Sophia-Antipolis, July 2018

Stable and Interpretable Features for Data using Topology

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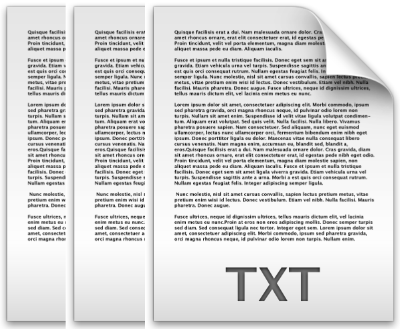
DataShape team, Inria Saclay

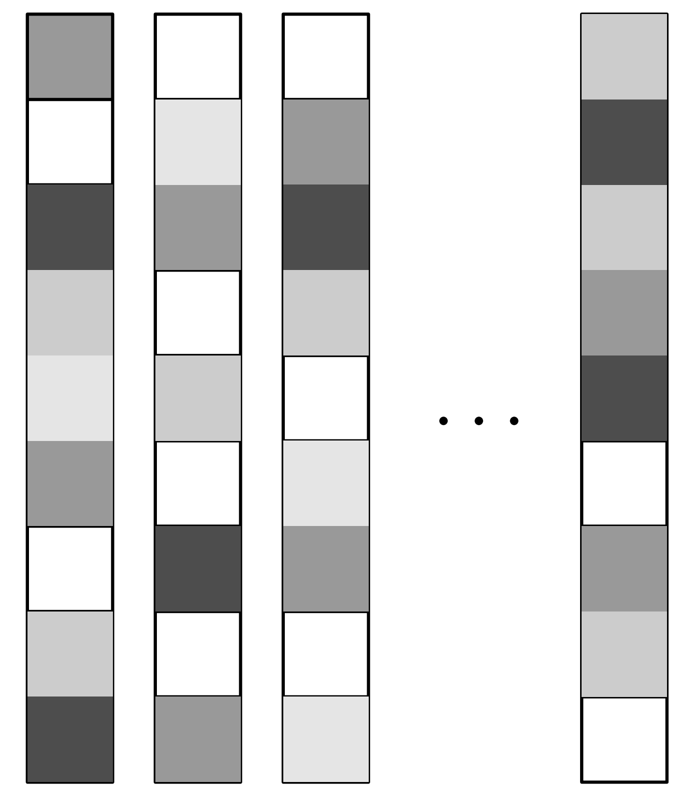
Features for data

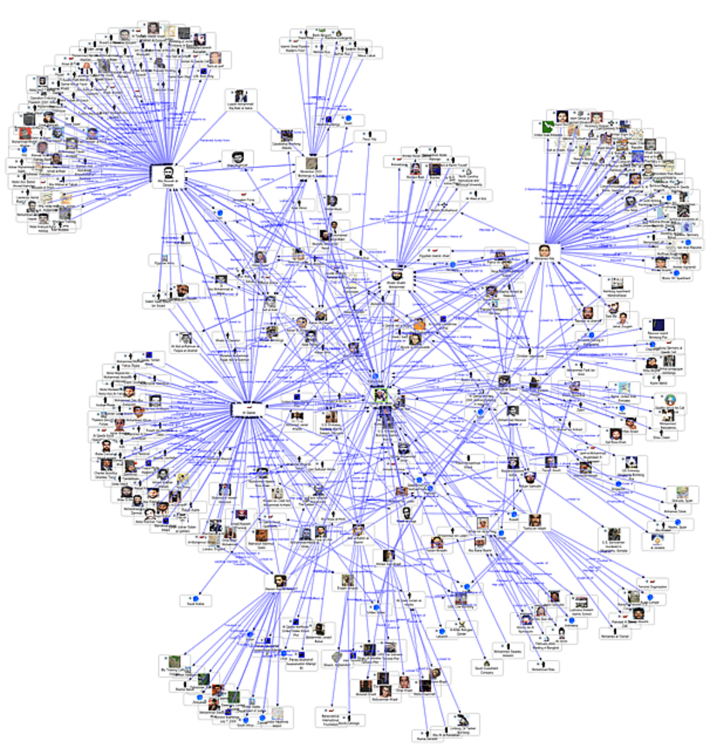


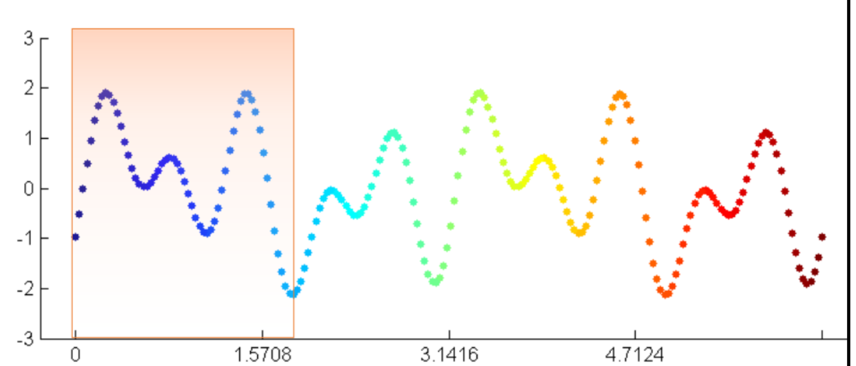
Data

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

(feature design or learning)







bag of words, word2vec

shape contexts, heat kernels

node2vec, Laplacian fact., rand. walks

sliding-window embeddings

metric embeddings, auto-encoders

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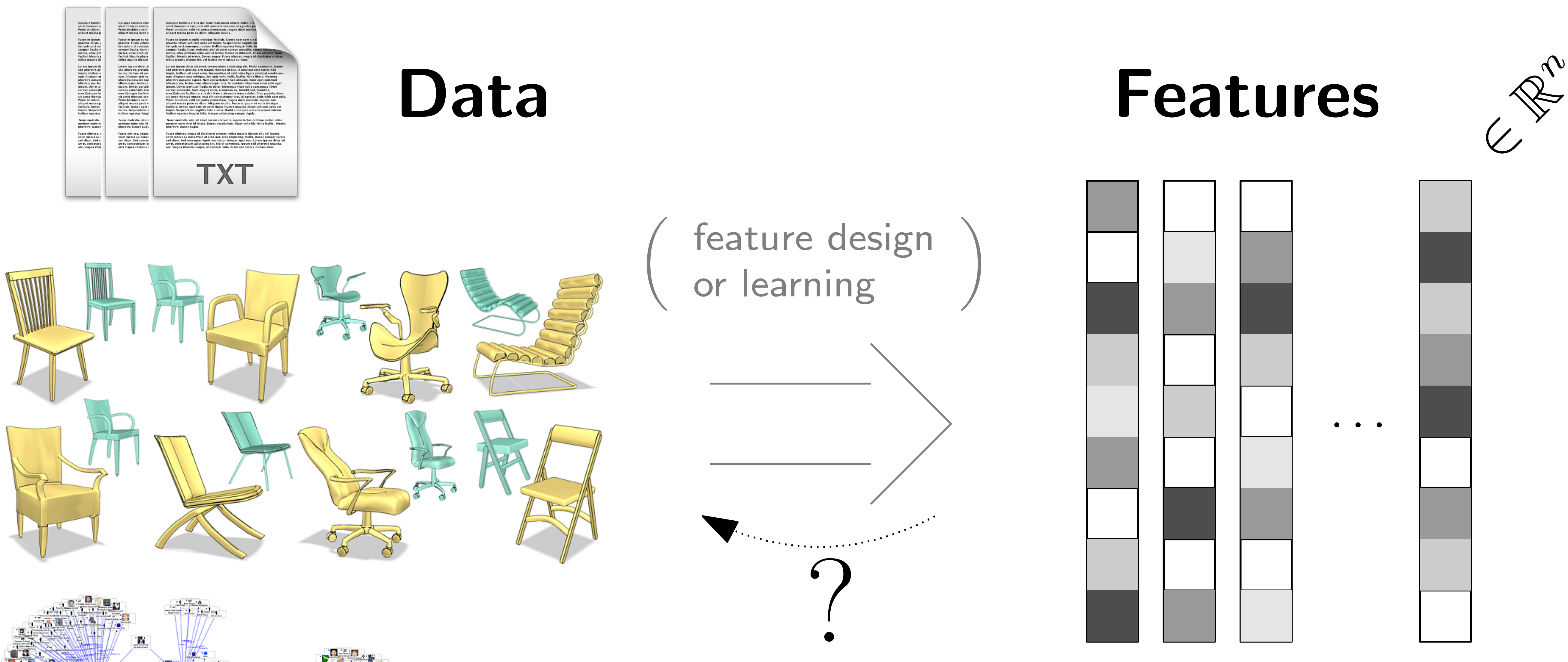


Is the feature map stable?

- continuity
- Lipschitz continuity
- differentiability

Can the feature map be inverted?

- Right inverse (∃ preimage): interpretable AI
- Left inverse (∃! preimage): reliable interpretation

Scenarios: dictionaries, deep layers, stats, etc.

bag of words, word2vec

shape contexts, heat kernels

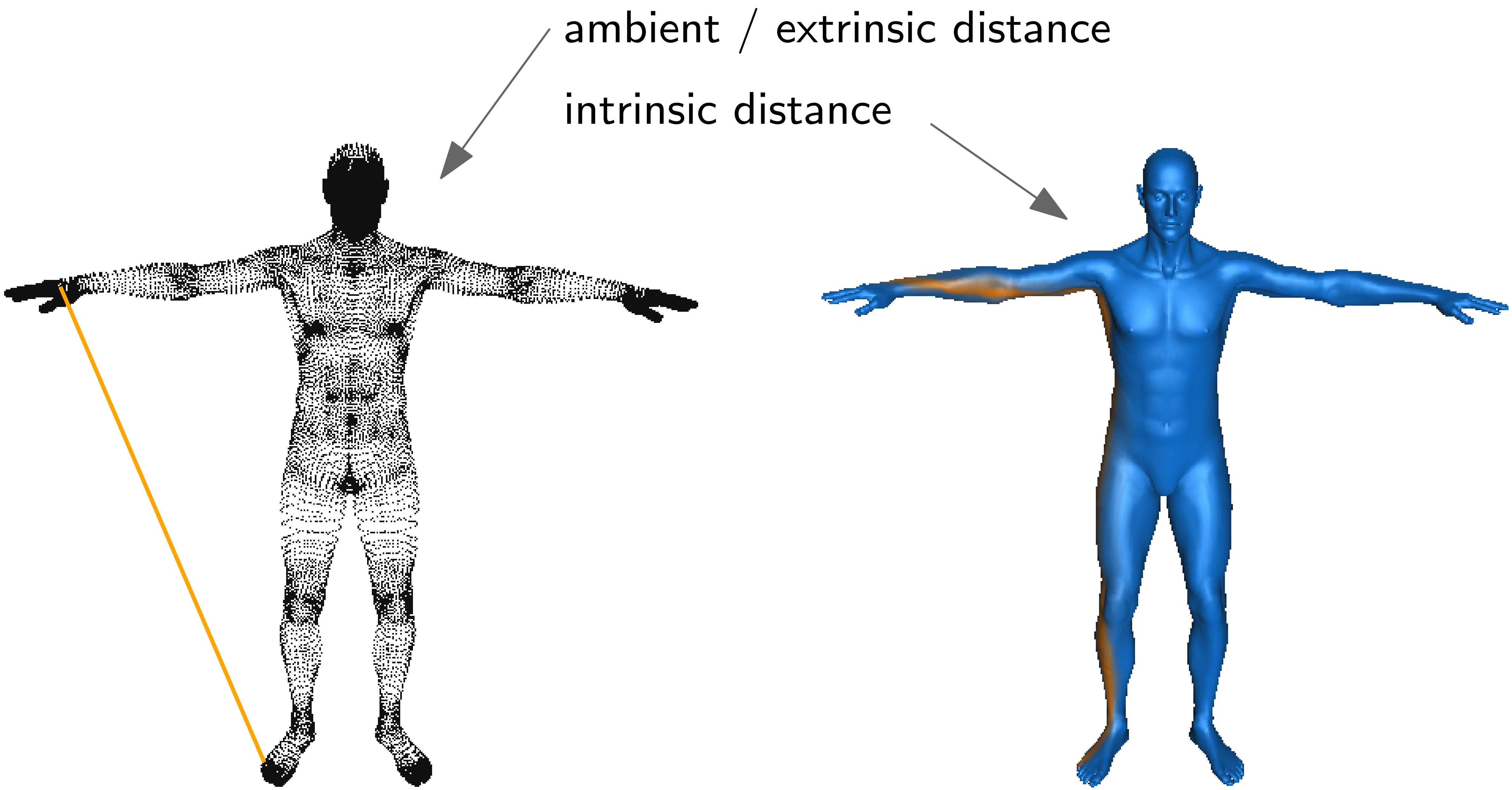
node2vec, Laplacian fact., rand. walks

sliding-window embeddings

metric embeddings, auto-encoders

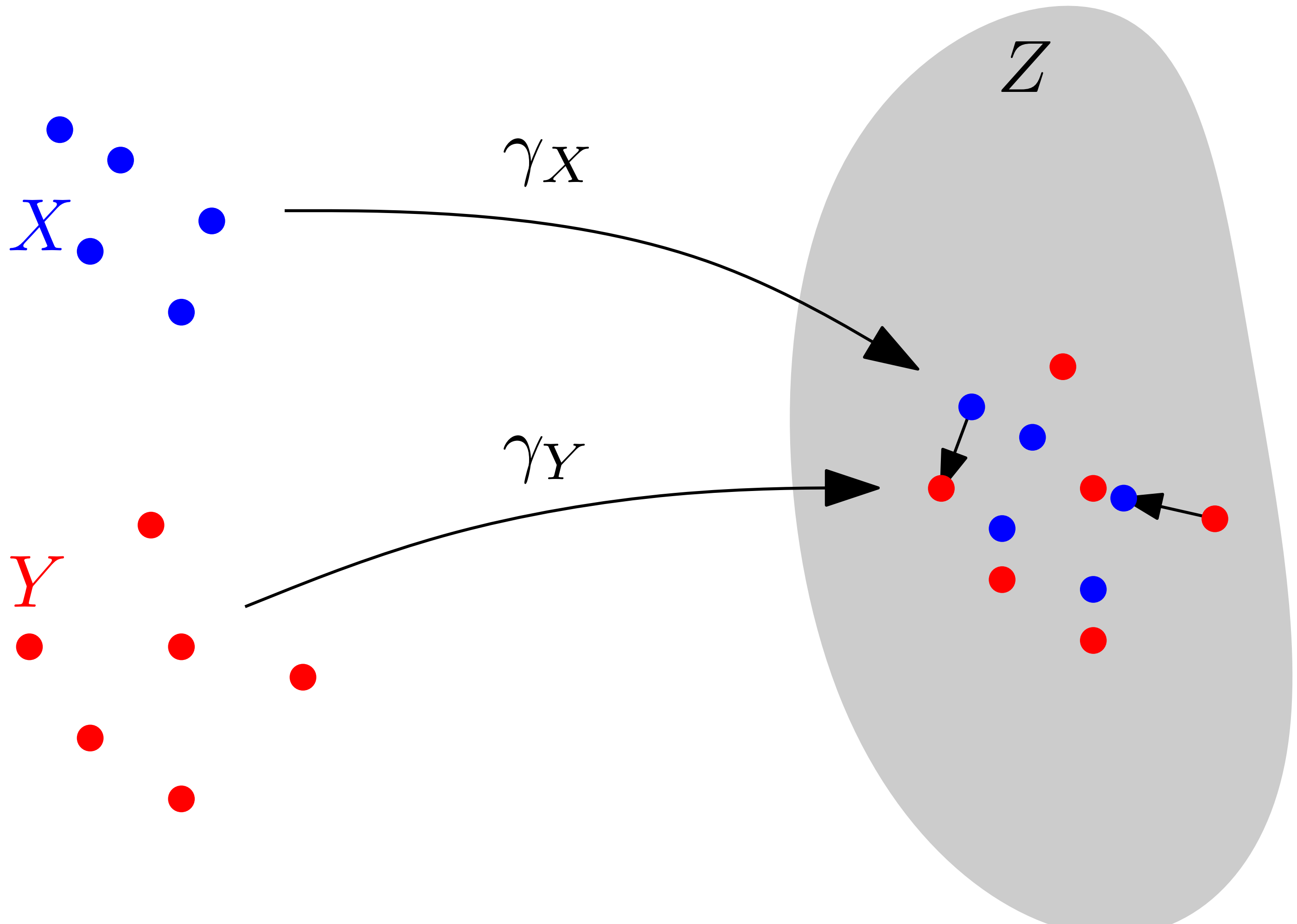
Mathematical framework

- data set / underlying space $\equiv$ compact metric / (dis-)similarity space



Mathematical framework

- data set / underlying space $\equiv$ compact metric / (dis-)similarity space
- distance between compact metric spaces $\equiv$ Gromov-Hausdorff (GH) distance



