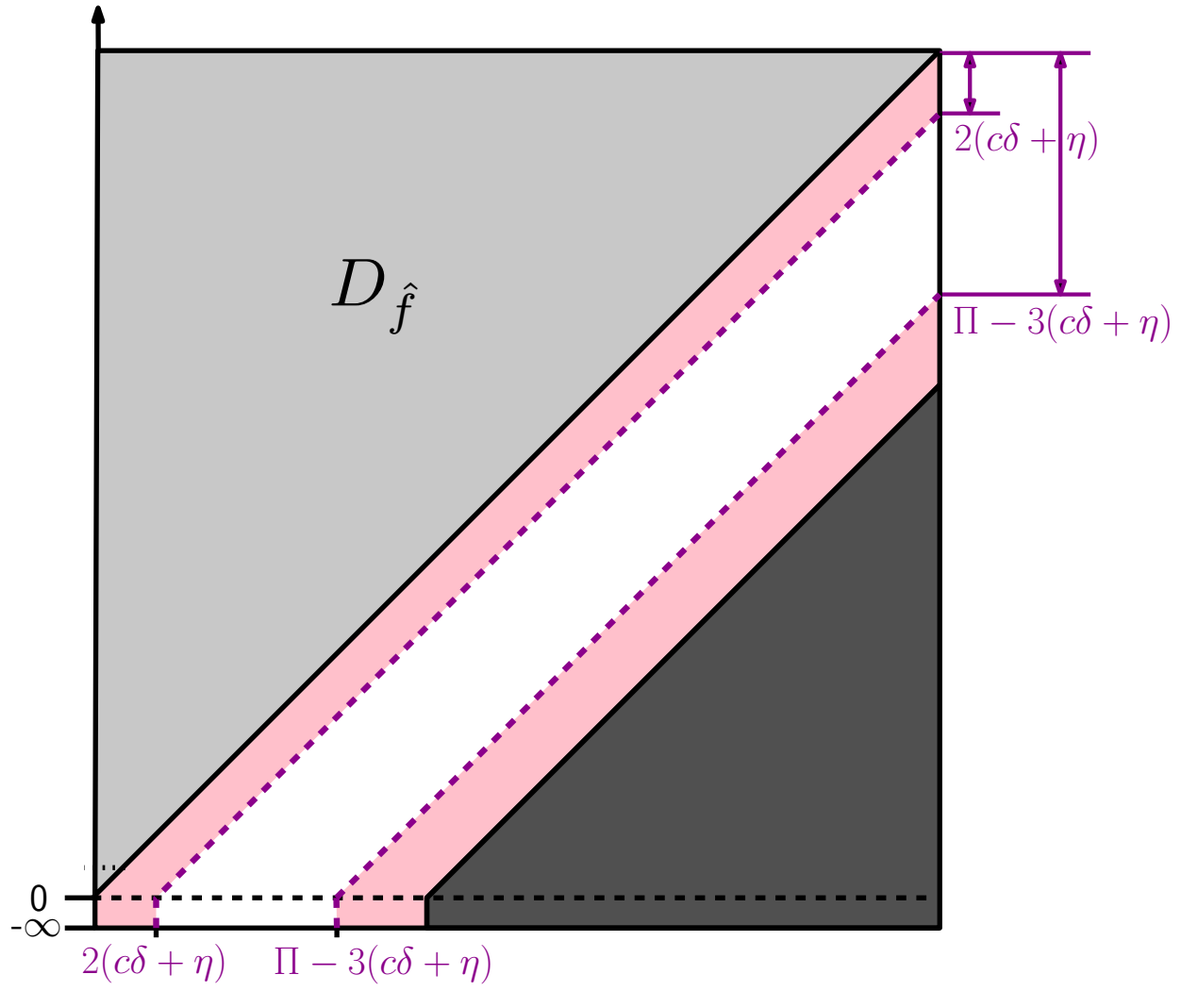
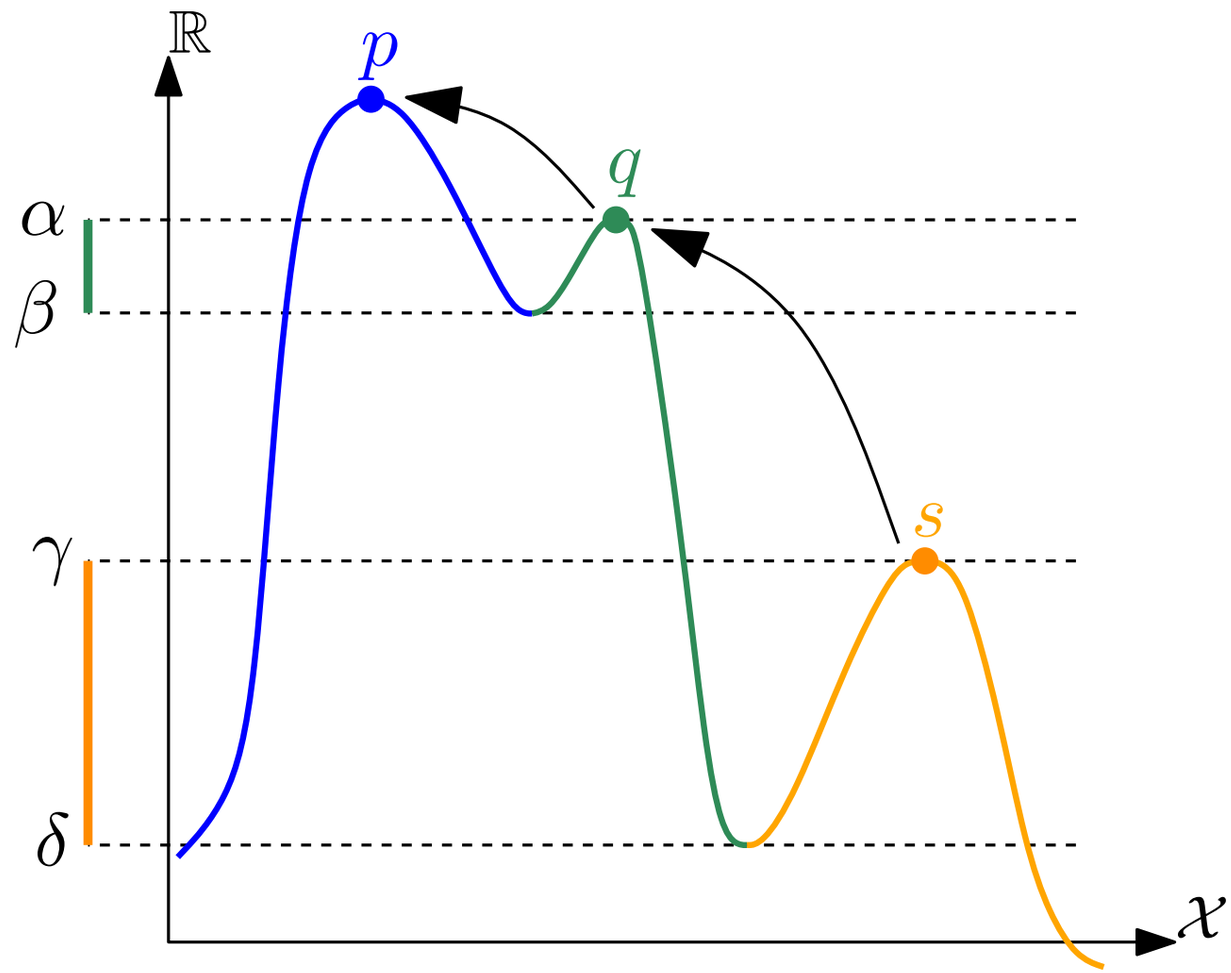




Proof's main ingredient: stability theorem for persistence diagrams

Merging clusters

- degree-0 persistence algo. builds a hierarchy of the peaks of $\hat{f}$ (merge tree)
- merge clusters according to the hierarchy (merge each cluster into its parent)



