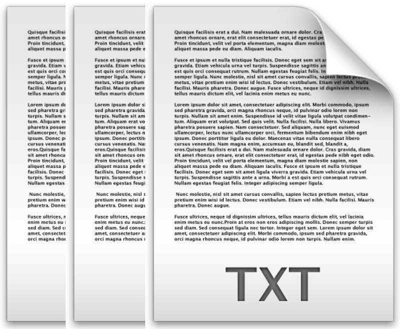
Journée statistique et informatique pour la science des données
IHES, January 2020

The pre-image problem from a topological perspective

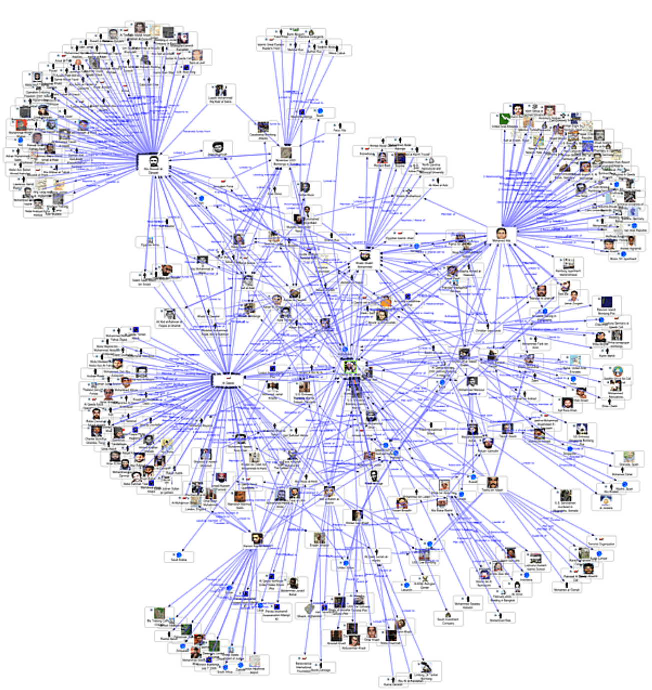
Steve Oudot

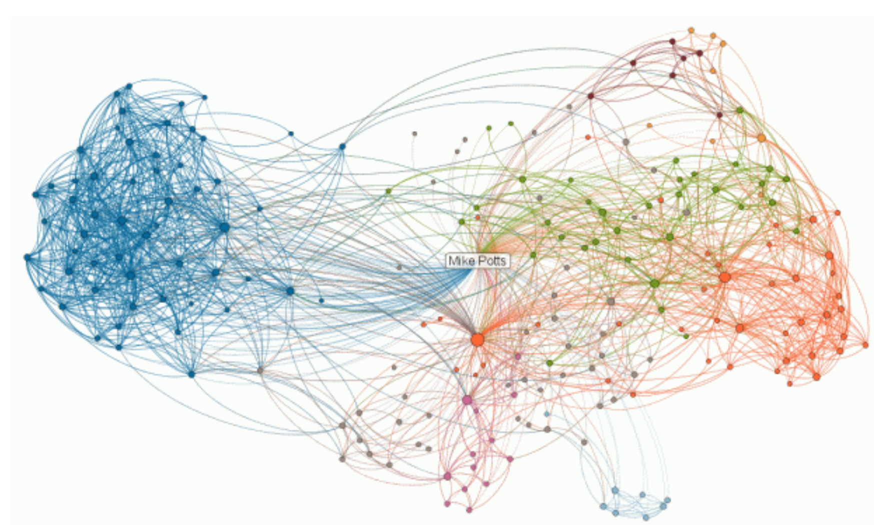
Inria

Preimage problem in data Sciences



Data

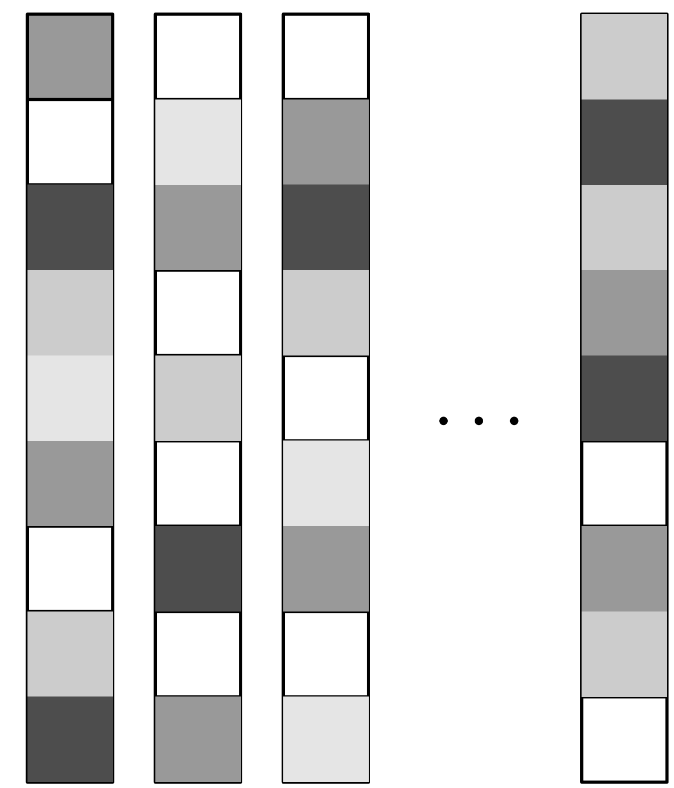




(feature design or learning)

$\Longrightarrow$

Features $\in \mathbb{R}^n$



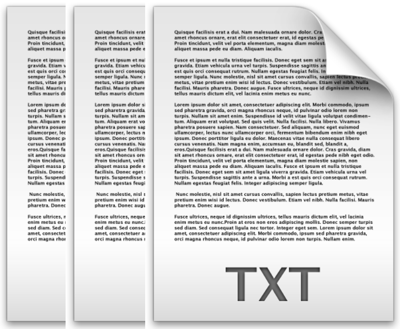
bag of words, word2vec

shape contexts, heat kernels

node2vec, Laplacian fact., rand. walks

dim. reduction, auto-encoders, etc.

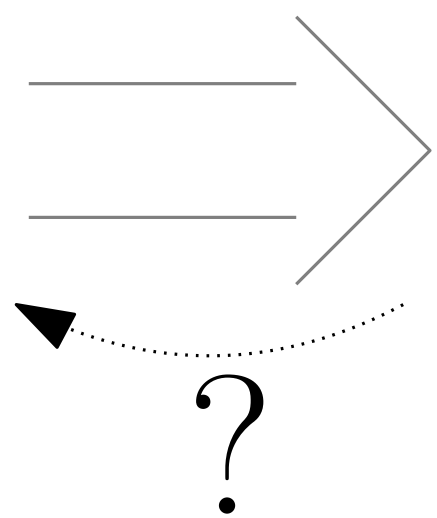
Preimage problem in data Sciences

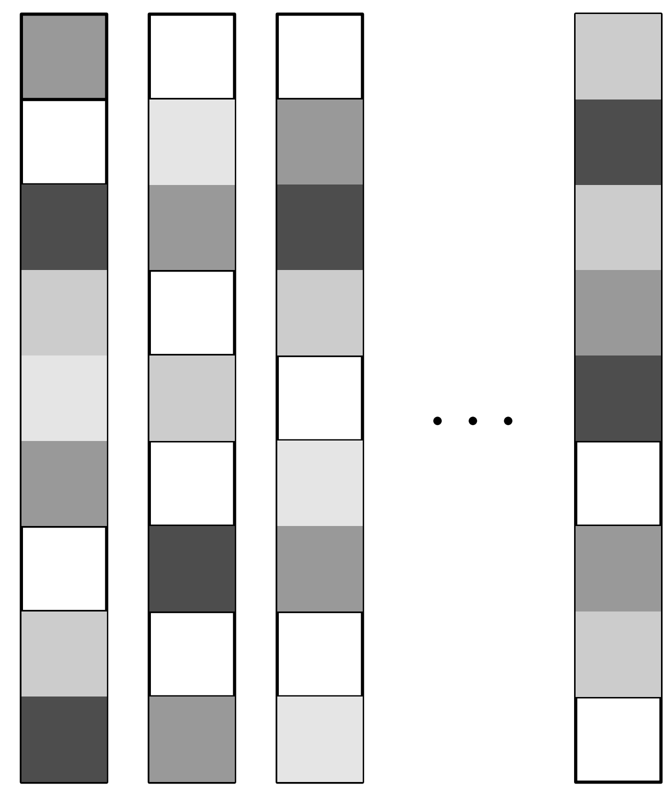


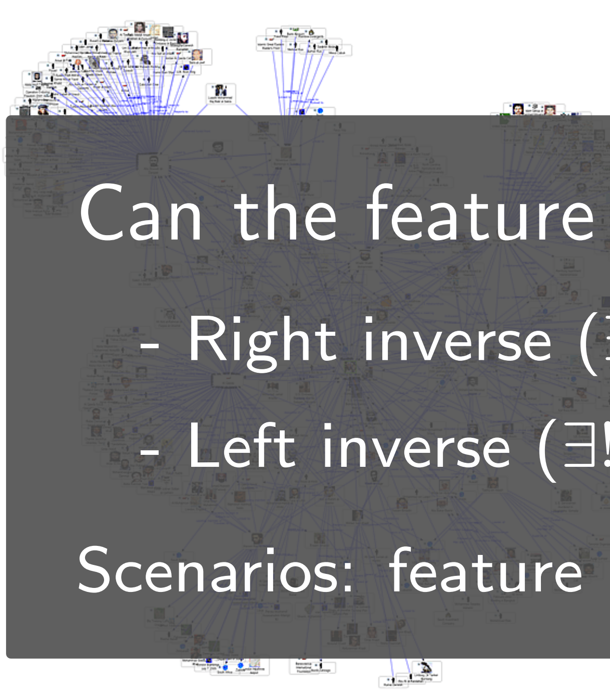
Data

Features $\in \mathbb{R}^n$

(feature design or learning)







Can the feature map be inverted?

- Right inverse ($\exists$ preimage): interpretable AI
- Left inverse ($\exists!$ preimage): reliable interpretation

Scenarios: feature interpretation, deep learning, inverse problems, etc.

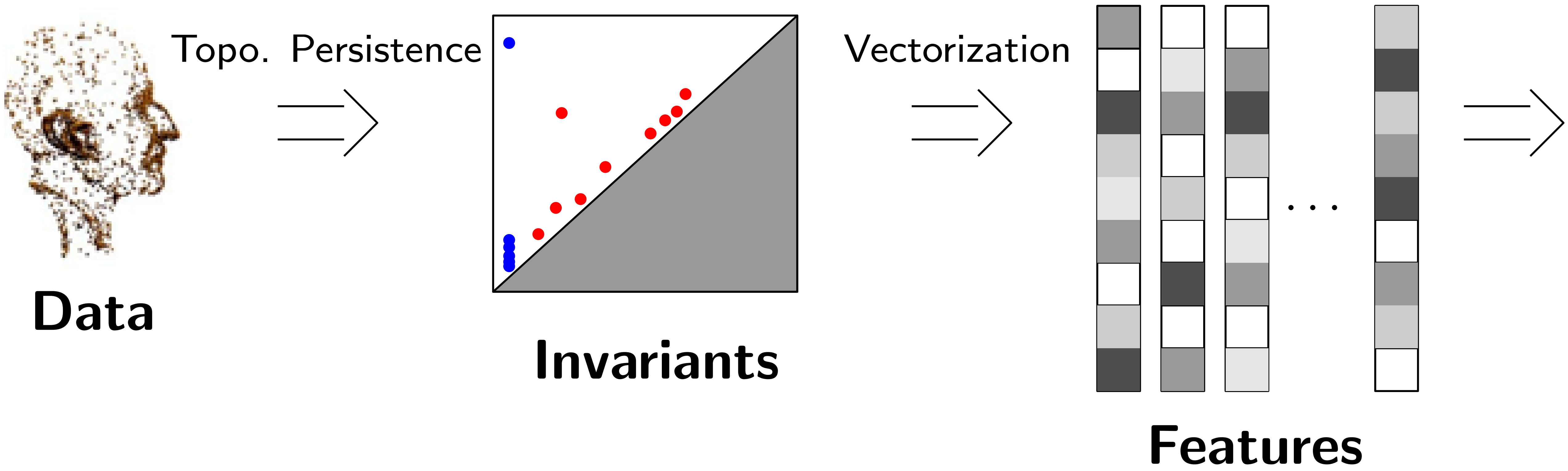
bag of words, word2vec

shape contexts, heat kernels

node2vec, Laplacian fact., rand. walks

dim. reduction, auto-encoders, etc.

Topological Data Analysis (TDA) pipeline



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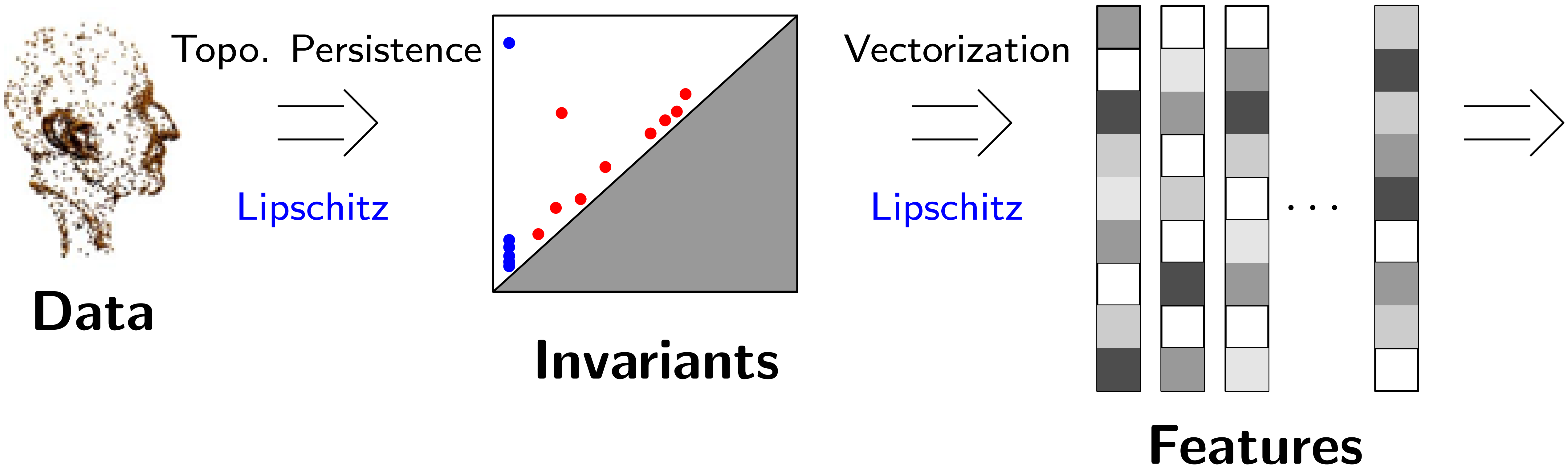
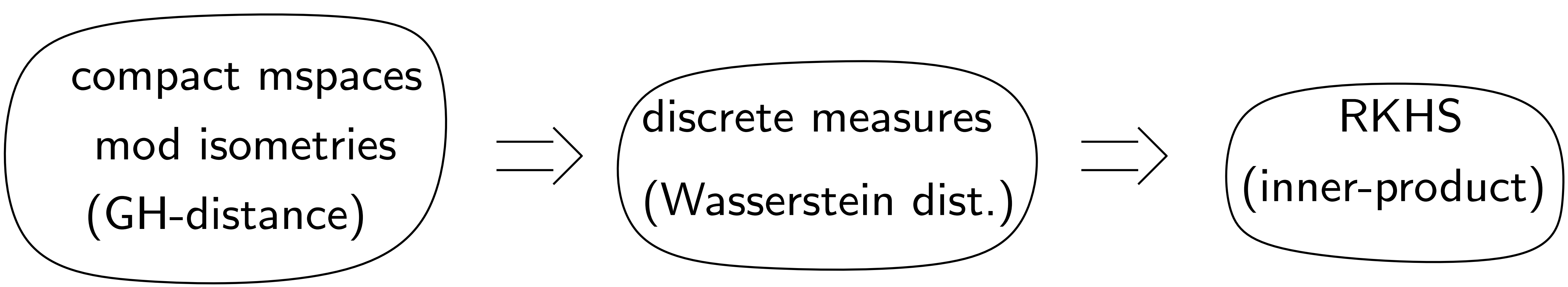


Mathematical framework:



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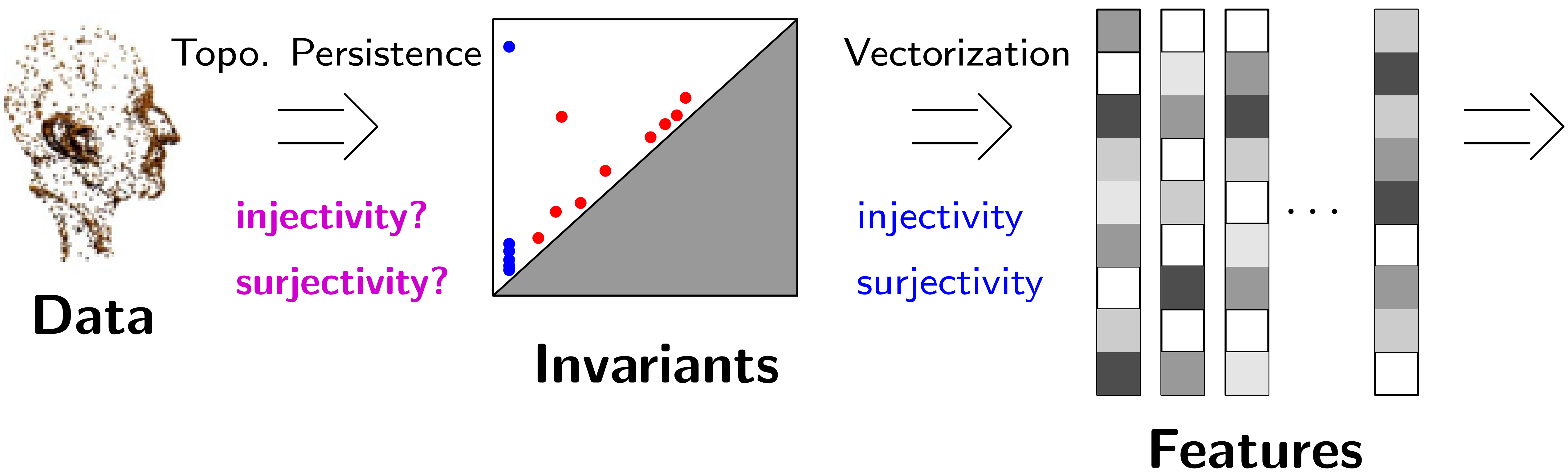

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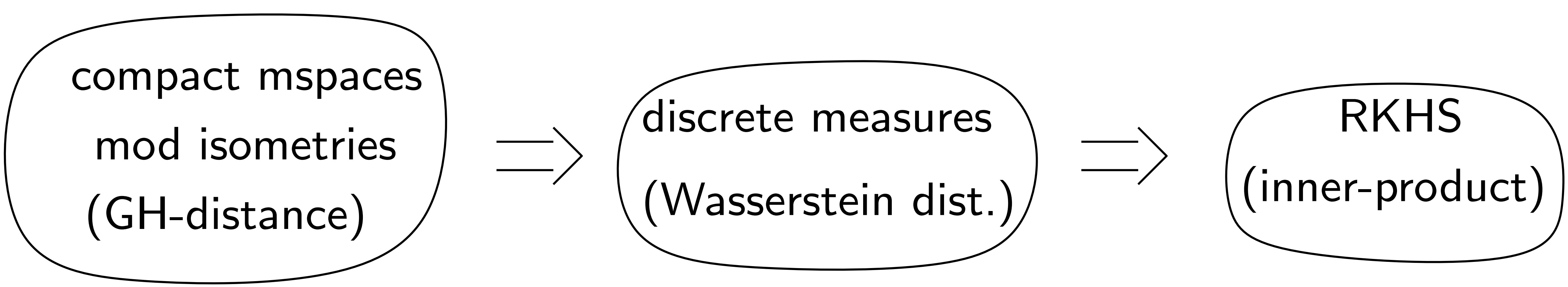

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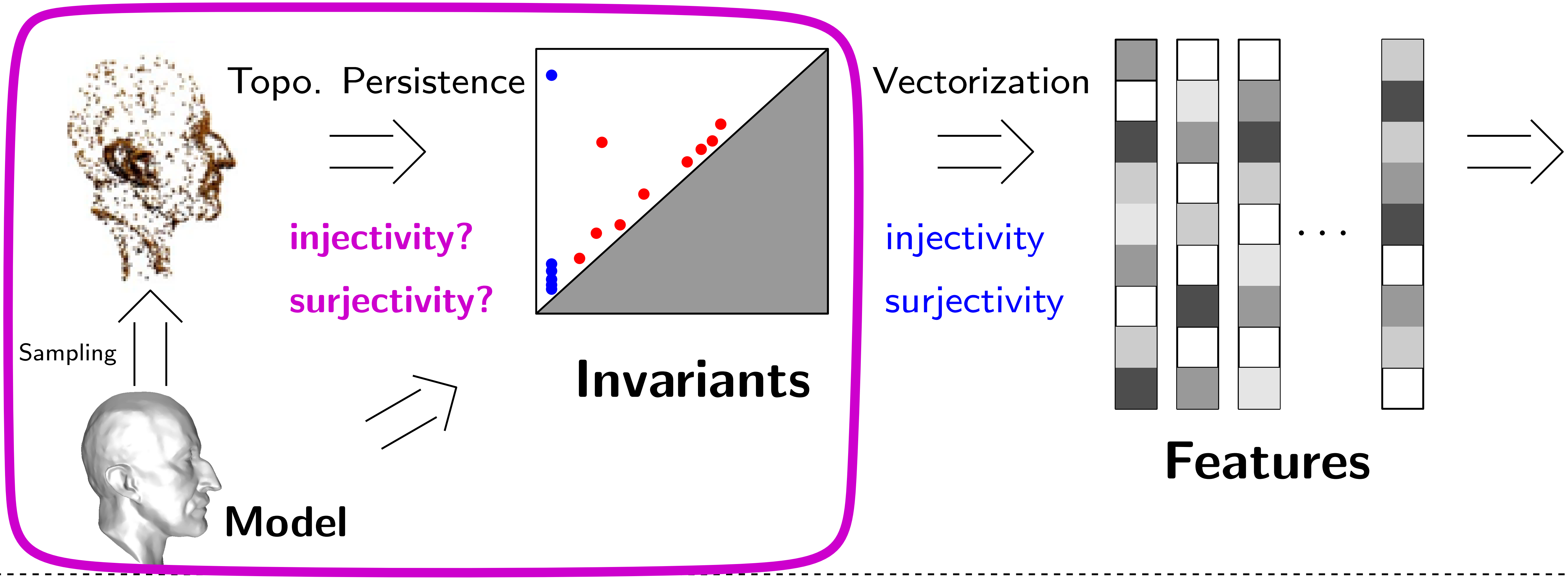


Mathematical framework:

compact mspaces mod isometries (GH-distance) ⟹ discrete measures (Wasserstein dist.) ⟹ RKHS (inner-product)

Topological Persistence (in a nutshell)

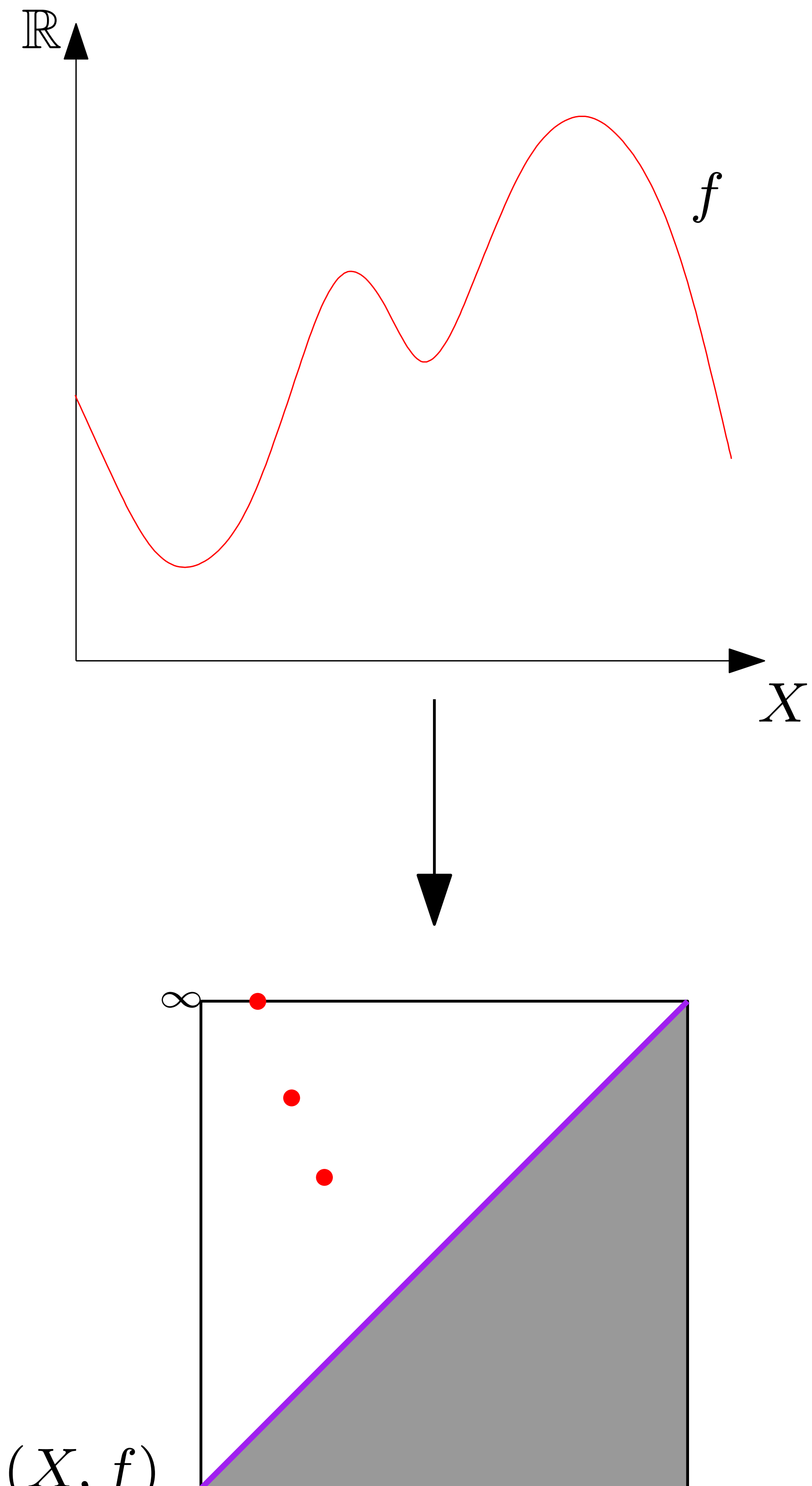
X topological space

$f : X \to \mathbb{R}$ (filter)