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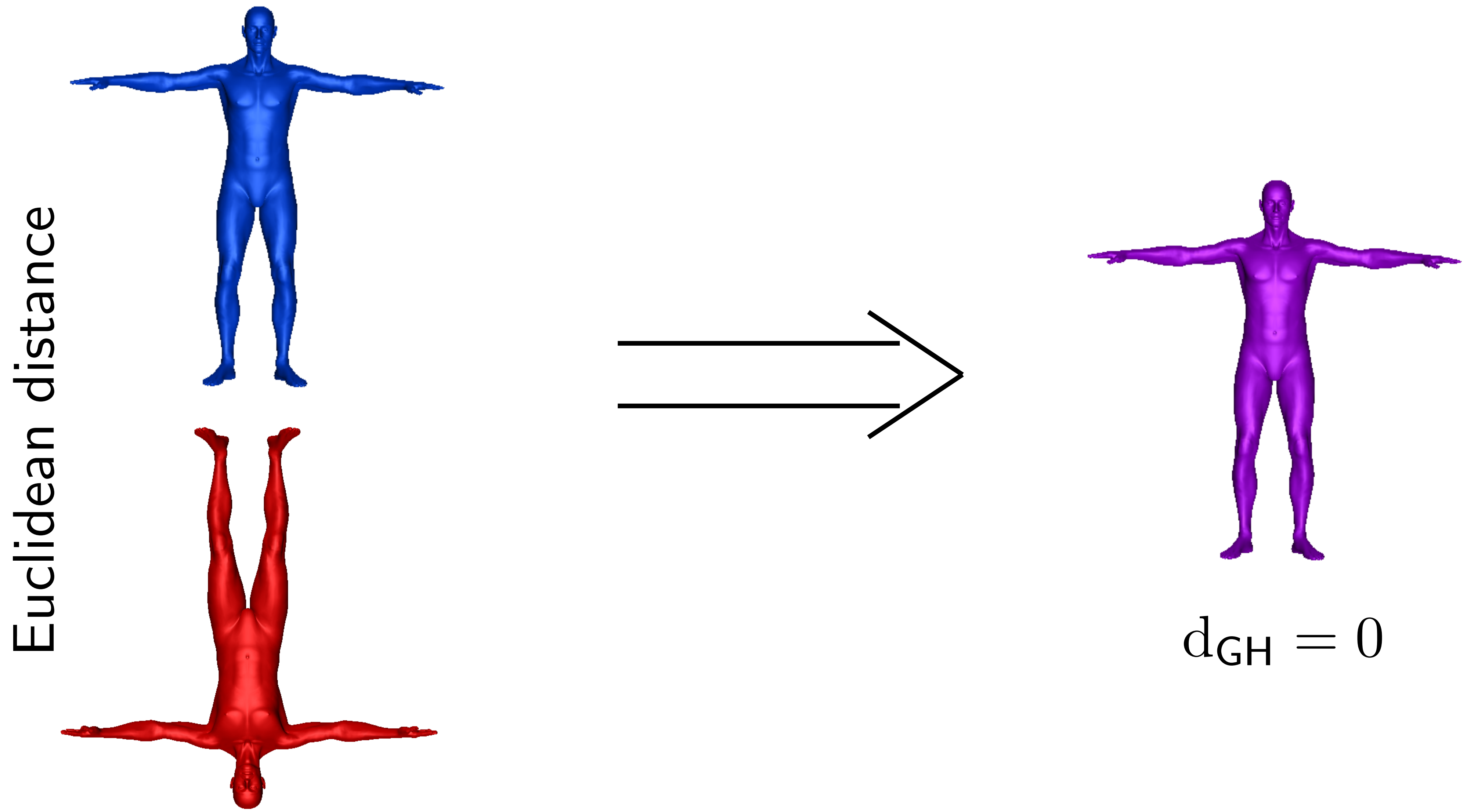

$d_{\mathsf{GH}} = 0$

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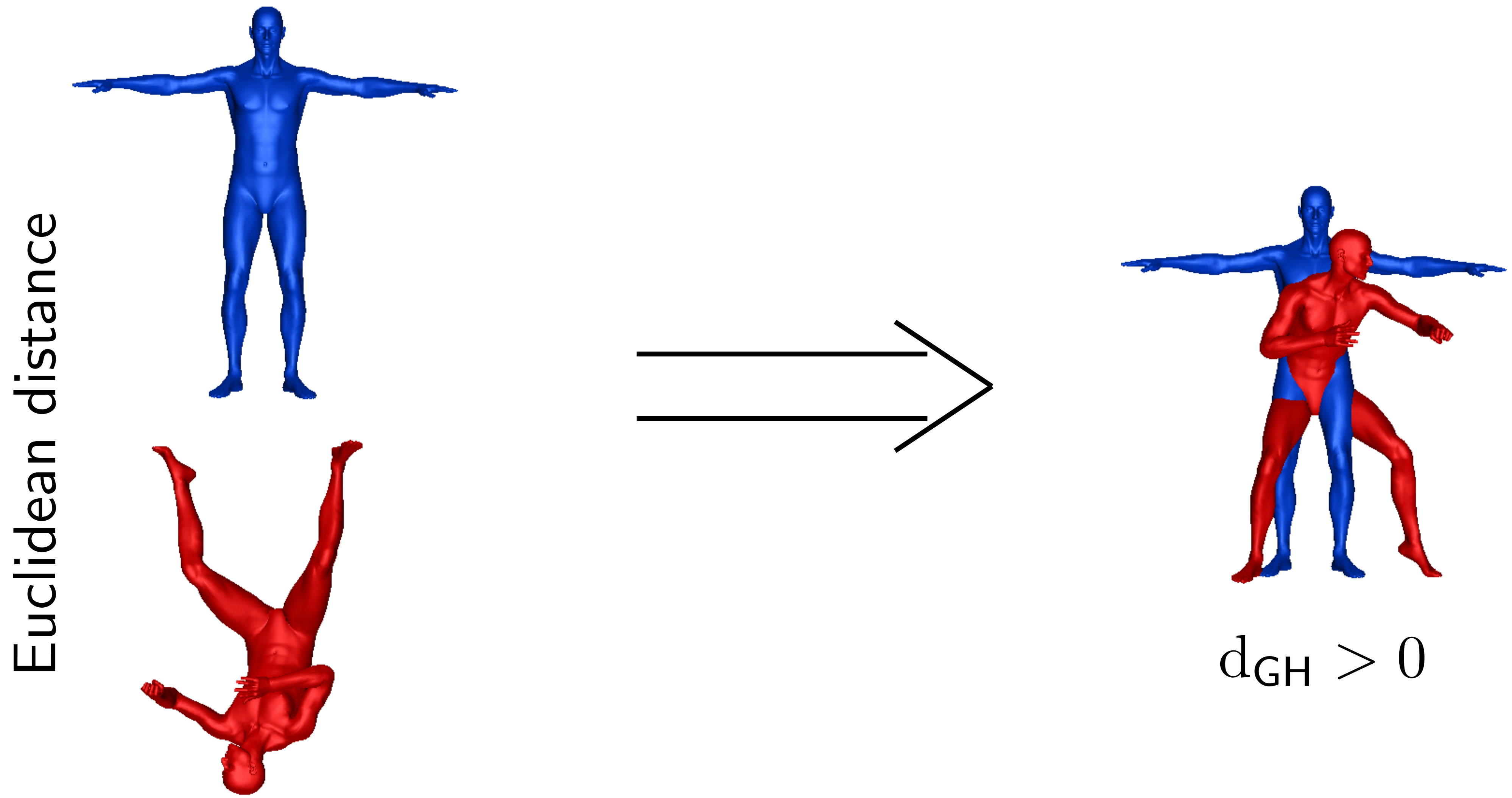

$d_{GH} > 0$

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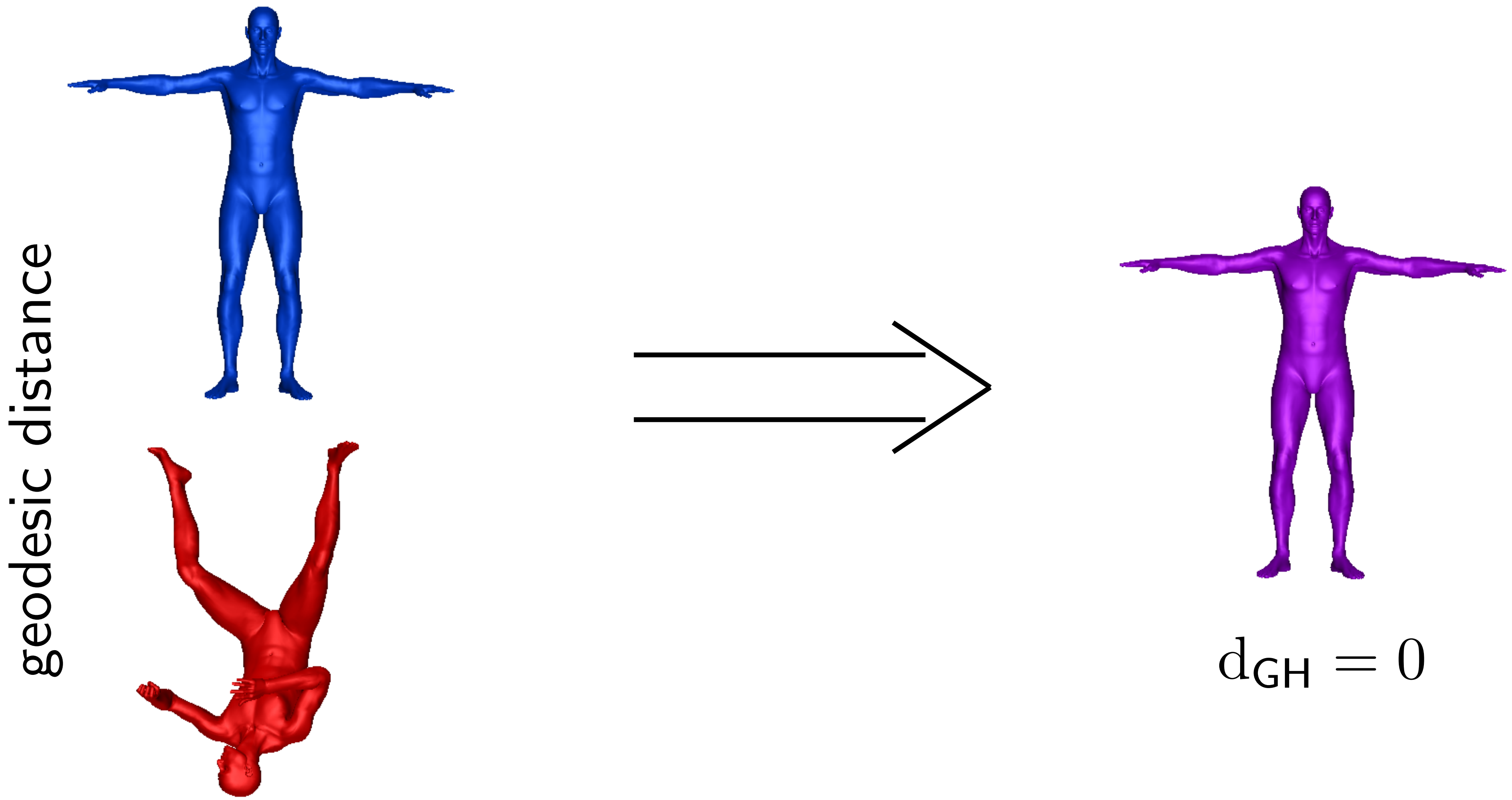
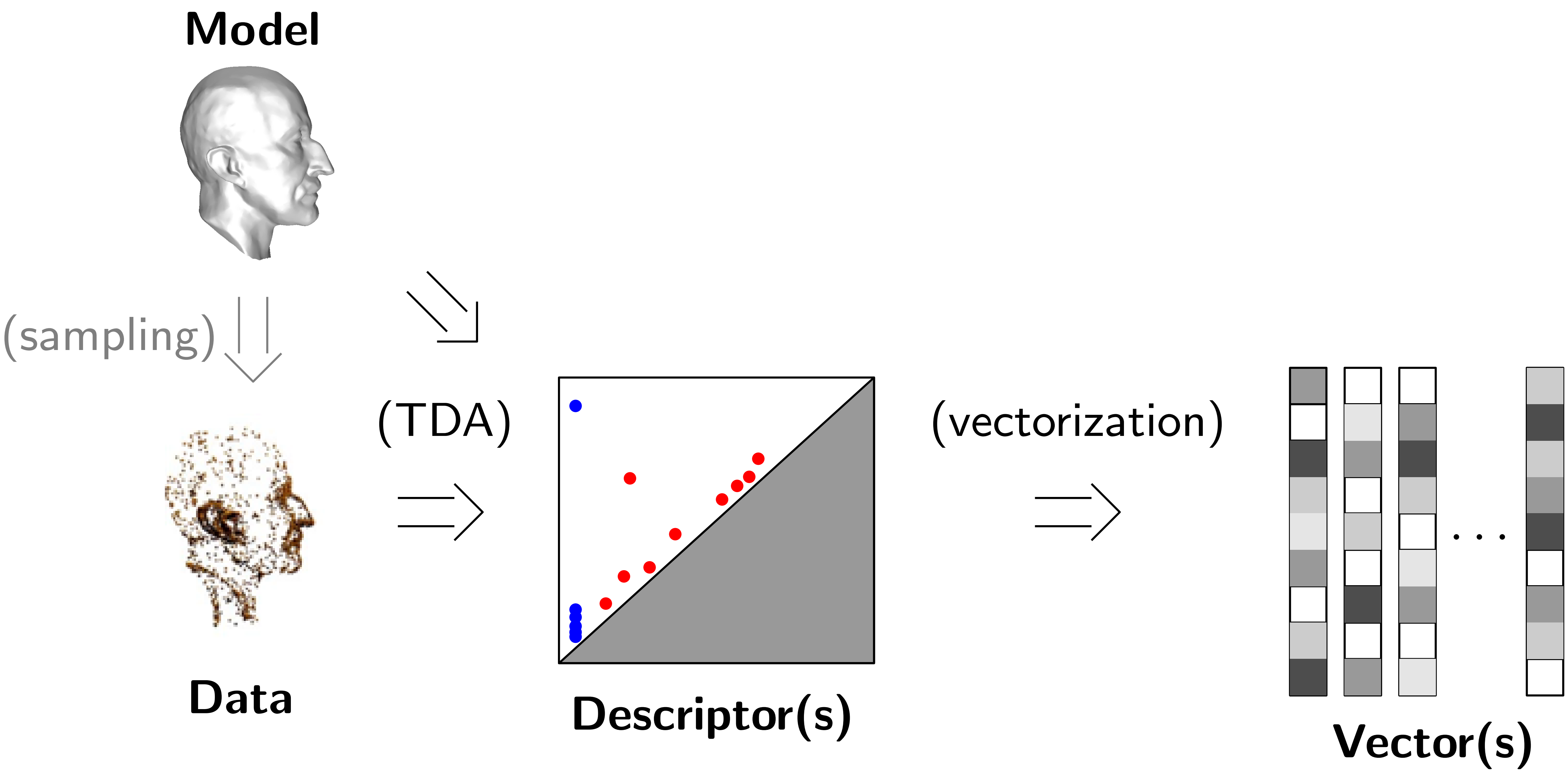


TDA for feature design



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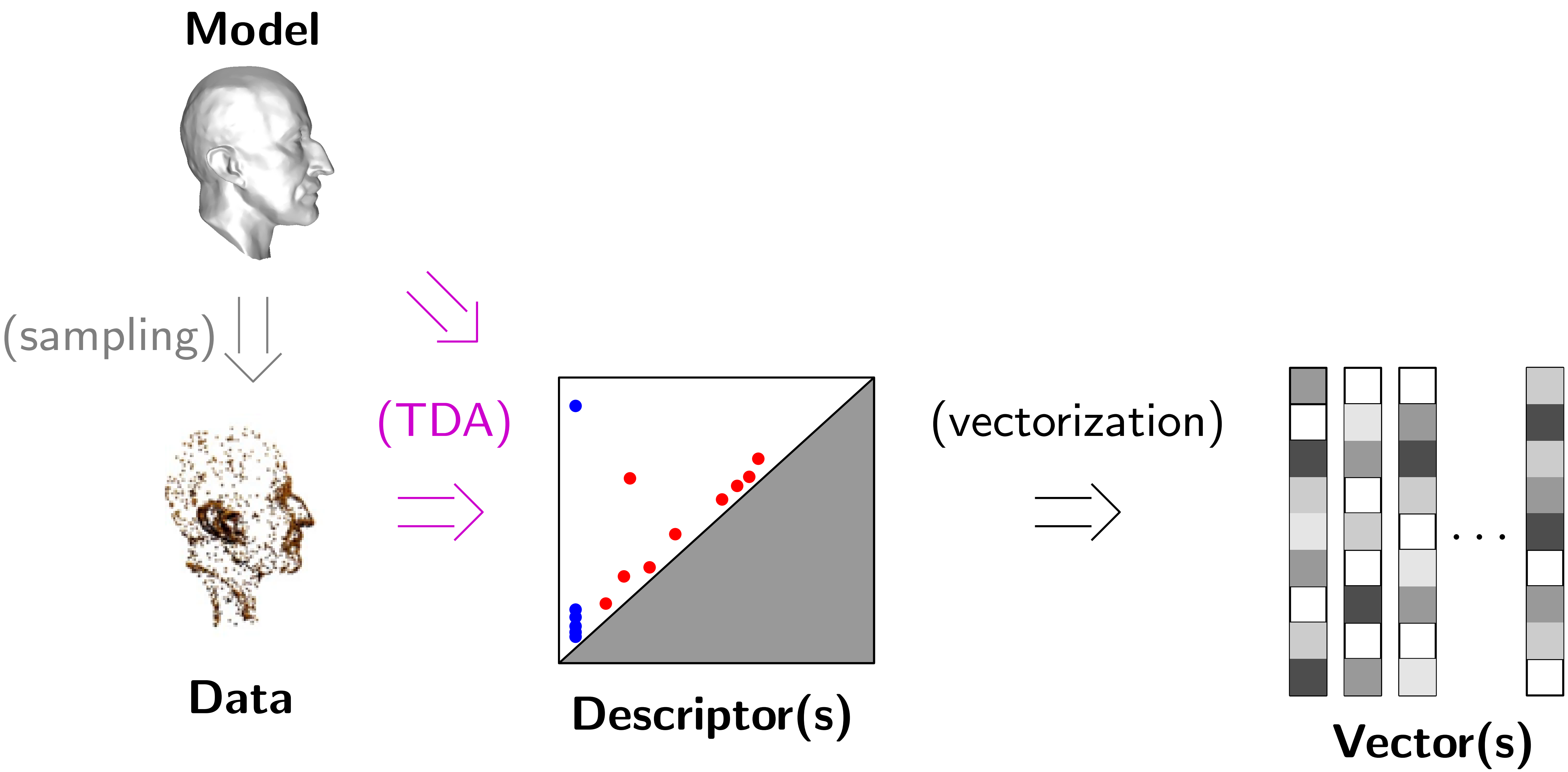