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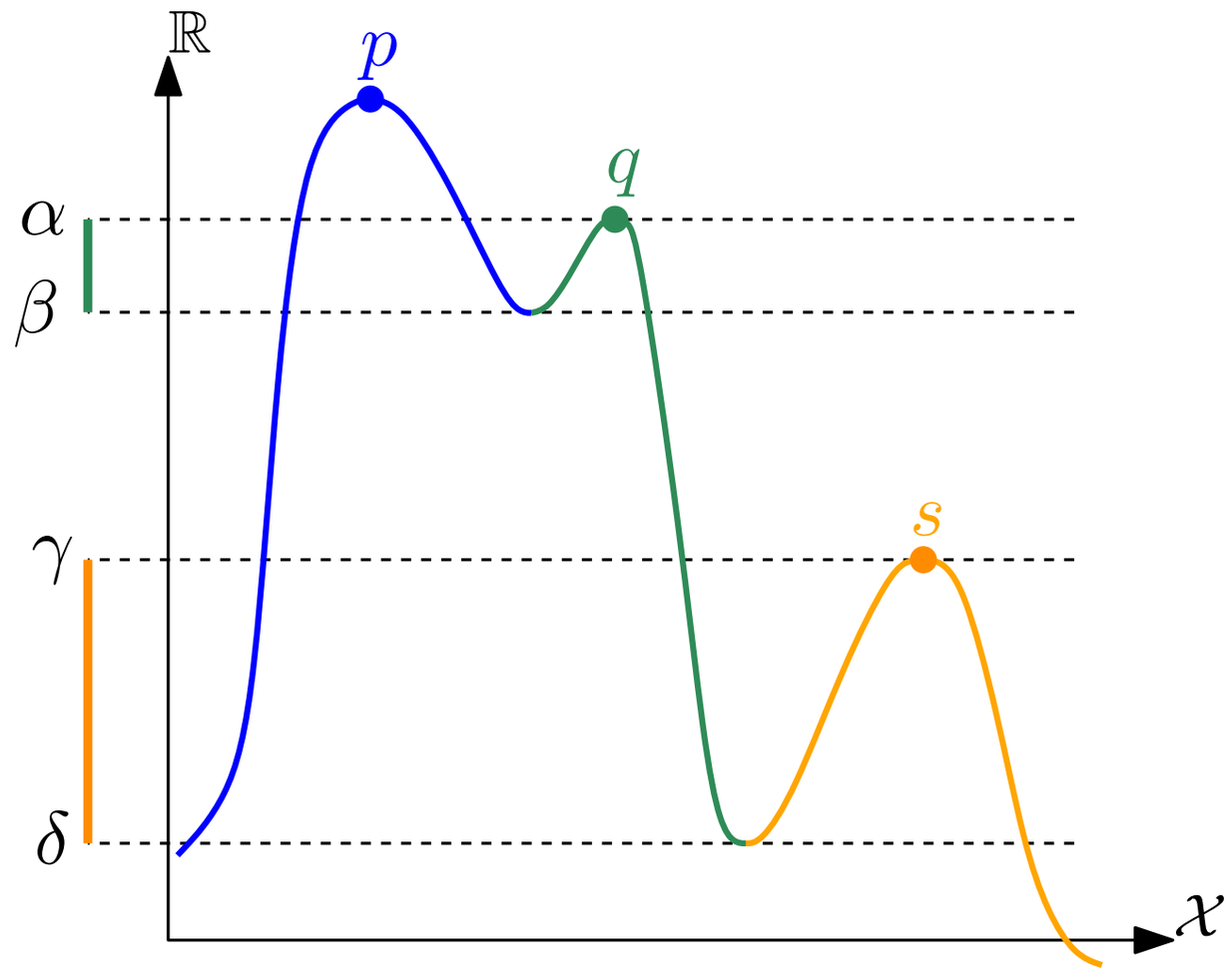
- given a fixed threshold $\tau \geq 0$, only merge those clusters of prominence $< \tau$

$$0 \leq \tau \leq \alpha - \beta$$



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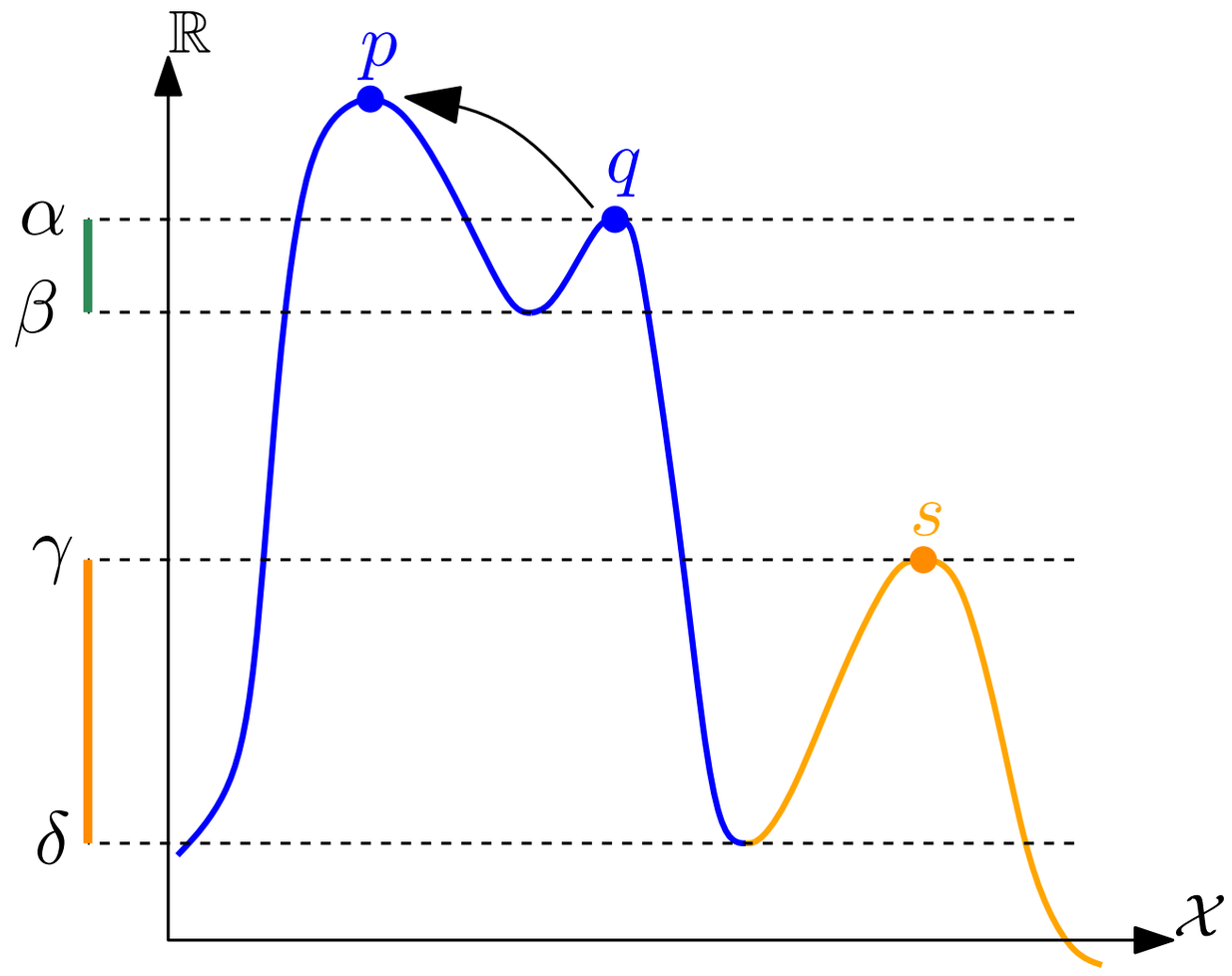
$$\alpha - \beta < \tau \leq \gamma - \delta$$



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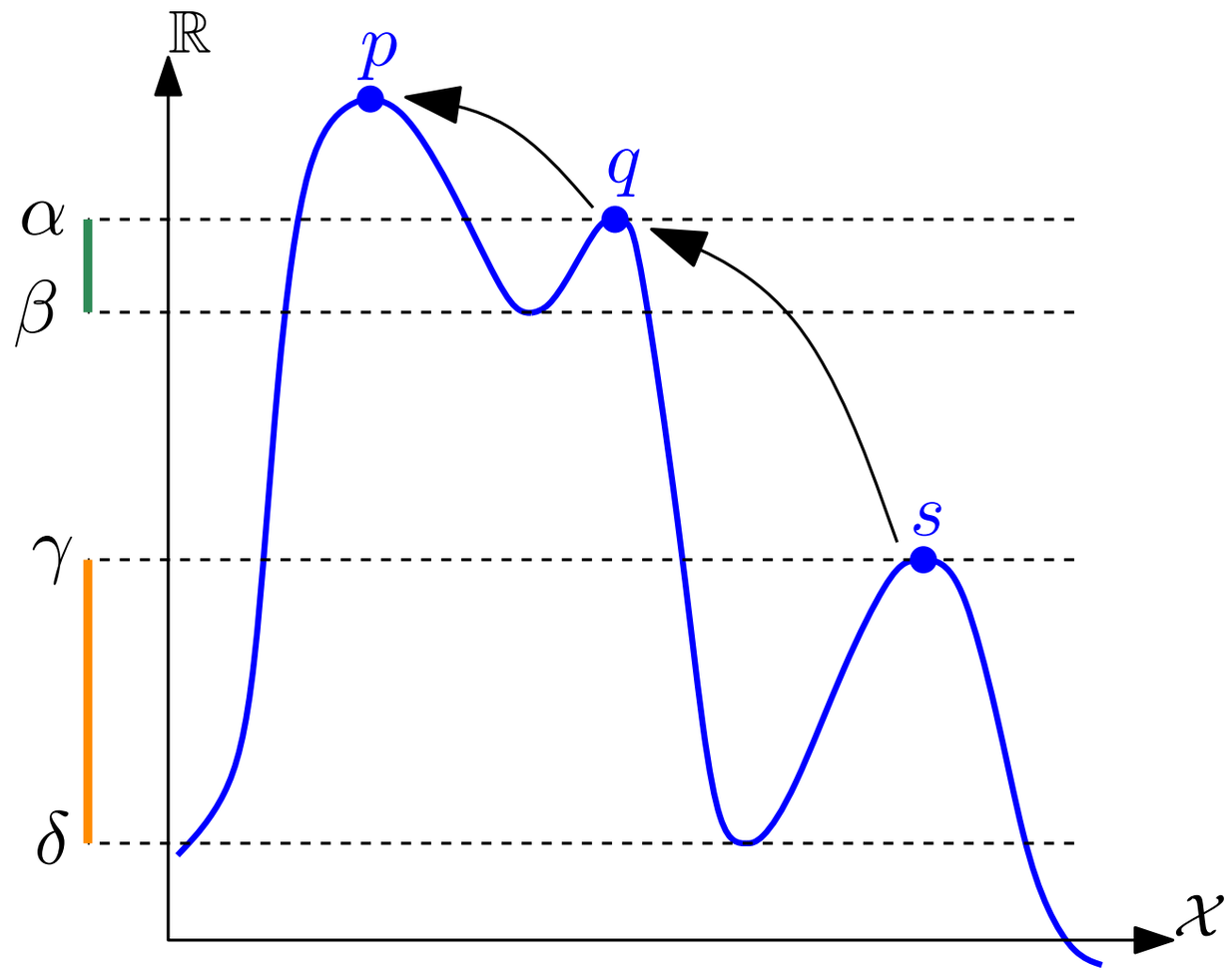