$\mathrm{Dgm}\, f$

signature: *persistence diagram*

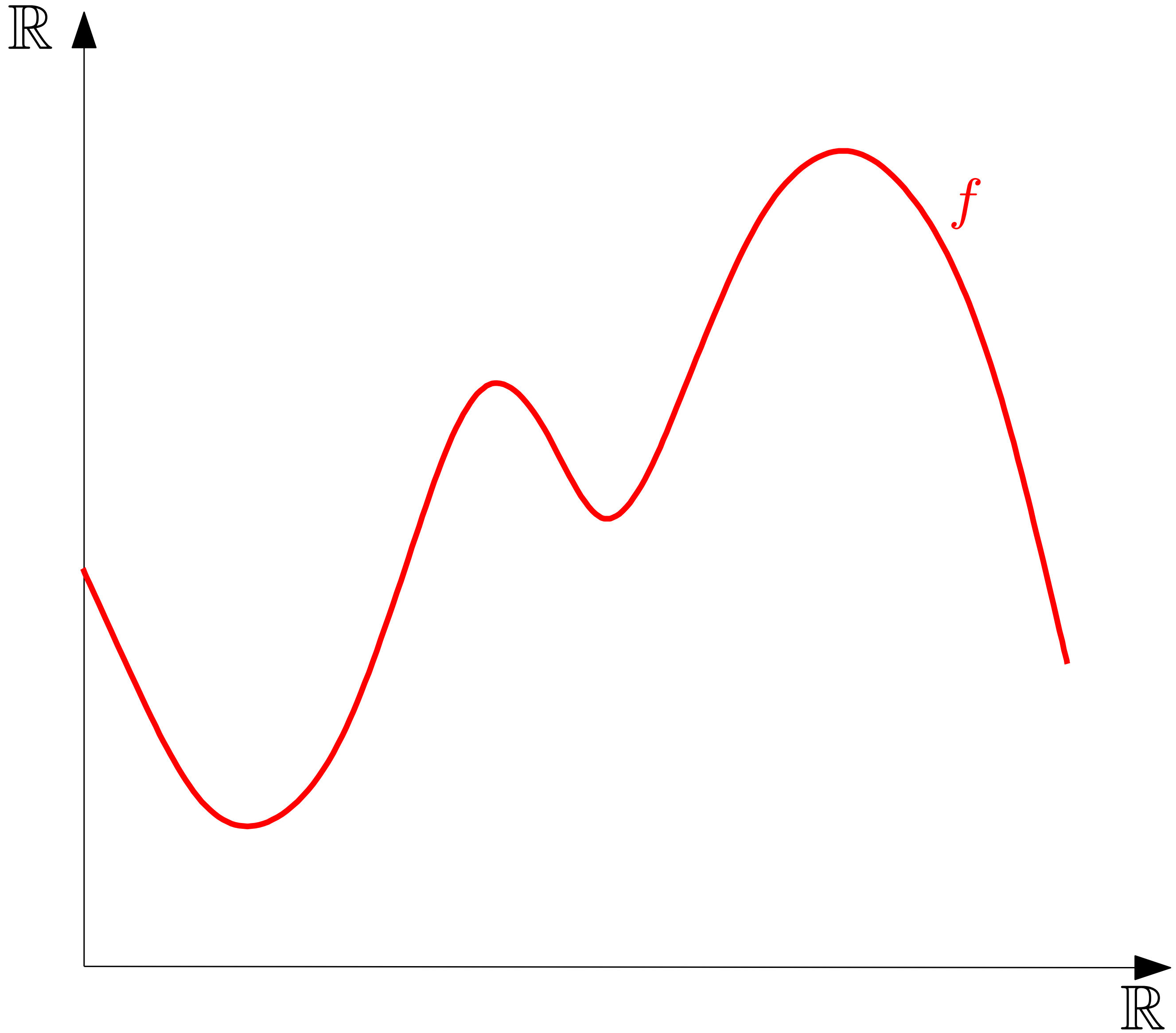
encodes the topological structure of the pair (X, f)



Topological Persistence (in a nutshell)

Inside the black box:

- Nested family (*filtration*) of sublevel-sets $f^{-1}((-\infty, \alpha])$ for α ranging over $\mathbb{R}$
- Track the evolution of the topology throughout the family (**homology**)



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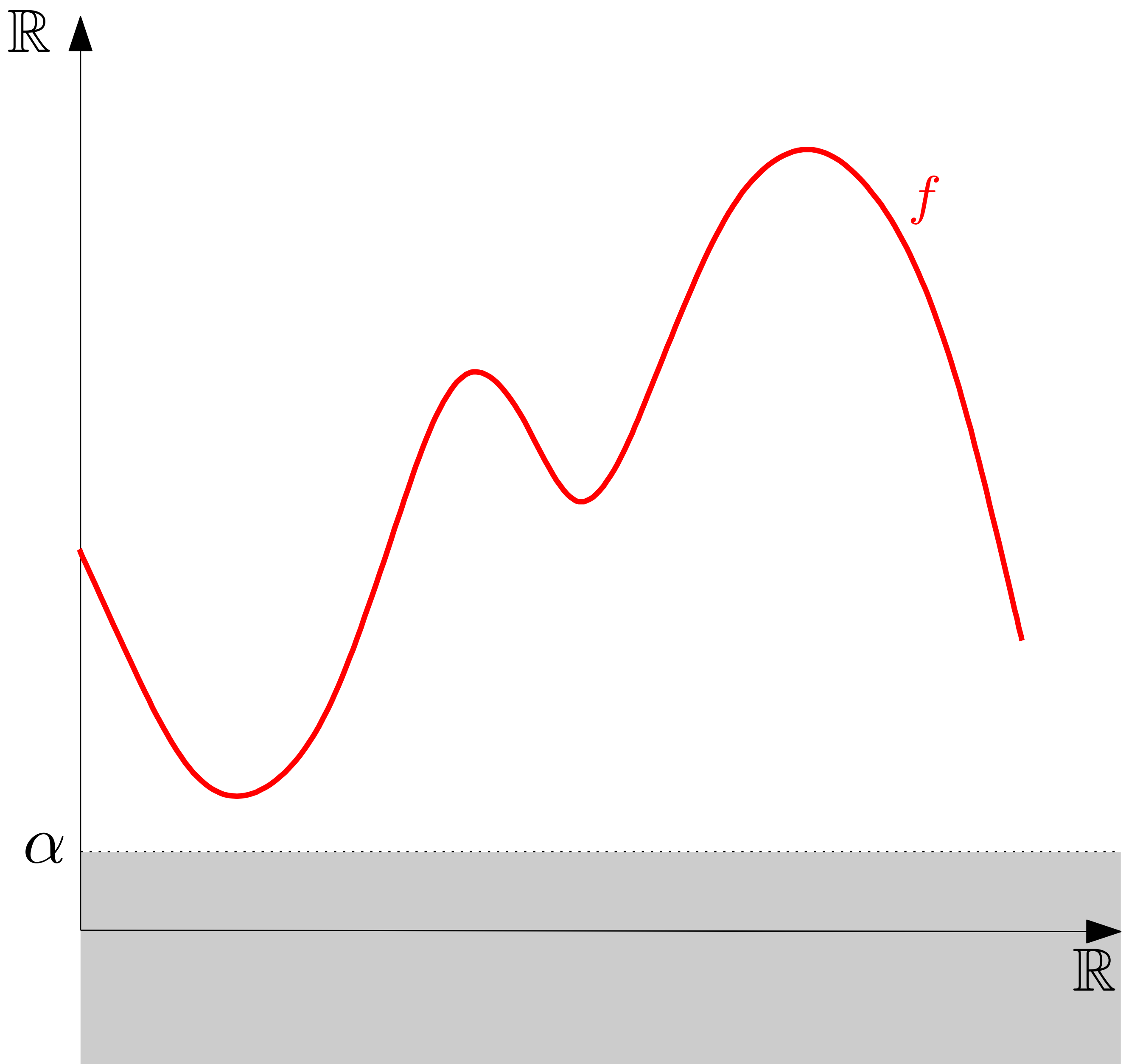

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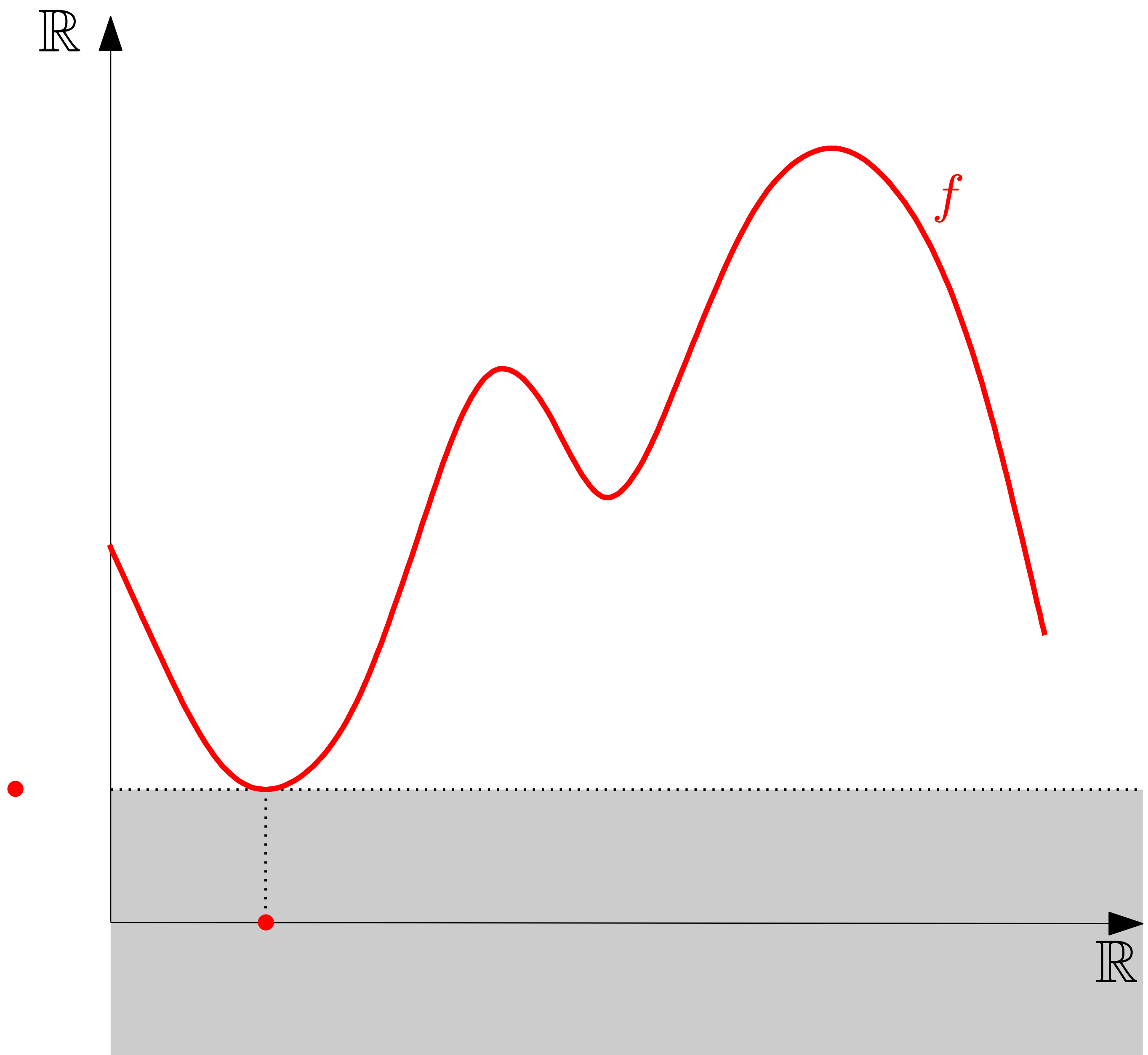

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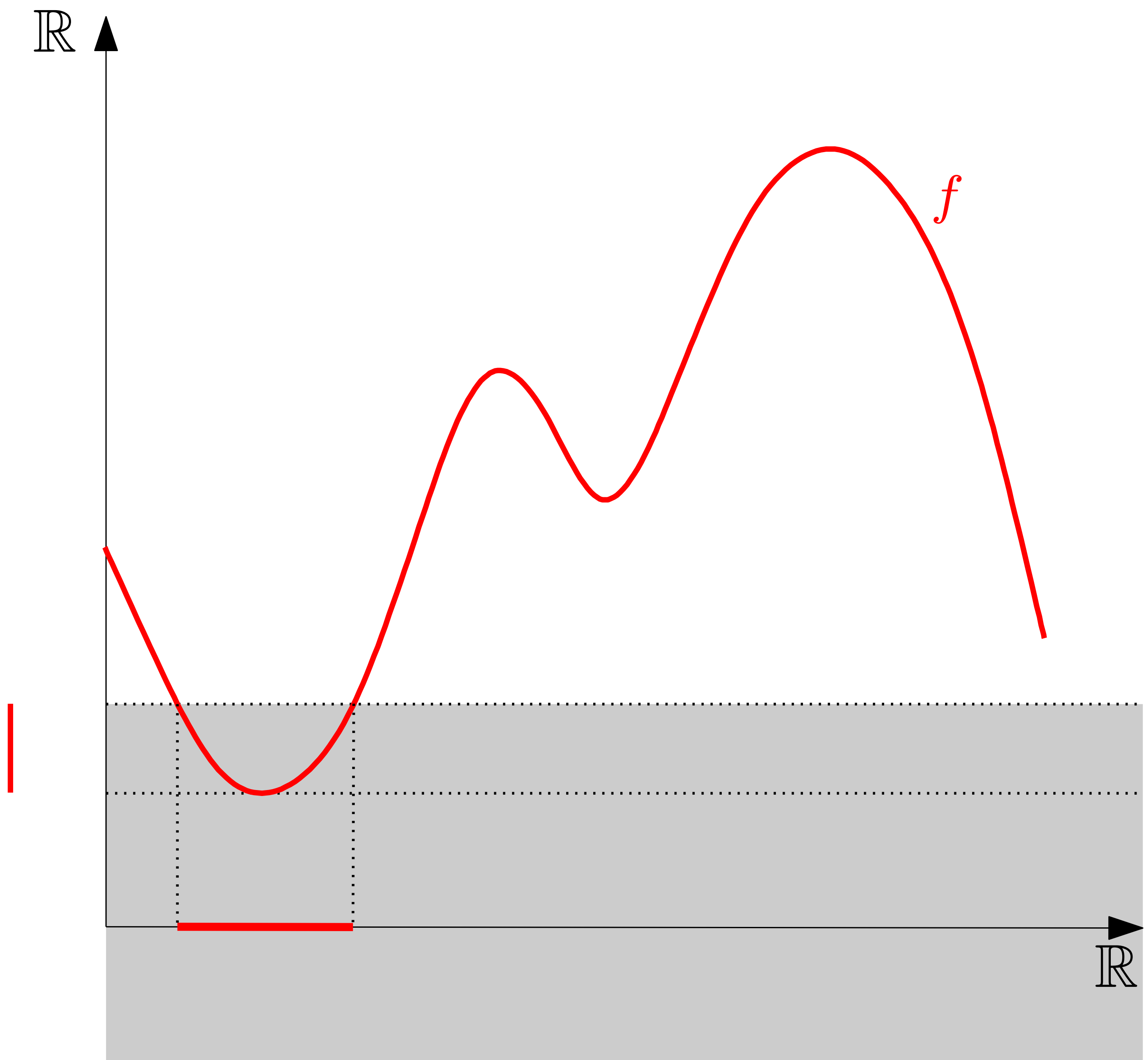

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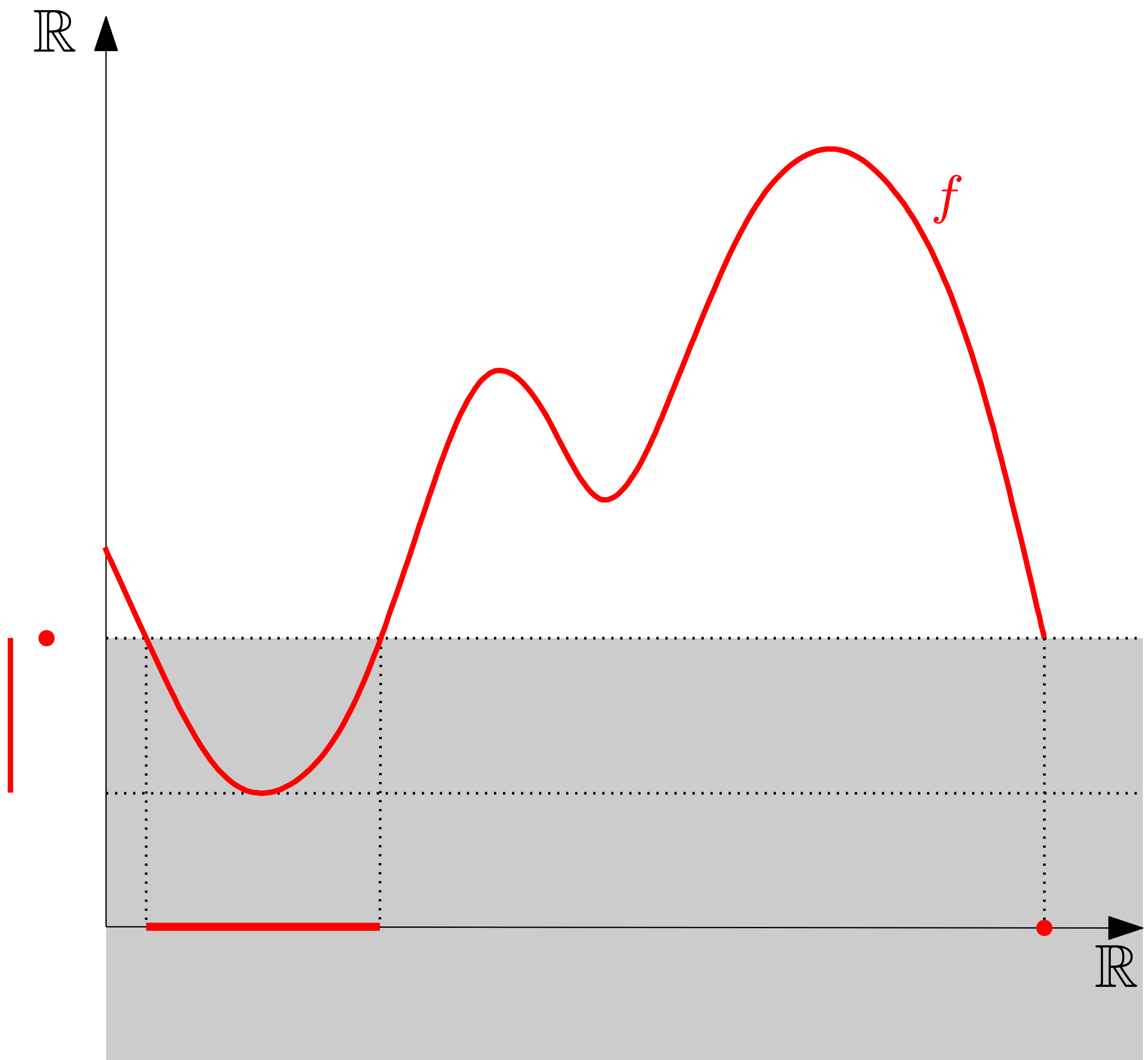

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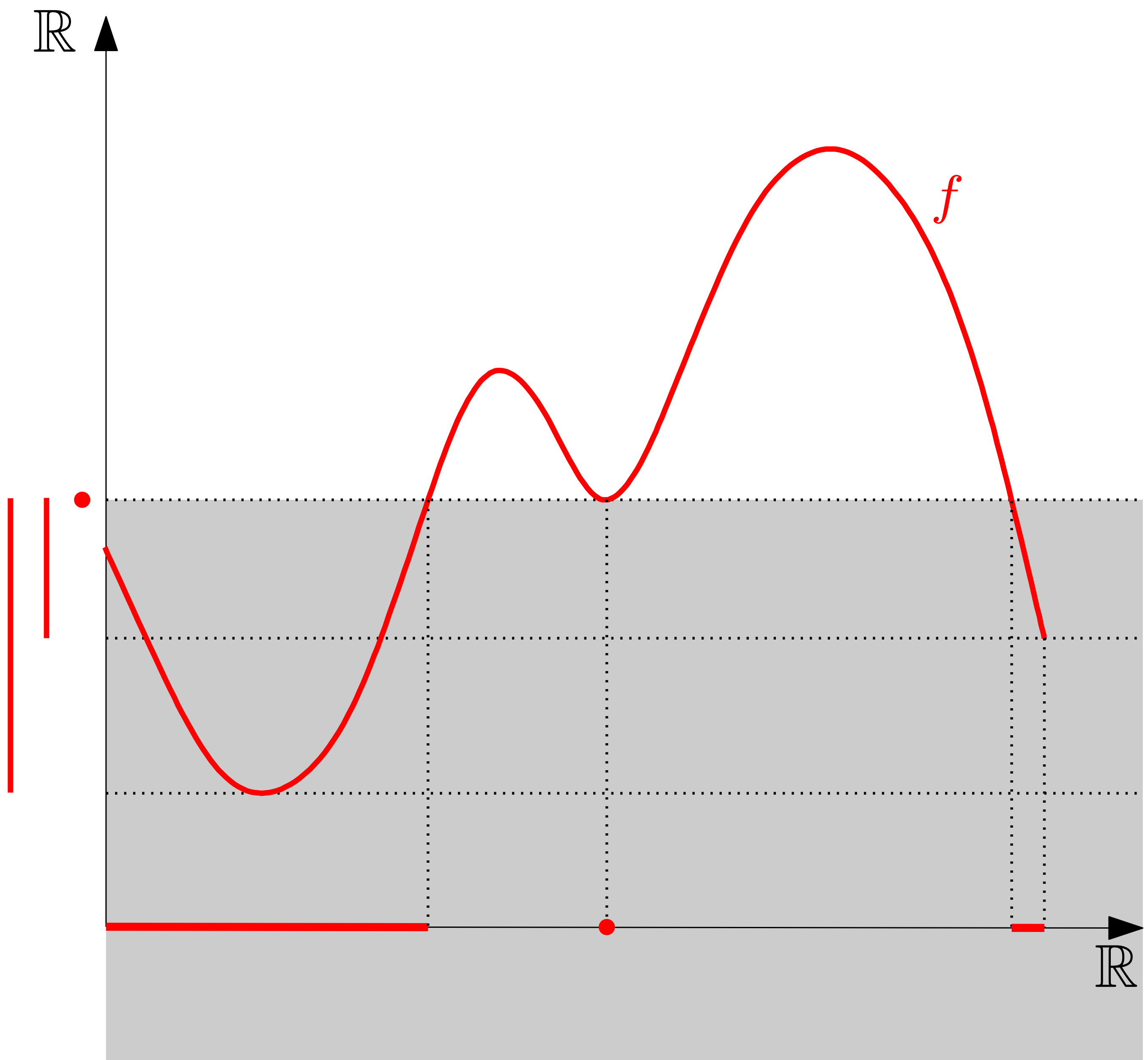