Persistent homology in a nutshell

X topological space

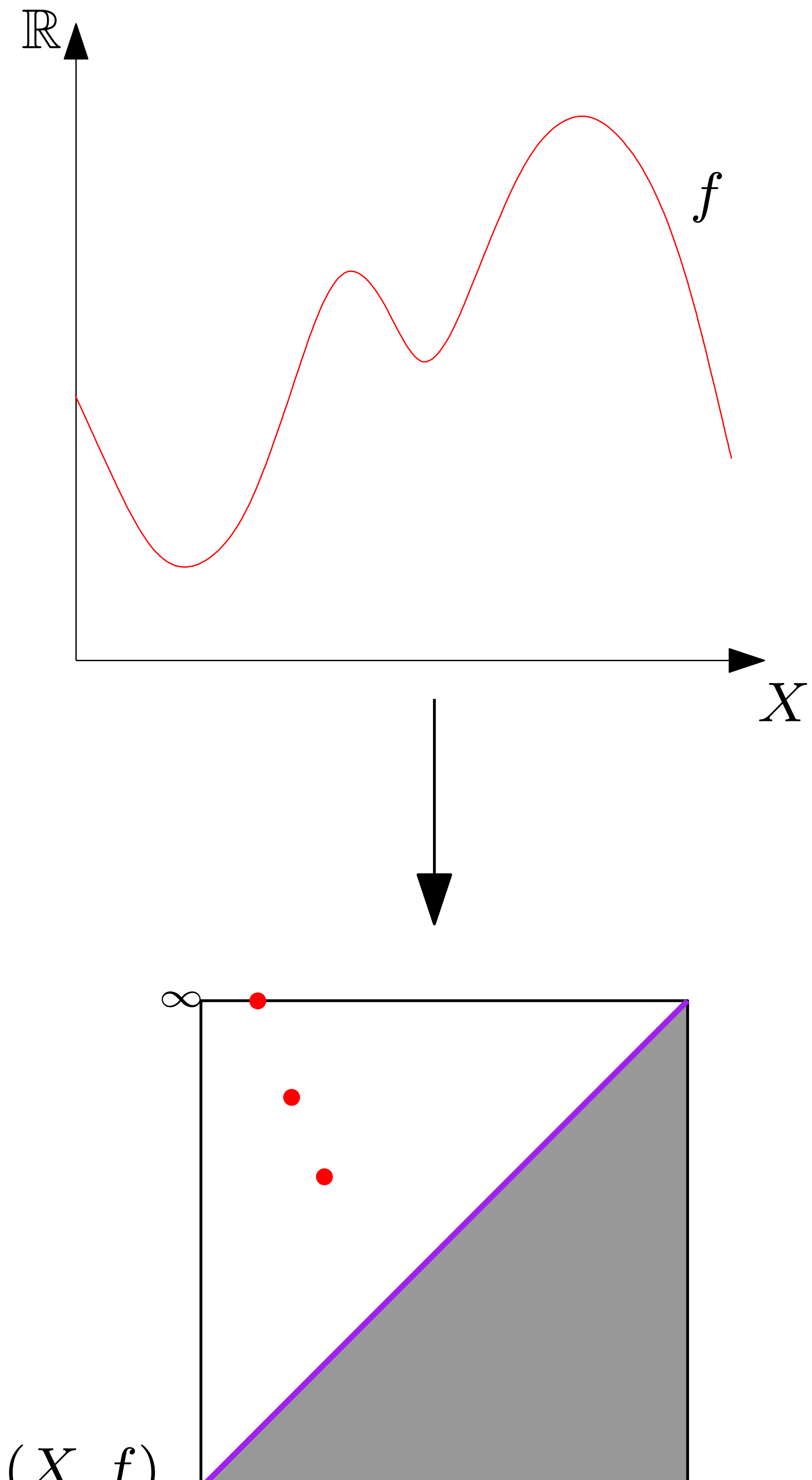
$f : X \to \mathbb{R}$

persistence

$\mathrm{dgm}\, f$

signature: *persistence diagram*

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



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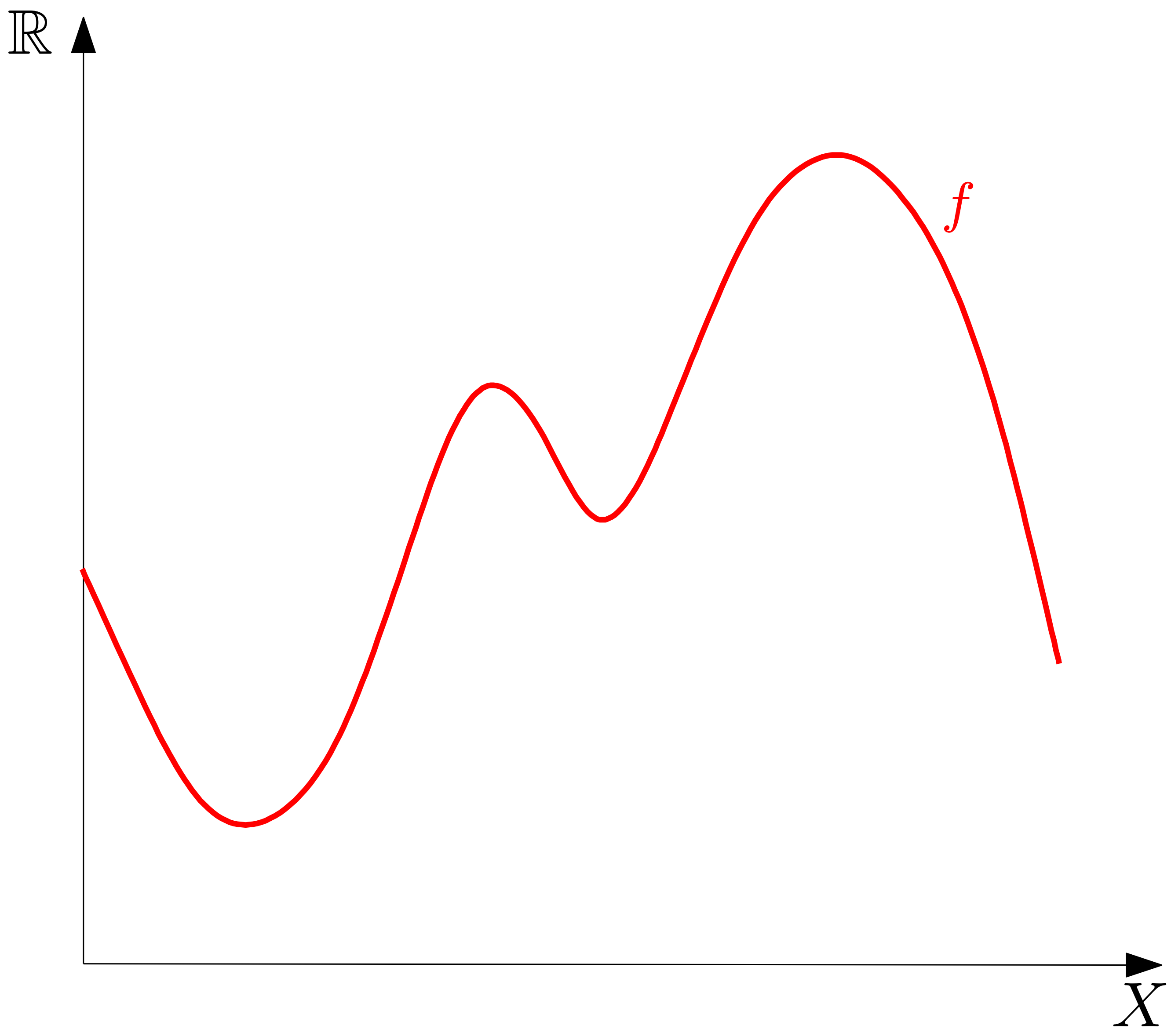
- Nested family (**filtration**) of sublevel-sets $f^{-1}((-\infty, t])$ for t ranging from $-\infty$ to $+\infty$
- Track the evolution of the topology (**homology**) throughout the family



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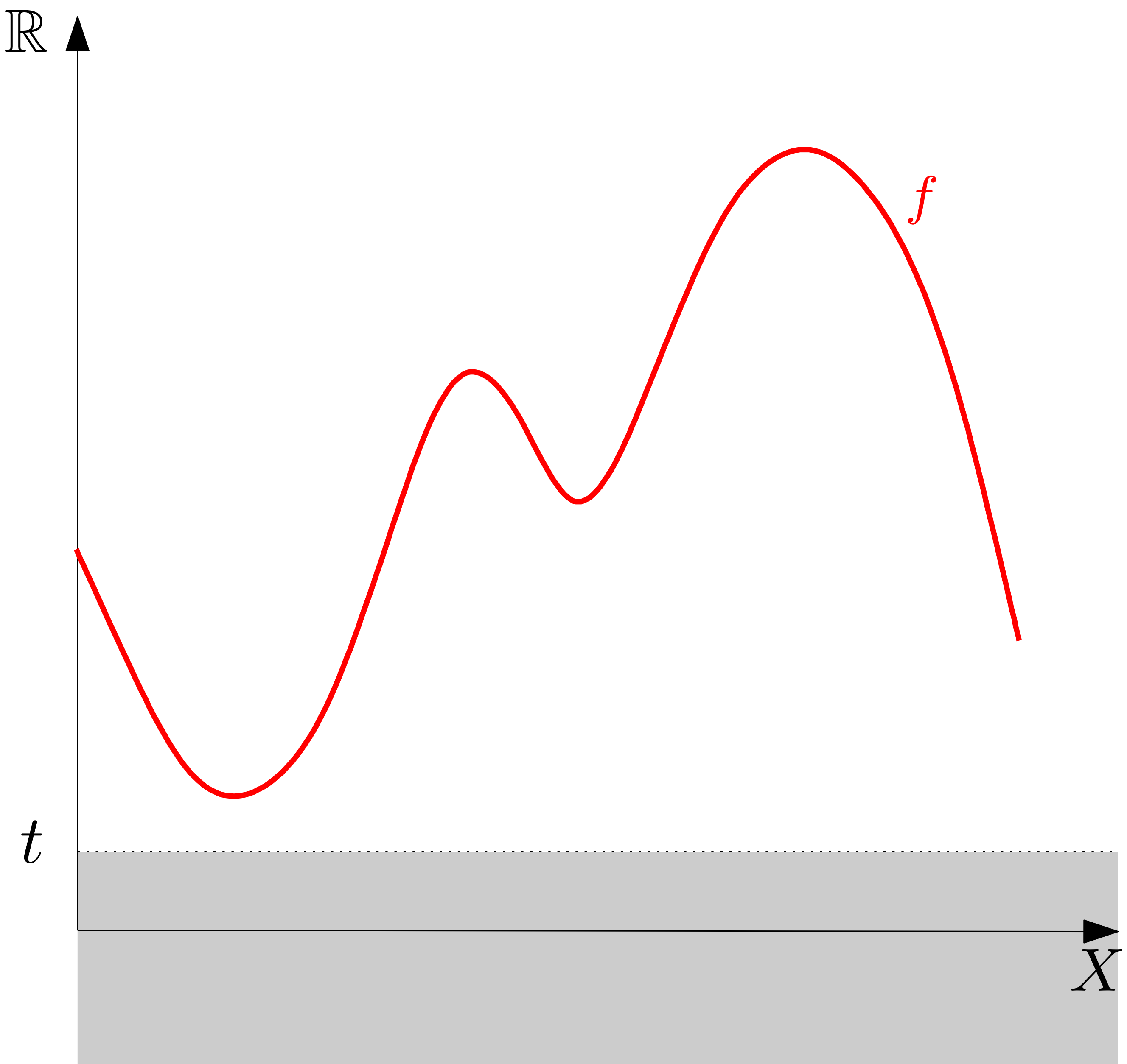

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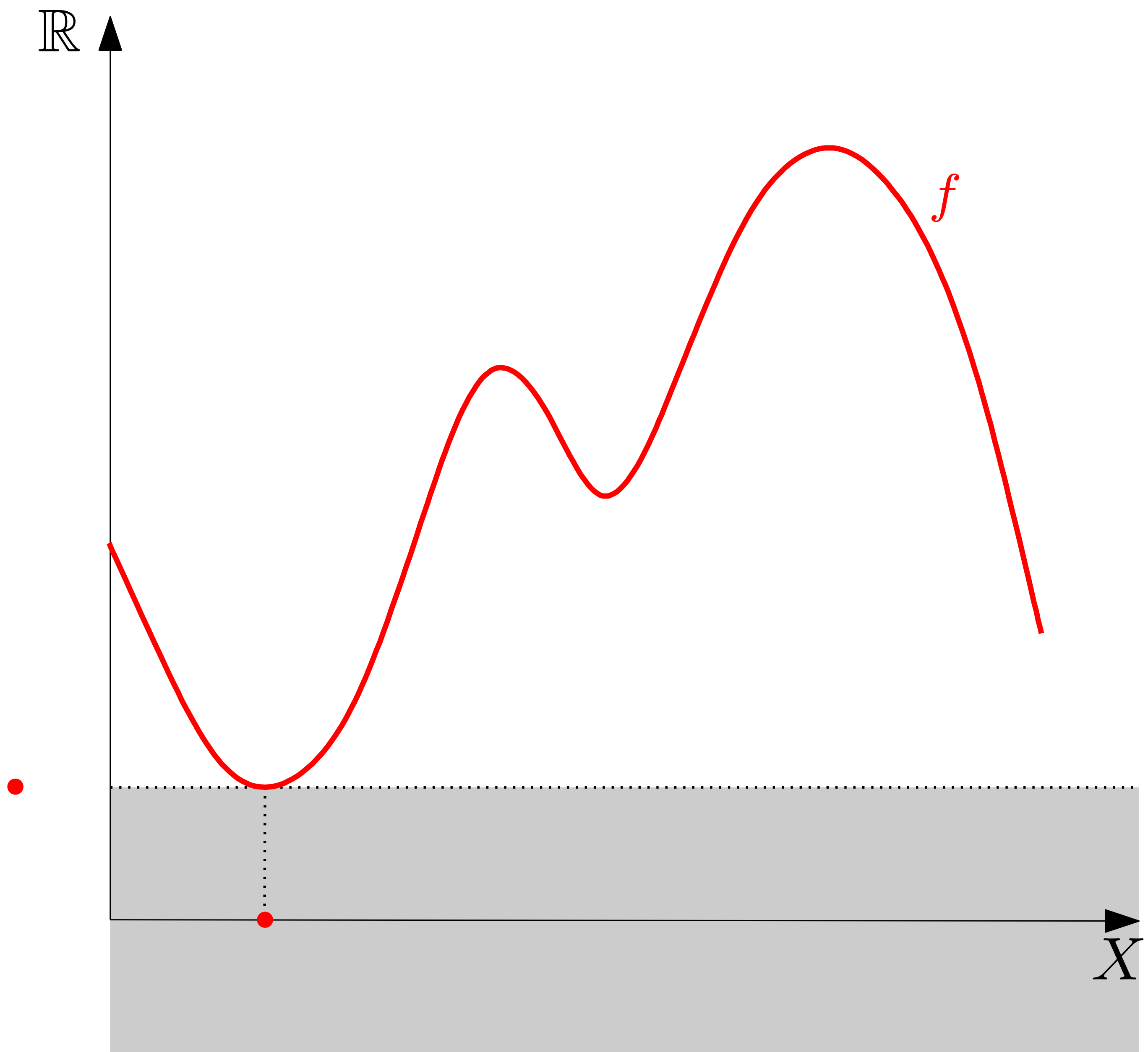