Pseudo-code

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

Sort the vertex indices $\{1, 2, \ldots, n\}$ 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: $\mathcal{U}.\texttt{MakeSet}(i)$;
        $r(e) \leftarrow i$ *// $r(e)$ stores the root vertex associated with the entry e*
    else *// vertex i is not a peak of $\hat{f}$ within G*
        $g(i) \leftarrow \operatorname{argmax}_{j \in \mathcal{N}} \hat{f}(j)$ *// $g(i)$ stores the approximate gradient at vertex i*
        $e_i \leftarrow \mathcal{U}.\texttt{Find}(g(i))$;
        Attach vertex i to the entry e_i: $\mathcal{U}.\texttt{Union}(i, e_i)$;
    for $j \in \mathcal{N}$ **do**
        $e \leftarrow \mathcal{U}.\texttt{Find}(j)$;
        if $e \neq e_i$ and $\min\{\hat{f}(r(e)),\ \hat{f}(r(e_i))\} < \hat{f}(i) + \tau$
            $\mathcal{U}.\texttt{Union}(e,\ e_i)$;
            $r(e \cup e_i) \leftarrow \operatorname{argmax}_{\{r(e),\ r(e_i)\}} \hat{f}$;
            $e_i \leftarrow e \cup e_i$;

graph-based hill-climbing (1976)

cluster merges with persistence (2013)

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

Complexity

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

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

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.

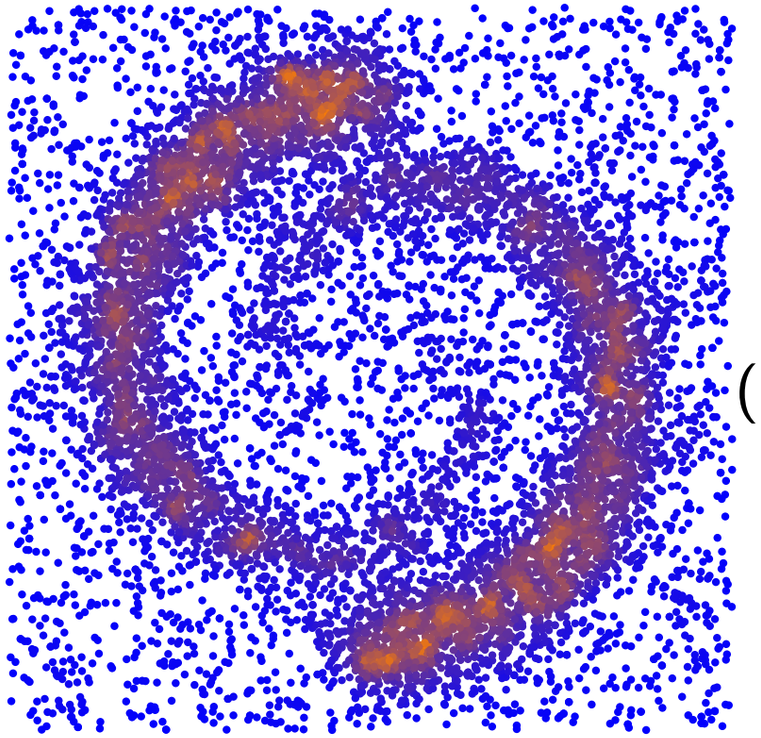
$\rightarrow$ Running time: $O(n \log n + (n + m)\alpha(n))$

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

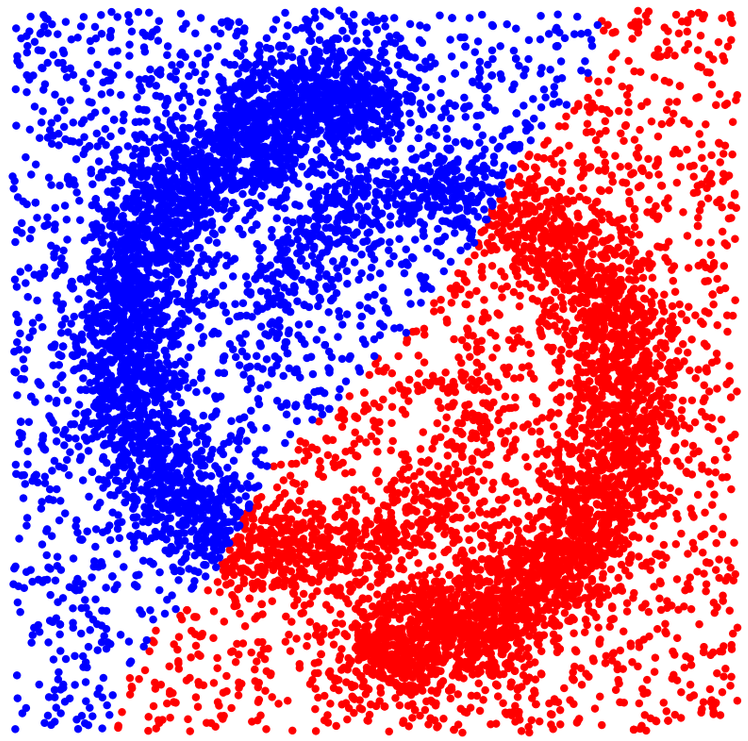
$\rightarrow$ Main memory usage: $O(n)$

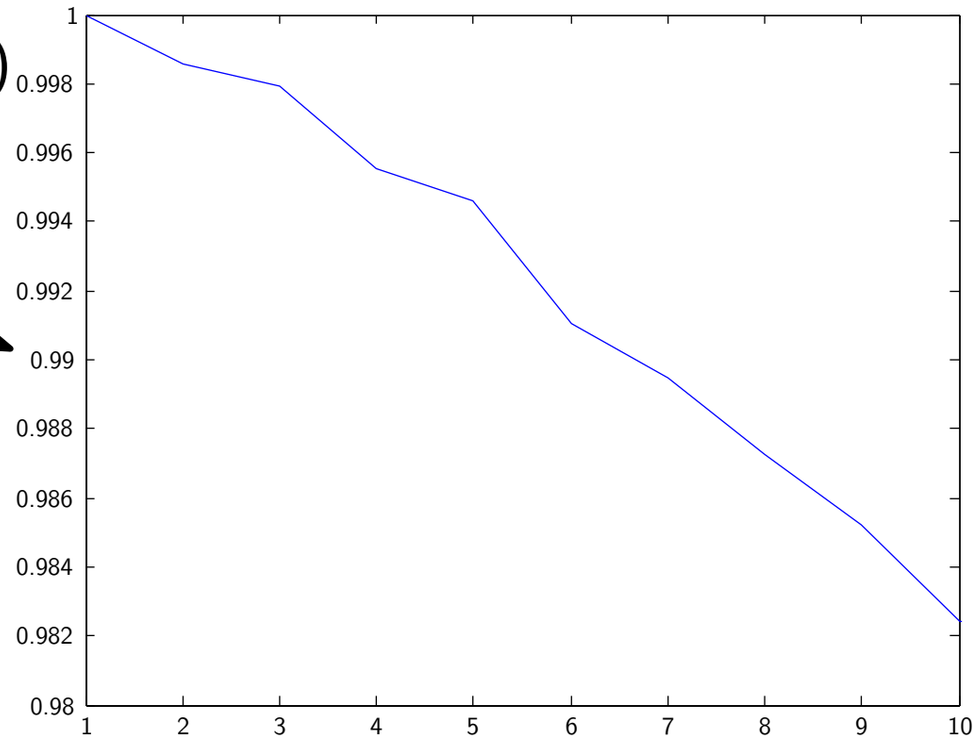
Experimental results

Synthetic Data



Spectral clustering
(k-means in eigenspace)