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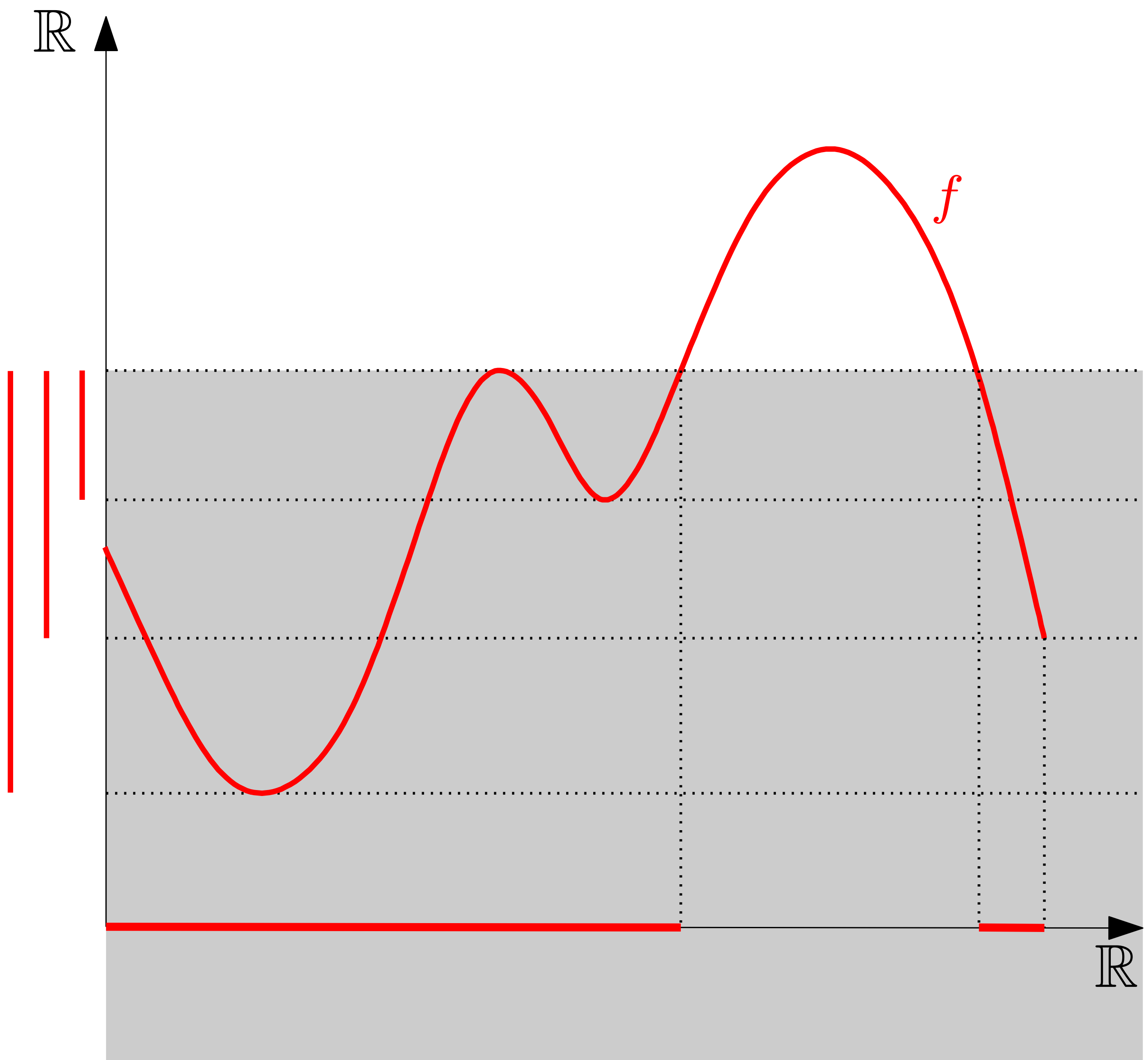

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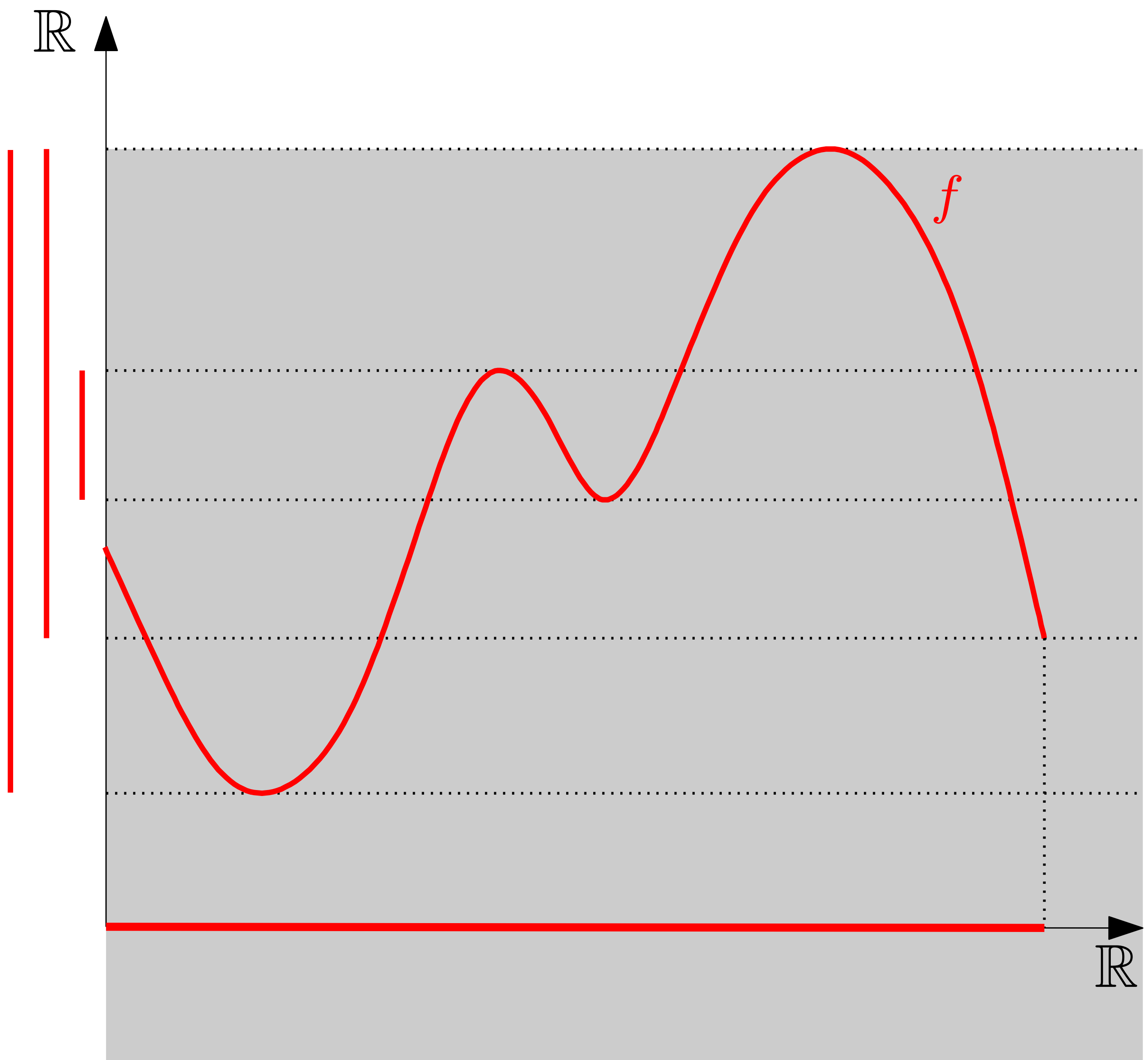
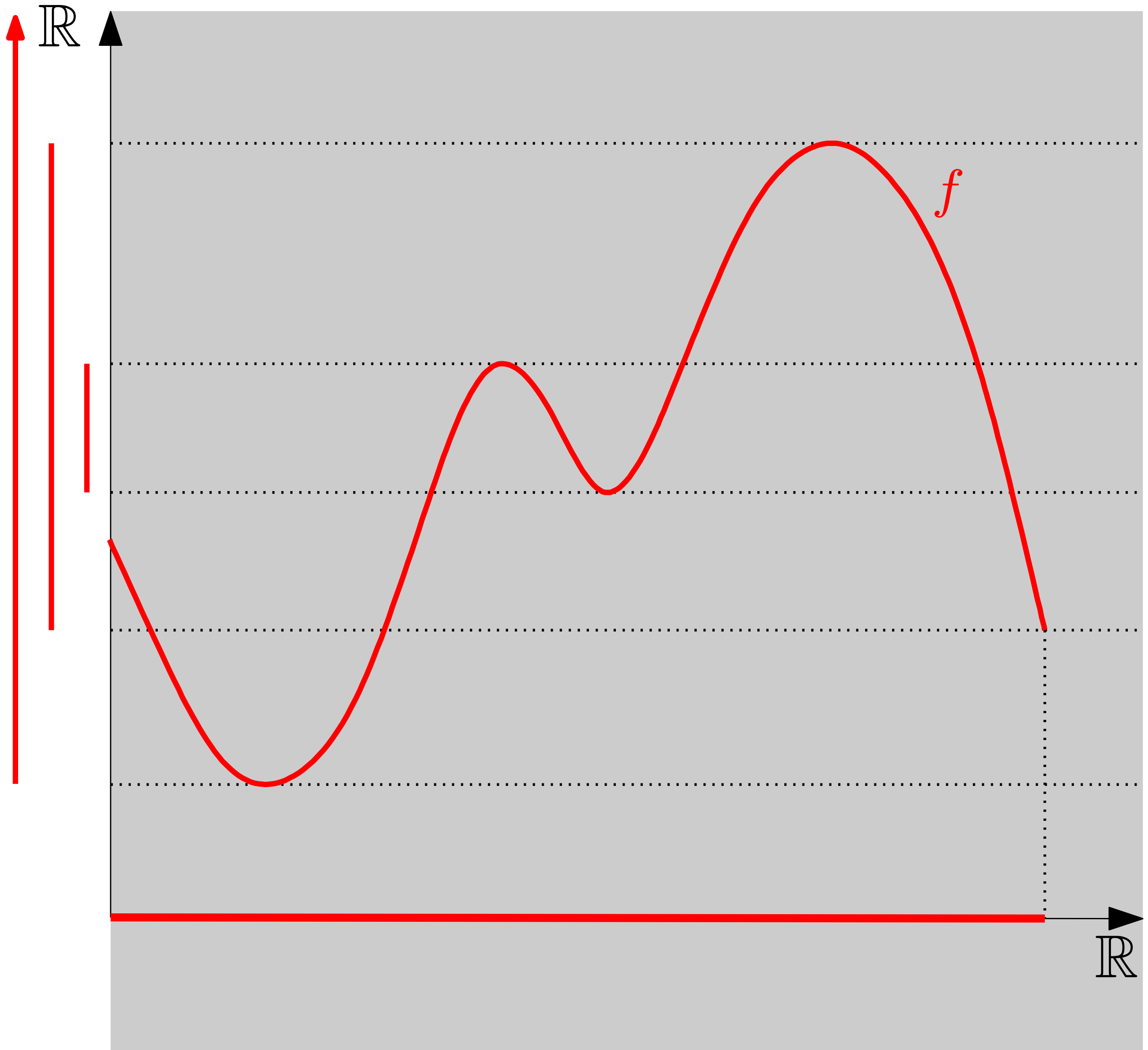


Topological Persistence (in a nutshell)

Inside the black box:

- Nested family (*filtration*) of sublevel-sets $f^{-1}((-\infty, \alpha])$ for α ranging over $\mathbb{R}$
- Track the evolution of the topology throughout the family (**homology**)
- Finite set of intervals (barcode) encodes births/deaths of topological features



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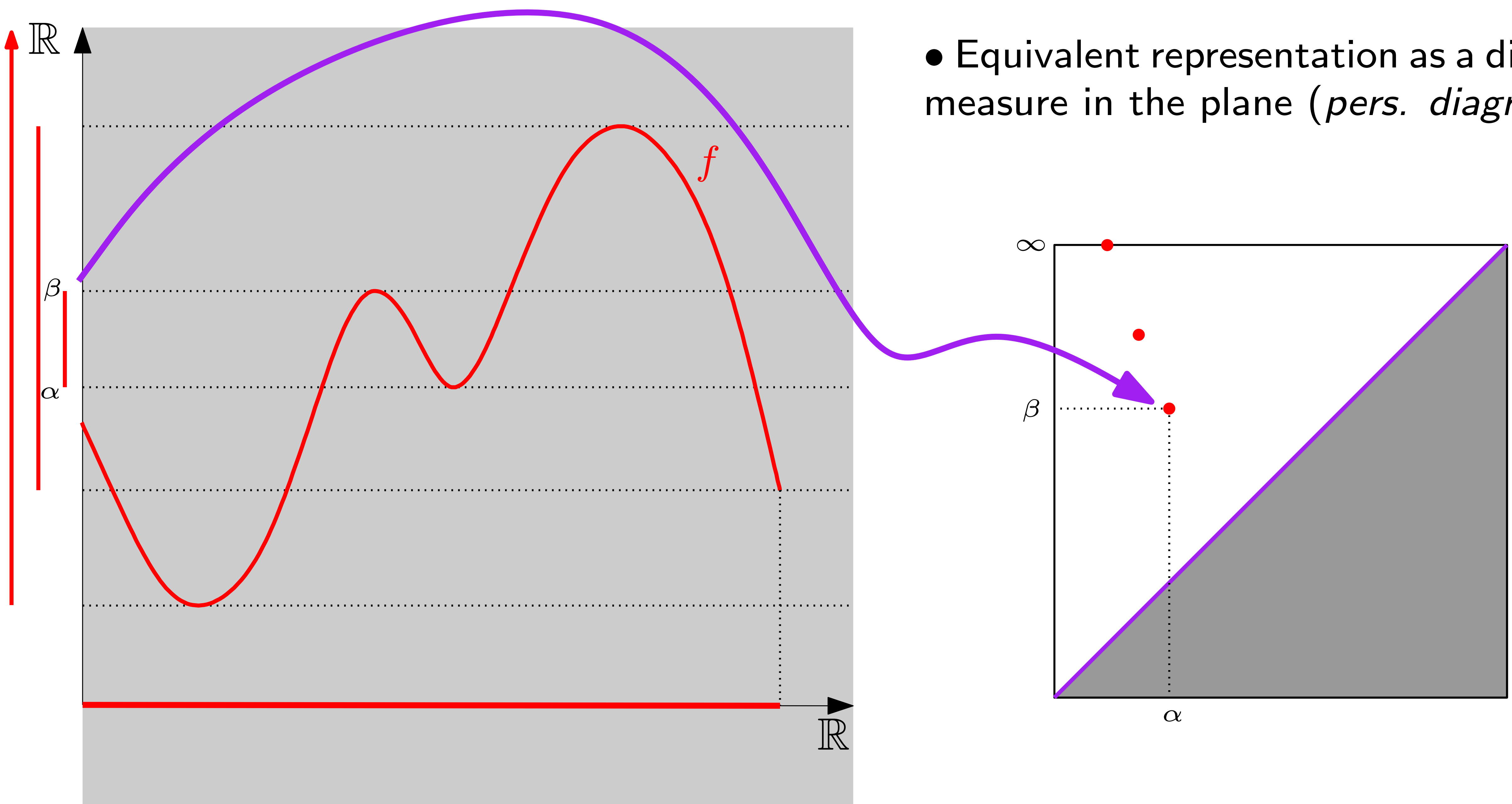
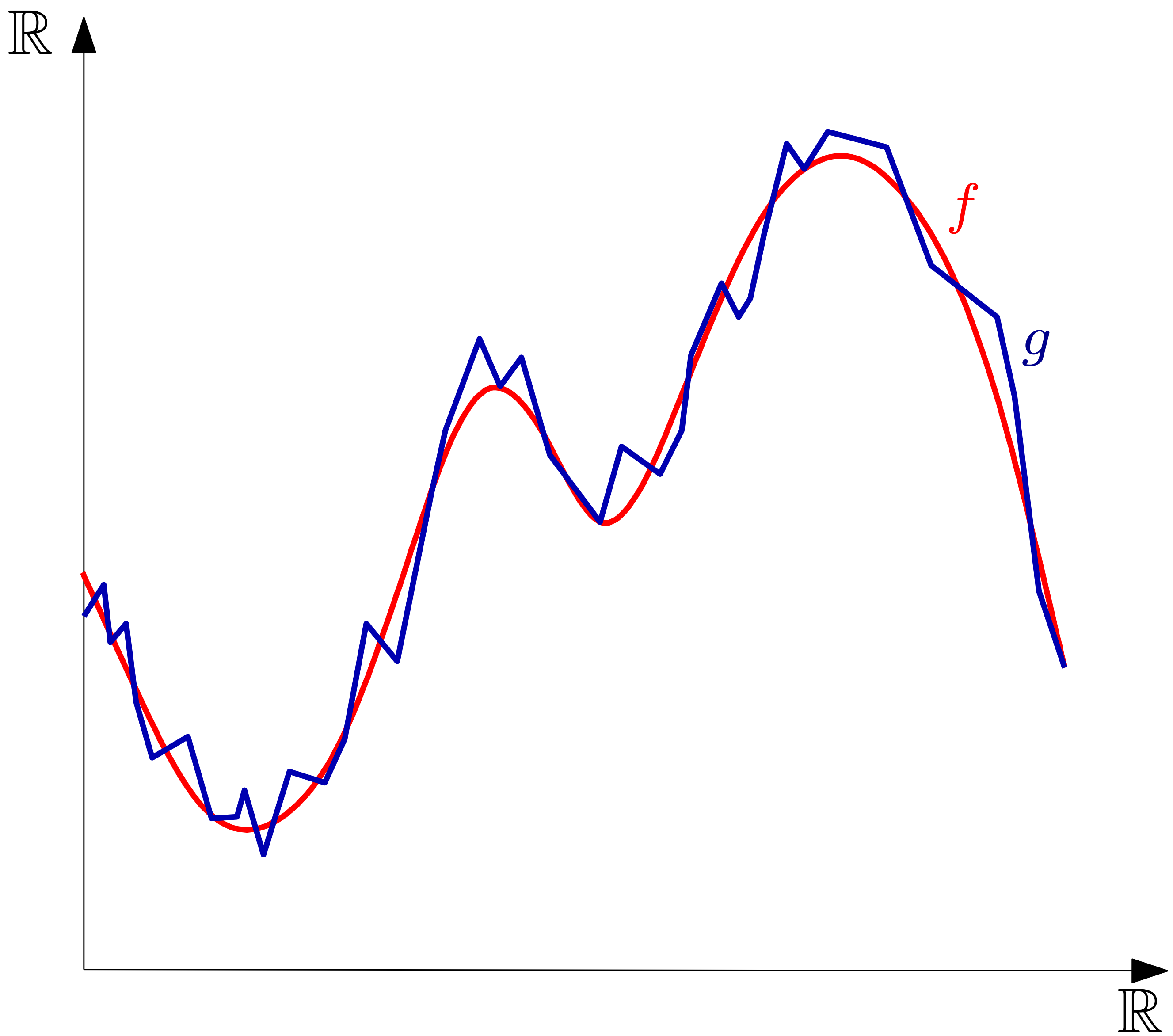
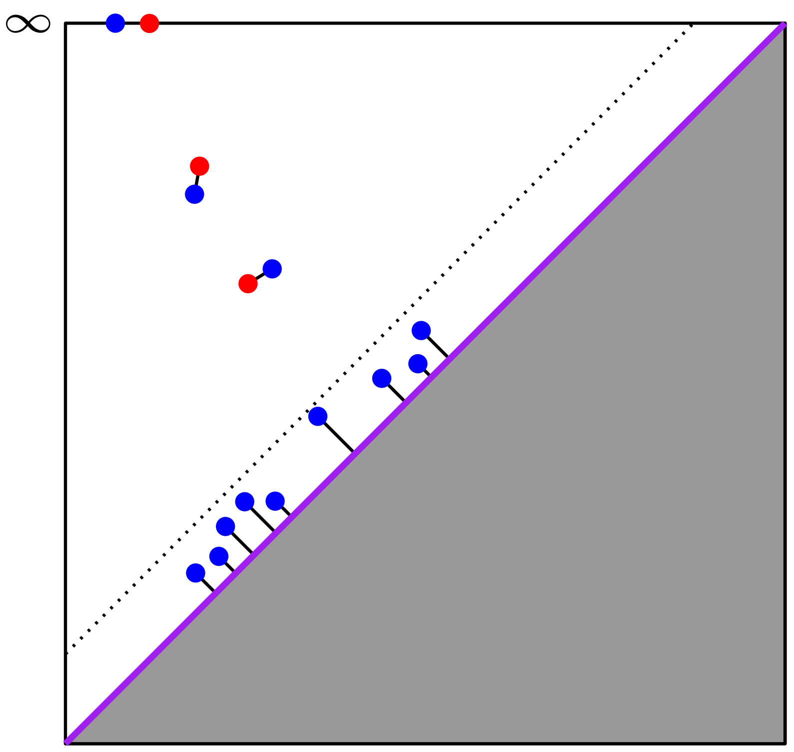
- Equivalent representation as a discrete measure in the plane (*pers. diagram*).



Topological Persistence (in a nutshell)

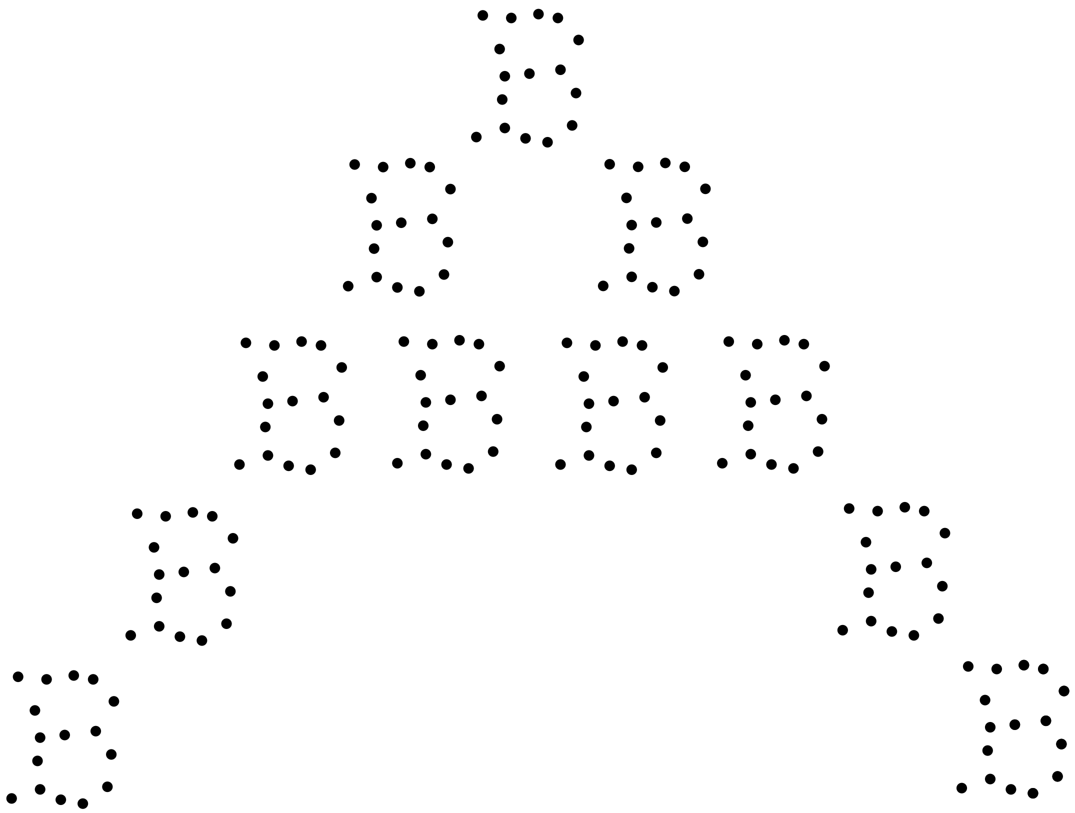
Theorem (Stability):
For any *tame* functions $f, g : X \to \mathbb{R}$, $\mathrm{d}_\mathrm{b}^\infty(\mathrm{Dgm}\, f, \mathrm{Dgm}\, g) \leq \|f - g\|_\infty$.