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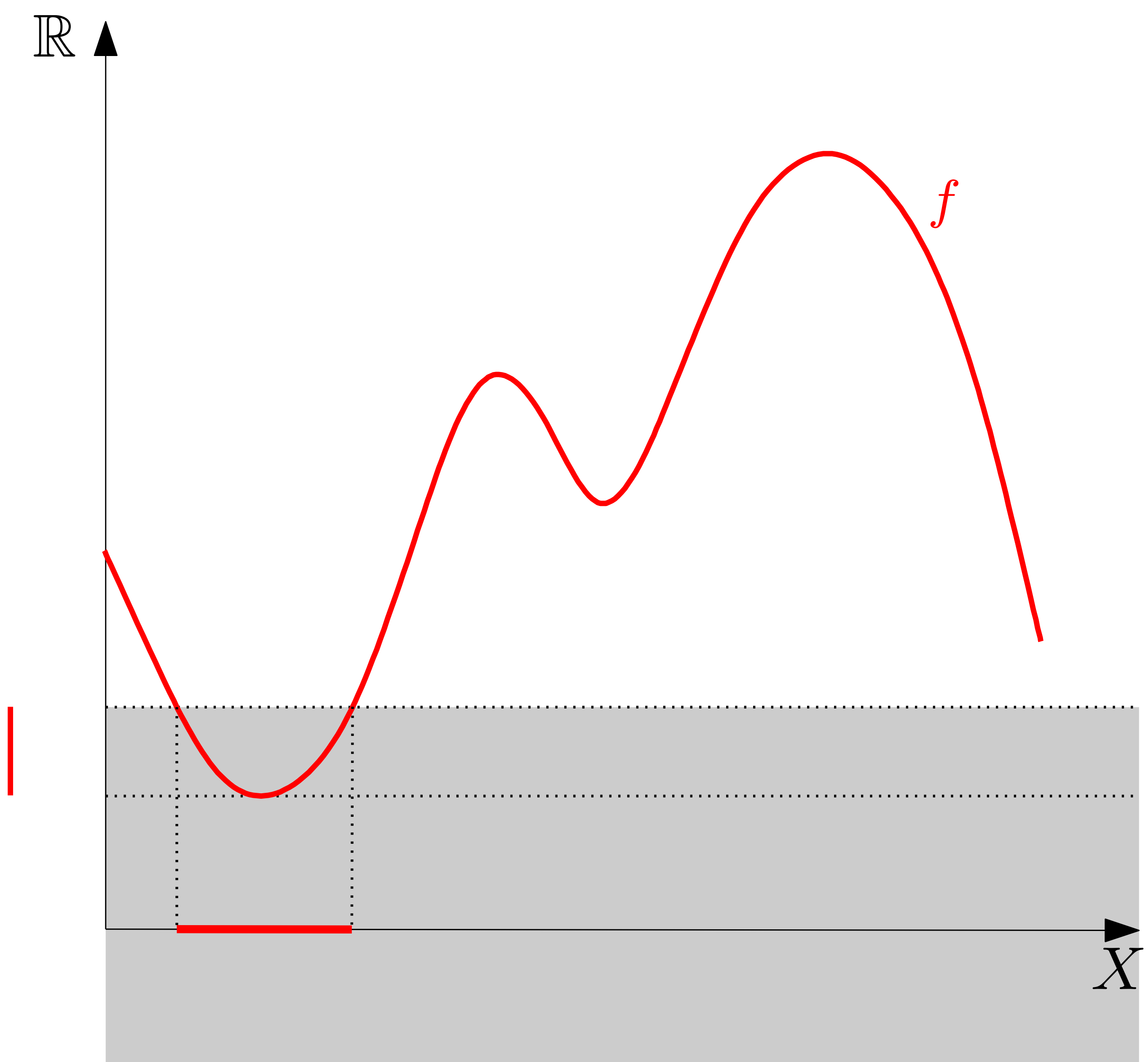

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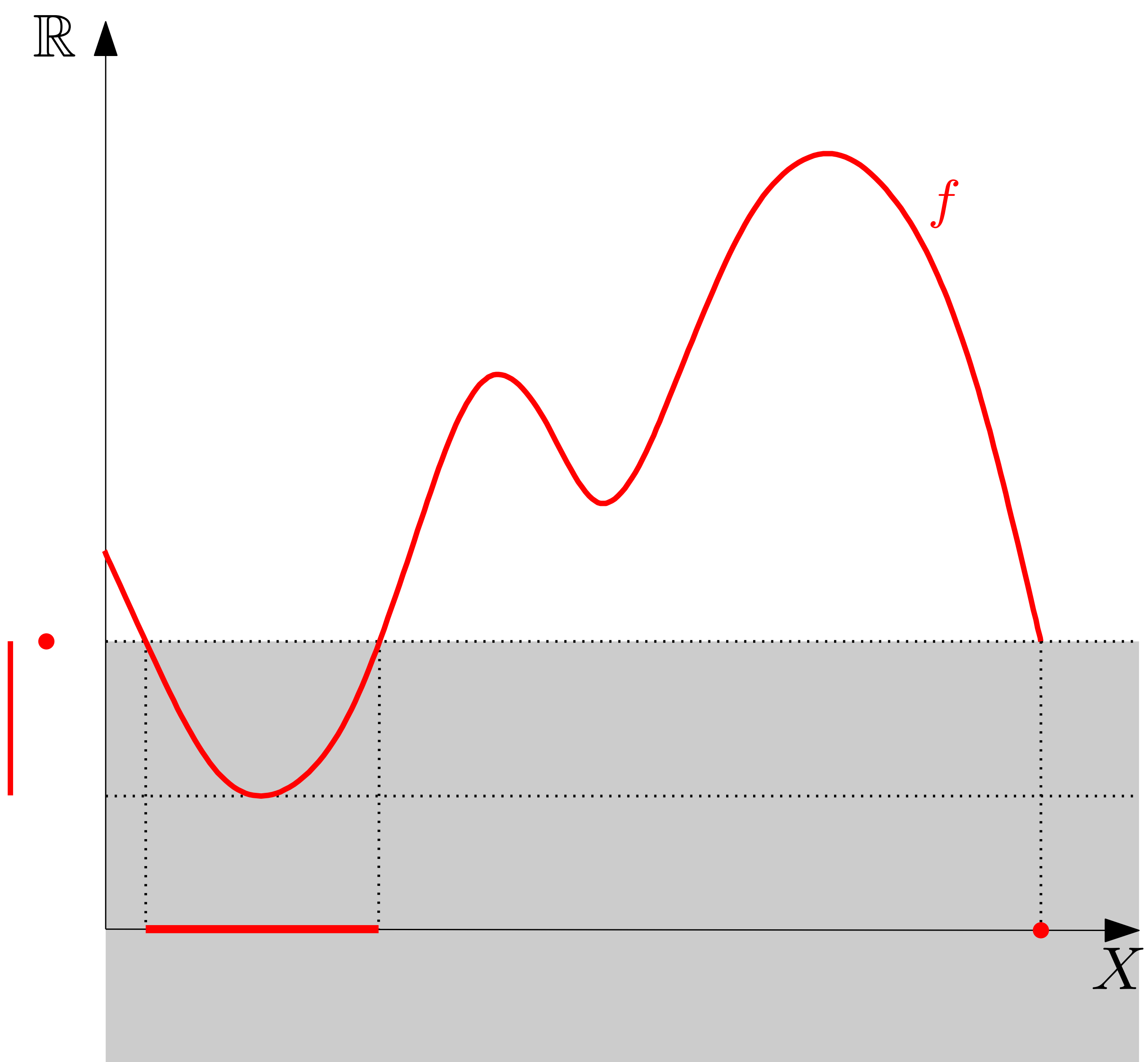

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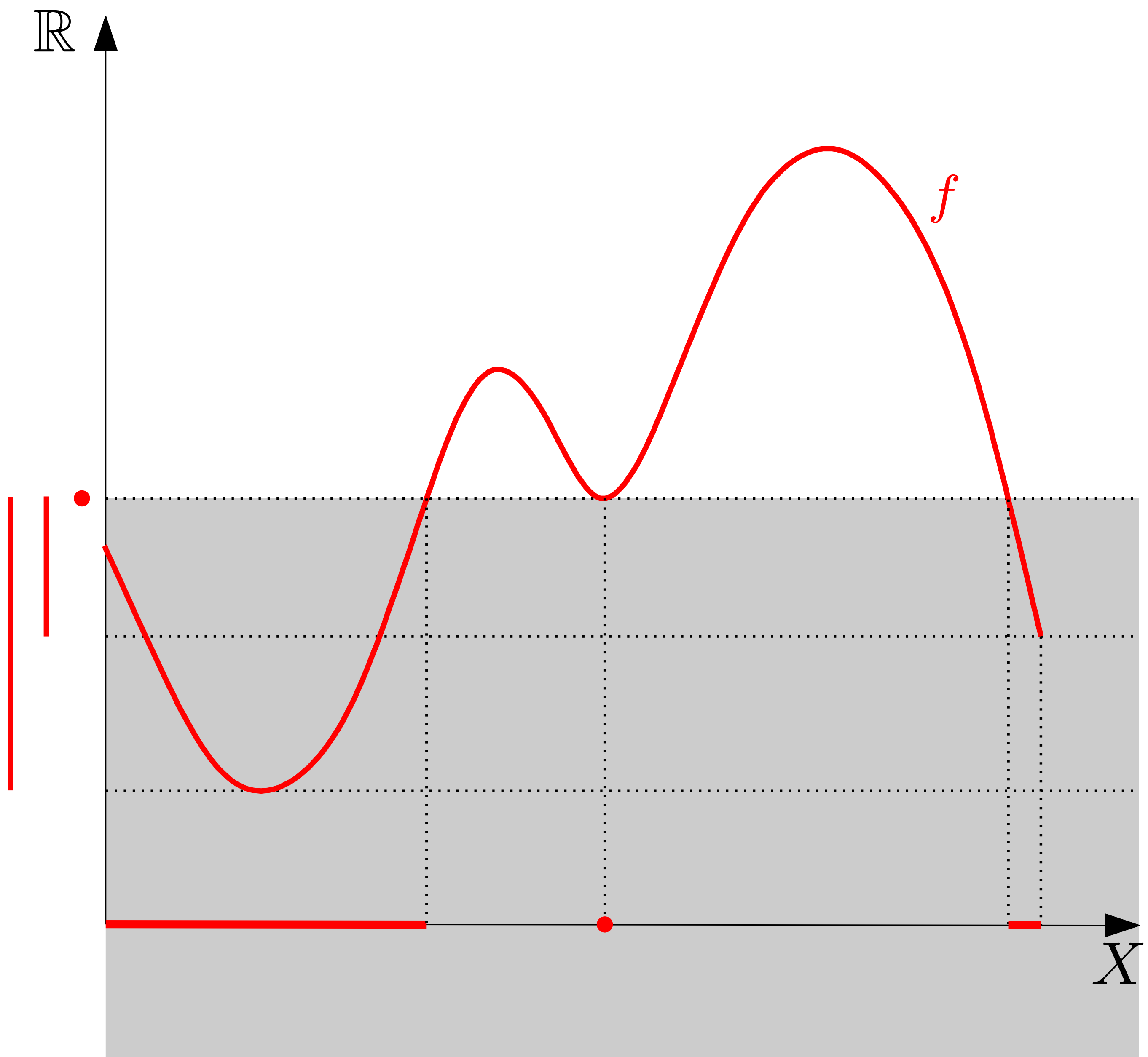

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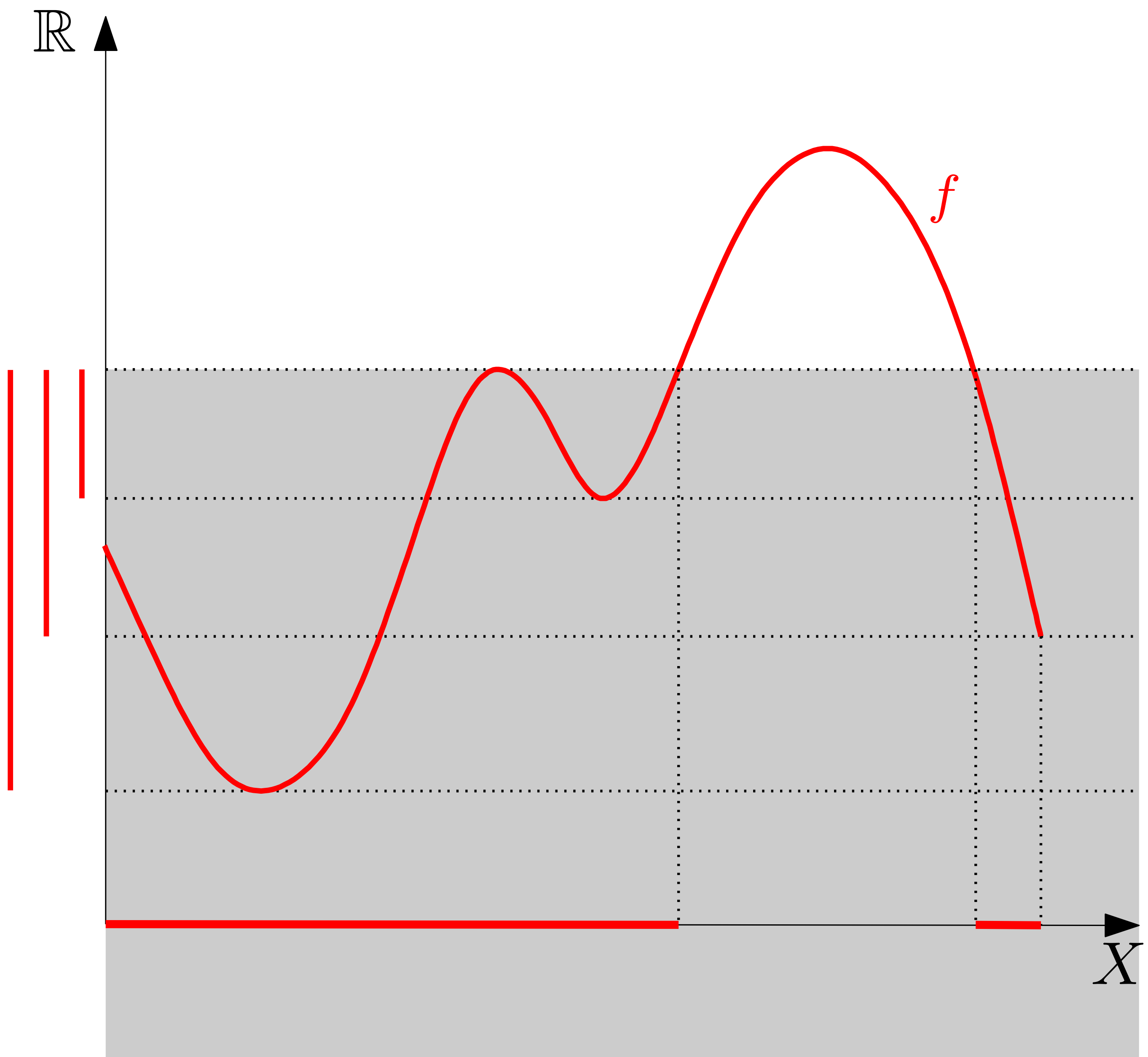

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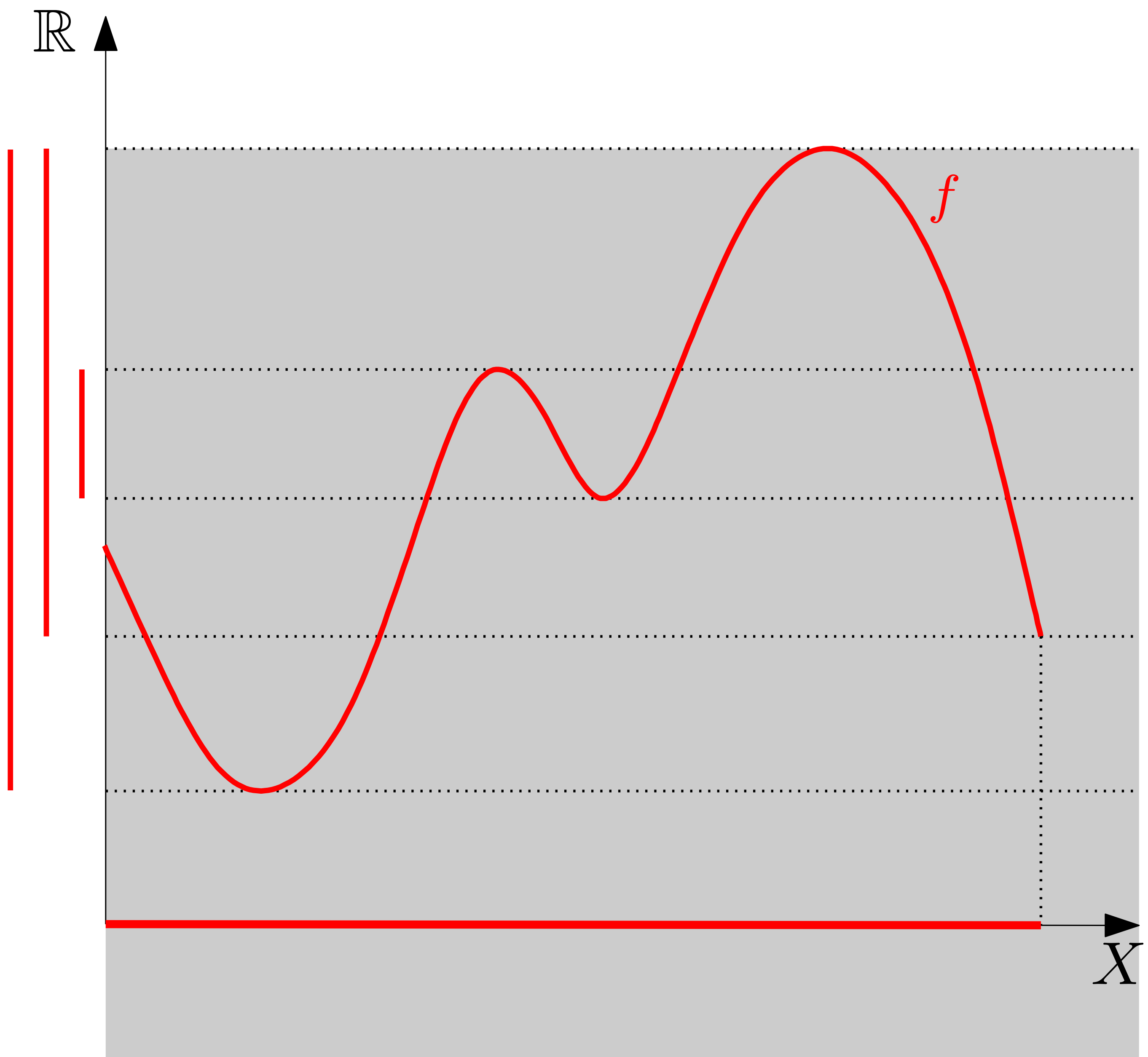