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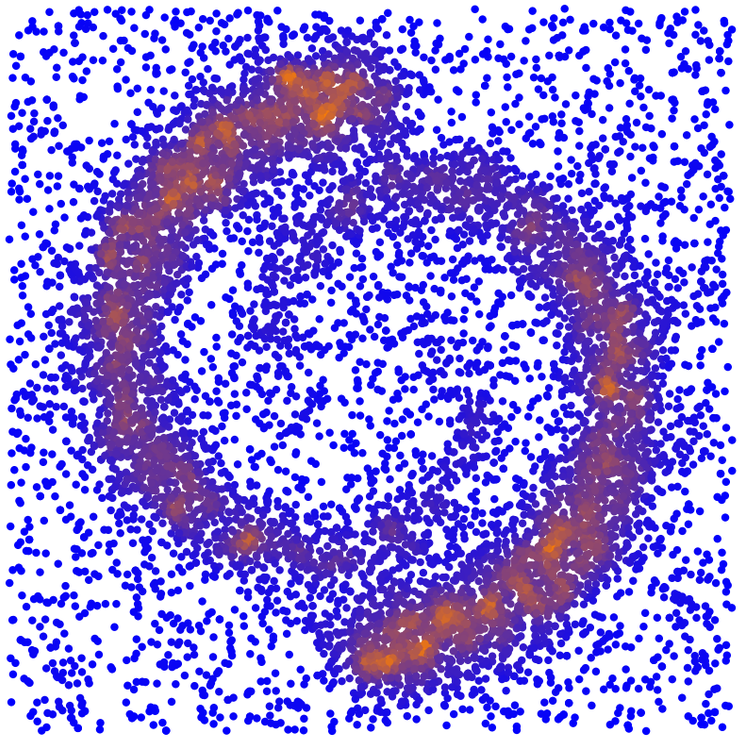
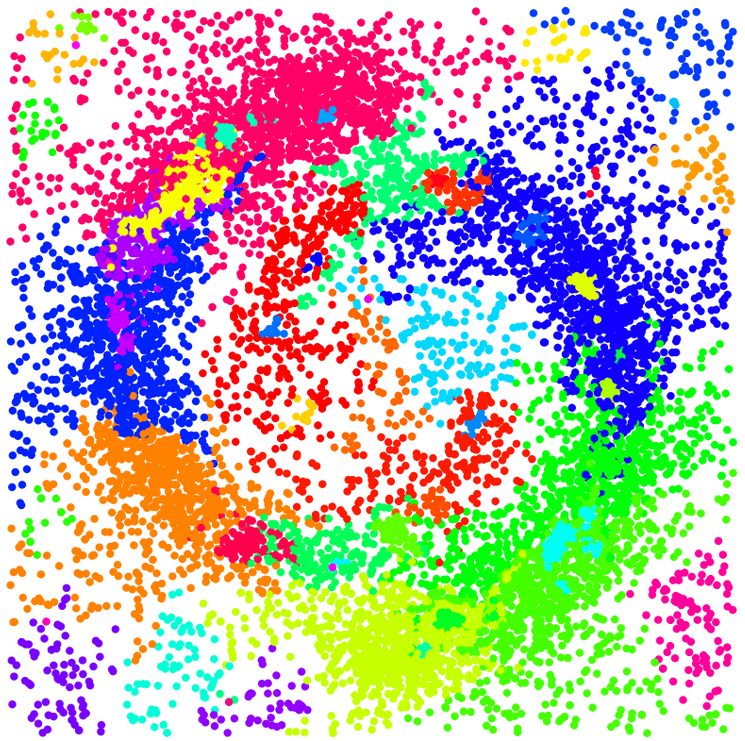
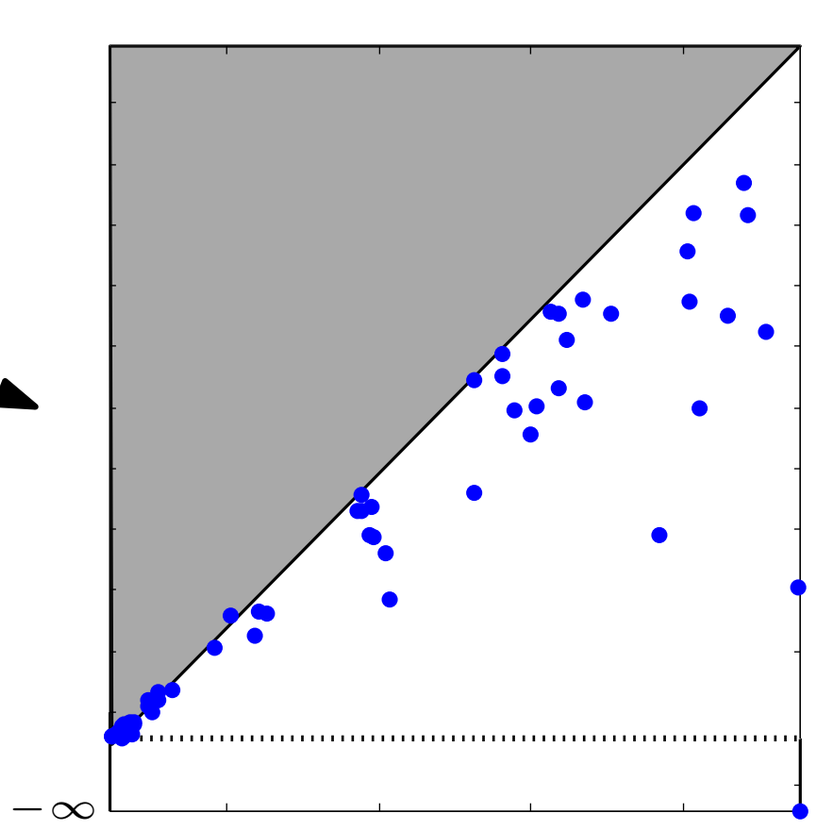


$\tau = 0$

ToMATo





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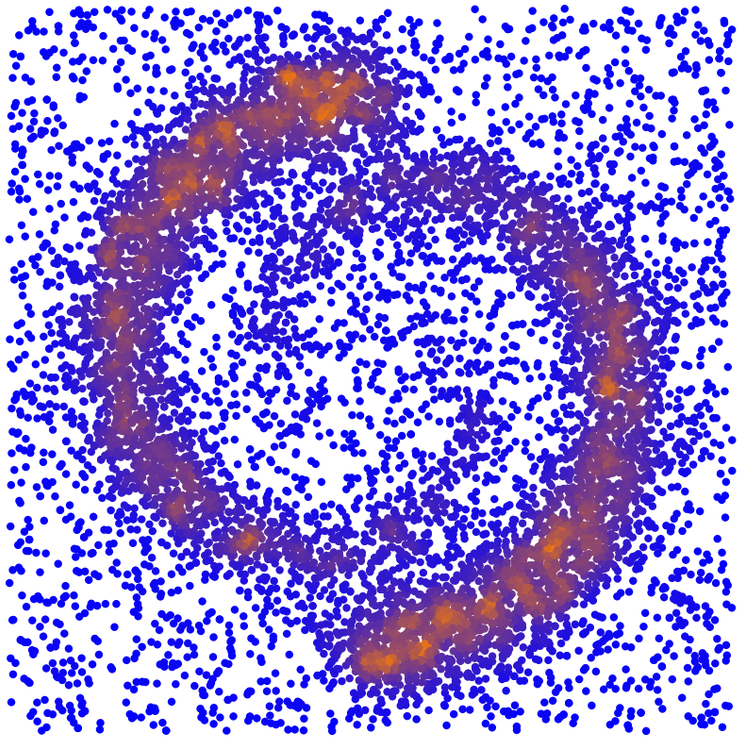