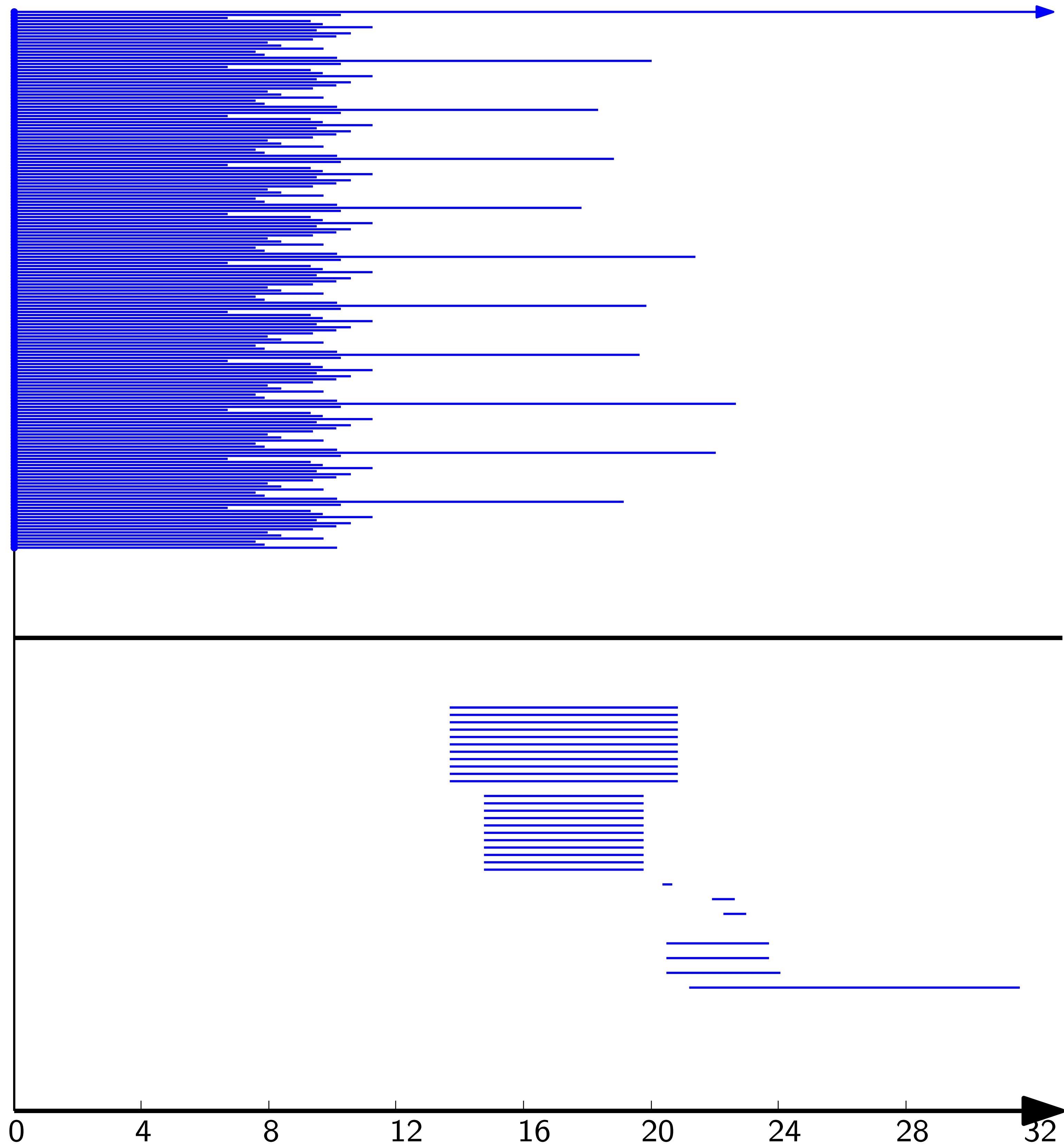




Example: distance function

$$f: \quad X = \mathbb{R}^d \to \mathbb{R}$$
$$x \mapsto \min_{p \in P} \|x - p\|_2$$





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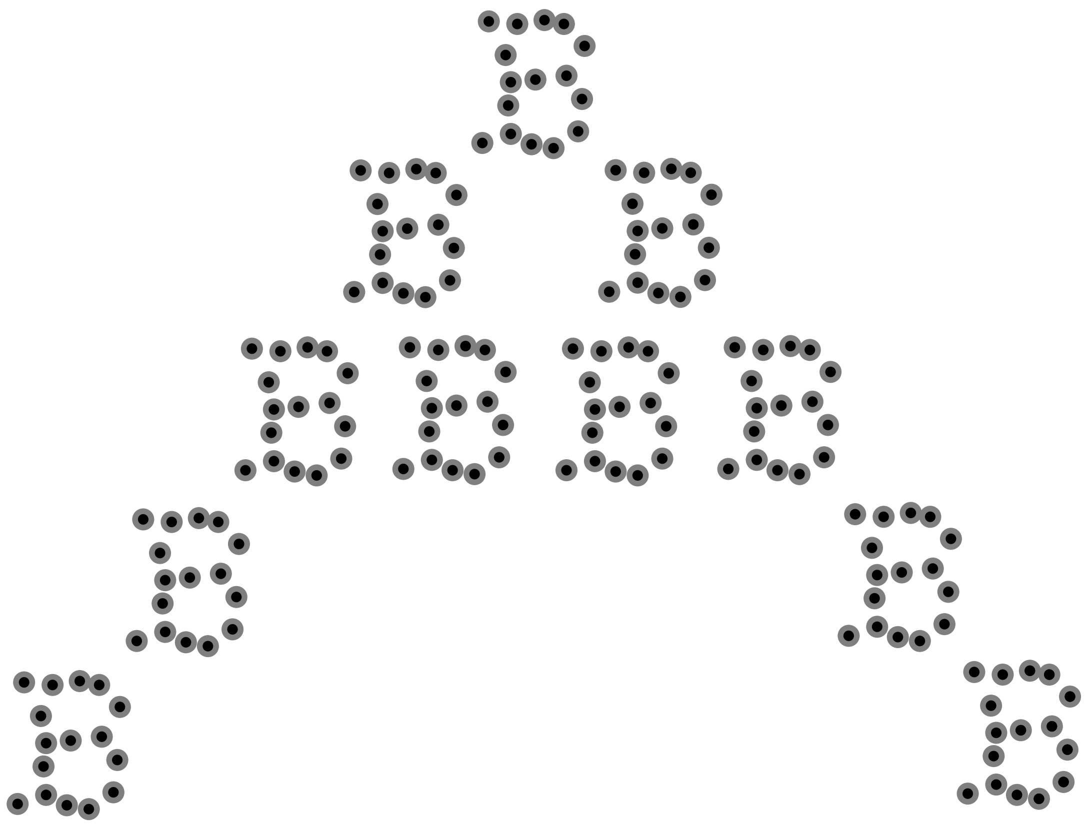

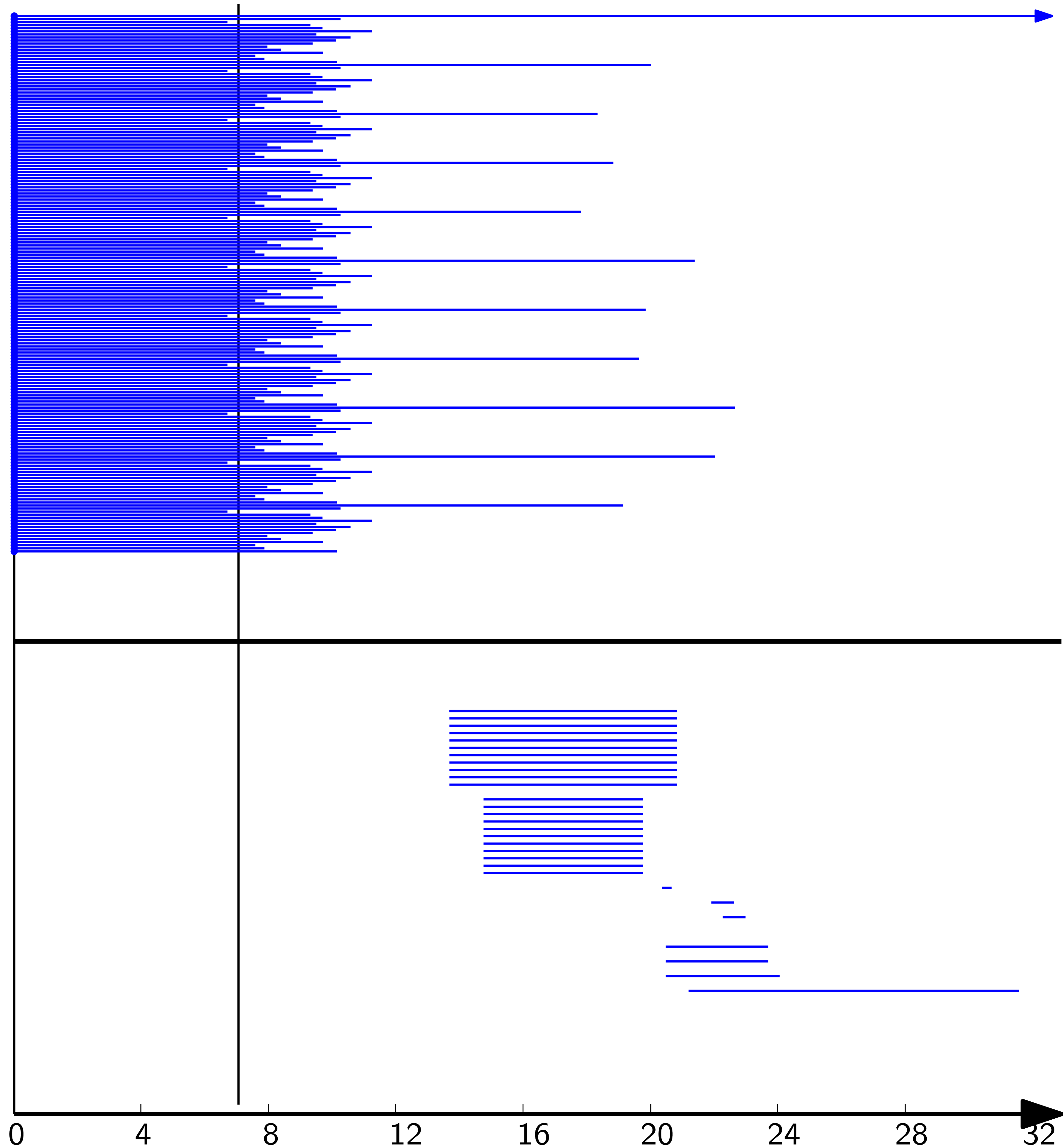

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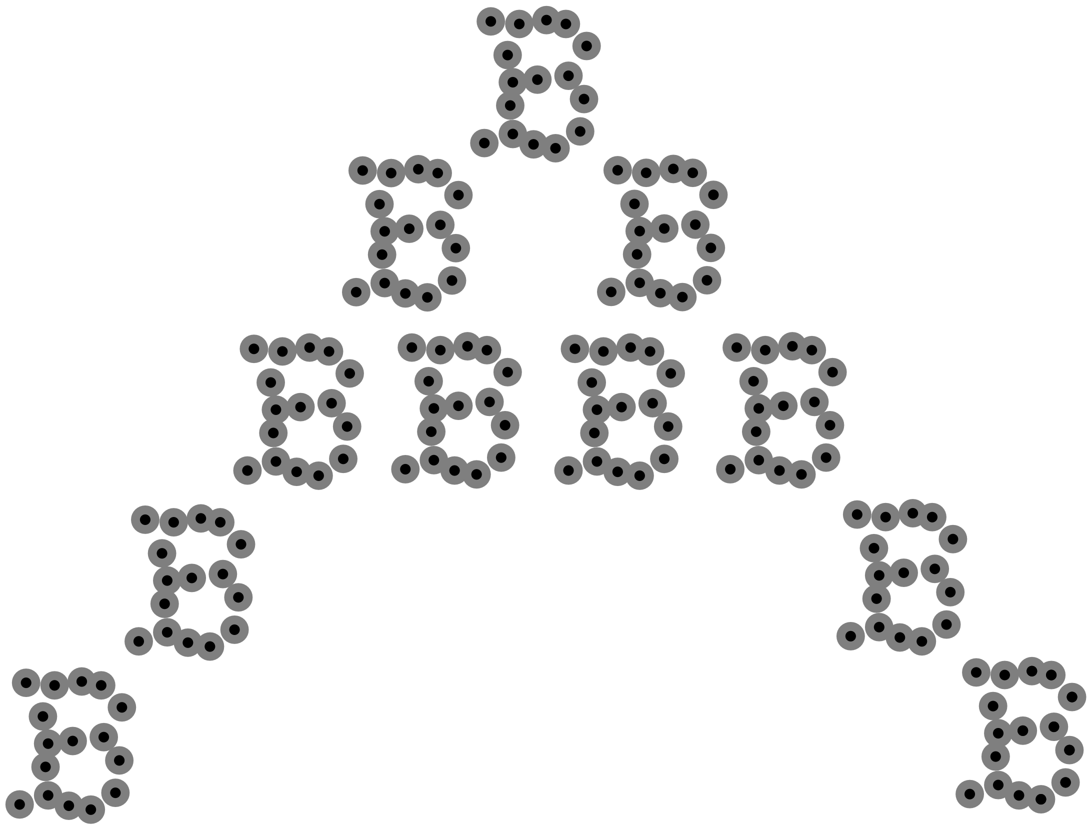

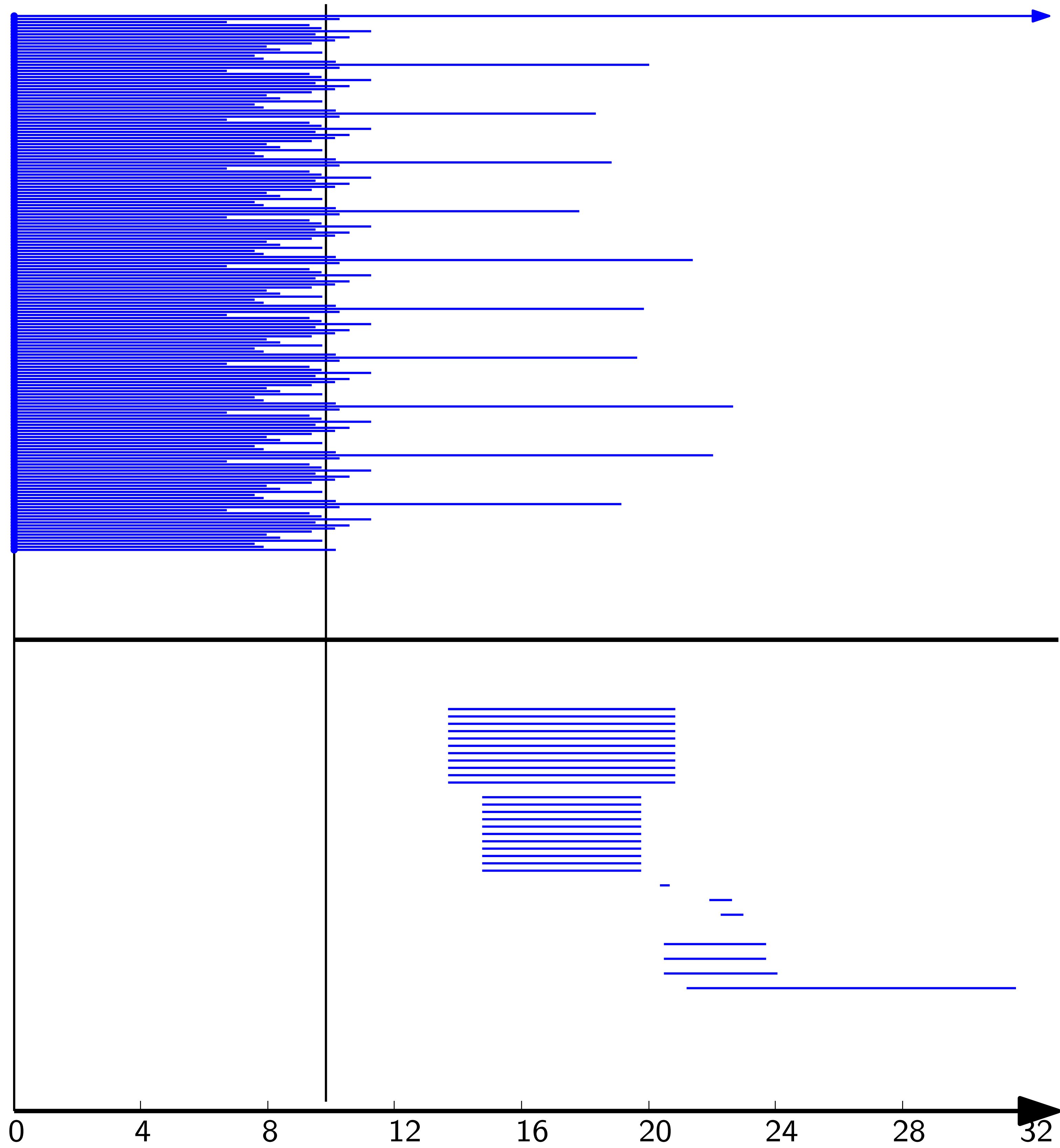

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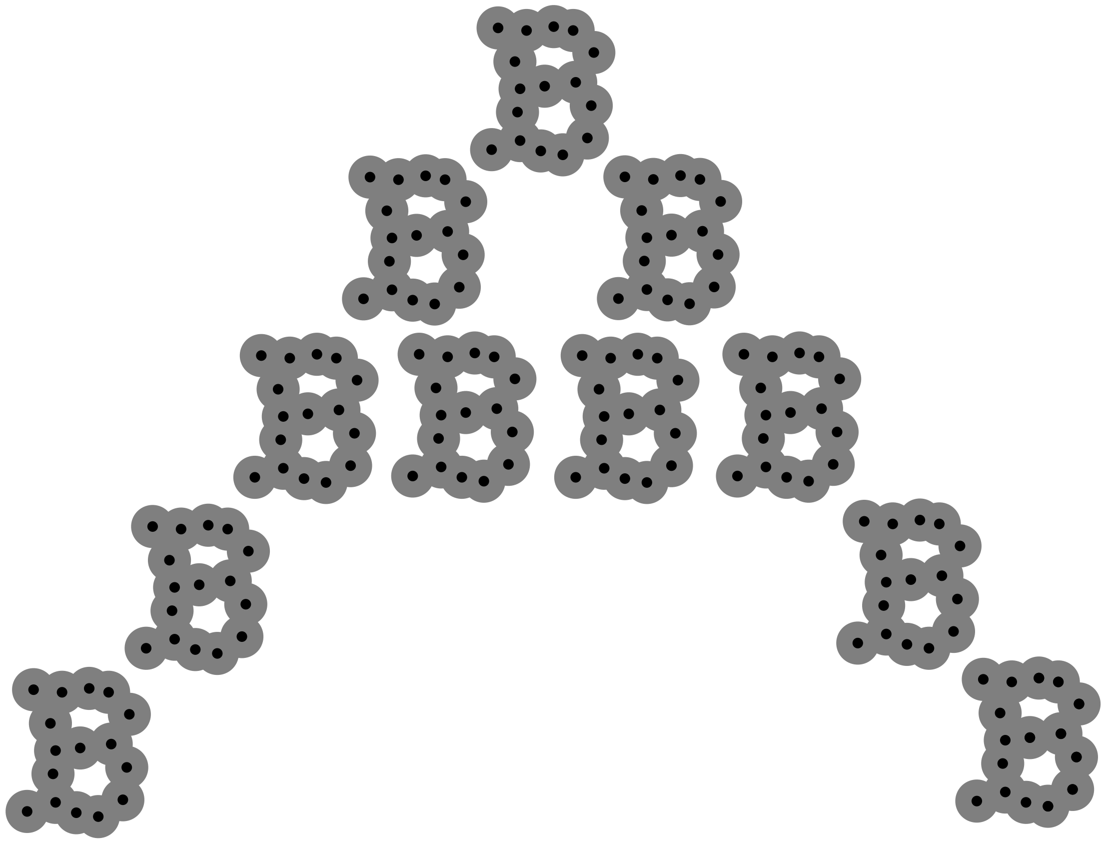

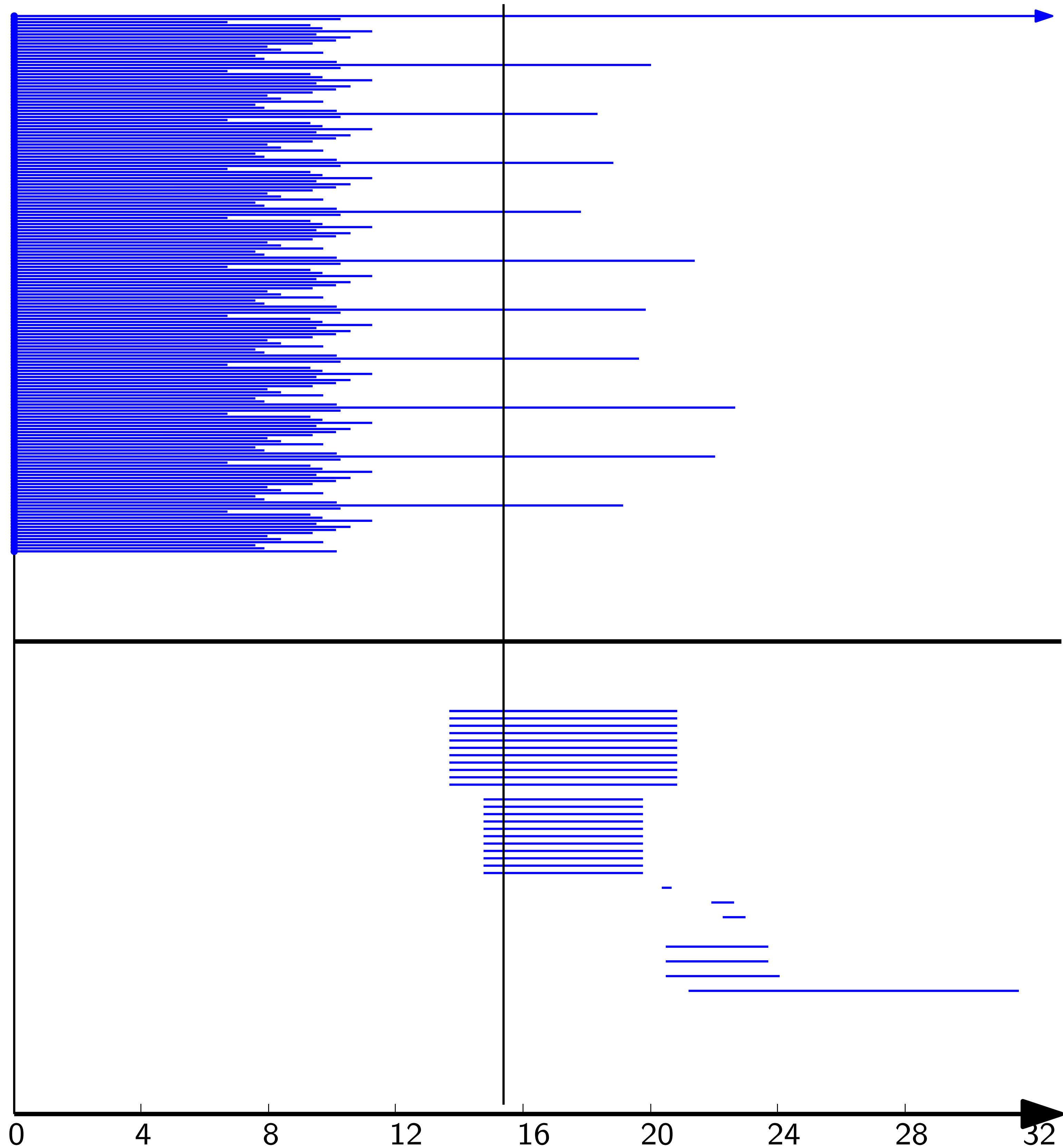

Example: distance function

$$
\begin{aligned}
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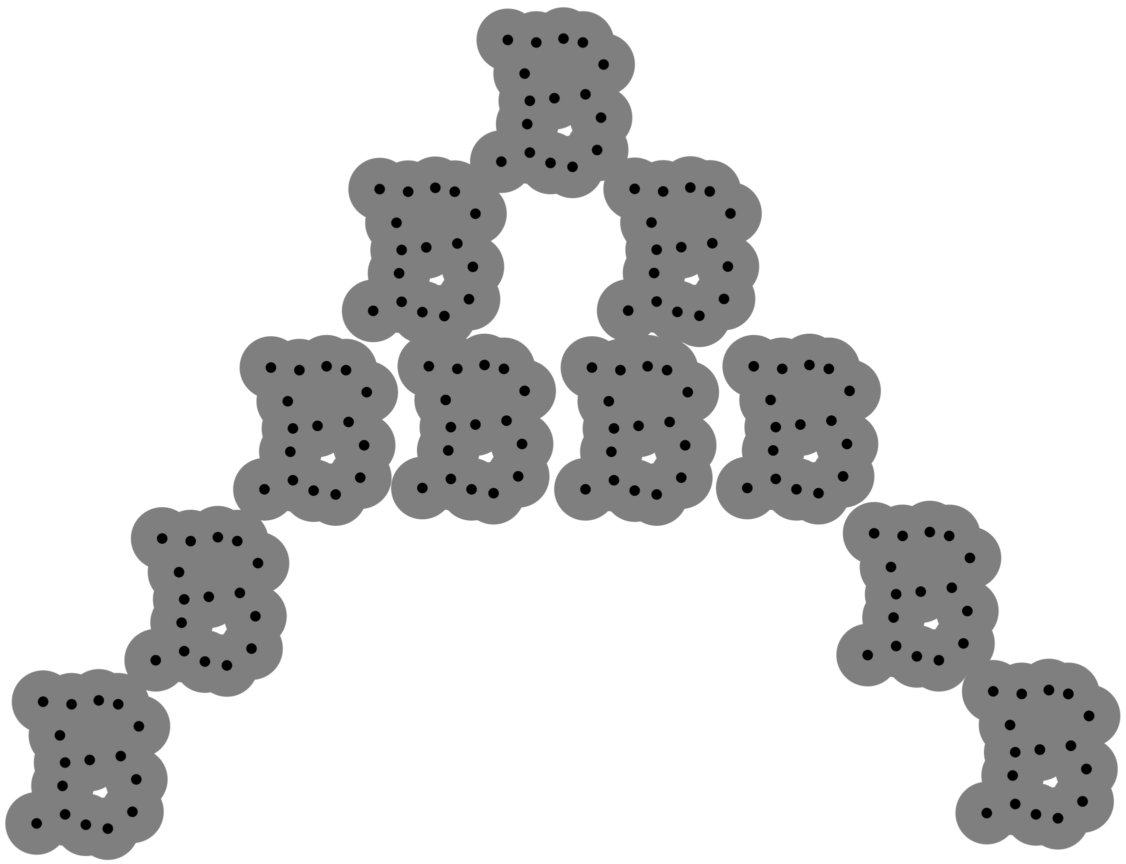
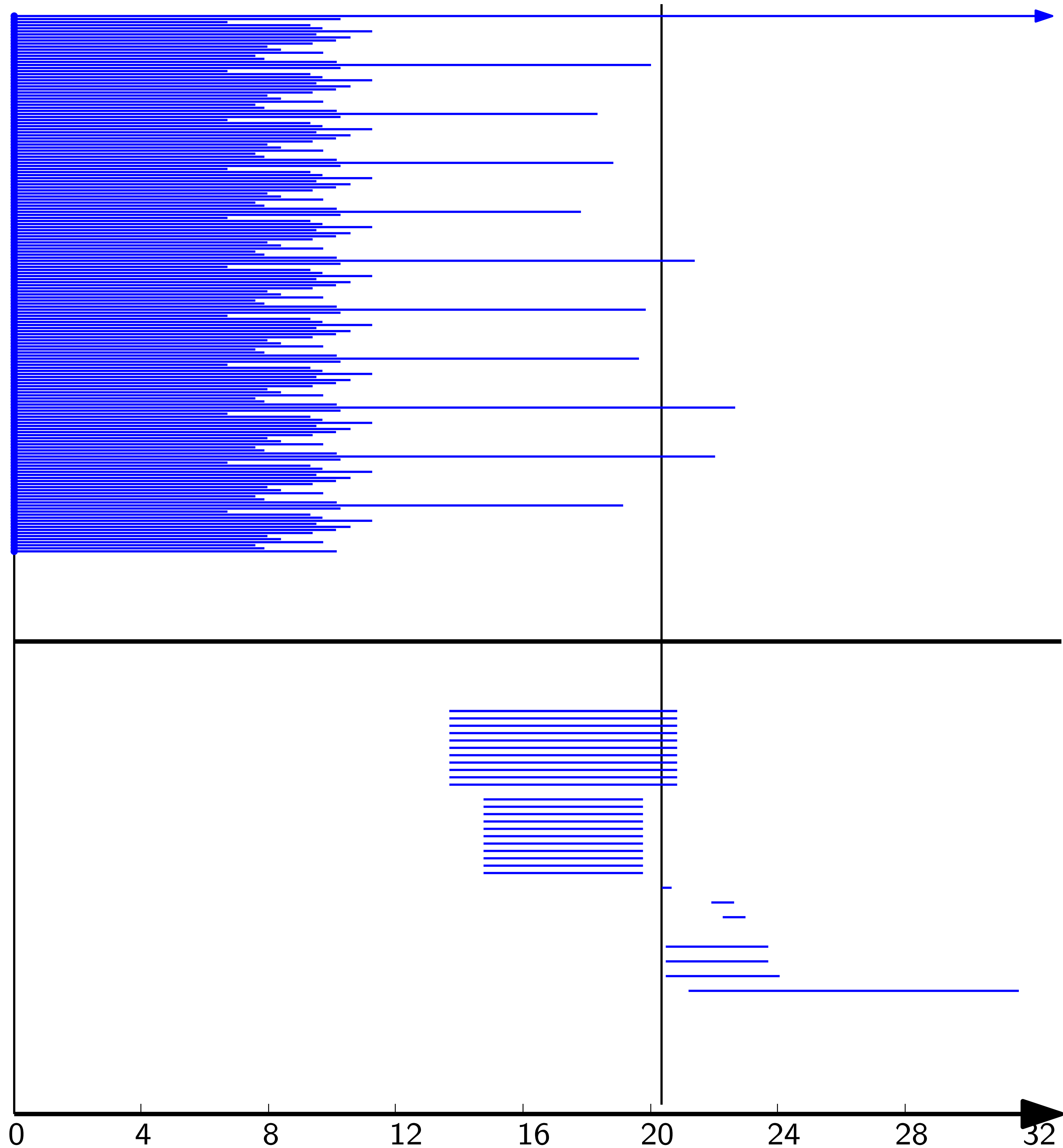
$$