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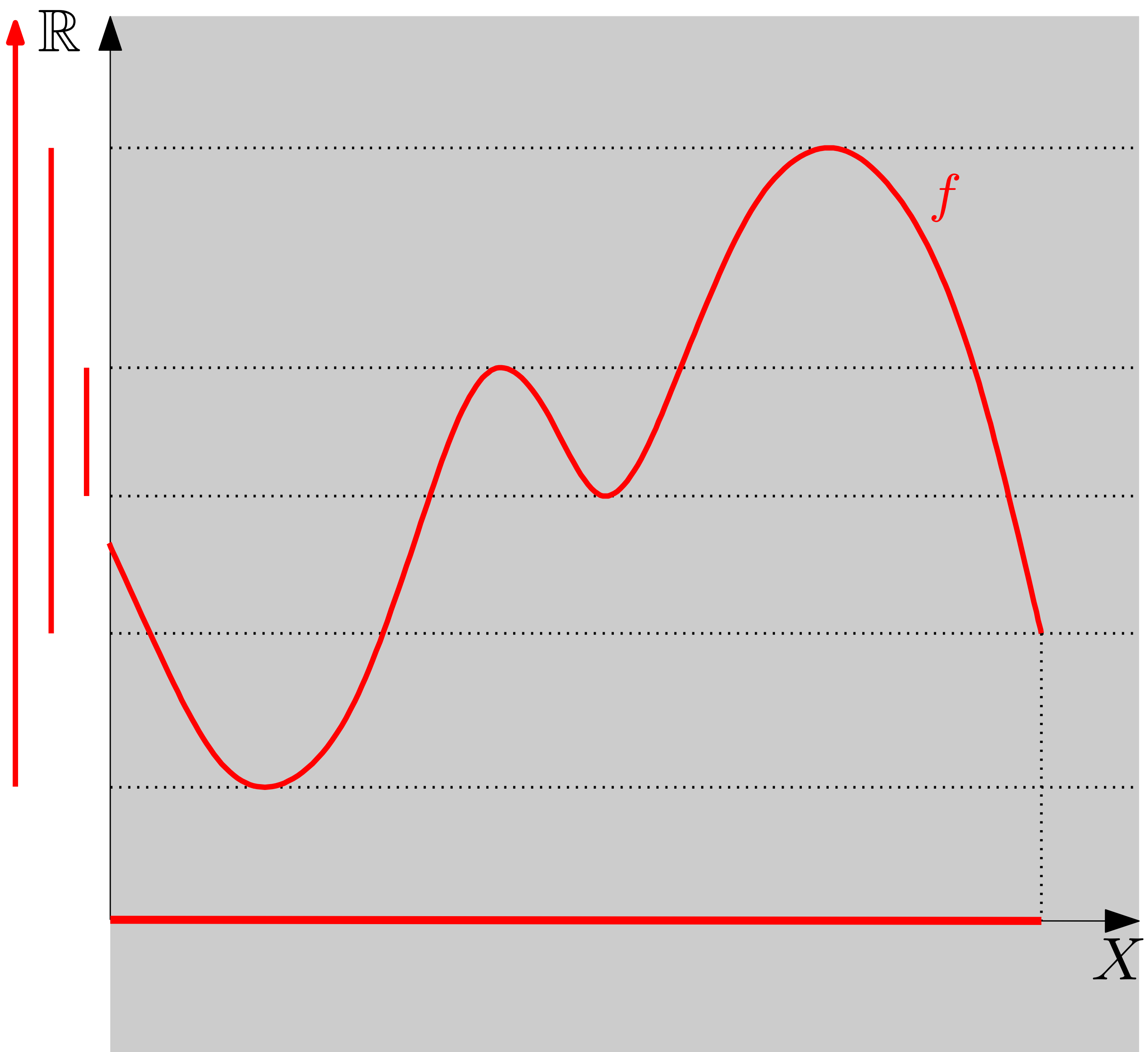
- Finite set of intervals (**barcode**) encodes births/deaths of topological features



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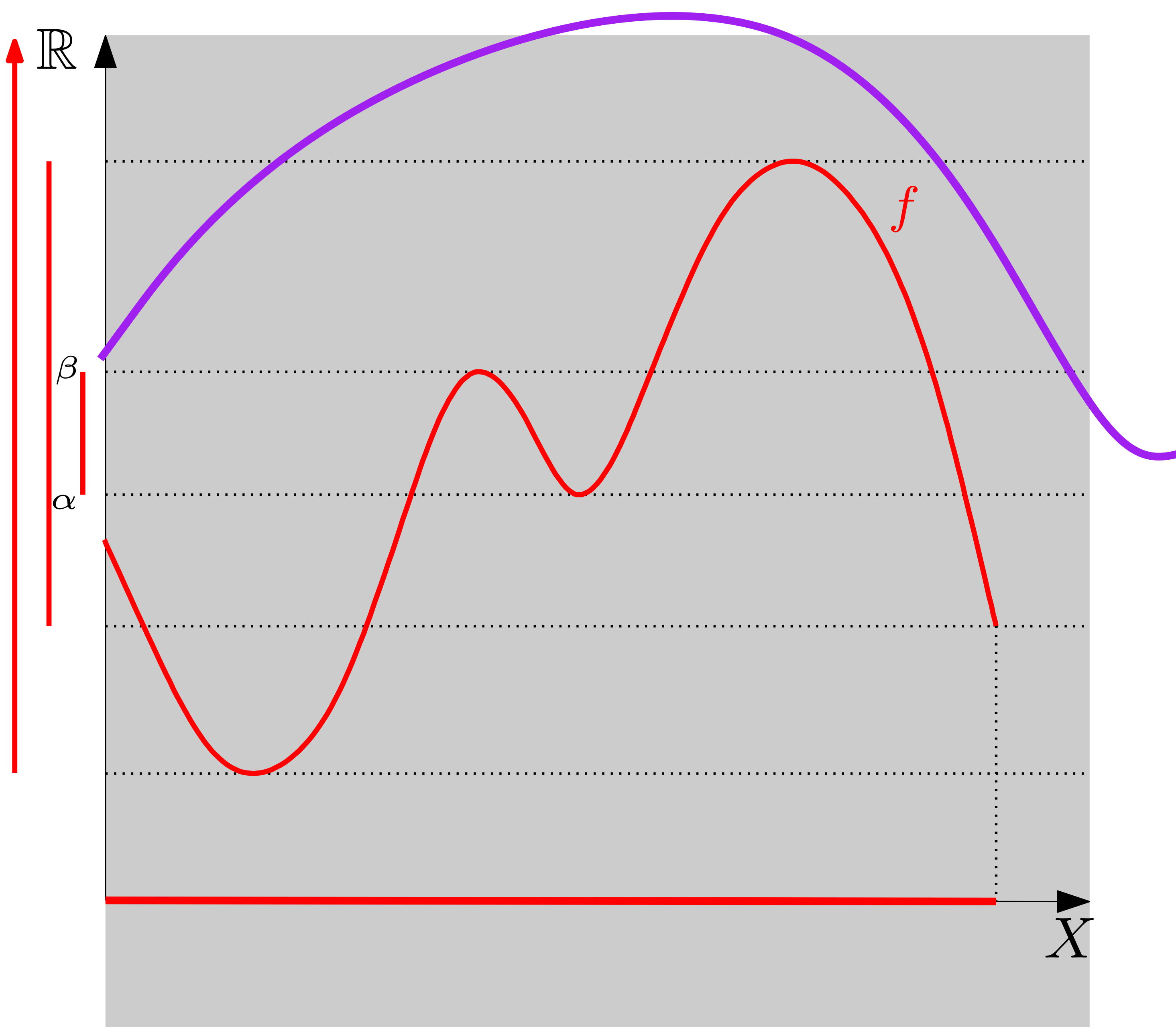
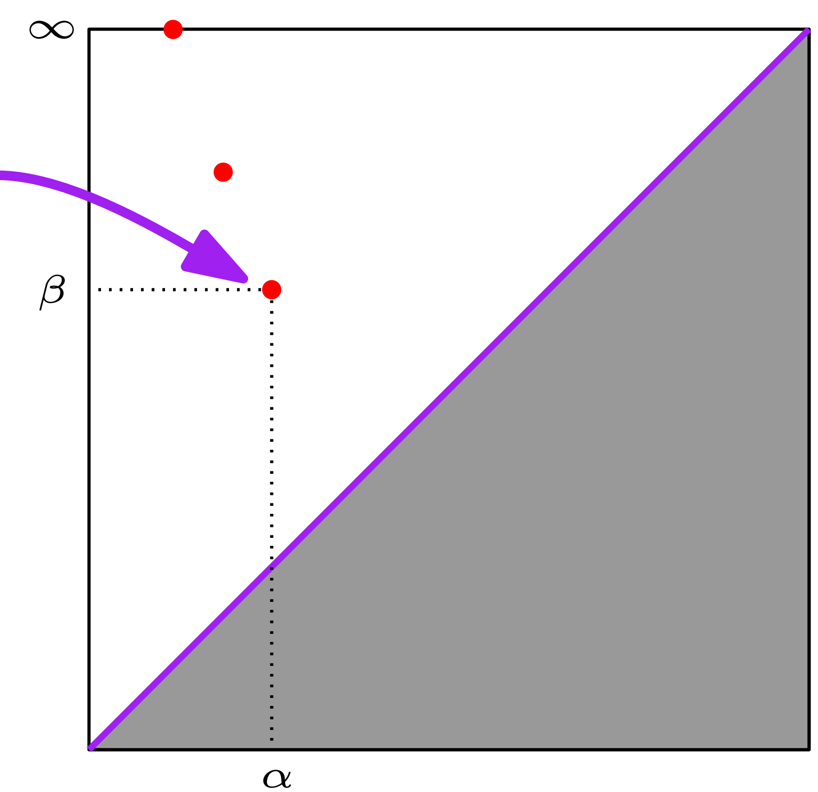


- Alternate representation as a multiset of points in the plane (**diagram**).



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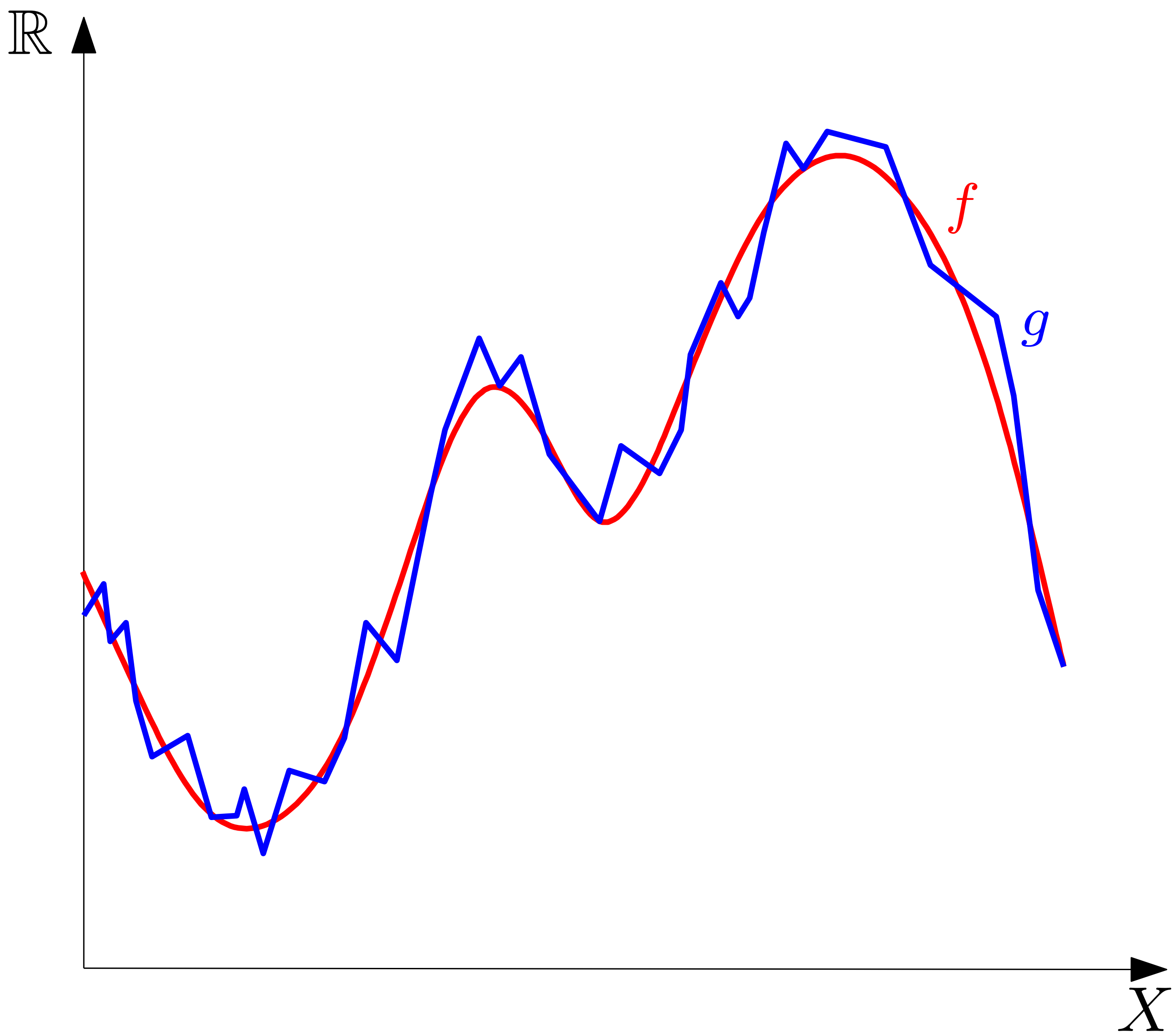

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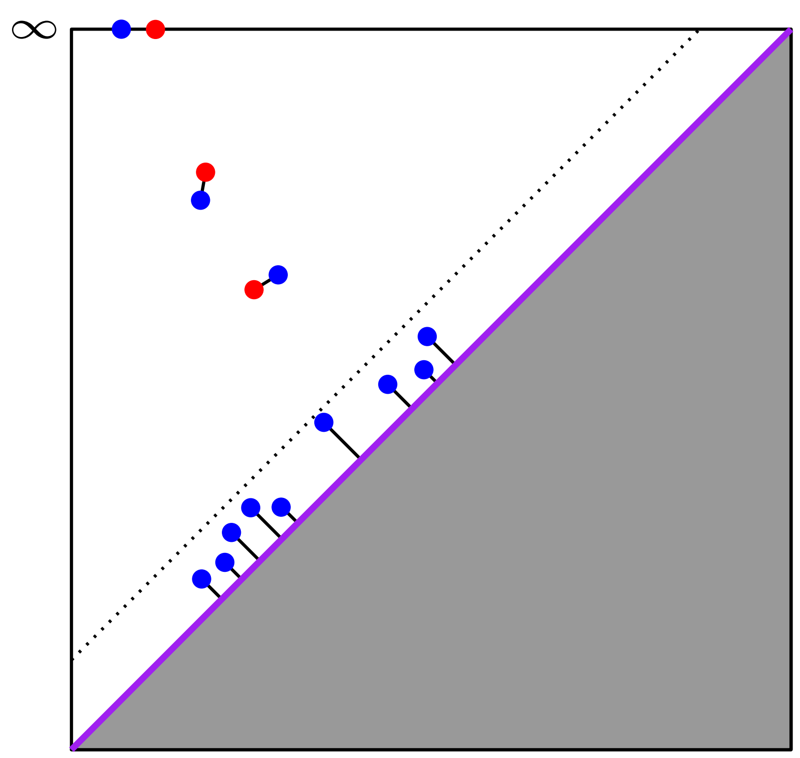
What if f is slightly perturbed?