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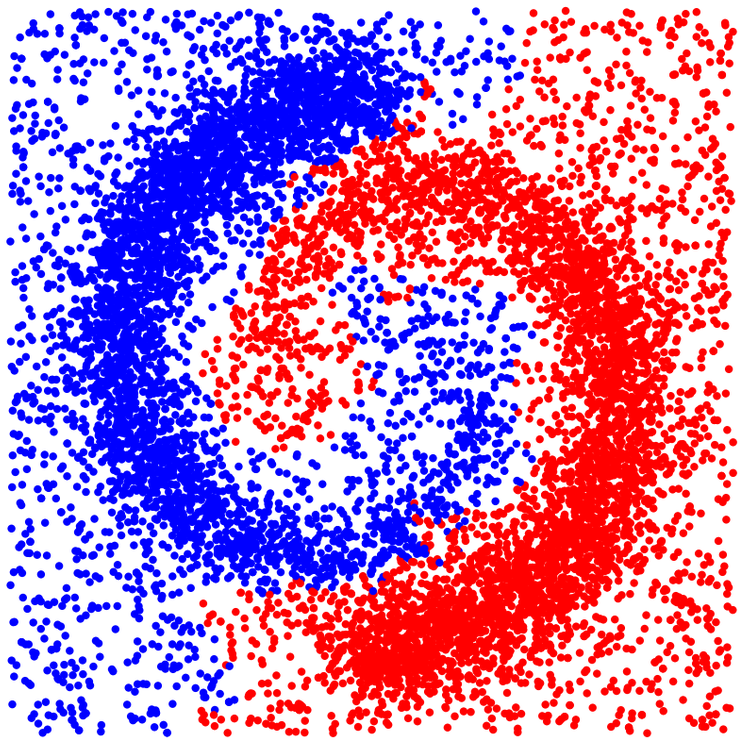

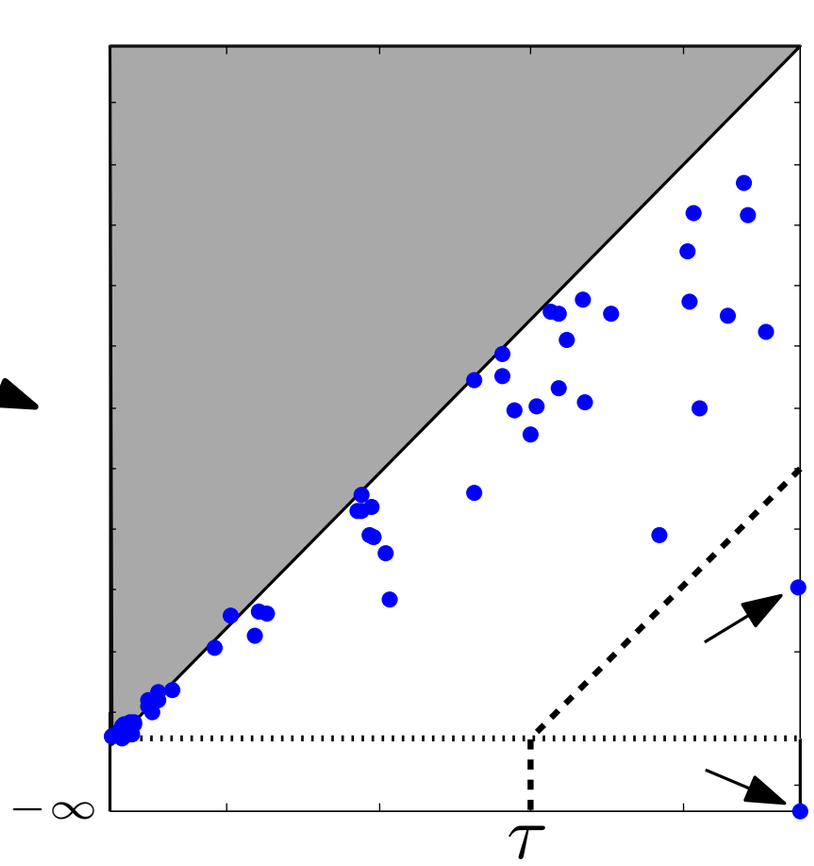

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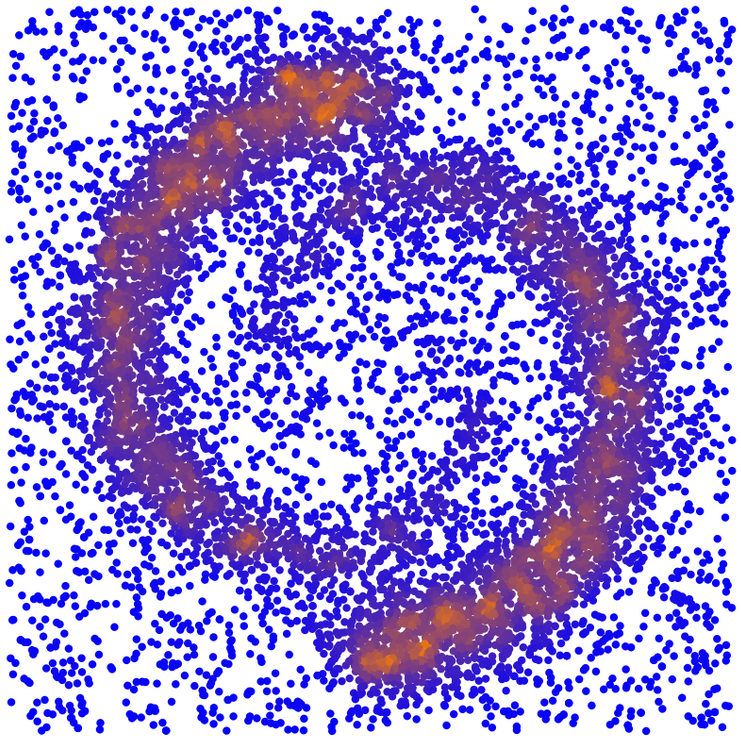
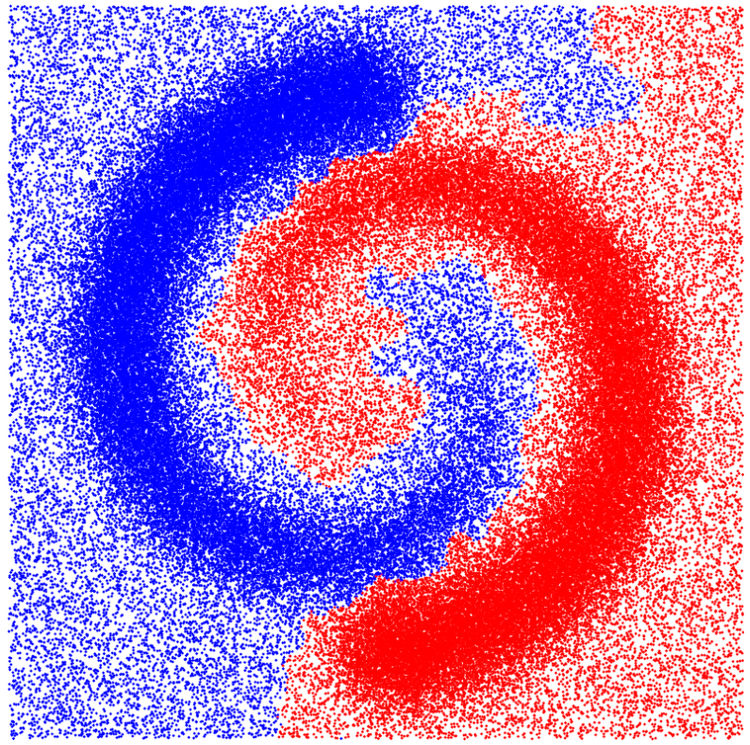
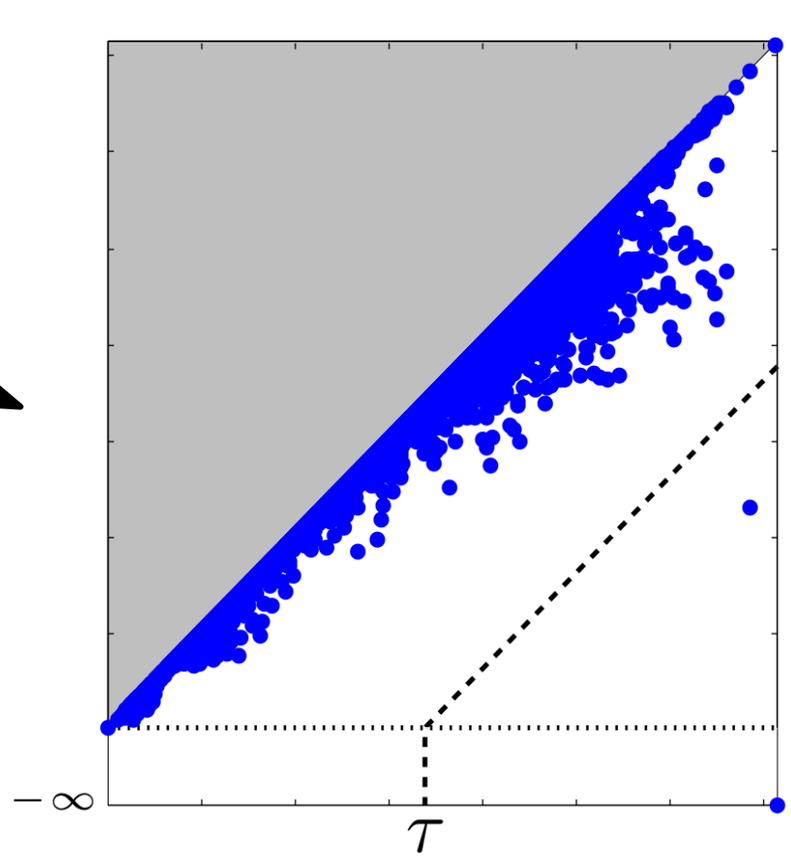