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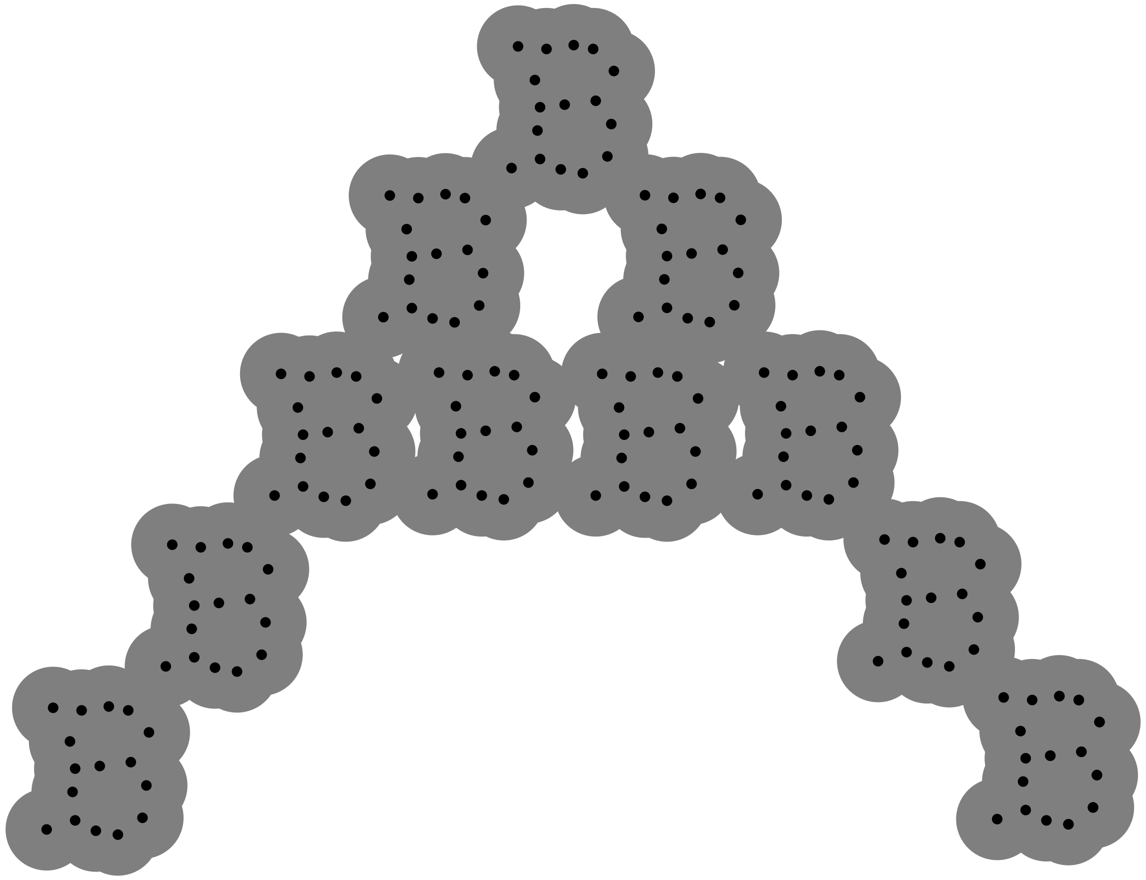

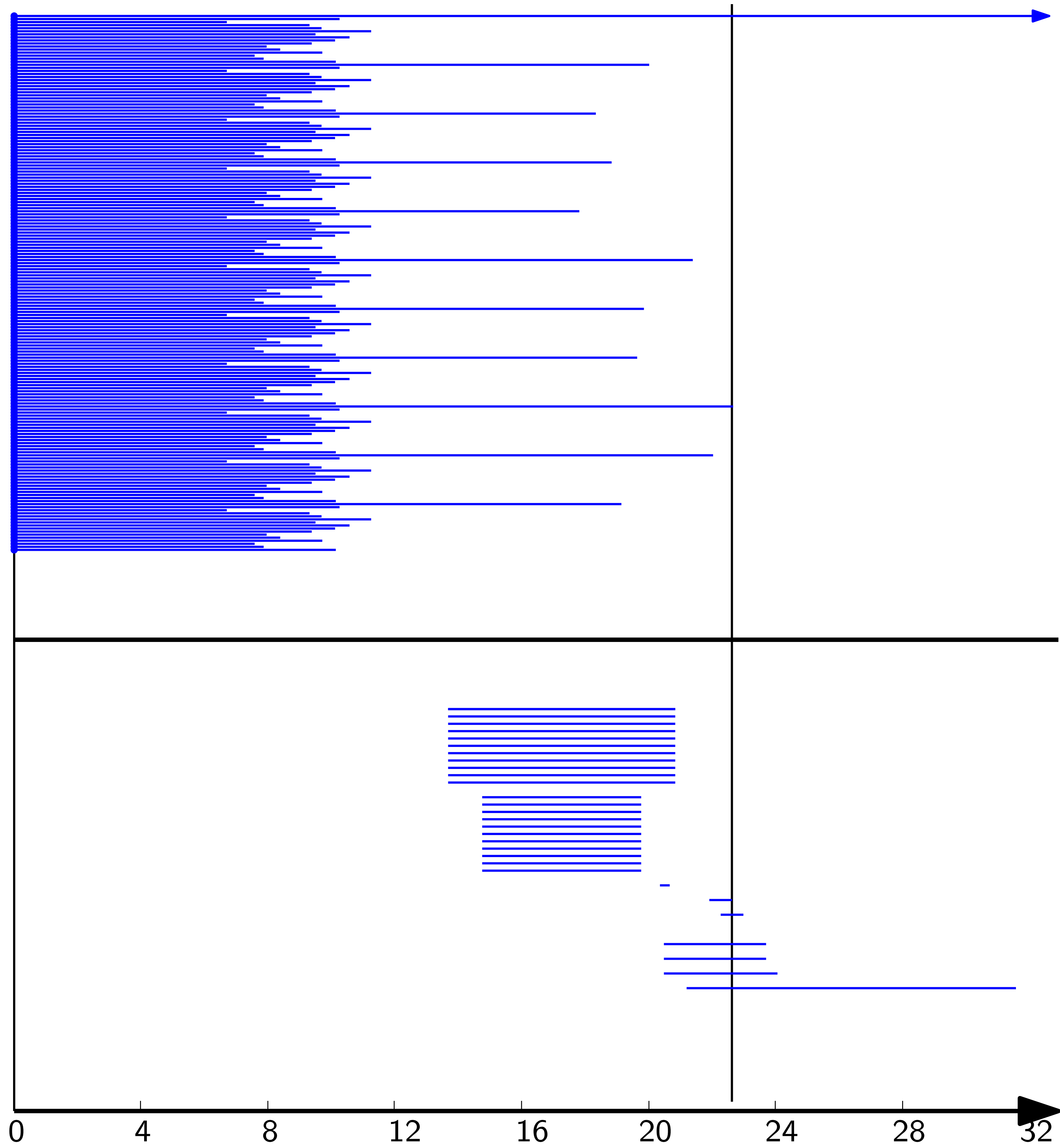

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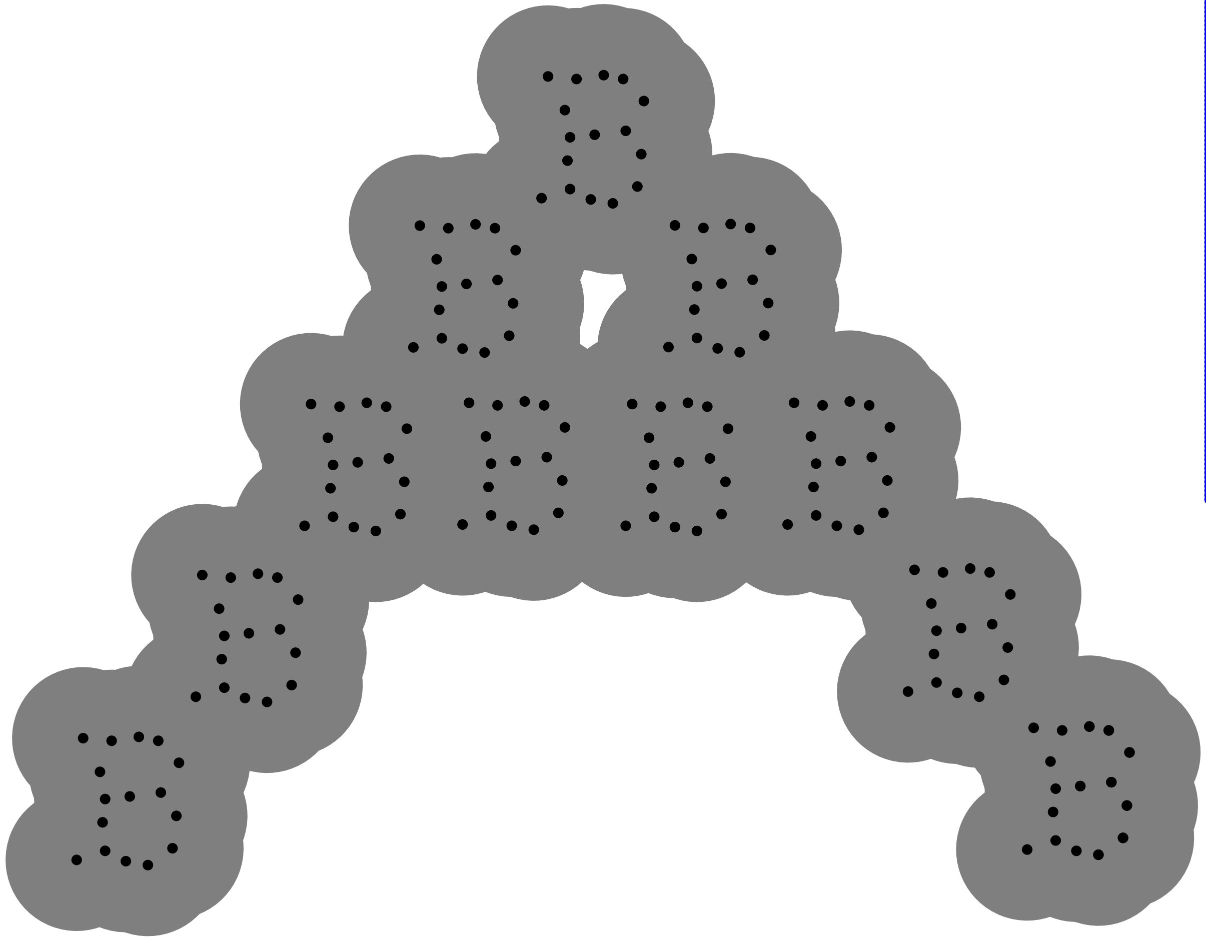

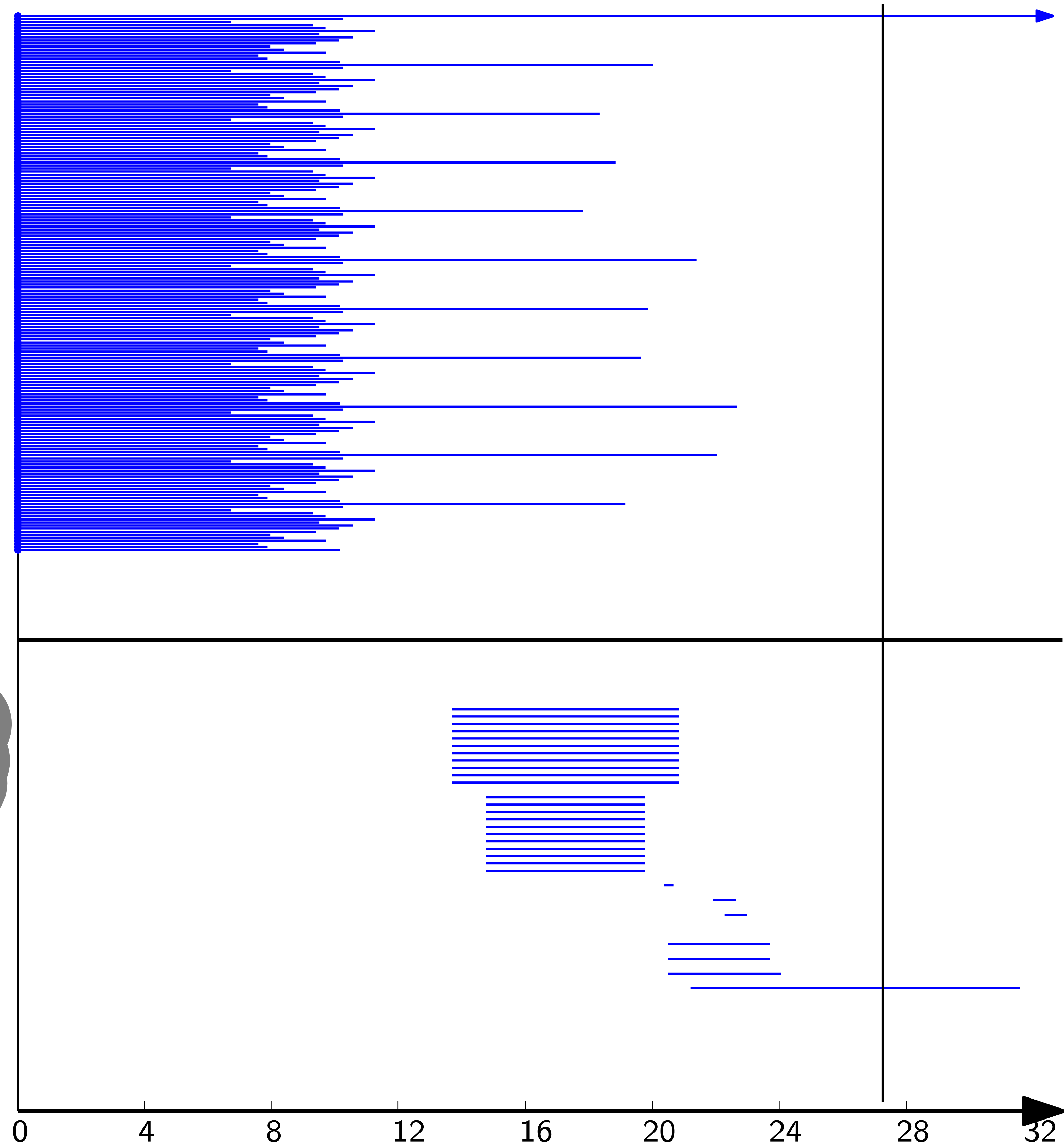

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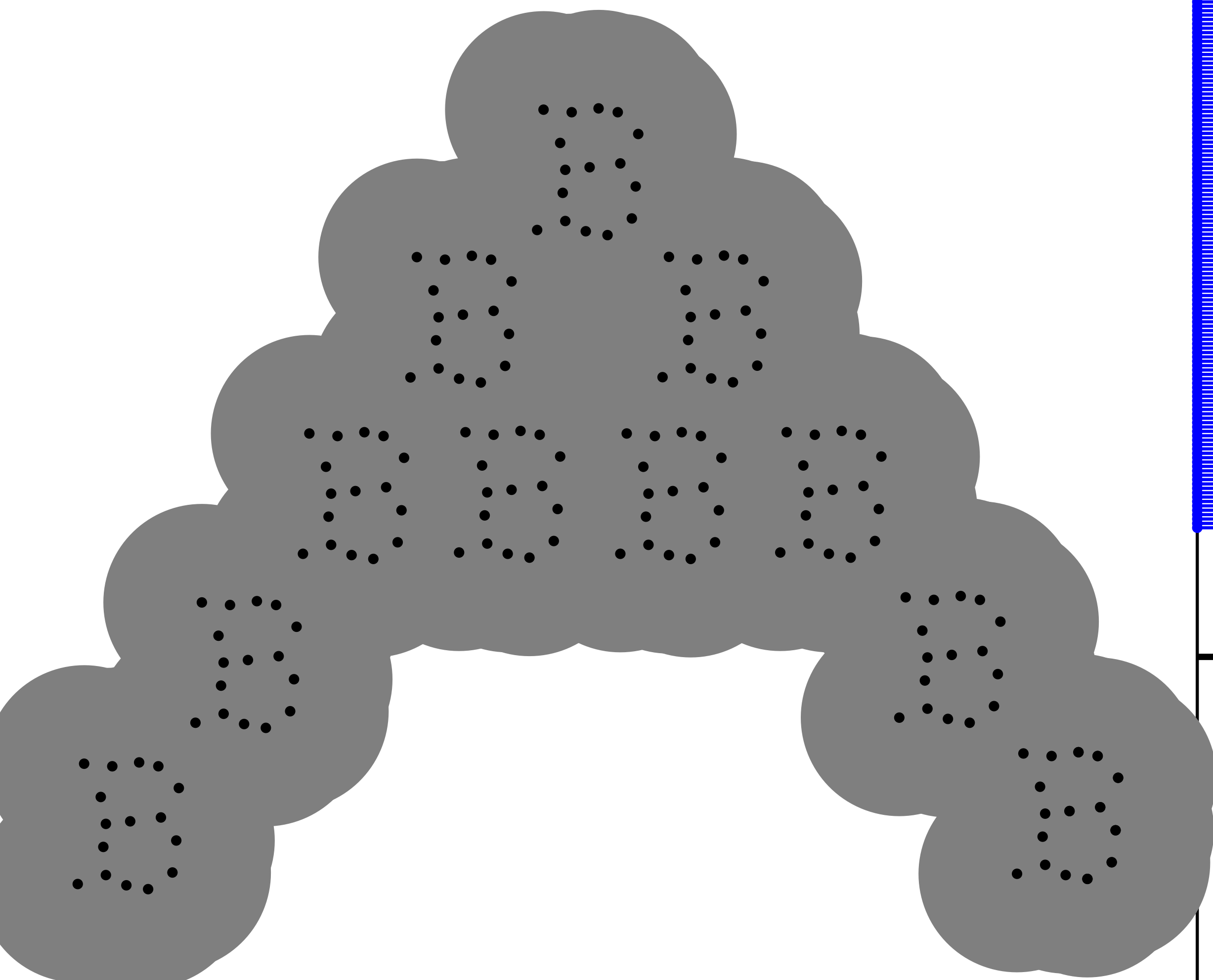
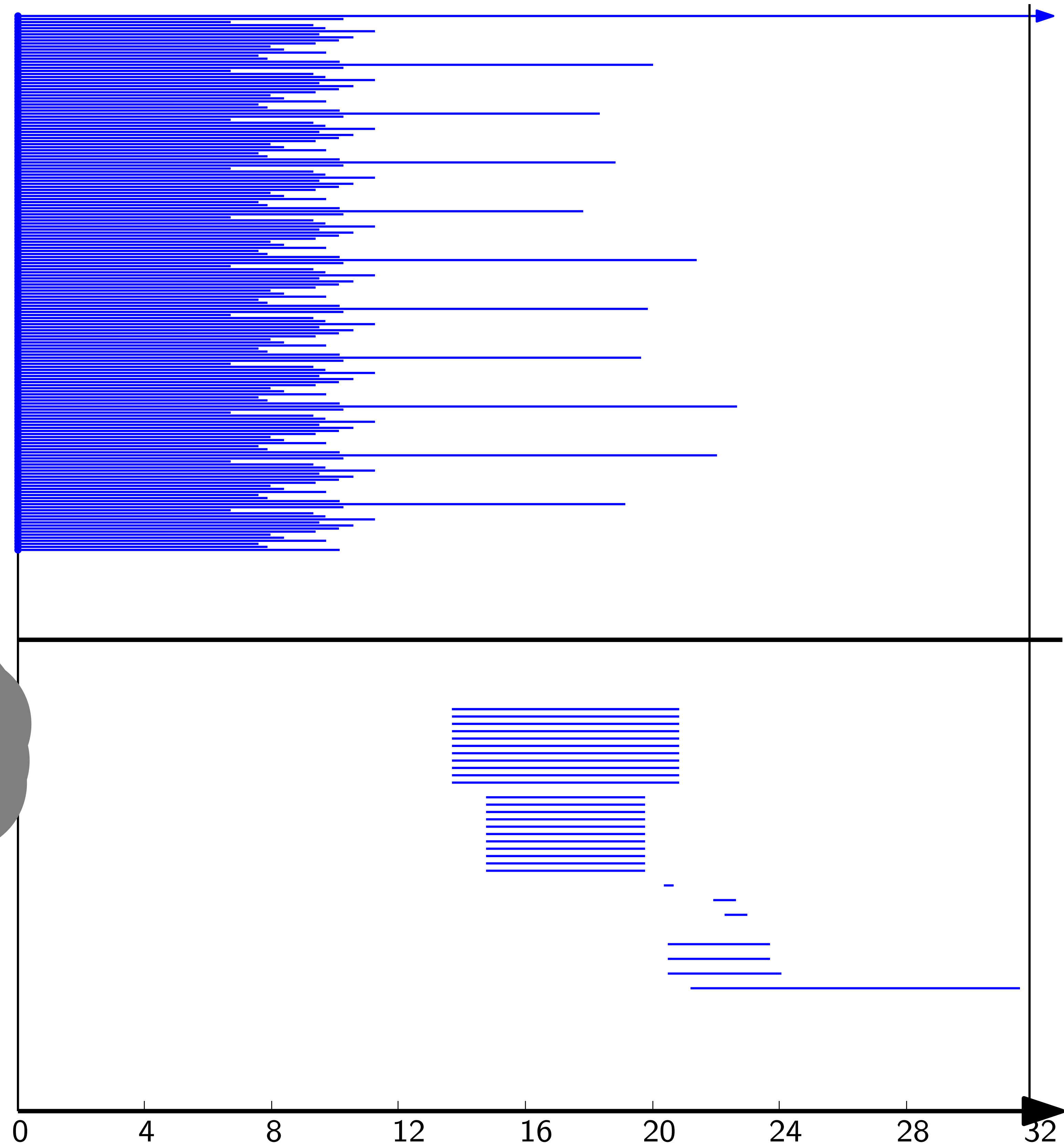
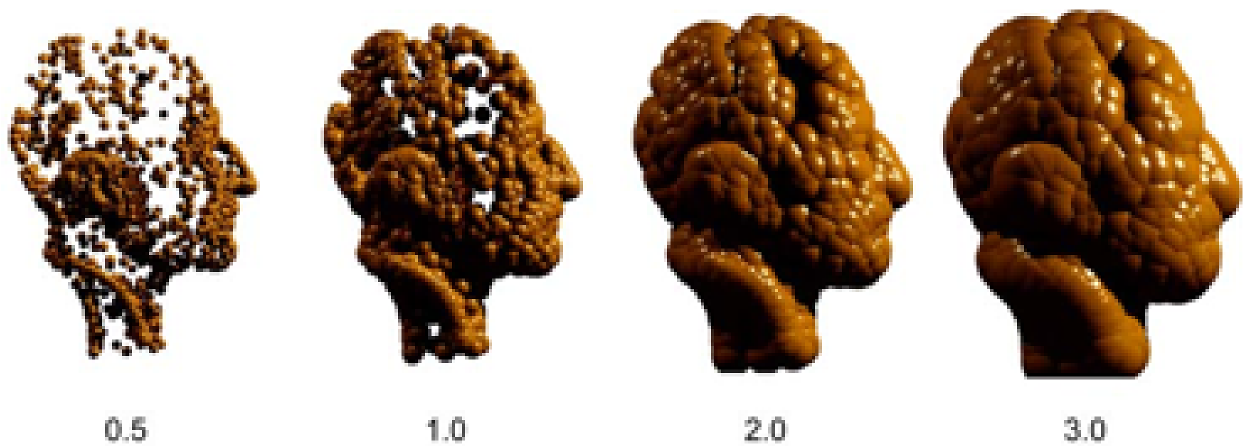




Vanilla pipeline

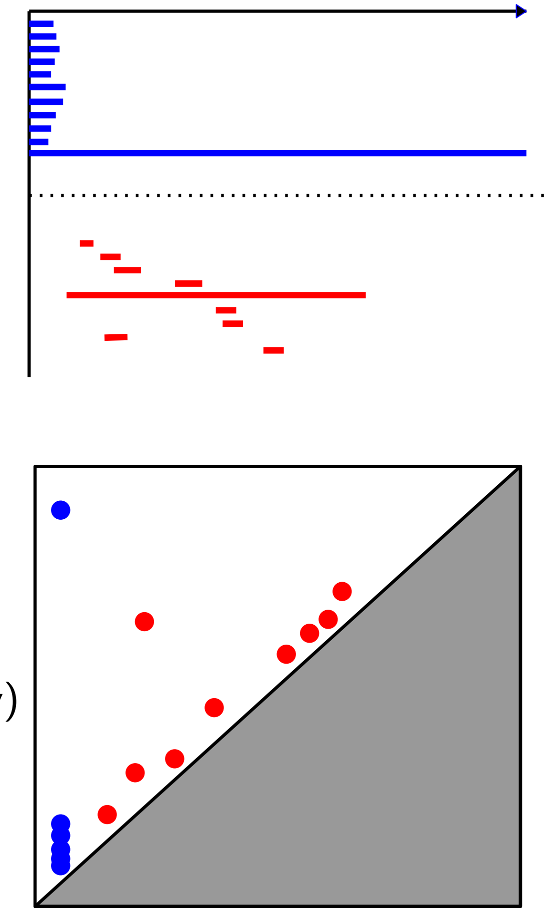
metric space (P, d)

$\Longrightarrow$ (geometry)



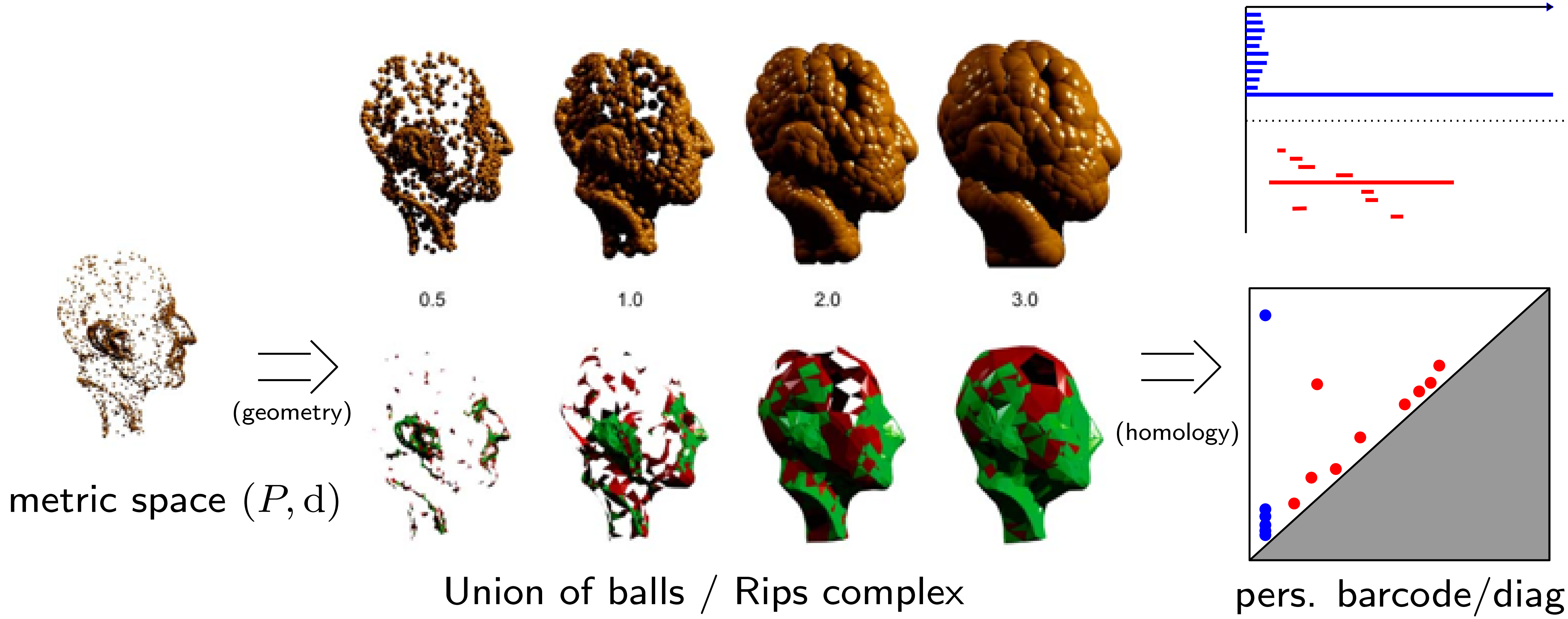
Union of balls

$\Longrightarrow$ (homology)



pers. barcode/diag.