Persistent homology in a nutshell

Theorem (Stability): [Cohen-Steiner et al. 2005, Chazal, O. et al. 2009]
For any *tame* functions $f, g : X \to \mathbb{R}$, $\mathrm{d}_\mathrm{B}^\infty(\mathrm{dgm}\, f, \mathrm{dgm}\, g) \leq \|f - g\|_\infty$.

partial matching $M : \mathrm{dgm}\, f \leftrightarrow \mathrm{dgm}\, g$

cost of a matched pair $(p, q) \in M$: $\|p - q\|_\infty$

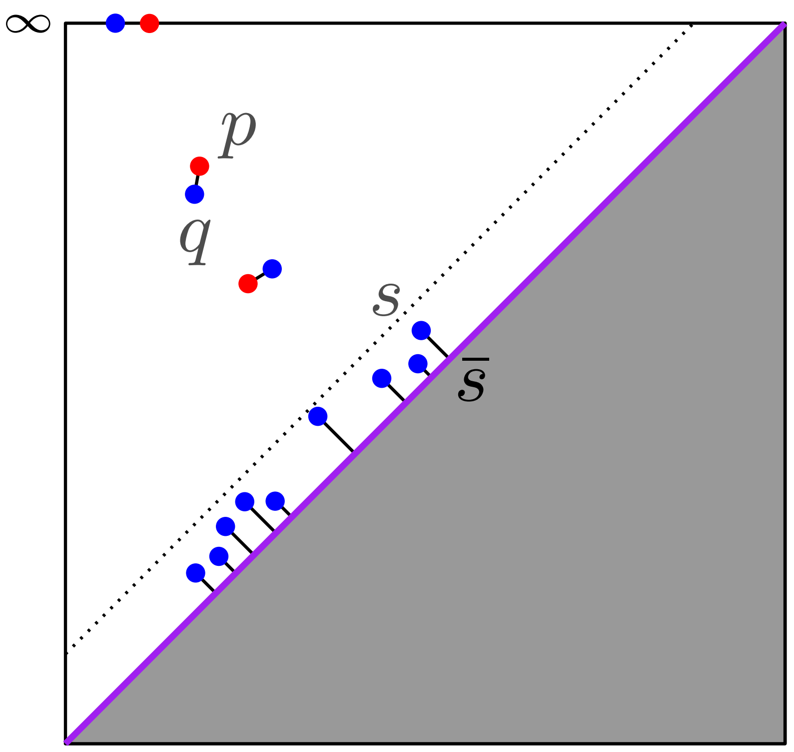
cost of an unmatched point $s \in \mathrm{dgm}\, f \sqcup \mathrm{dgm}\, g$: $\|s - \bar{s}\|_\infty$

cost of a matching:

$$\max \left\{ \sup_{(p,\,q)\ \text{matched}} \|p - q\|_\infty,\ \sup_{s\ \text{unmatched}} \|s - \bar{s}\|_\infty \right\}$$

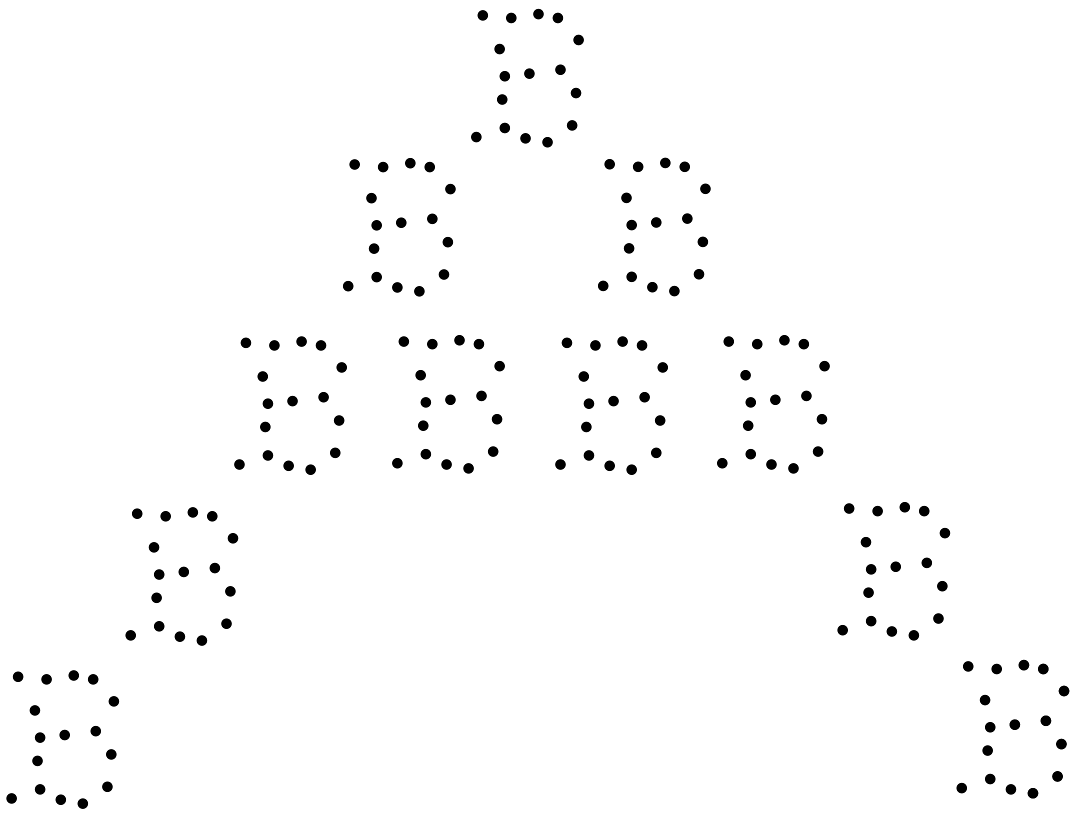
bottleneck distance:

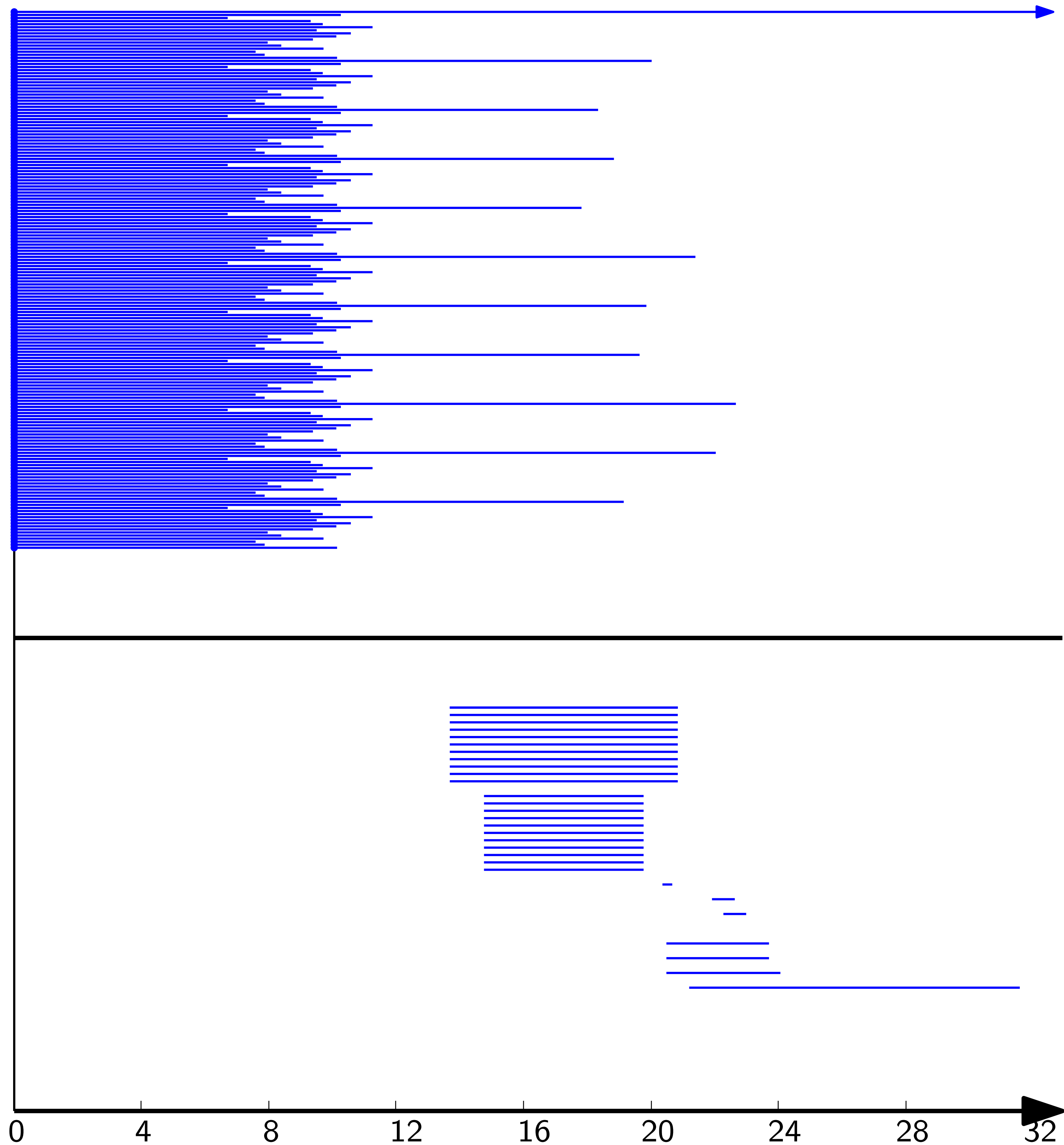
$$\mathrm{d}_\mathrm{B}^\infty(\mathrm{dgm}\, f, \mathrm{dgm}\, g) = \inf_{M : \mathrm{dgm}\, f \leftrightarrow \mathrm{dgm}\, g} \text{cost}(M)$$



Example: Distance Function

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





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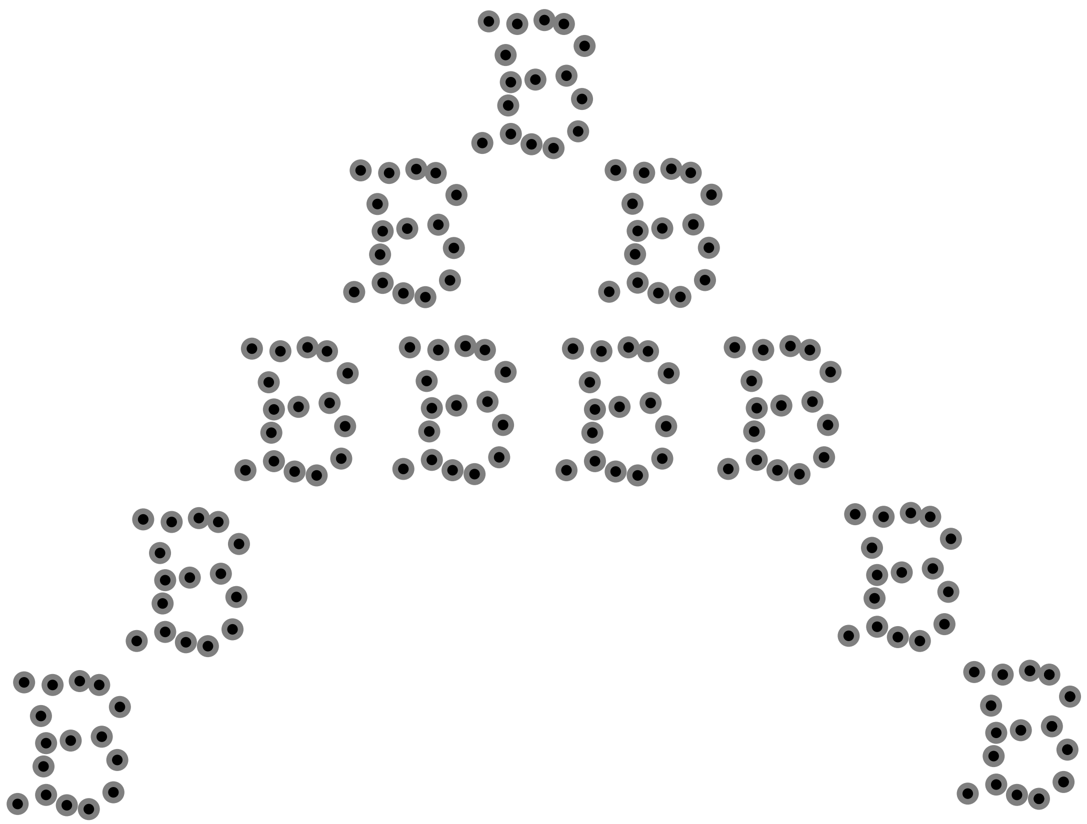

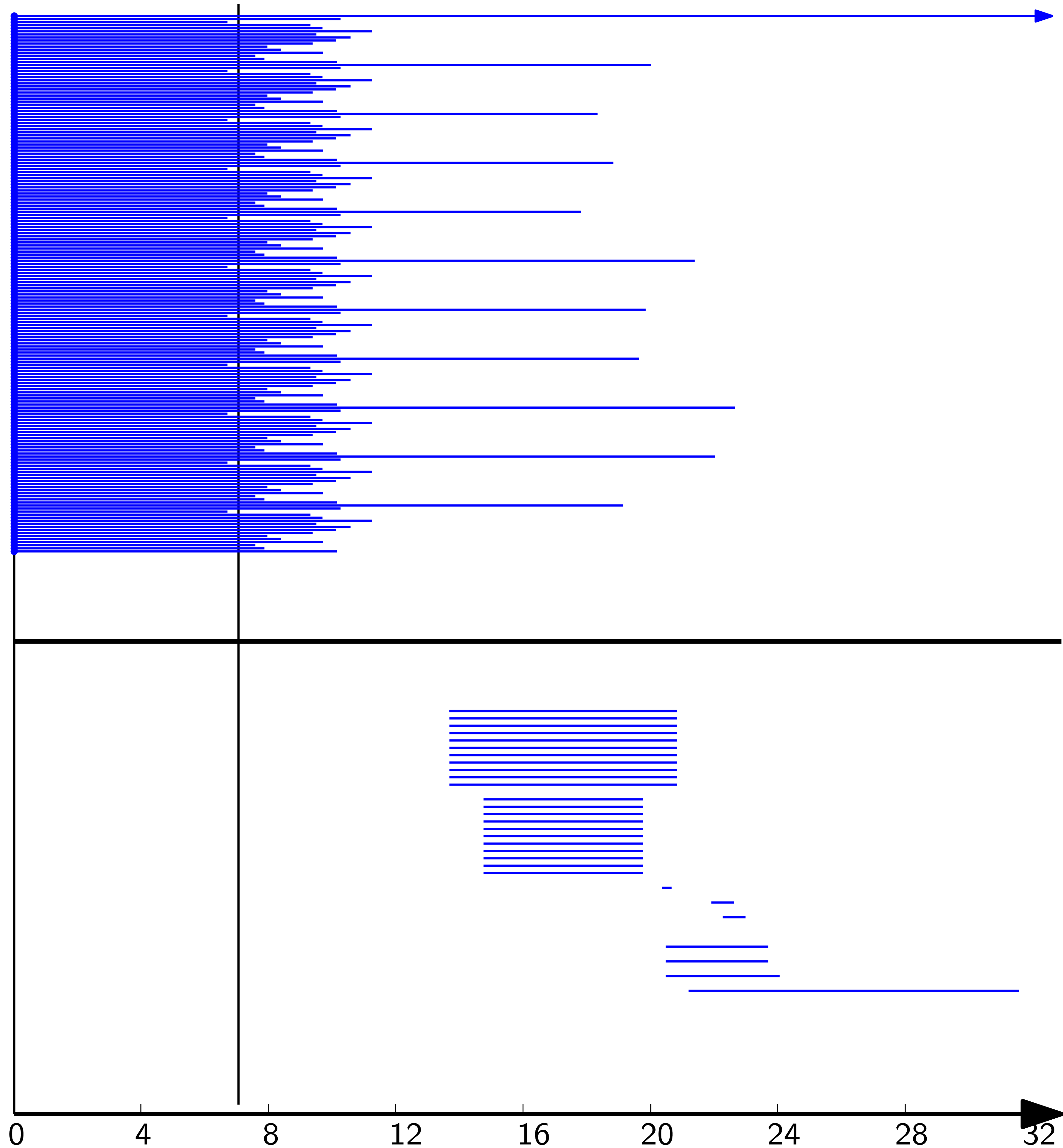

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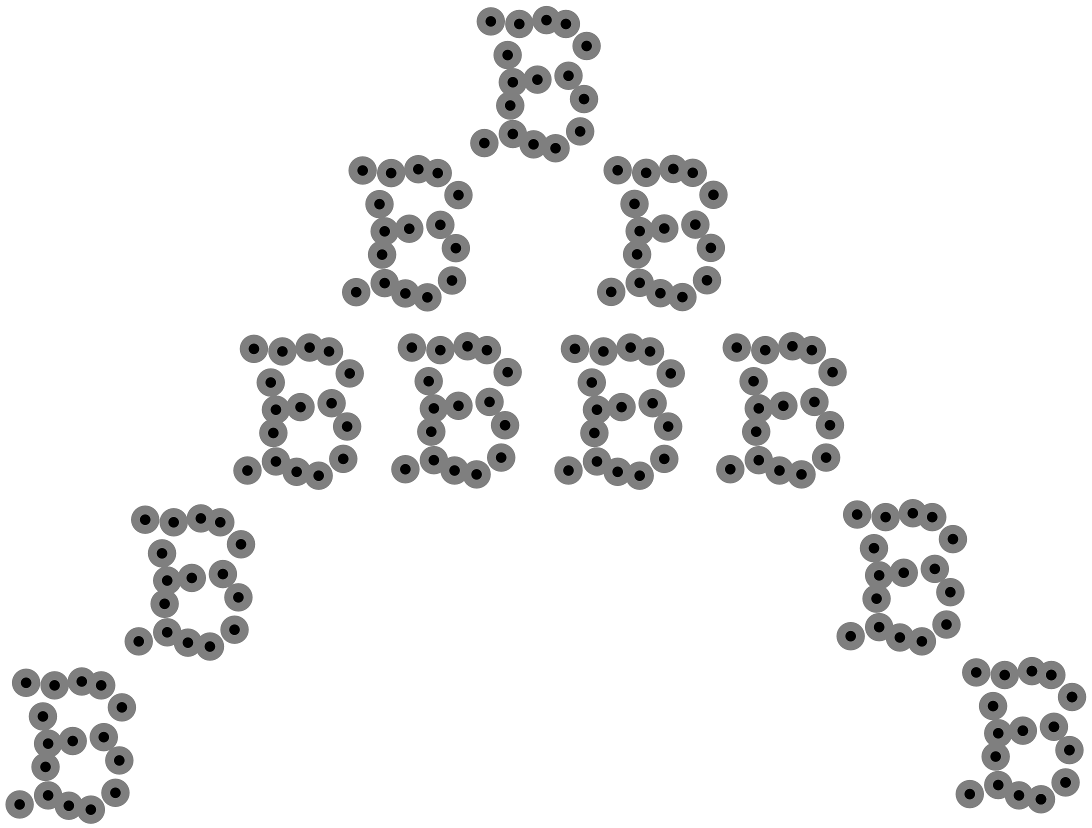