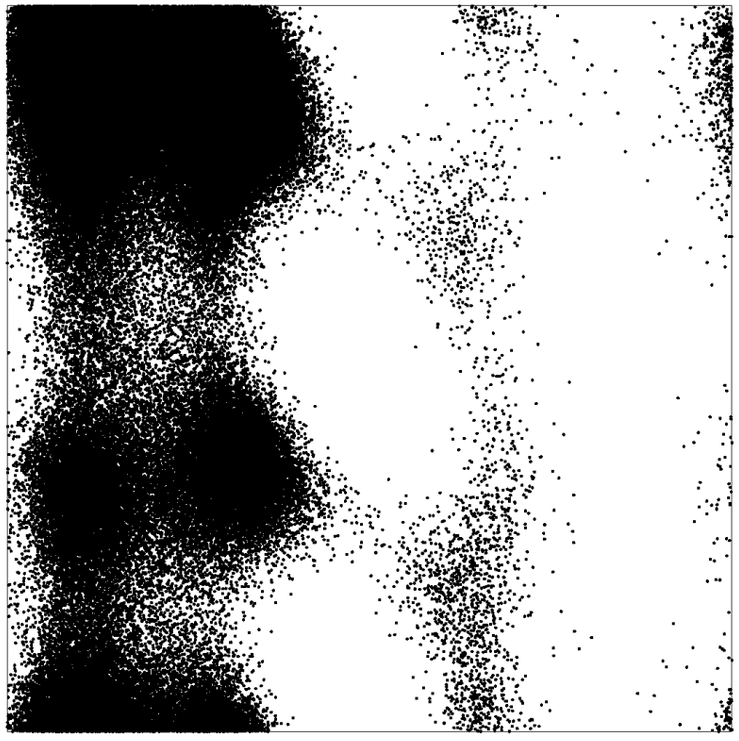


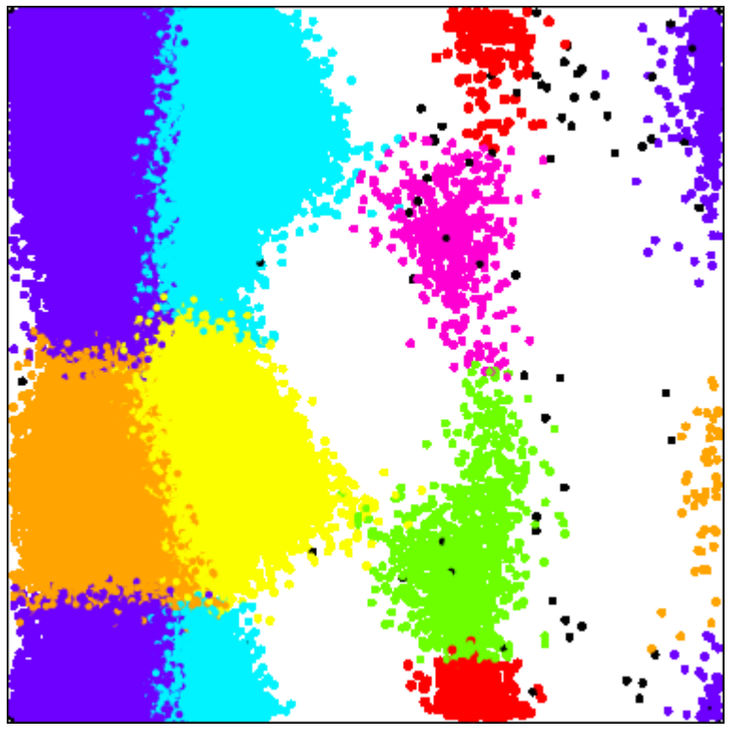
Experimental results

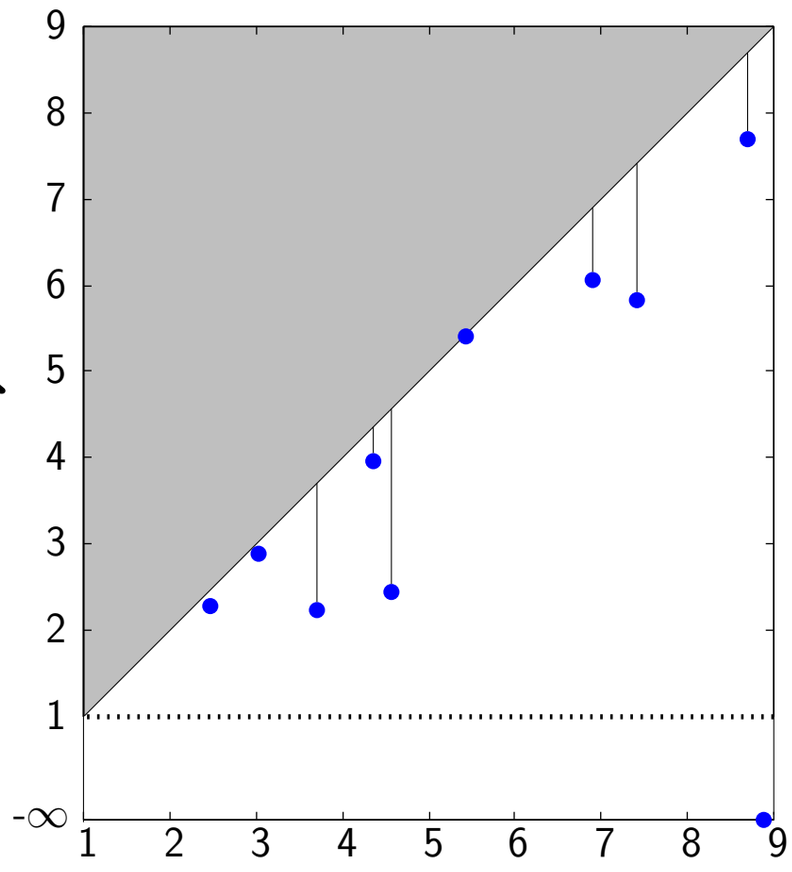
Biological Data

Alanine-Dipeptide conformations ($\mathbb{R}^{21}$)

RMSD distance (non-Euclidean)







Common belief: 6 metastable states

PD shows anywhere between 4 and 7 clusters

Experimental results

[*Topological methods for exploring low-density states in biomolecular folding pathways*, Yao, Sun, Huang, Bowman, Singh, Lesnick, Guibas, Pande, Carlsson, J. Chem. Phys., 2009]