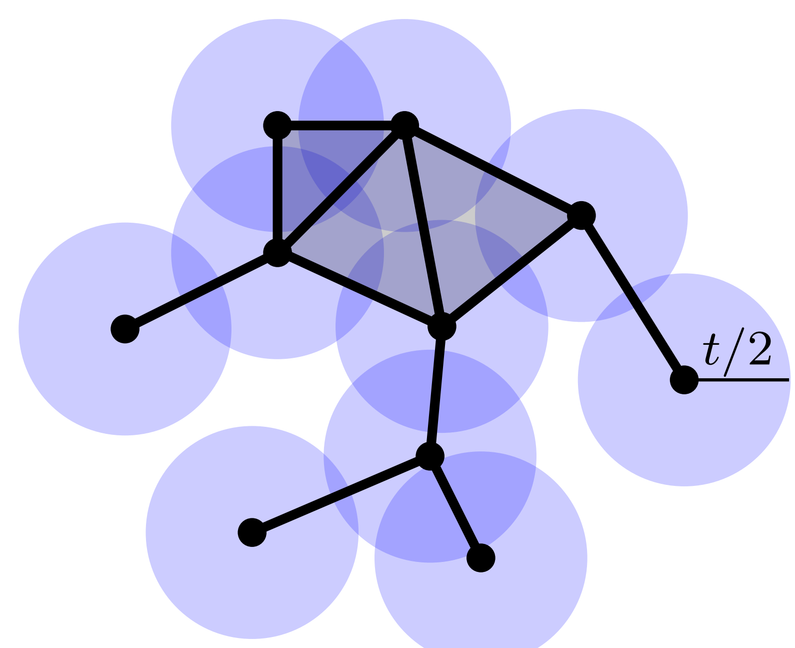
Vanilla pipeline



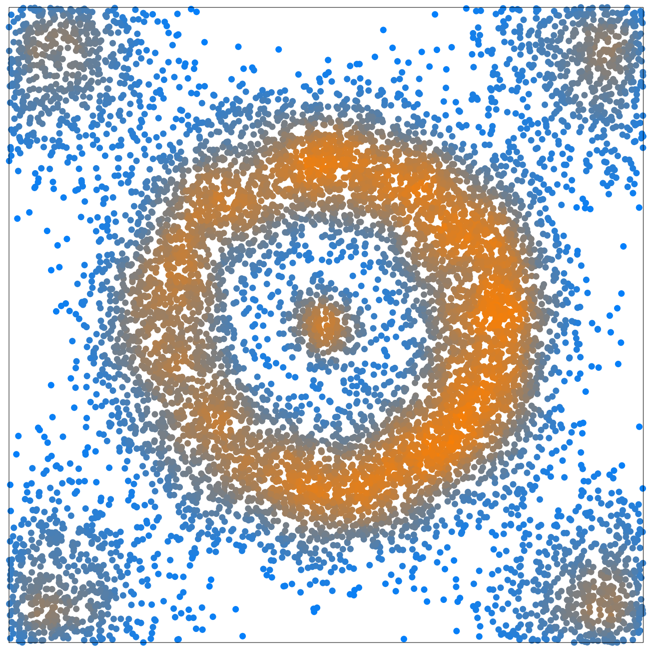
$$X = 2^P \setminus \{\emptyset\}$$

$$f : \sigma = \{p_0, \cdots, p_k\} \mapsto \max_{1 \leq i < j \leq k} \mathrm{d}(p_i, p_j)$$

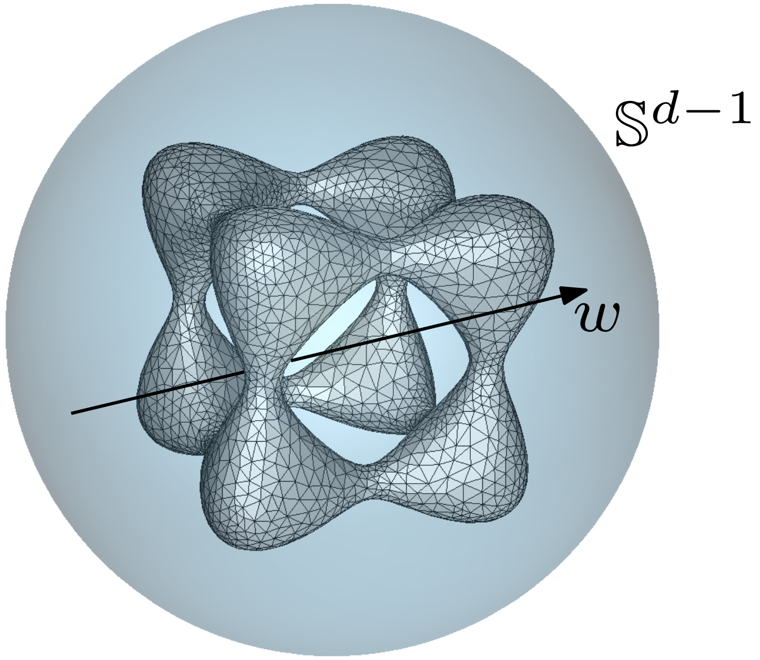
Rips filtration $\mathcal{R}(P)$: $R_t(P) := f^{-1}((-\infty, t])$



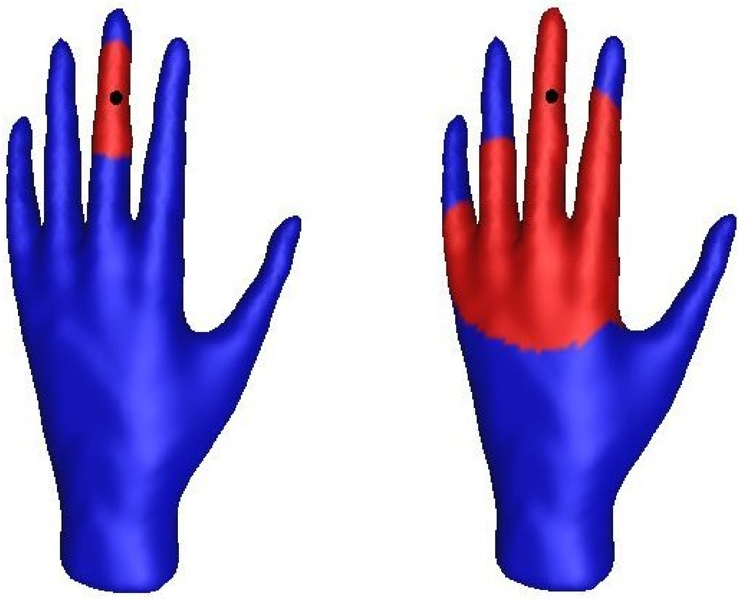
Many variants (filters, topological constructions, approximations)



density estimators



projections

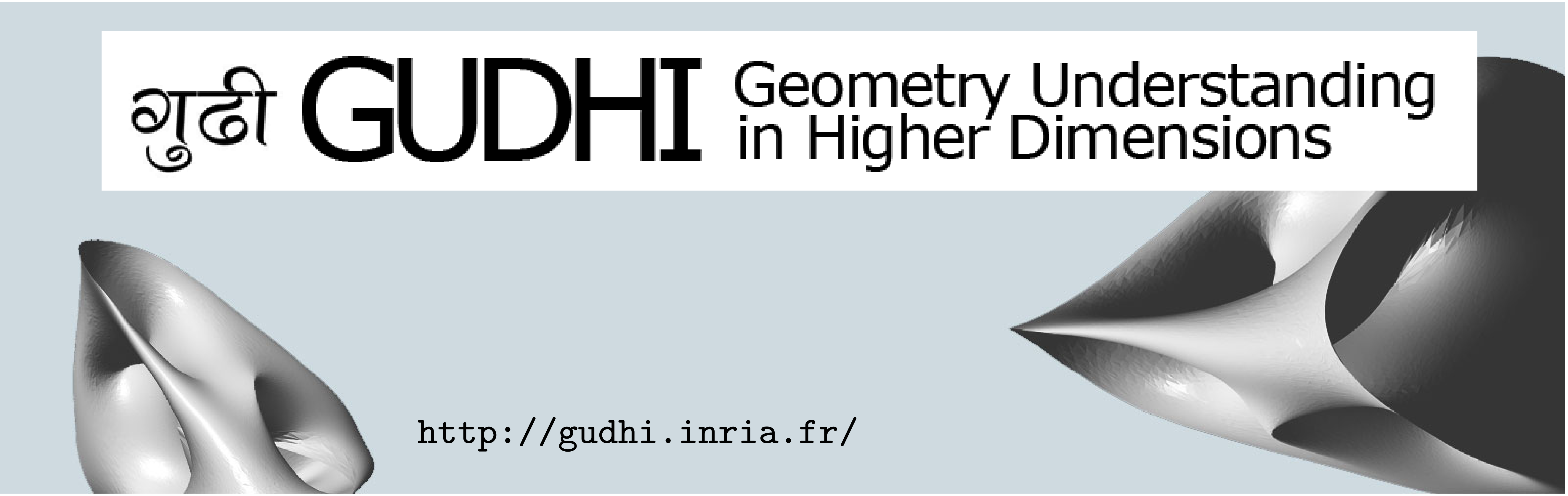


single-source distances

others:

- non-linear projections
- curvature measures
- PDE solutions (heat, wave)
- etc.

Software



- reference library in TDA (encompasses all aspects)
- 60k downloads in the last 12 months
- developers community, editorial board
- competitors (specialized on specific aspects of the TDA pipeline):

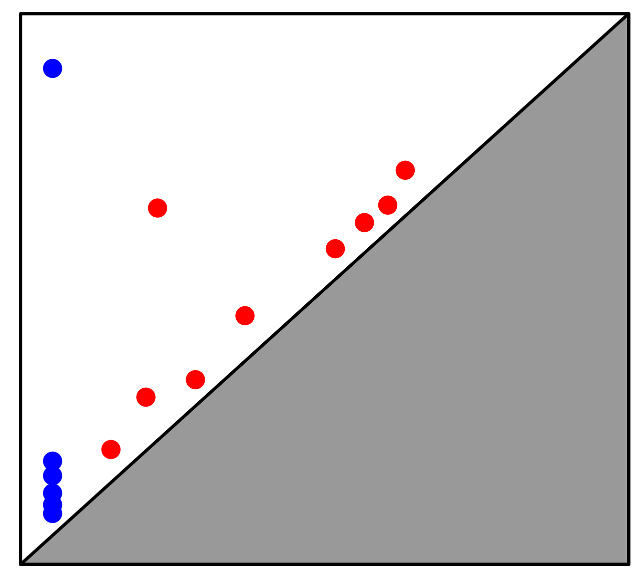
  DIONYSUS, PHAT, DIPHA, RIPSER, EIRENE

The problem

compact metric space

persistence barcode/diagram

Lipschitz op (filter)

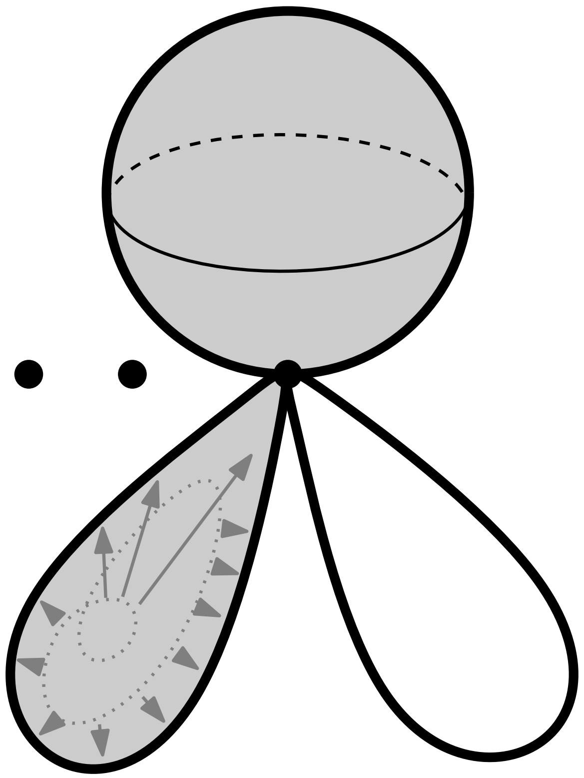


right inverse: realize barcode as the PH of some isom. class

left inverse: characterize isometry class uniquely

Right inverses for Topological Persistence

Fact: [Moore spaces] Any finitely generated Abelian group can be realized as the (reduced) homology of some topological space.

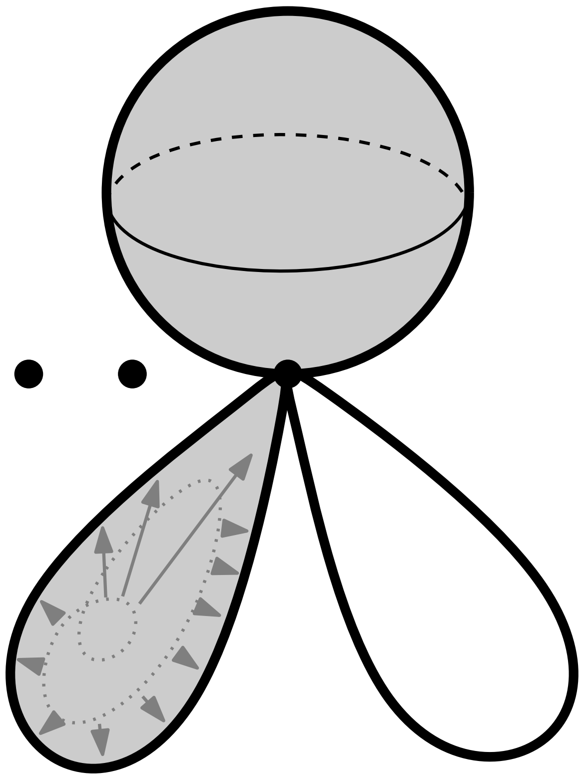


bouquets of spheres

Right inverses for Topological Persistence

Fact: [Moore spaces] Any finitely generated Abelian group can be realized as the (reduced) homology of some topological space.

Thm: Any locally finite point cloud in $\mathbb{R}^2$ can be realized as the (extended) persistence diagram of some function on a topological space.



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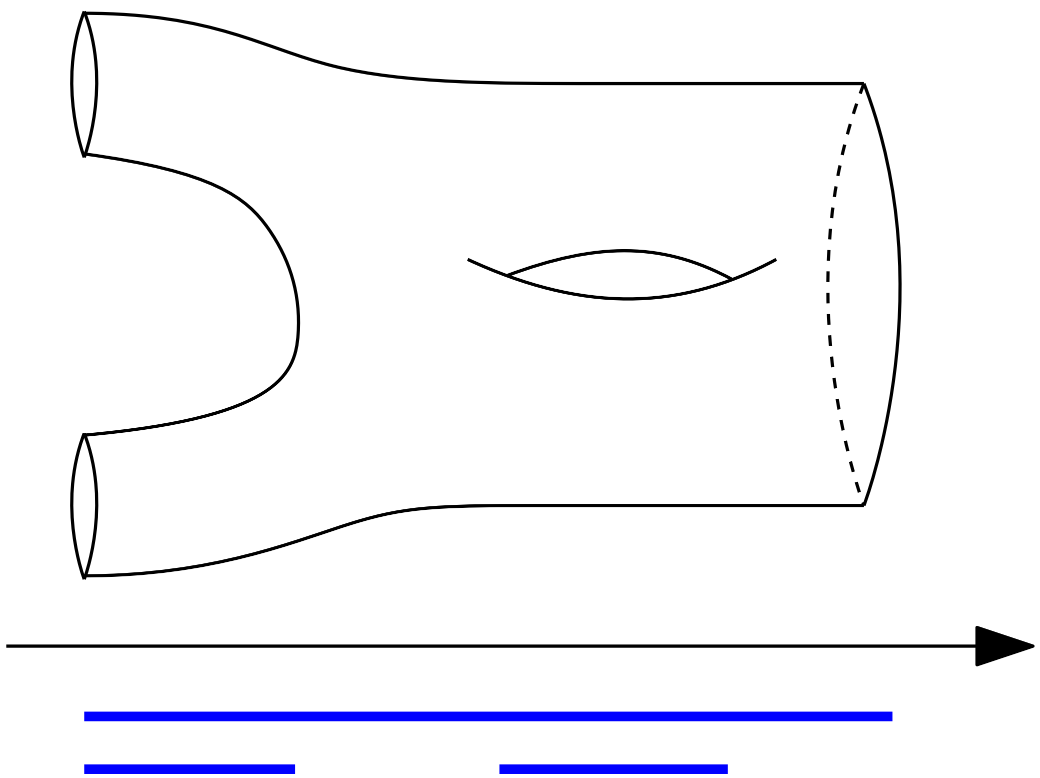


handlebody theory

Local right inverses

point cloud Rips filtration barcode

Local right inverses

point cloud Rips filtration barcode

$P \in \mathbb{R}^{nd}$ $\longmapsto$ $v \in \mathbb{R}^{2m+n}$

ordered point clouds
with n points in $\mathbb{R}^d$

ordered barcodes
with m bounded and
n unbounded intervals
($\nexists$ **smooth structure on** Bar)

Local right inverses

point cloud Rips filtration barcode

$$P \in \mathbb{R}^{nd} \longmapsto v \in \mathbb{R}^{2m+n}$$

Thm: [Gameiro, Hiraoka, Obayashi '16]

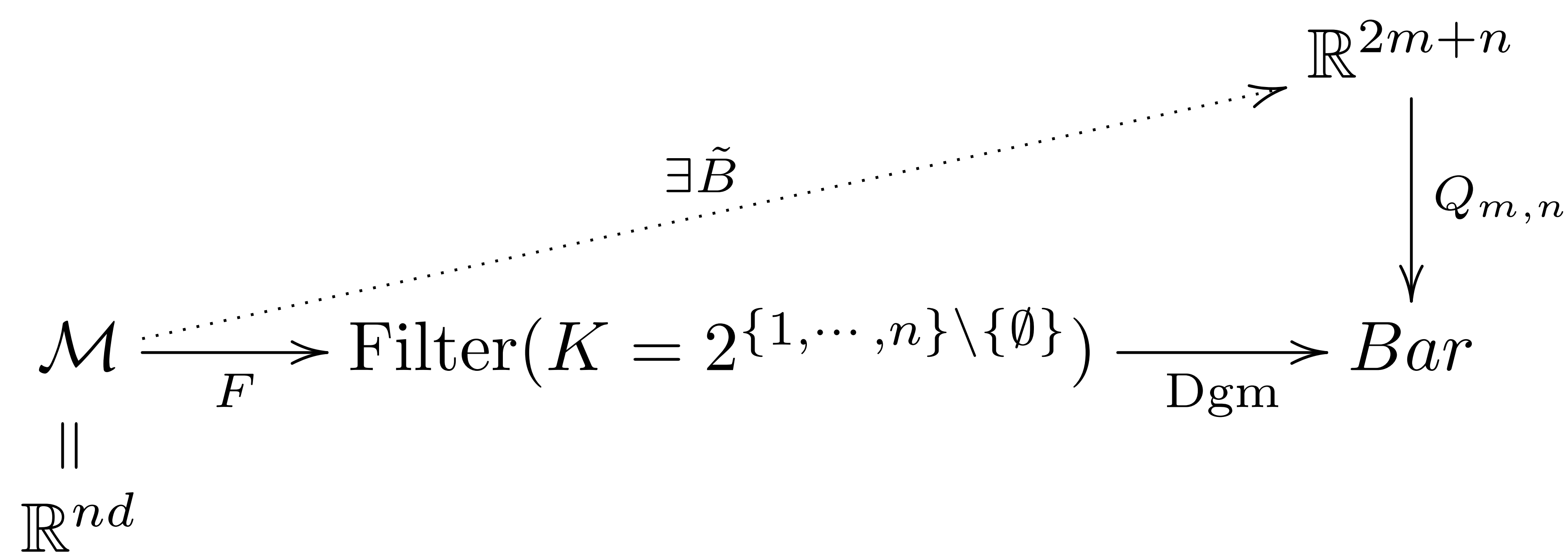
(i) *Generic* point cloud $\Rightarrow \exists U \ni P$ in $\mathbb{R}^{nd}$ over which the mapping $P \mapsto v$ can be extended to a function $\tilde{B} : U \to \mathbb{R}^{2m+n}$ computing ordered barcodes.

(ii) For U small enough, $\tilde{B}$ is of class C^∞.

Observation: order of distances is constant in small enough U.

Local right inverses

Local lift:



Thm: [Gameiro, Hiraoka, Obayashi '16]

(i) *Generic* point cloud $\Rightarrow \exists U \ni P$ in $\mathbb{R}^{nd}$ over which the mapping $P \mapsto v$ can be extended to a function $\tilde{B} : U \to \mathbb{R}^{2m+n}$ computing ordered barcodes.

(ii) For U small enough, $\tilde{B}$ is of class C^{∞}.

Observation: order of distances is constant in small enough U.