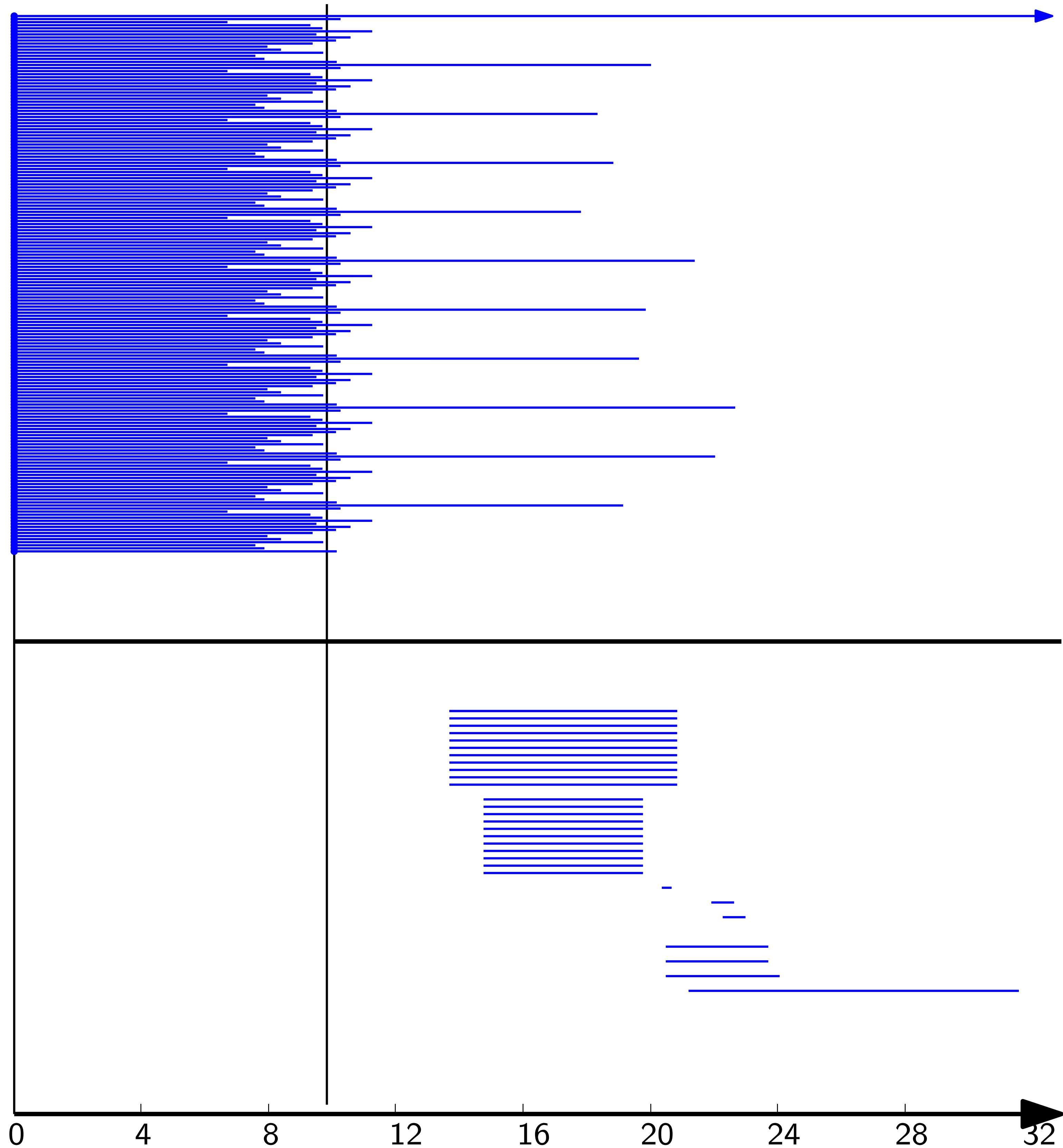

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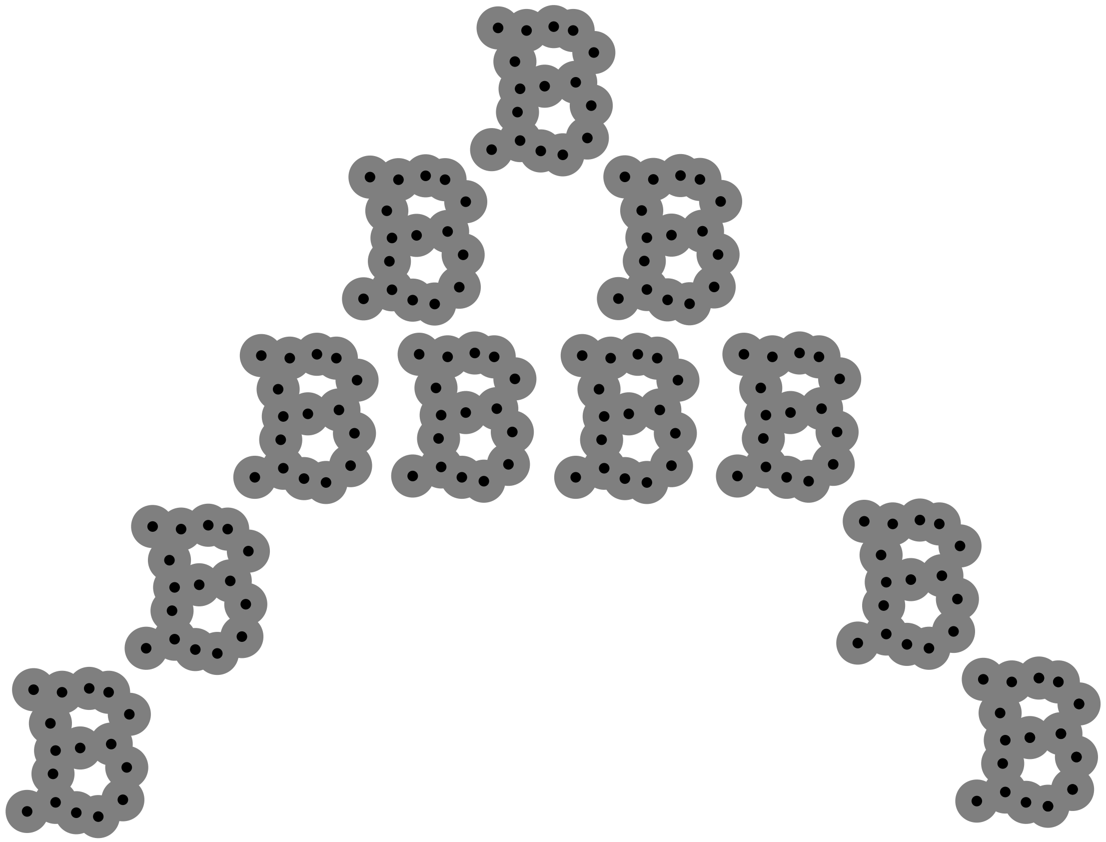

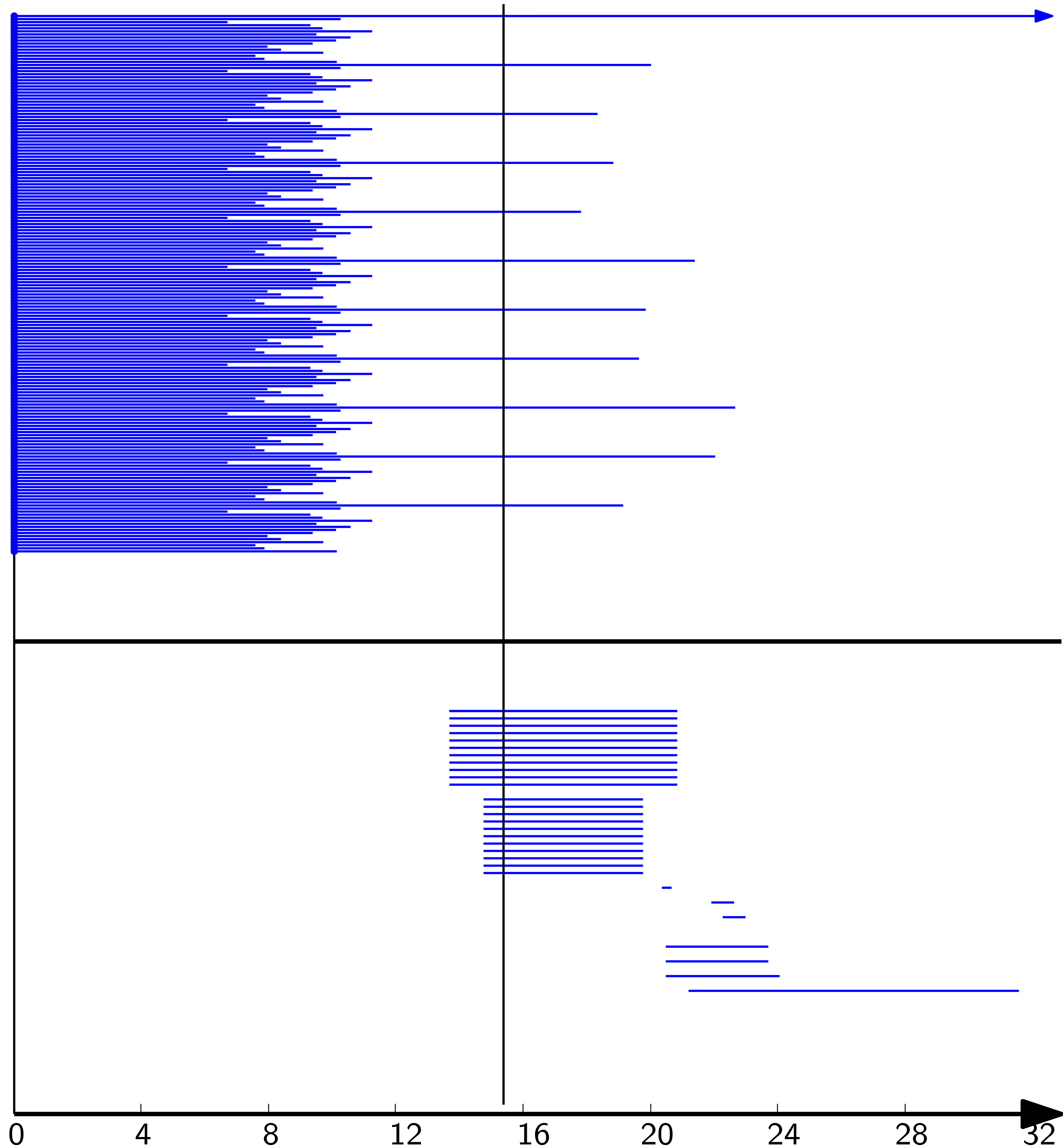

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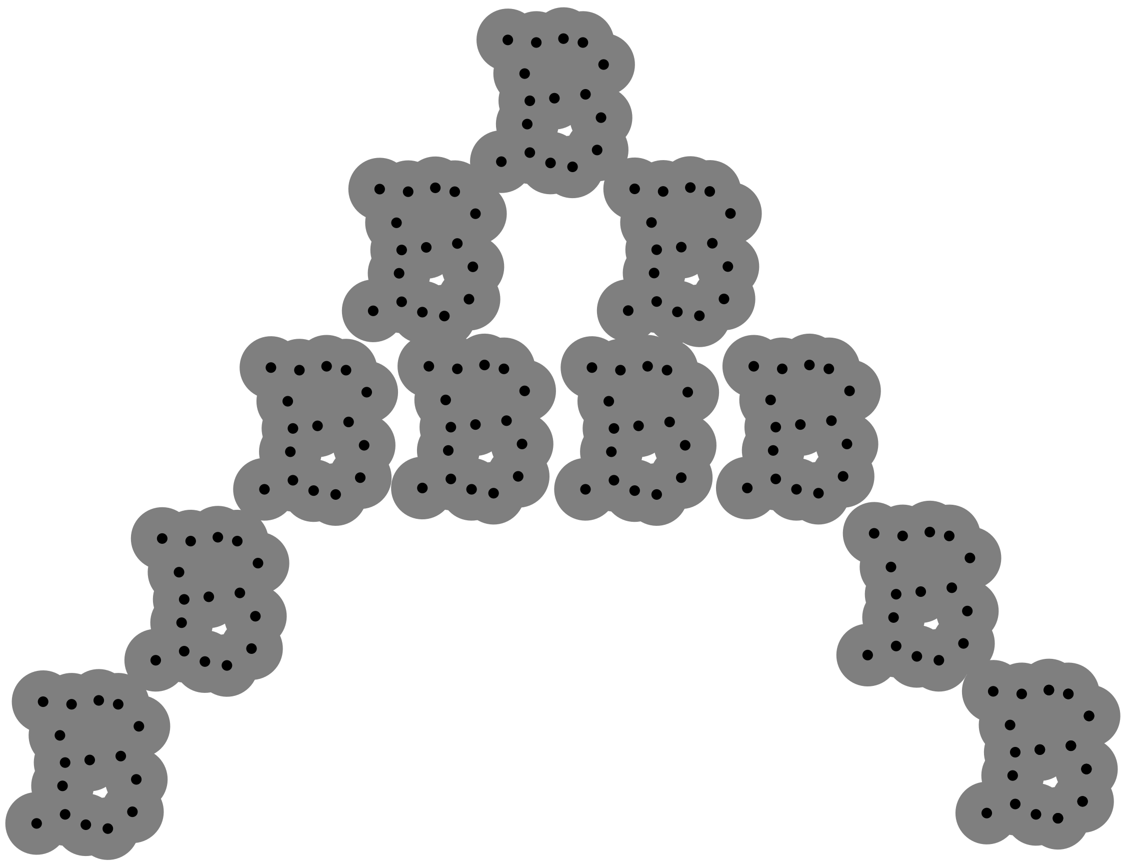