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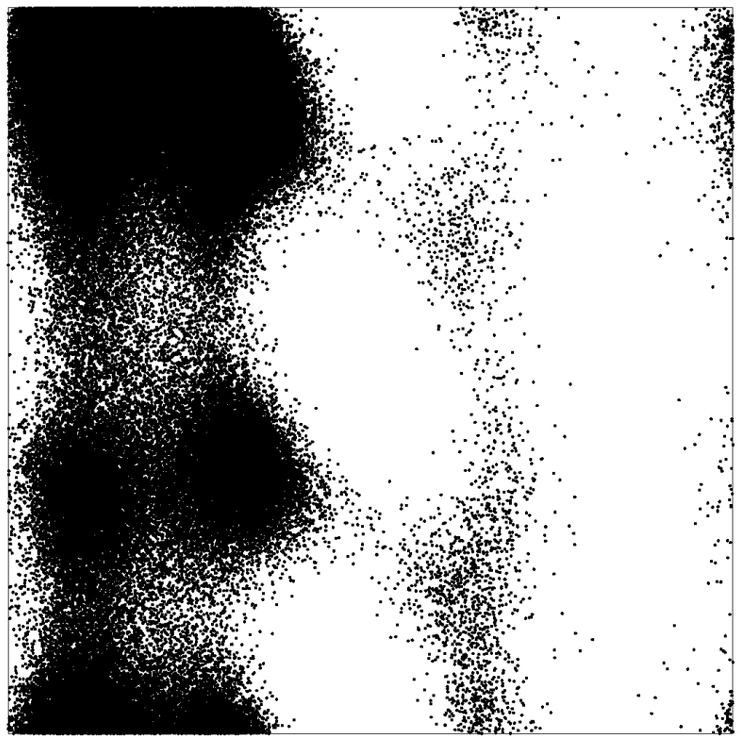
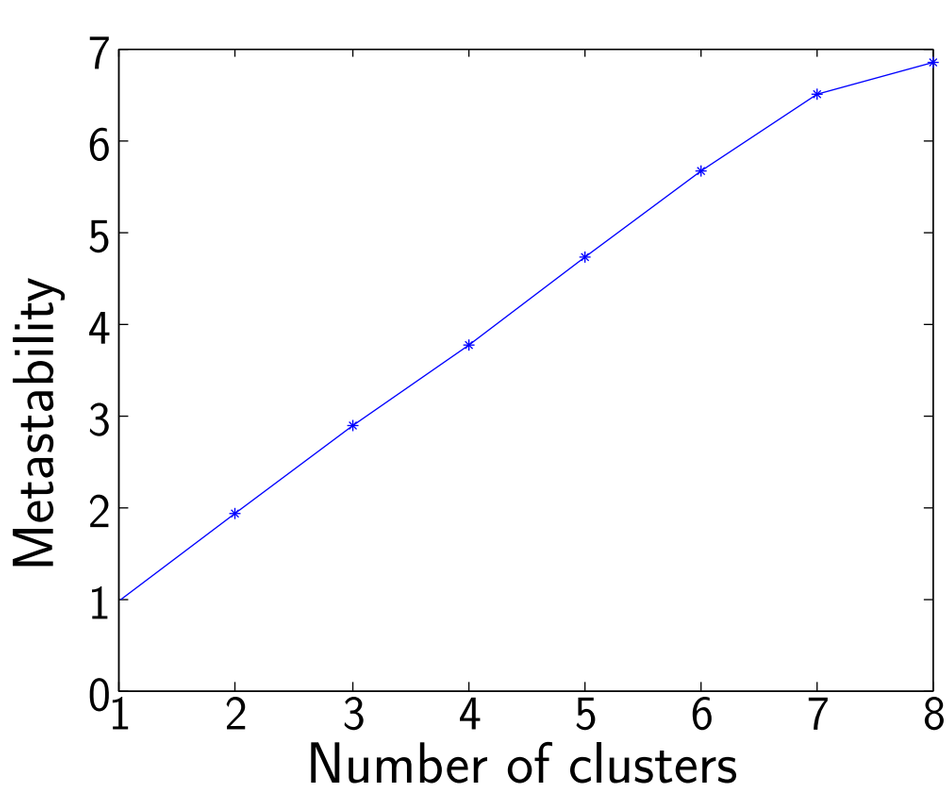


Rank	Prominence	Metastability
1	$+\infty$	0.99982
2	3827	1.91865
3	1334	2.8813
4	557	3.76217
5	85	4.73838
6	32	5.65553
7	26	6.50757
8	7.2	6.8193
9	3.0	-
10	2.2	-



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Measures of metastability confirm this insight

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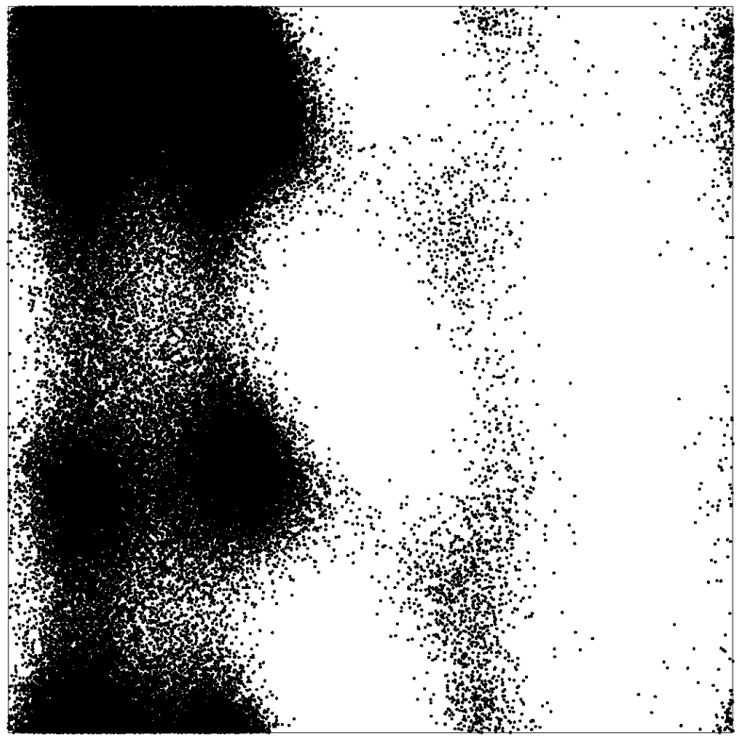


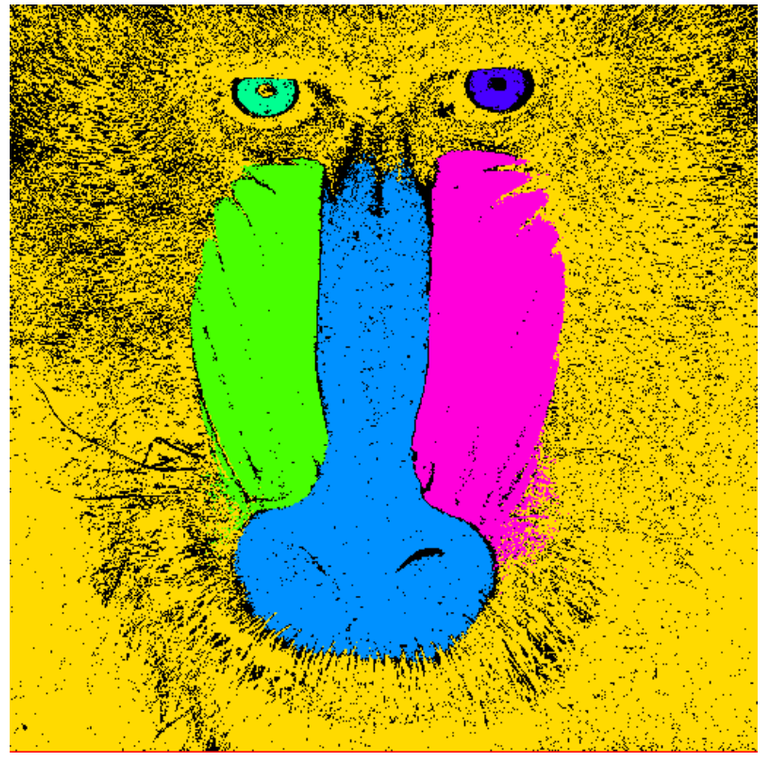
Note: Spectral Clustering takes a week of tweaking, while ToMATo runs out-of-the-box in a few minutes

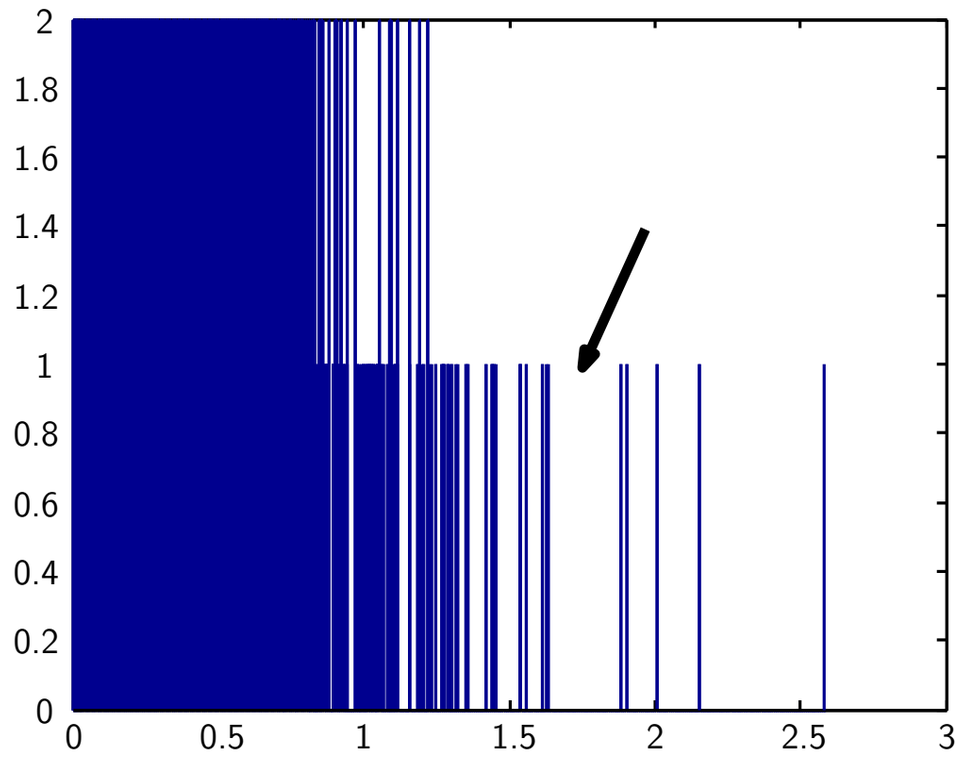
Experimental results

Image Segmentation

Density is estimated in 3D color space (Luv)