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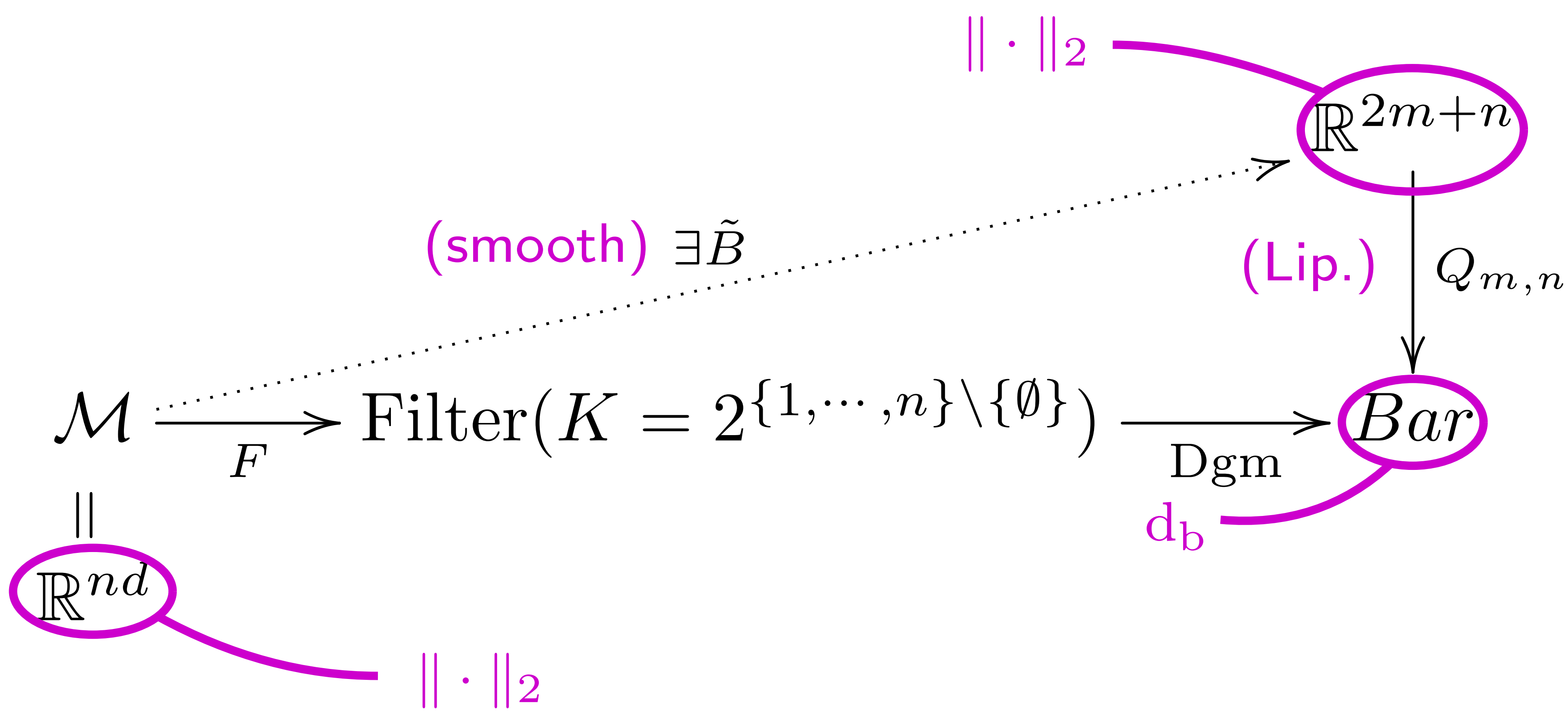

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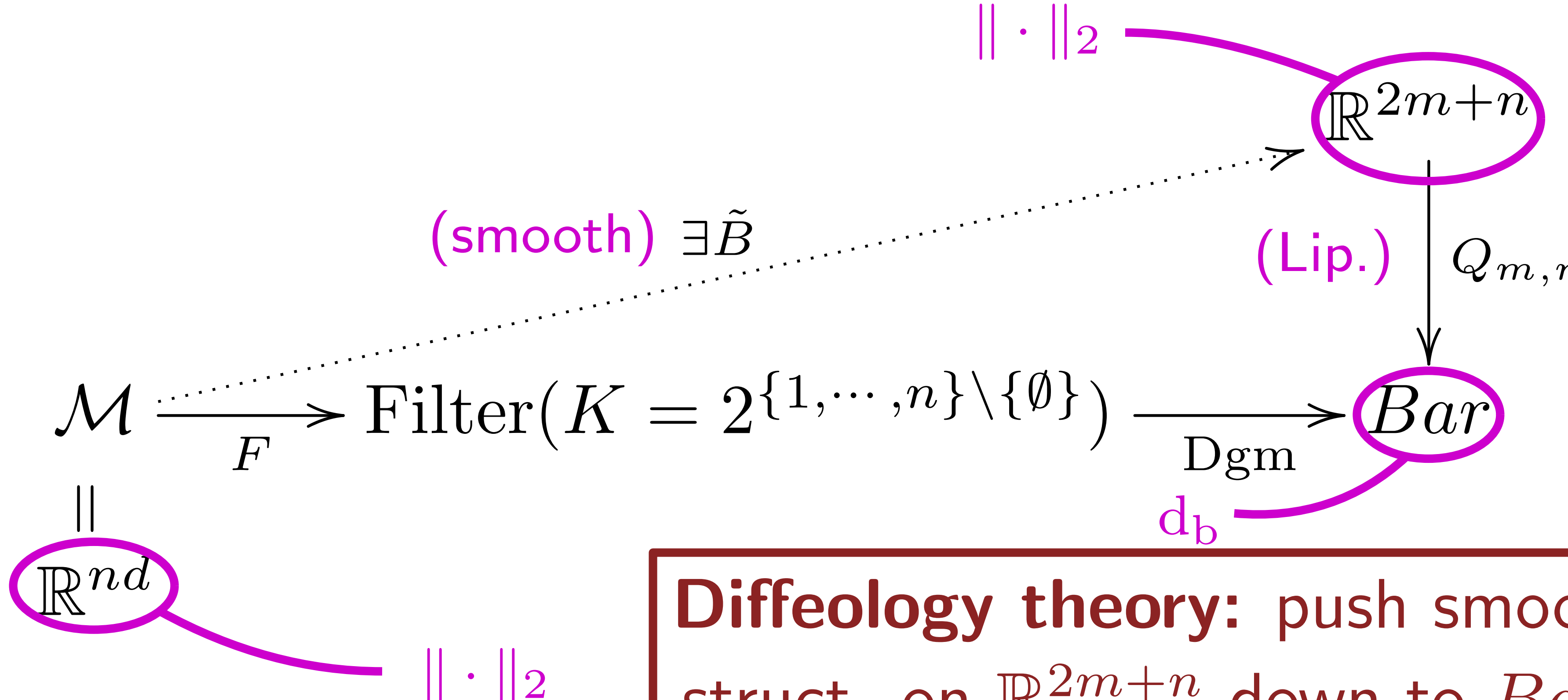

Diffeology theory: push smooth struct. on $\mathbb{R}^{2m+n}$ down to Bar

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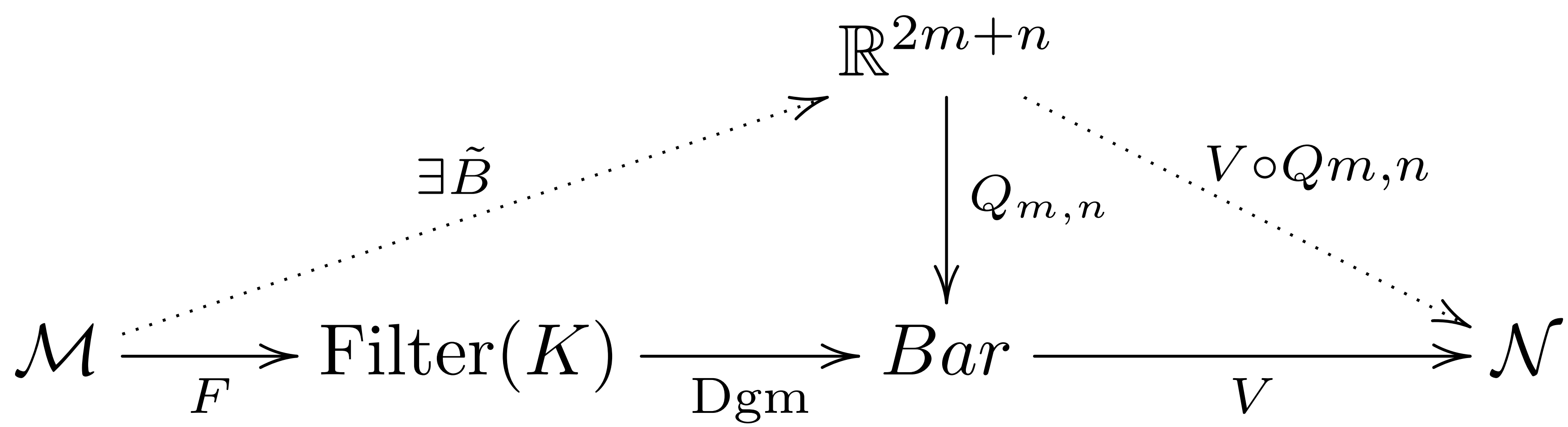


Thm: [Leygonie, O., Tillmann '19]

If F is C^r on some generic subset of $\mathcal{M}$, then so is $\text{Dgm} \circ F$.

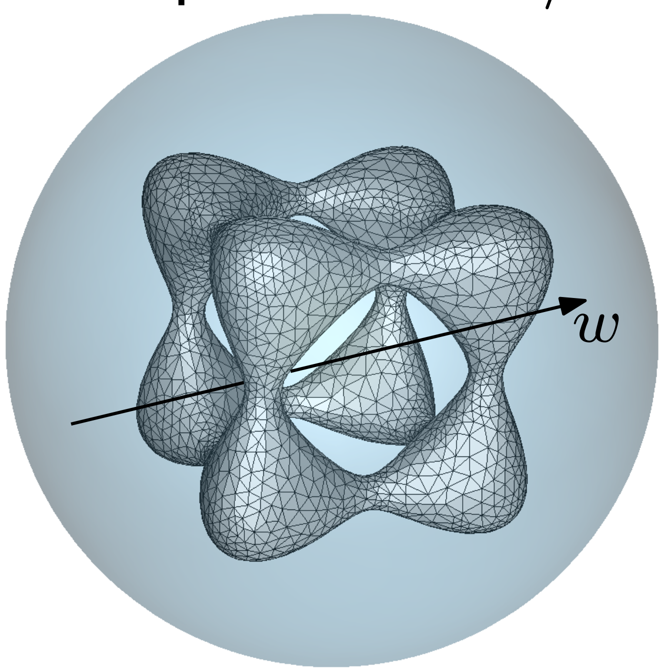
Prop: [Chain Rule]

If $\text{Dgm} \circ F$ and V are r-differentiable, then $V \circ \text{Dgm} \circ F$ is C^r and $d_\theta(V \circ \text{Dgm} \circ F) = d_{\tilde{B}(\theta)}(V \circ Q_{m,n}) \circ d_\theta \tilde{B}$ is independent of lift

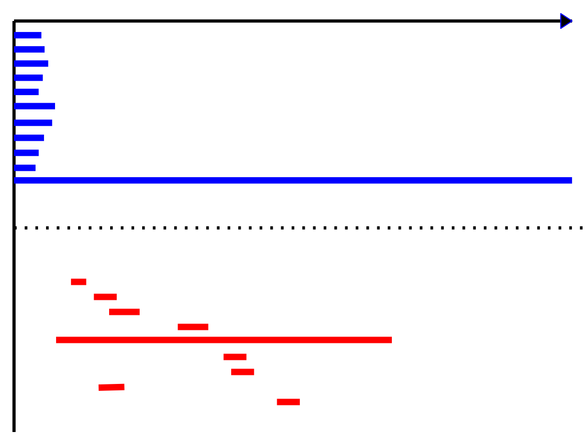
Local right inverses

Applications:

Optimization / ML: (gradient back-propagation)



$\Longrightarrow$



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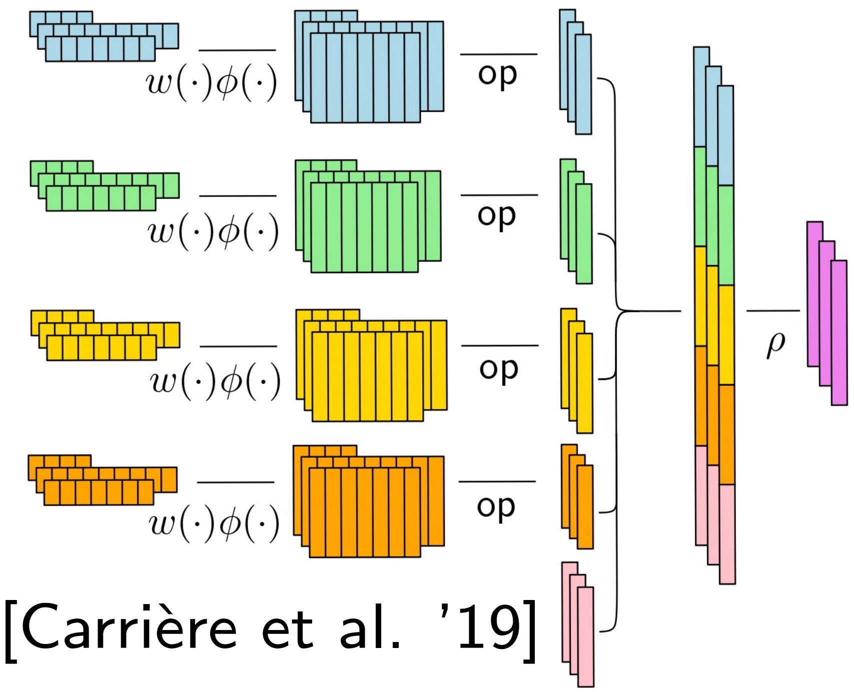

[Carrière et al. '19]

Local right inverses

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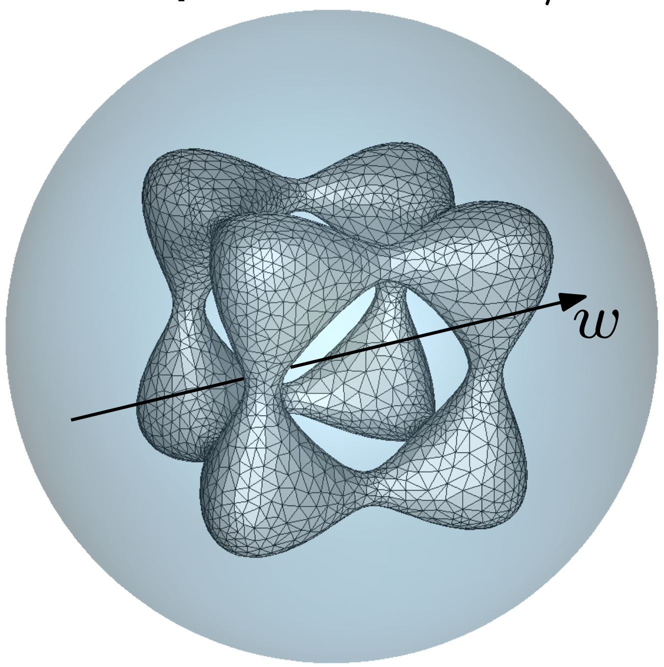
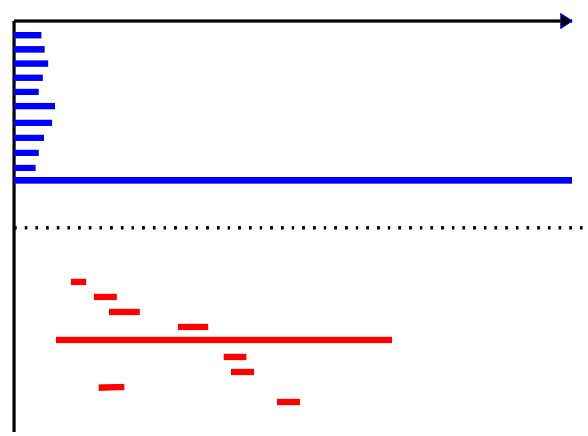
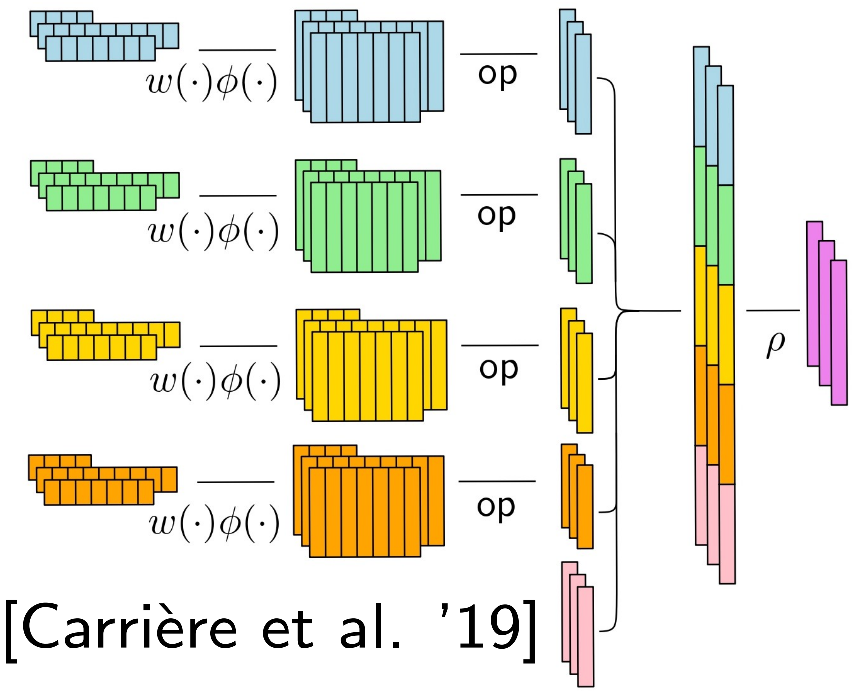
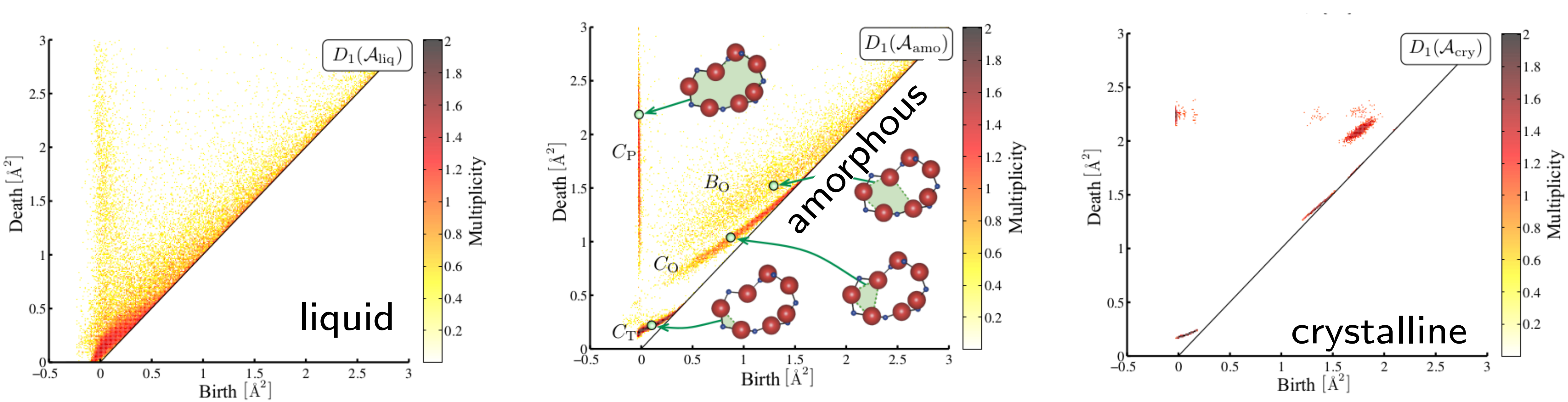






[Carrière et al. '19]

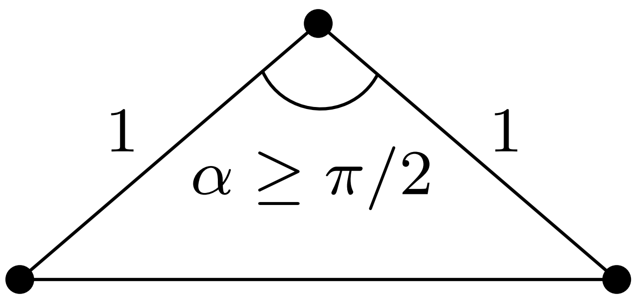
Continuation / inverse problems: (Newton-Raphson)



[Nakamura et al. '15]

Left inverses?

- distance functions



$$\operatorname{Dgm} \mathcal{R}(P) = \{(0, +\infty)\} \sqcup \{(0, 1)\} \sqcup \{(0, 1)\}$$

$\Rightarrow$ diagrams for different values of α are indistinguishable

Left inverses?

- distance functions

Prop: For any *metric tree* (P, d):

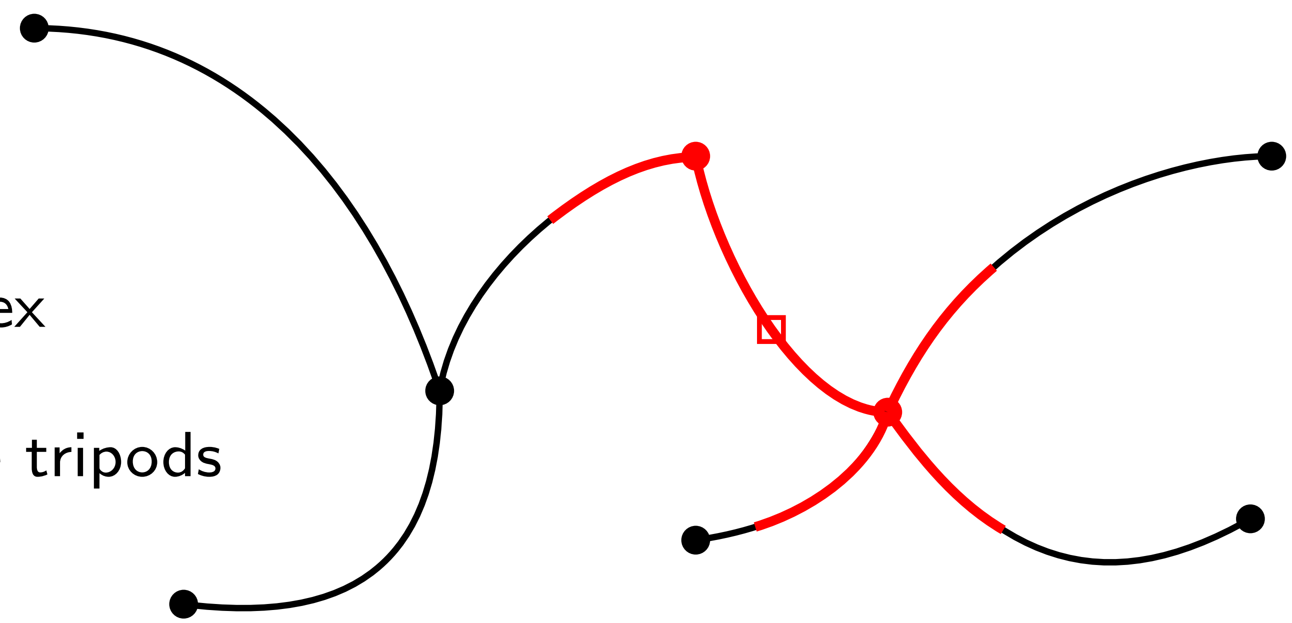
$$\mathrm{Dgm}\, \mathcal{R}(P) = \{(0, +\infty)\}$$

$\Rightarrow$ no information on the metric

X is 0-hyperbolic

$\Rightarrow$ metric balls are convex

$\Rightarrow$ geodesic triangles are tripods



Left inverses?