Neighborhood graph is built in image domain



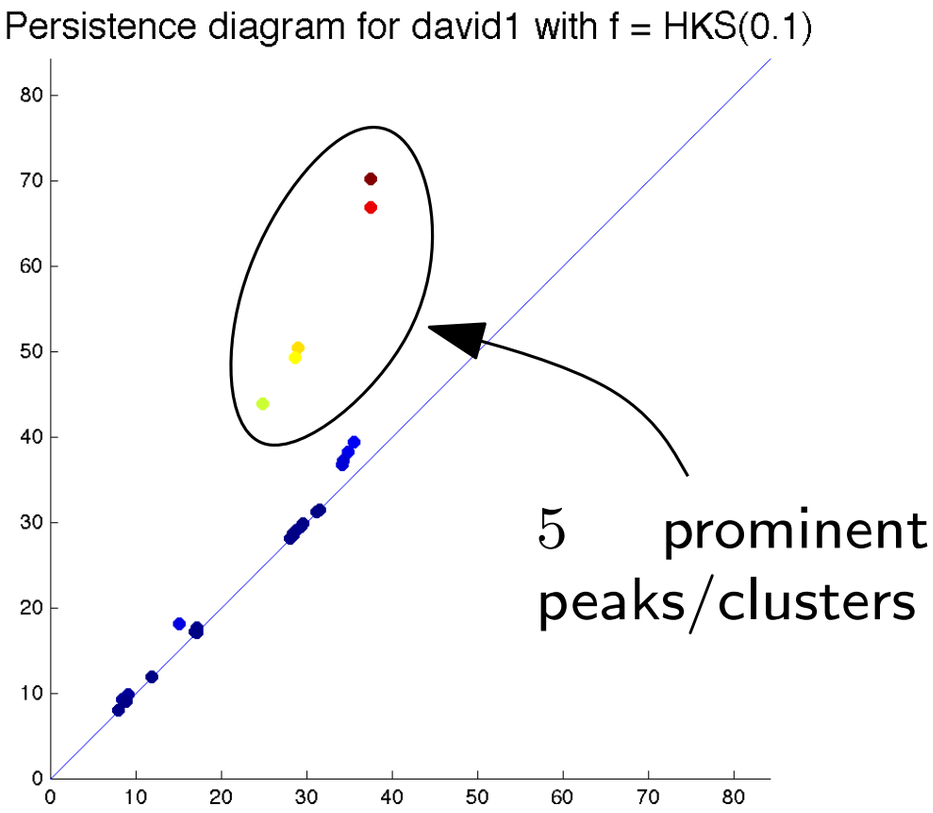


Distribution of prominences does not usually show a clear unique gap

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

Application to non-rigid shape segmentation

[*Persistence-Based Segmentation of Deformable Shapes*, Skraba, Ovsjanikov, Chazal, Guibas, Proc. CVPR 2010]



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

[*Persistence-Based Segmentation of Deformable Shapes*, Skraba, Ovsjanikov, Chazal, Guibas, Proc. CVPR 2010]

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.

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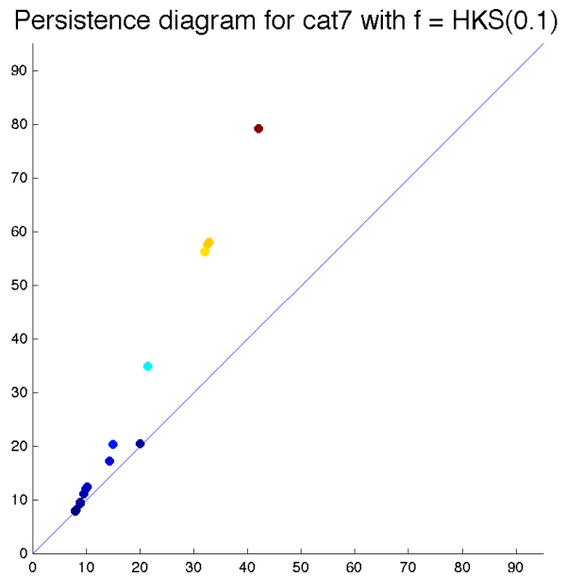
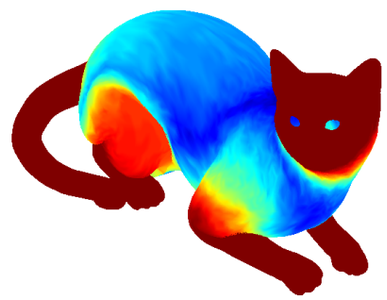
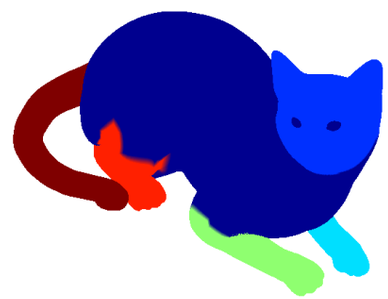
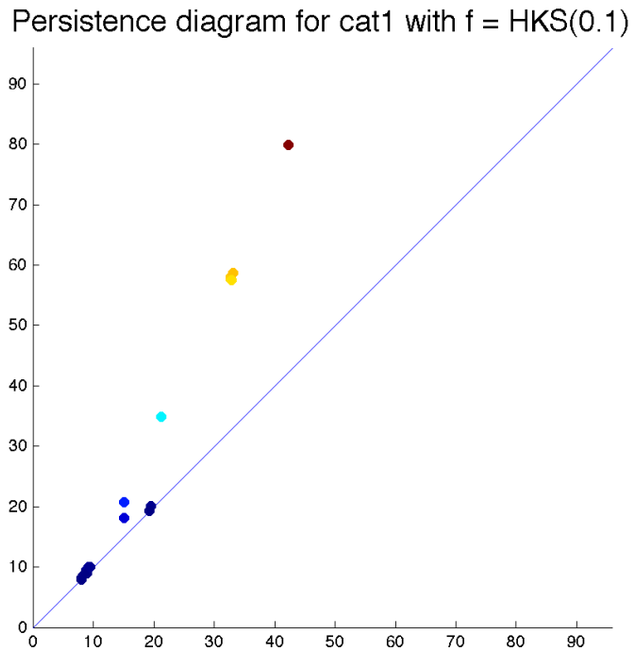
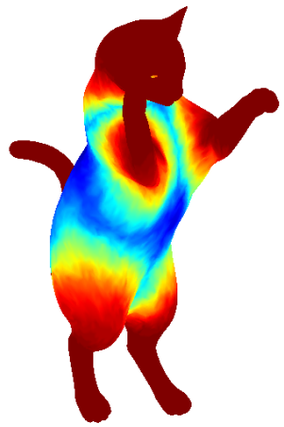








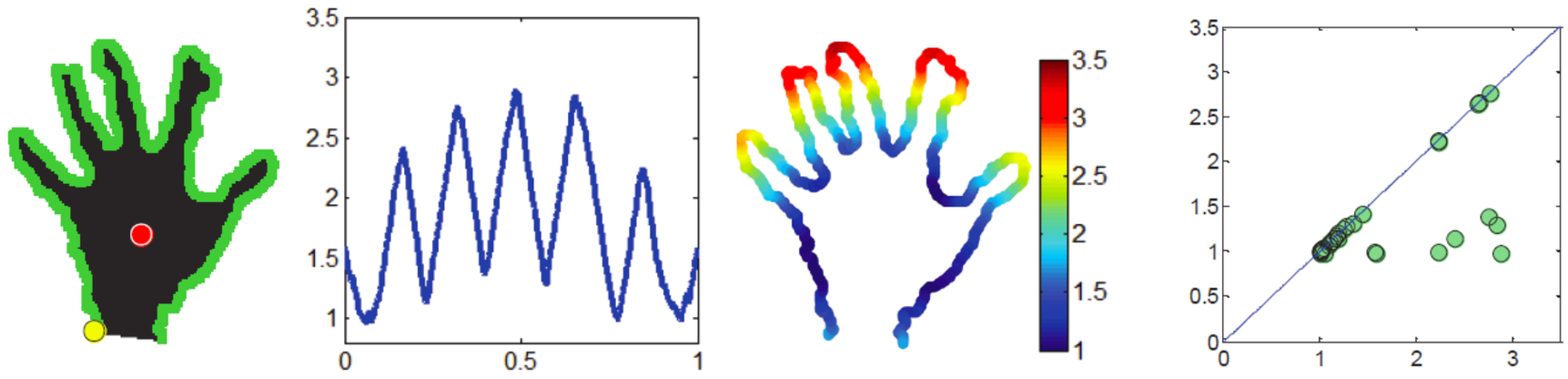


Other applications: classification, object recognition

Examples:

- Hand gesture recognition

[*Persistence-based structural recognition*, Li, Ovsjanikov, Chazal, Proc. CVPR, 2014]



- Persistence-based pooling for shape recognition

[*Persistence-based Pooling for Shape Pose Recognition*, Bonis, Ovsjanikov, Oudot, Chazal, 2015]