- distance functions

Prop: For any *metric tree* (P, d):

$$\mathrm{Dgm}\,\mathcal{R}(P) = \{(0, +\infty)\}$$

$\Rightarrow$ no information on the metric

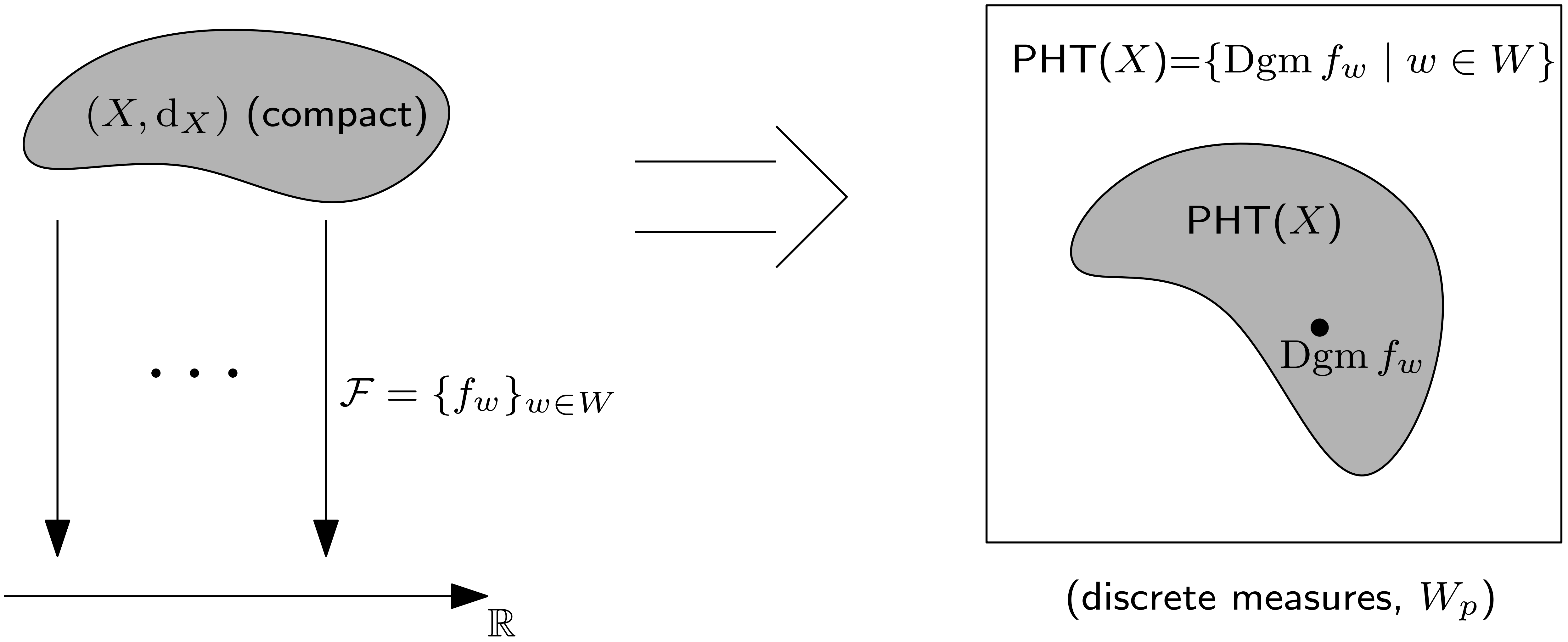
- real-valued functions

Prop: For any $f : X \to \mathbb{R}$ and $h : Y \to X$ homeomorphism:

$$\mathrm{Dgm}\, f \circ h = \mathrm{Dgm}\, f$$

$\Rightarrow$ Invariance under homeomorphisms, not just isometries

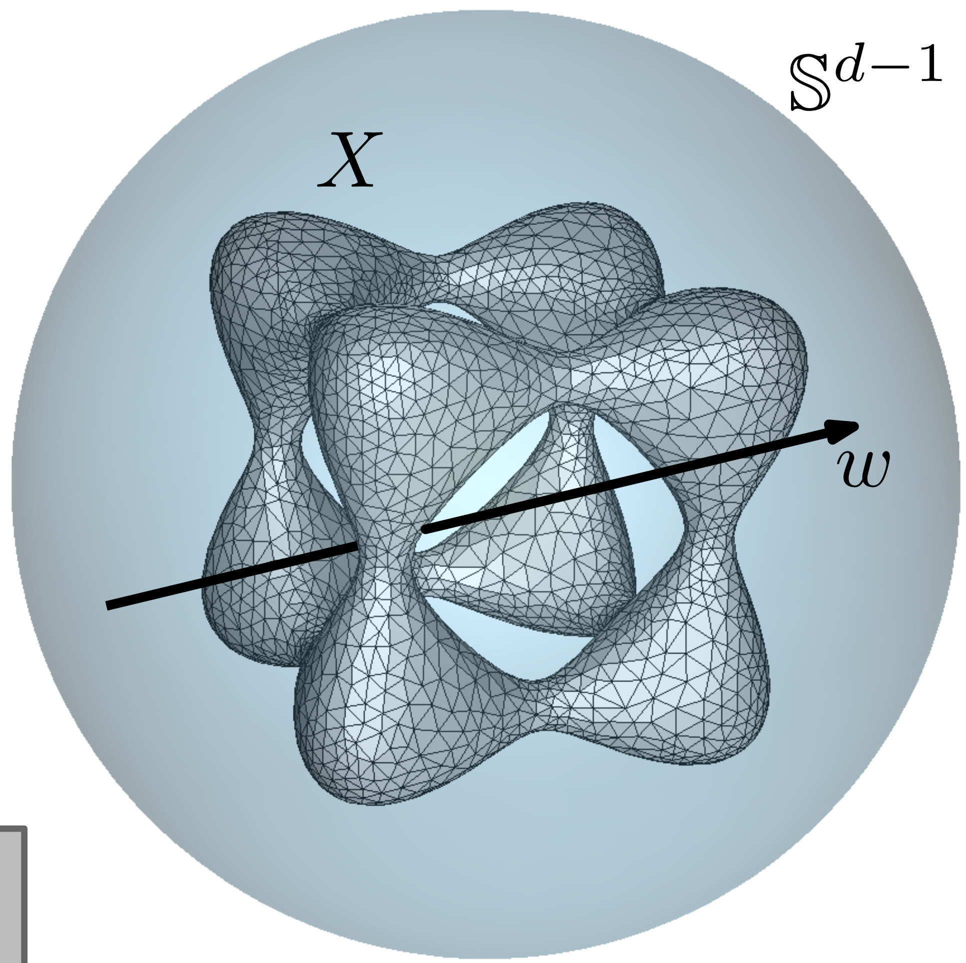
Persistent Homology Transform (PHT)



PHT for compact subanalytic sets in $\mathbb{R}^d$

Focus: compact subanalytic sets in $\mathbb{R}^d$

PHT: $\mathcal{F} = \{f_w\}_{w \in \mathbb{S}^{d-1}}$ where $f_w = \langle \cdot, w \rangle$



Thm: [Boyer, Curry, Mukherjee, Turner 2014, 2018] [Ghrist, Levanger, Mai 2018]
With $\mathcal{F} = \{\langle \cdot, w \rangle\}_{w \in \mathbb{S}^{d-1}}$, PHT is injective on the class of compact subanalytic sets in $\mathbb{R}^d$.

Still true for a finite ($O(2^d)$) set of directions if we restrict to geometric simplicial complexes.

PHT for compact subanalytic sets in $\mathbb{R}^d$

Formalism: $M \subset \mathbb{R}^d$ $\rightsquigarrow$ $\mathbb{1}_M : \mathbb{R}^d \to \mathbb{Z}$

compact subanalytic constructible

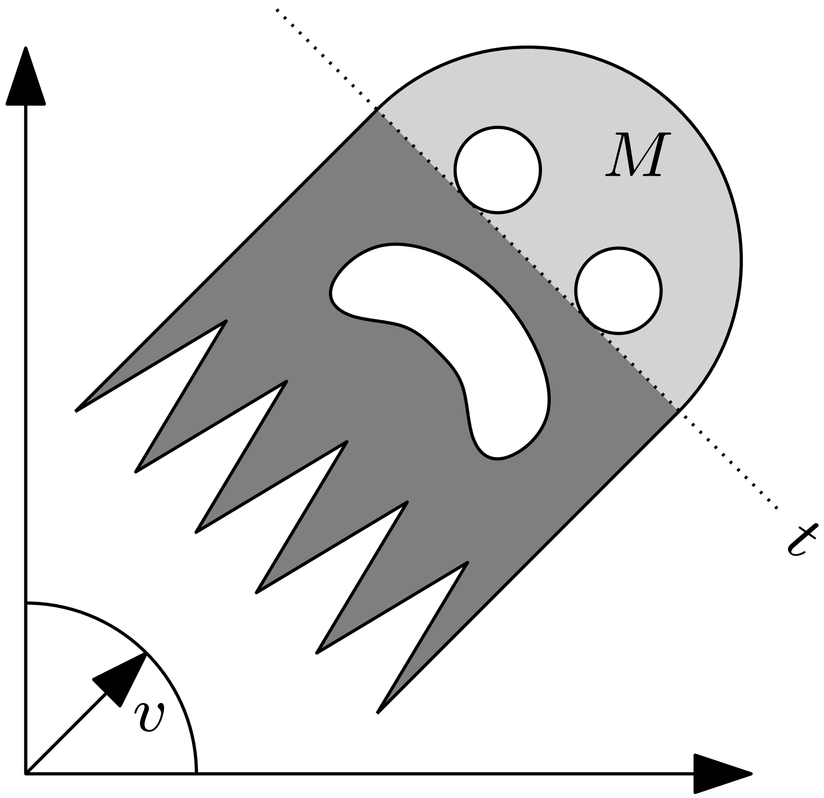
PHT for compact subanalytic sets in $\mathbb{R}^d$

Formalism: $M \subset \mathbb{R}^d$ $\rightsquigarrow$ $\mathbb{1}_M : \mathbb{R}^d \to \mathbb{Z}$

compact subanalytic → constructible

$\mathrm{CF}(\mathbb{R}^d) \ni \mathbb{1}_M$ —PHT→ $(\mathbb{S}^{d-1} \to Bar)$

$\mathrm{CF}(\mathbb{R}^d) \ni \mathbb{1}_M$ —ECT→ $(\mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}))$



ECT$(\mathbb{1}_M)$:

$$\begin{array}{|l} \mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}) \\ v \longmapsto \left(t \mapsto \int \mathbb{1}_M \, \mathbb{1}_{x\cdot v \leq t} \, \mathrm{d}\chi = \chi(M \cap \{x \in \mathbb{R}^d \mid x \cdot v \leq t\})\right) \end{array}$$

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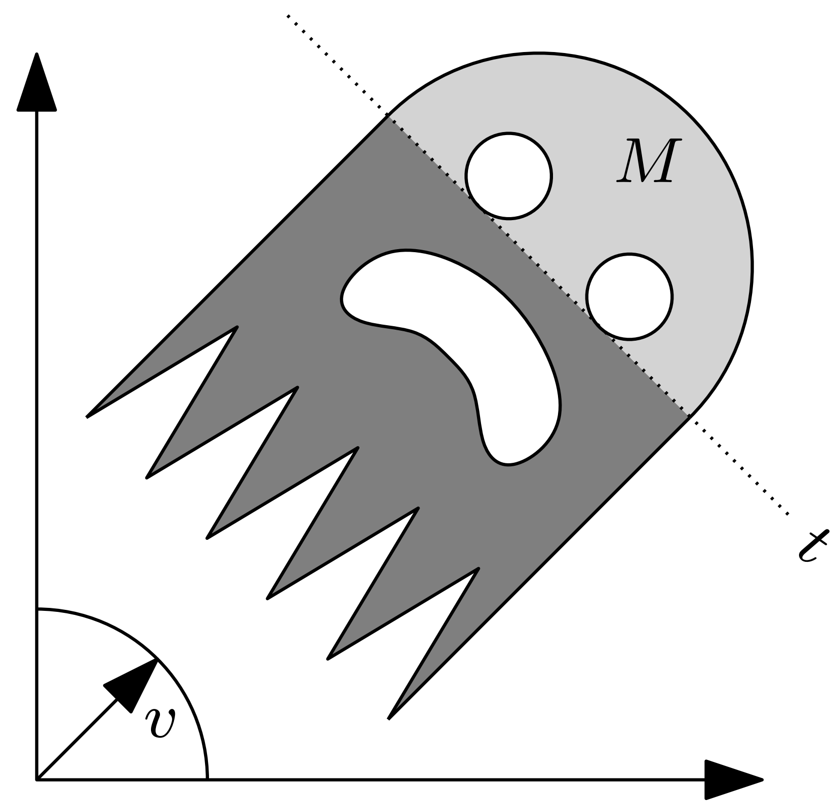
Formalism: $M \subset \mathbb{R}^d \rightsquigarrow \mathbb{1}_M : \mathbb{R}^d \to \mathbb{Z}$

compact subanalytic $\qquad$ constructible

$$\begin{array}{ccc} \mathrm{CF}(\mathbb{R}^d) & \xrightarrow{\text{PHT}} & (\mathbb{S}^{d-1} \to Bar) \\ \cup & \searrow^{\text{ECT}} & \downarrow \pi \\ \mathbb{1}_M & & (\mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R})) \end{array}$$



$$\text{ECT}(\mathbb{1}_M) : \left| \begin{array}{l} \mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}) \\ v \longmapsto \left(t \mapsto \int \mathbb{1}_M \, \mathbb{1}_{x \cdot v \leq t} \, \mathrm{d}\chi = \chi(M \cap \{x \in \mathbb{R}^d \mid x \cdot v \leq t\}) \right) \end{array} \right.$$

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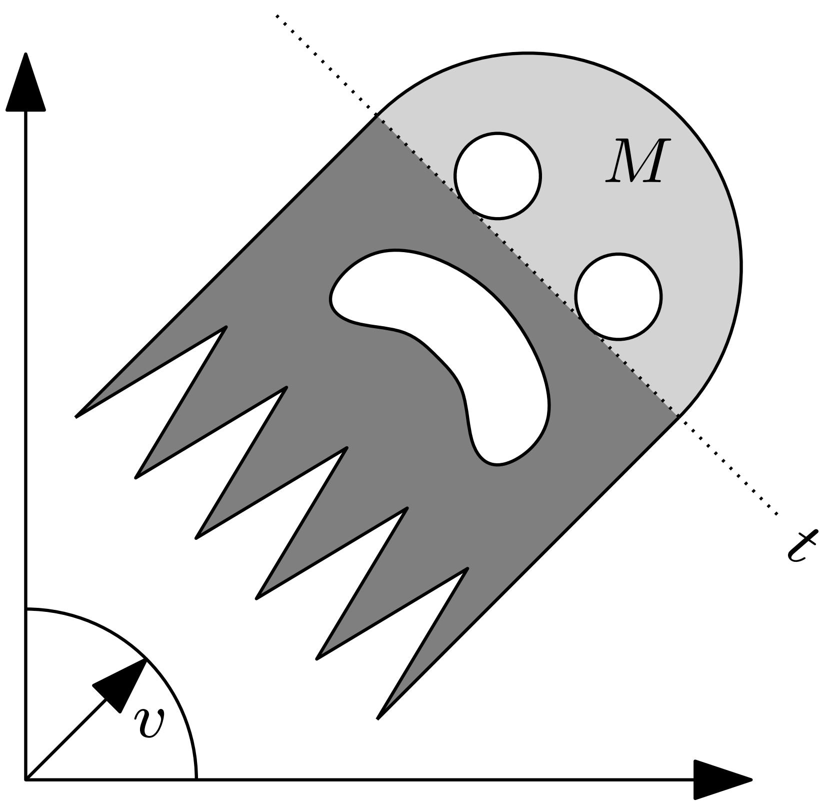
compact subanalytic $\quad$ constructible

$$\mathrm{CF}(\mathbb{R}^d) \ni \mathbb{1}_M \xrightarrow{\text{PHT}} (\mathbb{S}^{d-1} \to Bar) \xrightarrow{\pi} (\mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}))$$

$$\mathrm{CF}(\mathbb{R}^d) \xrightarrow{\text{ECT}} (\mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}))$$



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Thm: For $\mathbb{1}_M, \mathbb{1}_N \in \mathrm{CF}(\mathbb{R}^d)$: $\text{ECT}(\mathbb{1}_M) = \text{ECT}(\mathbb{1}_N) \Rightarrow \mathbb{1}_M = \mathbb{1}_N$

PHT for compact subanalytic sets in $\mathbb{R}^d$

Formalism: $M \subset \mathbb{R}^d$ (compact subanalytic) $\rightsquigarrow$ $\mathbb{1}_M : \mathbb{R}^d \to \mathbb{Z}$ (constructible)

$$\mathrm{CF}(\mathbb{R}^d) \xrightarrow{\text{PHT}} (\mathbb{S}^{d-1} \to Bar)$$

$$\mathrm{CF}(\mathbb{R}^d) \ni \mathbb{1}_M$$

$$(\mathbb{S}^{d-1} \to Bar) \xrightarrow{\pi} (\mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}))$$

$$\mathrm{CF}(\mathbb{R}^d) \xrightarrow{\text{ECT}} (\mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}))$$

Radon transform

$\mathrm{CF}(\mathbb{R}^d) \to \mathrm{CF}(\mathrm{AffGr}_d)$

inversion theorem

[Schapira 1995]

$$\mathsf{ECT}(\mathbb{1}_M) : \left| \begin{array}{l} \mathbb{S}^{d-1} \to \mathrm{CF}(\mathbb{R}) \\ v \longmapsto \left(t \mapsto \int \mathbb{1}_M \, \mathbb{1}_{x\cdot v \le t} \, \mathrm{d}\chi = \chi(M \cap \{x \in \mathbb{R}^d \mid x \cdot v \le t\}) \right) \end{array} \right.$$

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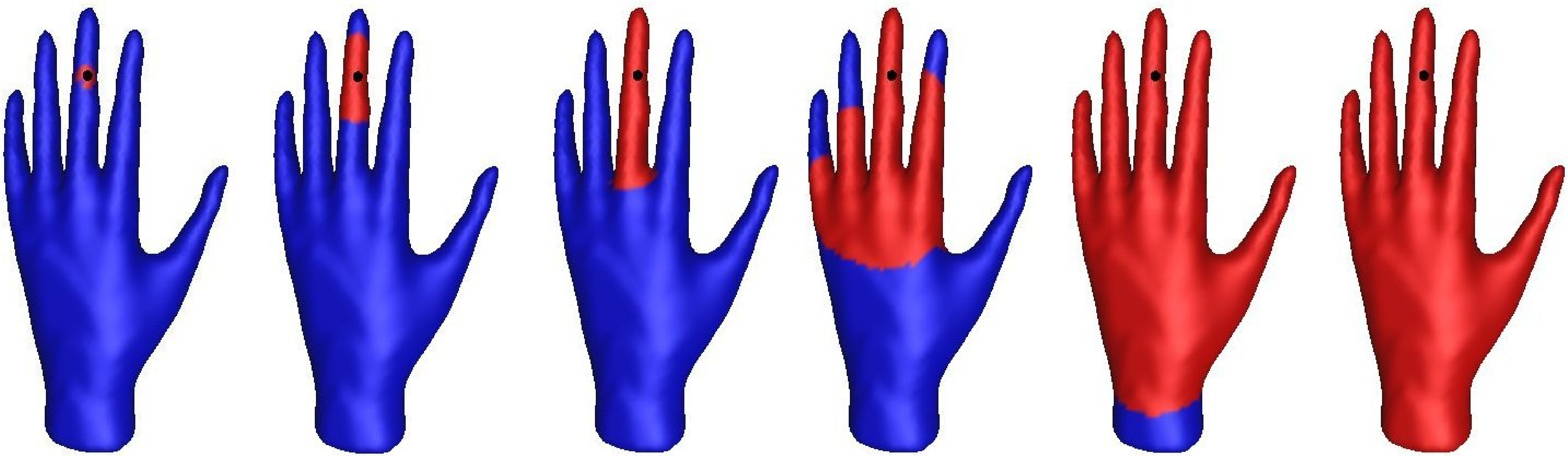
PHT for compact length spaces

Focus: compact length spaces (X, d_X)

PHT: $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$



PHT for metric graphs

Focus: compact metric graphs (1-dimensional stratified length spaces)

PHT: $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$

Thm (stability): [Dey, Shi, Wang 2015]
For any compact metric graphs X, Y,

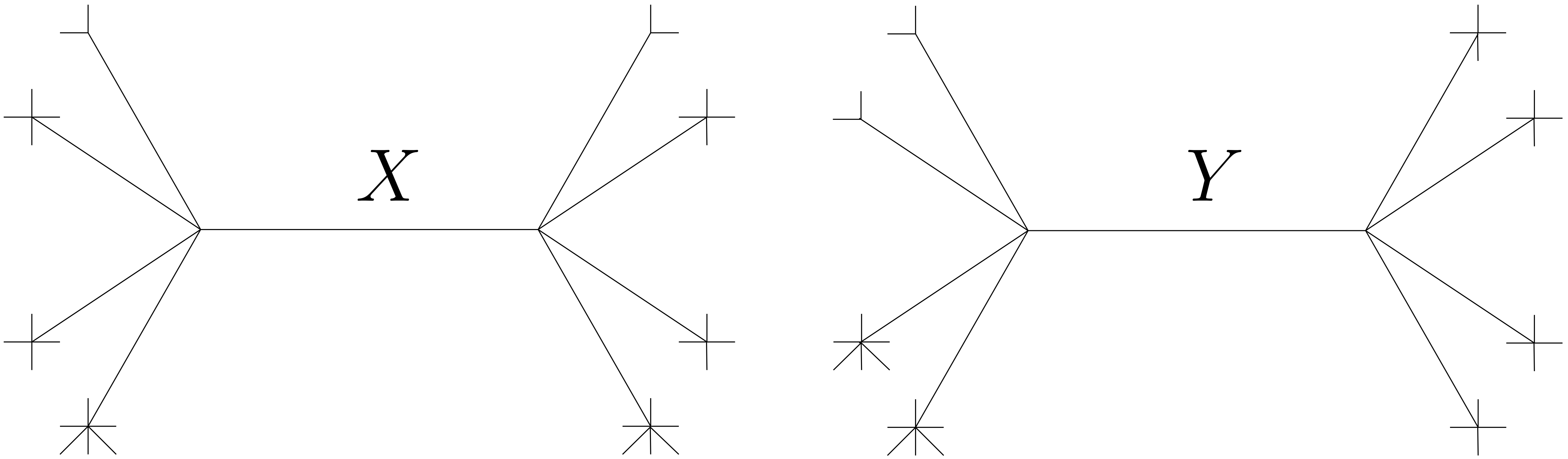
$$\mathrm{d}_{\mathrm{H}}(\mathsf{PHT}(X), \mathsf{PHT}(Y)) \leq 18\, \mathrm{d}_{\mathrm{GH}}(X, Y).$$

Thm (density): [Gromov]
Compact metric graphs are GH-dense among the compact length spaces.

Q: injectivity of PHT on metric graphs?

PHT for metric graphs

Bad news: PHT is not injective on all compact metric graphs



$$\text{PHT}(X) = \text{PHT}(Y) \text{ while } X \not\simeq Y$$

PHT for metric graphs

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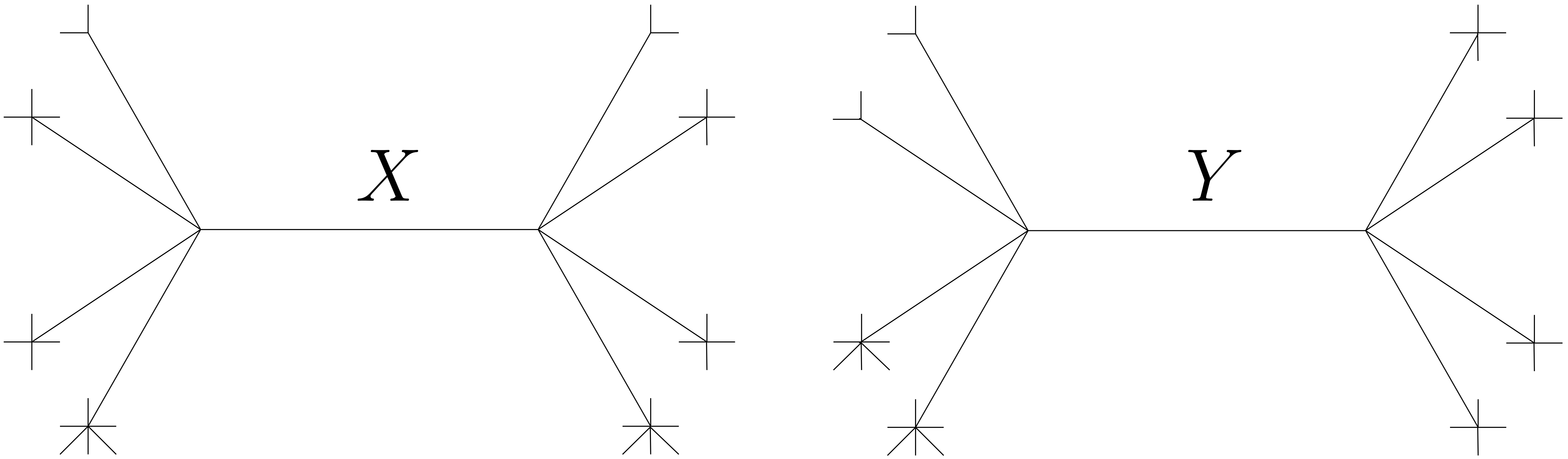

$\mathsf{PHT}(X) = \mathsf{PHT}(Y)$ while $X \not\simeq Y$

Note: $\mathrm{Aut}(X)$ is non-trivial, hence $\Psi_X : x \mapsto \mathrm{Dgm}\, \mathrm{d}_X(\cdot, x)$ is not injective

PHT for metric graphs

Let $\mathsf{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

Thm: (injectivity) [O., Solomon '18]

- PHT is GH-*locally* injective on compact metric graphs.
- PHT is injective on Inj_Ψ.
- Inj_Ψ is generic among the compact metric graphs.

$\Longrightarrow$ PHT is injective on a dense subset of the compact length spaces

PHT for compact metric measure spaces

Let (X, d, μ) be a compact metric (Borel) measure space

Distance kernel operator:

$$D^X : L^2(X) \to L^2(X)$$
$$(D^X f)(x) := \int_X f(y)\mathrm{d}(x,y)d\mu(y)$$

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Hilbert-Schmidt op. $\Rightarrow$ eigenvalues $|\lambda_1| \geq |\lambda_2| \geq \cdots$, assumed simple wlog

Choose unit eigenfunctions $\phi_1, \phi_2, \cdots$, such that $\langle \phi_i, |\phi_i| \rangle > 0$

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Mapping: $\Phi^X : X \to \mathbb{C}^\infty$

$$\Phi^X := (\sqrt{\lambda_1}\phi_1, \sqrt{\lambda_2}\phi_2, \cdots)$$

$\Phi^X_k := \Phi^X_{|\mathbb{C}^k}$

note:

$$\mathrm{d}(x,y) = \sum_{i\in\mathbb{N}} \lambda_i \phi_i(x)\phi_i(y)$$

$$= \sum_{i\in\mathbb{N}} \sqrt{\lambda_i}\phi_i(x)\sqrt{\lambda_i}\phi_i(y)$$

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Let (X, d, μ) be a compact metric (Borel) measure space

Thm: [Maria, O., Solomon '19] If μ is strictly positive on open sets, then $\Phi^X : X \to \mathbb{C}^\infty$ is a topological embedding

Thm: [Maria, O., Solomon '19] Let d, d' be metrics on X, and let μ, μ' be strictly positive measures on X such that μ is absolutely continuous w.r.t. μ'. Then,

$$\Phi^{(X,\mathrm{d},\mu)}(X) = \Phi^{(X,\mathrm{d}',\mu')}(X) \quad \Longrightarrow \quad \mathrm{d} = \mathrm{d}'$$

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Pb: the Euclidean PHT and ECT apply only to finite-dimensional spaces

PHT for compact metric measure spaces

Let (X, d, μ) be a compact metric (Borel) measure space

Fix $k \in \mathbb{N}$.

$\Phi_k^X : X \to \mathbb{C}^k \simeq \mathbb{R}^{2k}$ **may not be an embedding**... but it doesn't matter

PHT for compact metric measure spaces

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$X \mapsto \Phi^X$ **may not be injective**... but we can bound its fibers:

Thm: [Maria, O., Solomon '19] Assume $\Phi_k^X(X) = \Phi_k^Y(Y)$, under the same conditions as previously. Then, $\mathrm{d}_{\mathrm{GH}}(X, Y) \leq E_{X,k} + E_{Y,k}$, where $E_{X,k}$ measures the sup-norm difference between d and its order-k eigenfunction expansion $(x, y) \mapsto \sum_{i=1}^k \lambda_i \phi_i(x) \phi_i(y)$.

Cor: [Maria, O., Solomon '19] Assume $\Phi_k^X(X) = \Phi_k^Y(Y)$, where X, Y are finite or have finite non-zero spectrum. Then, under the same conditions as previously, and for k large enough, X and Y are isometric.

Thank you