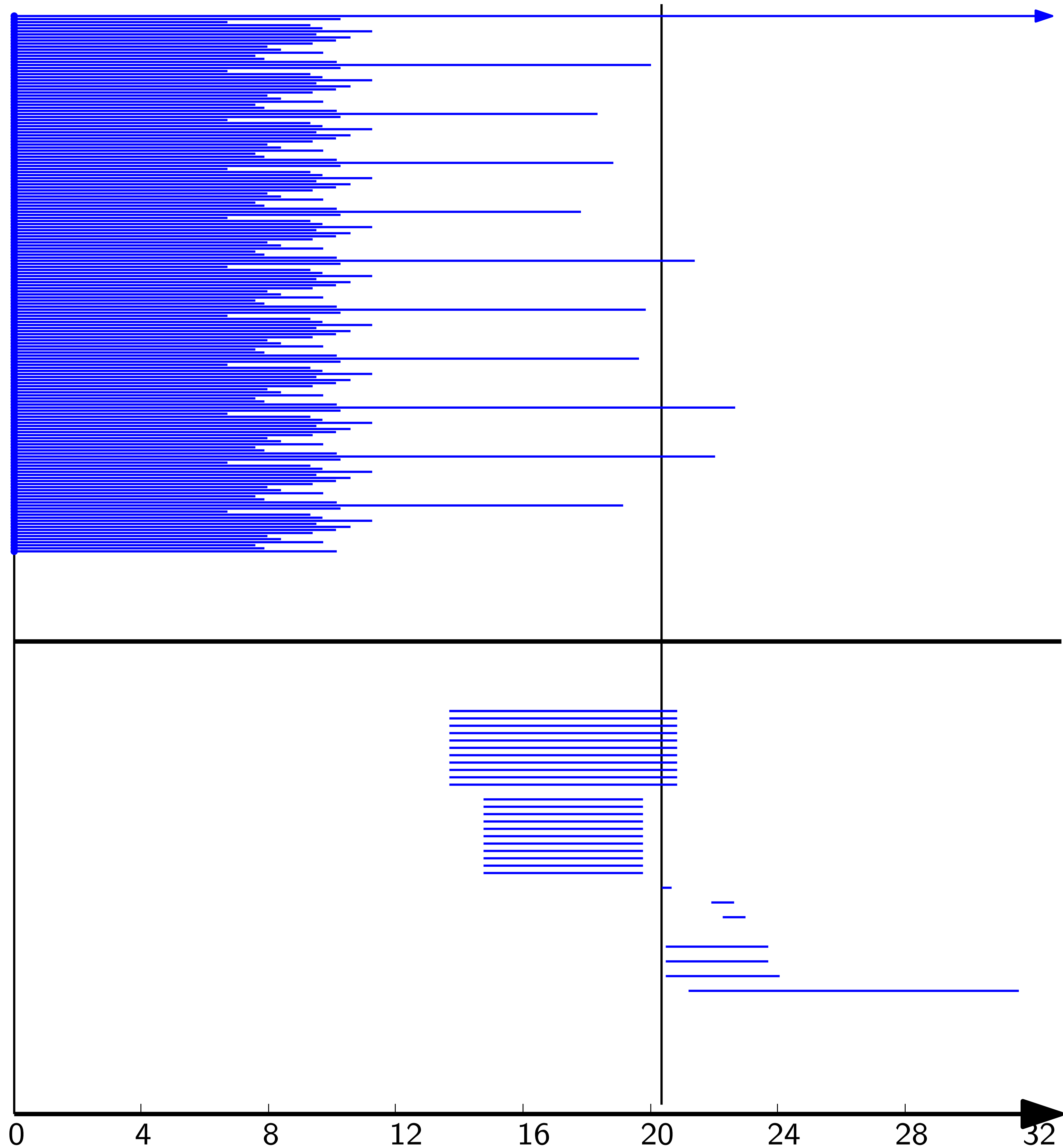

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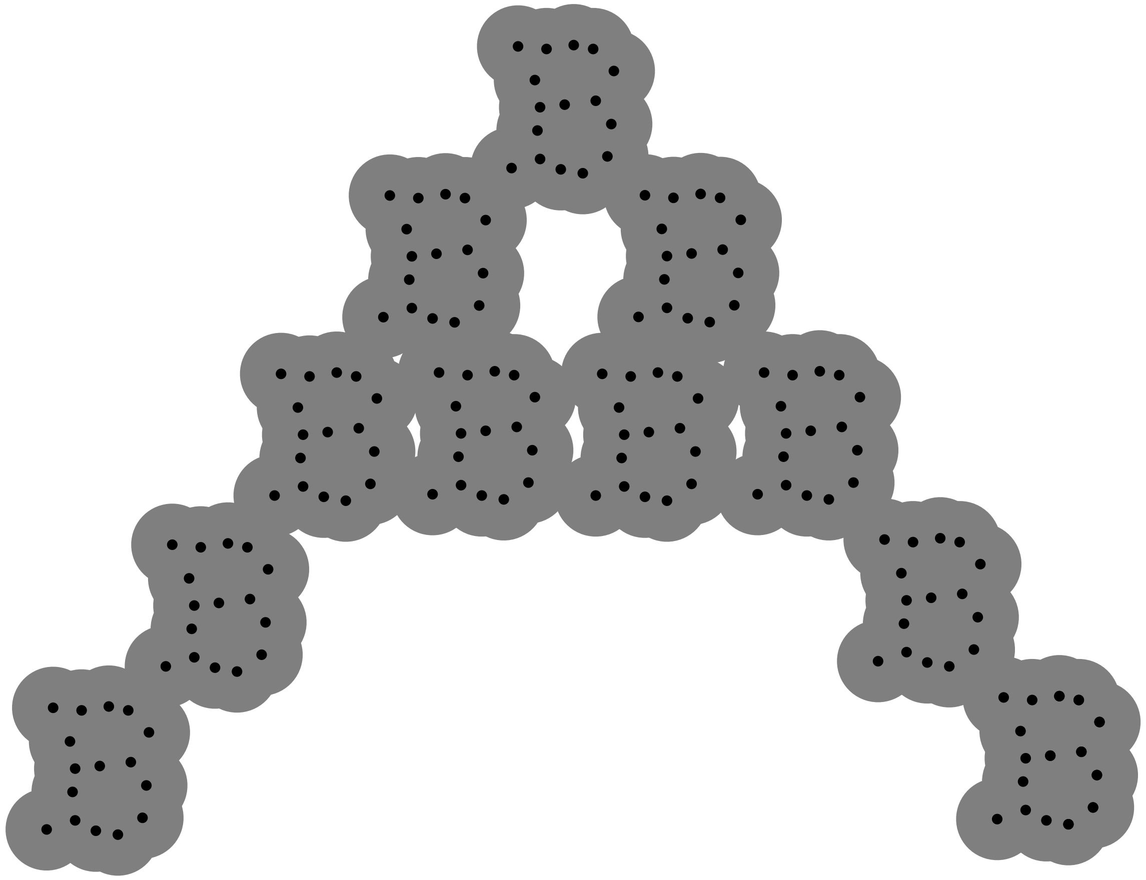

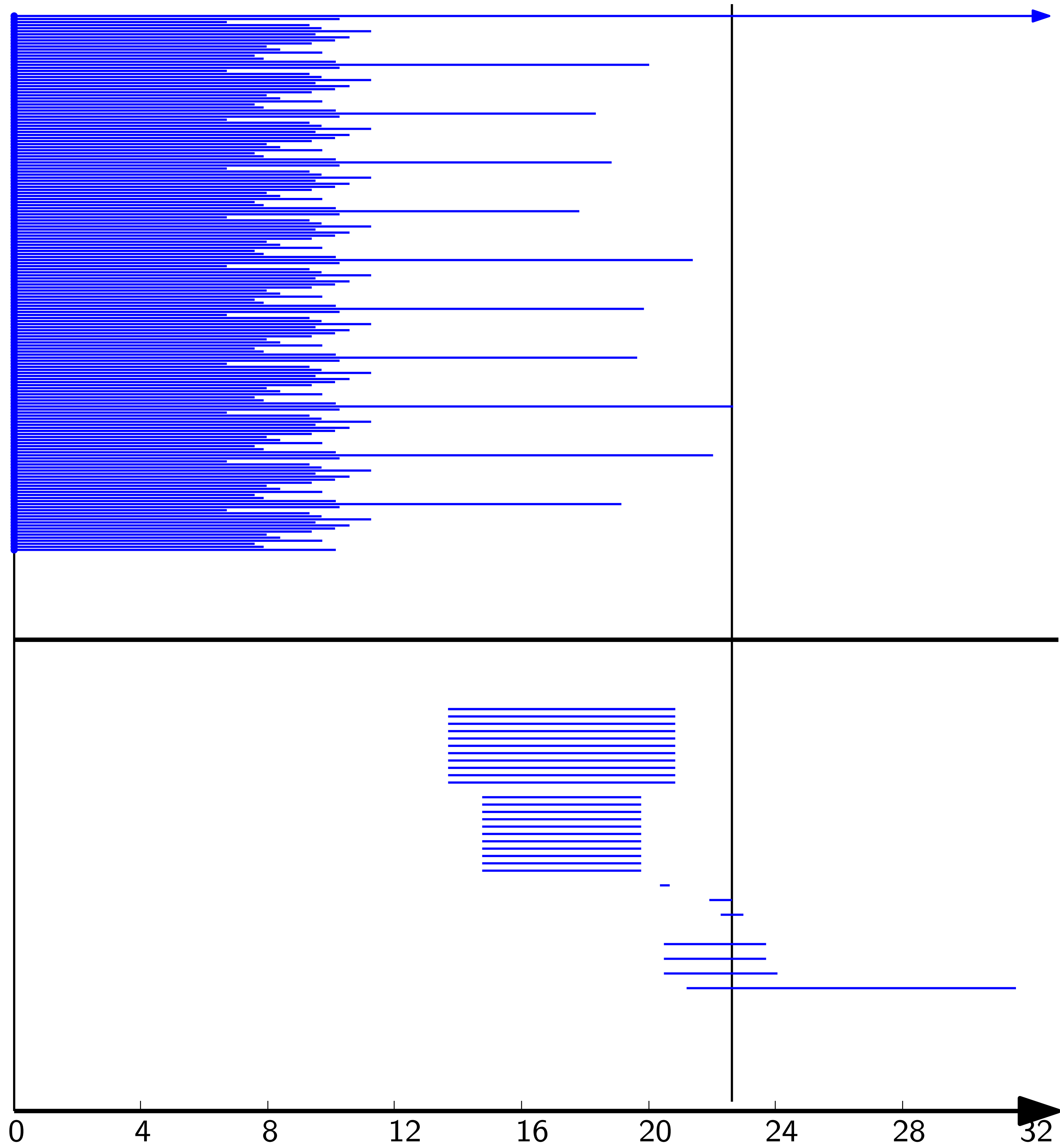

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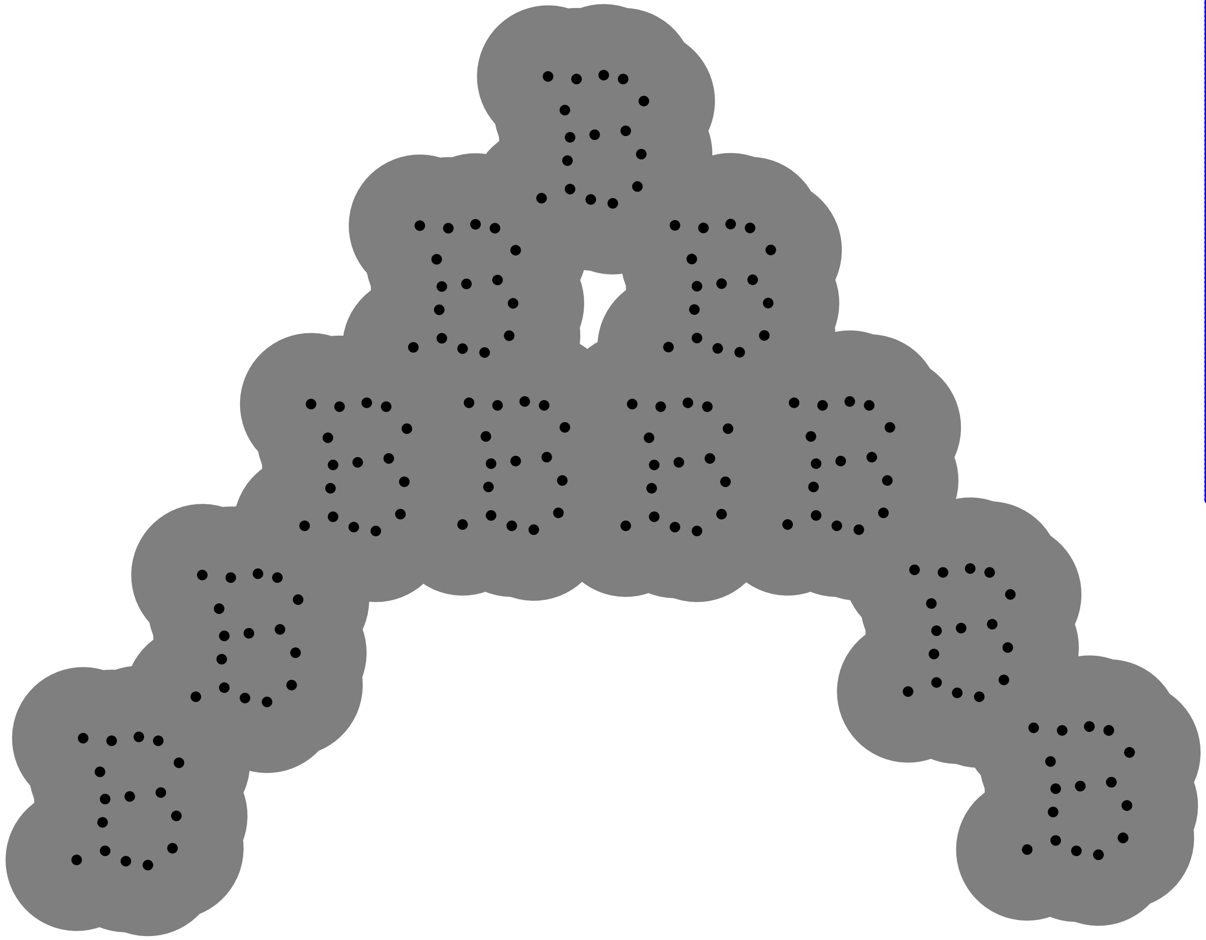

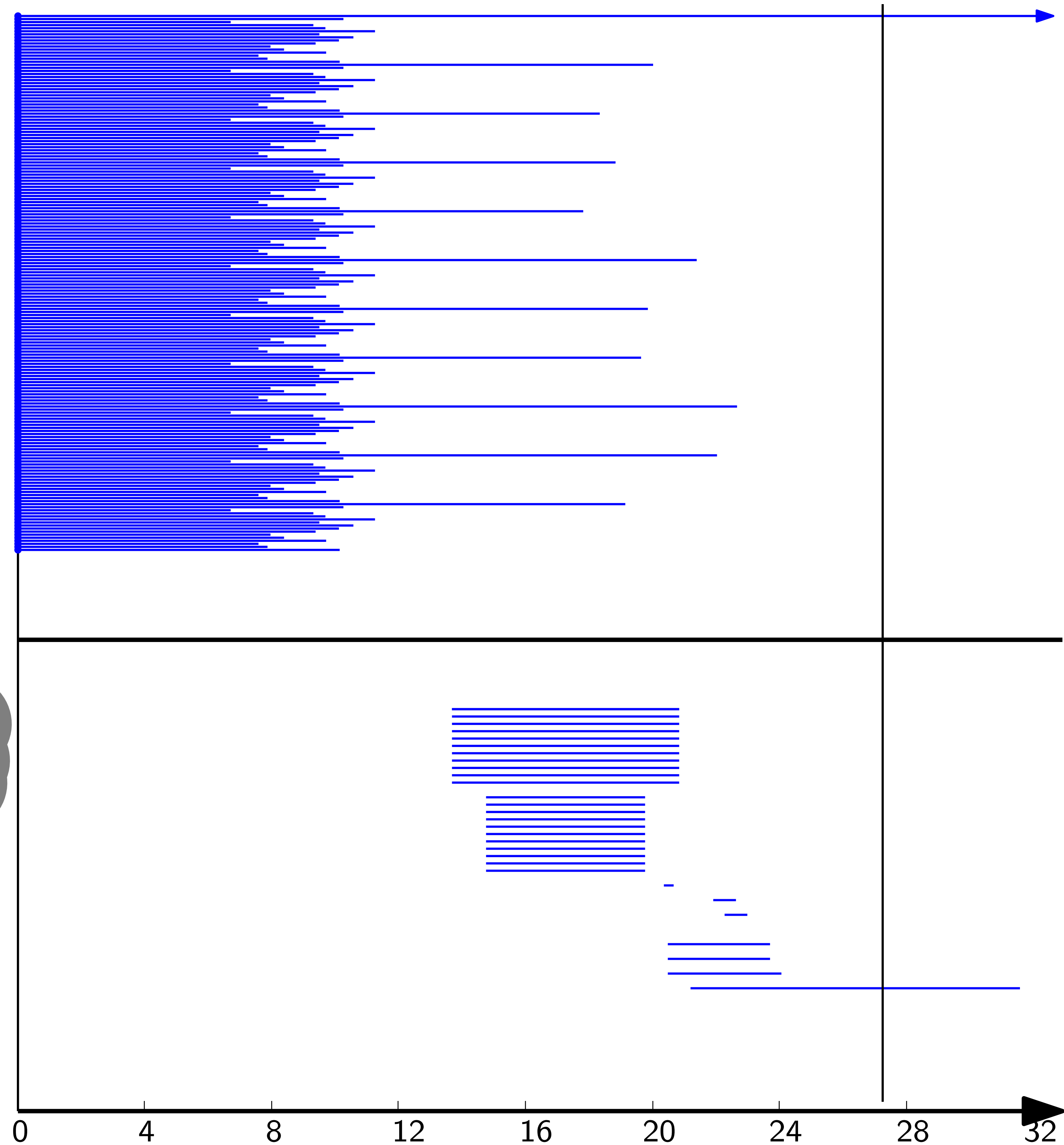

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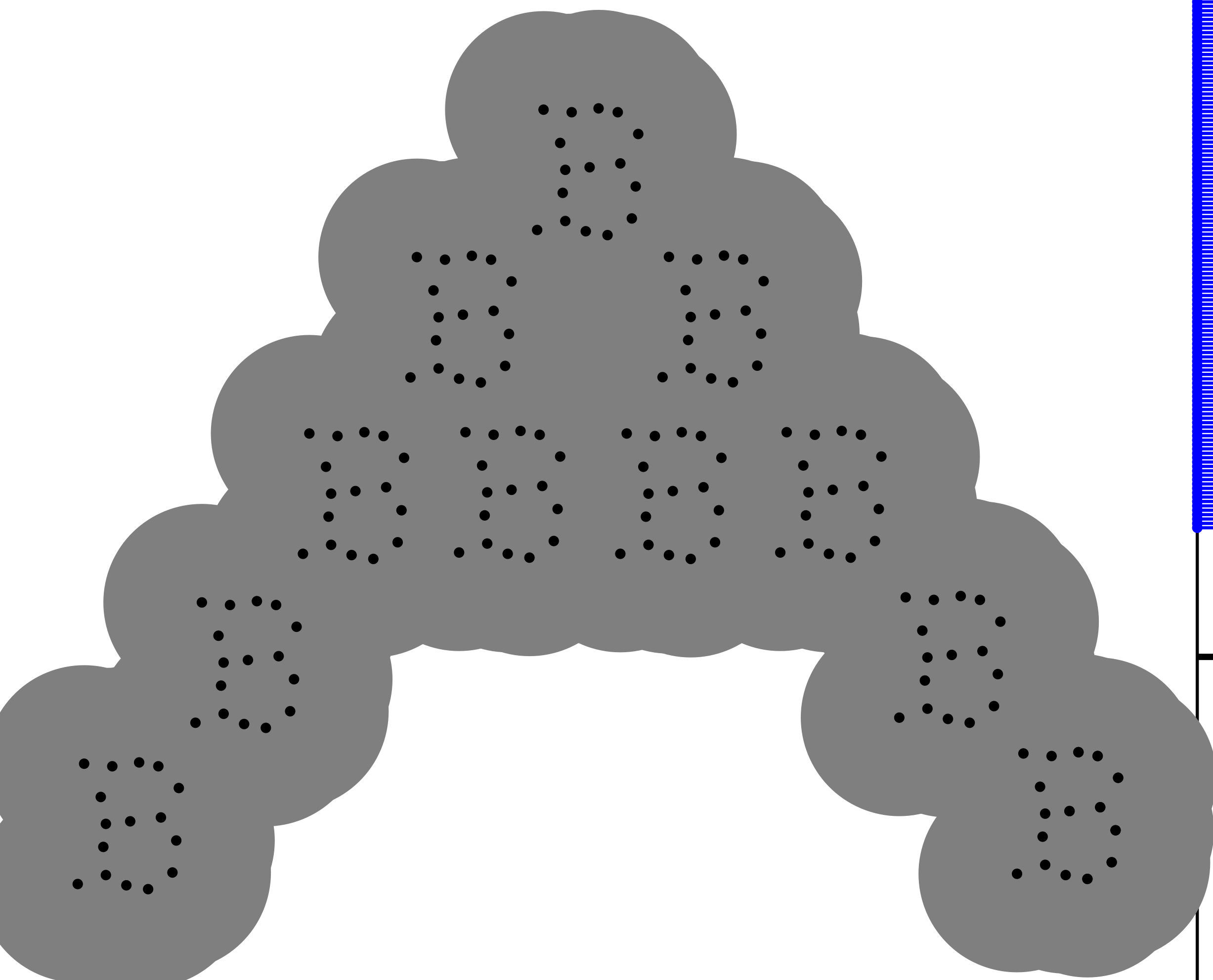
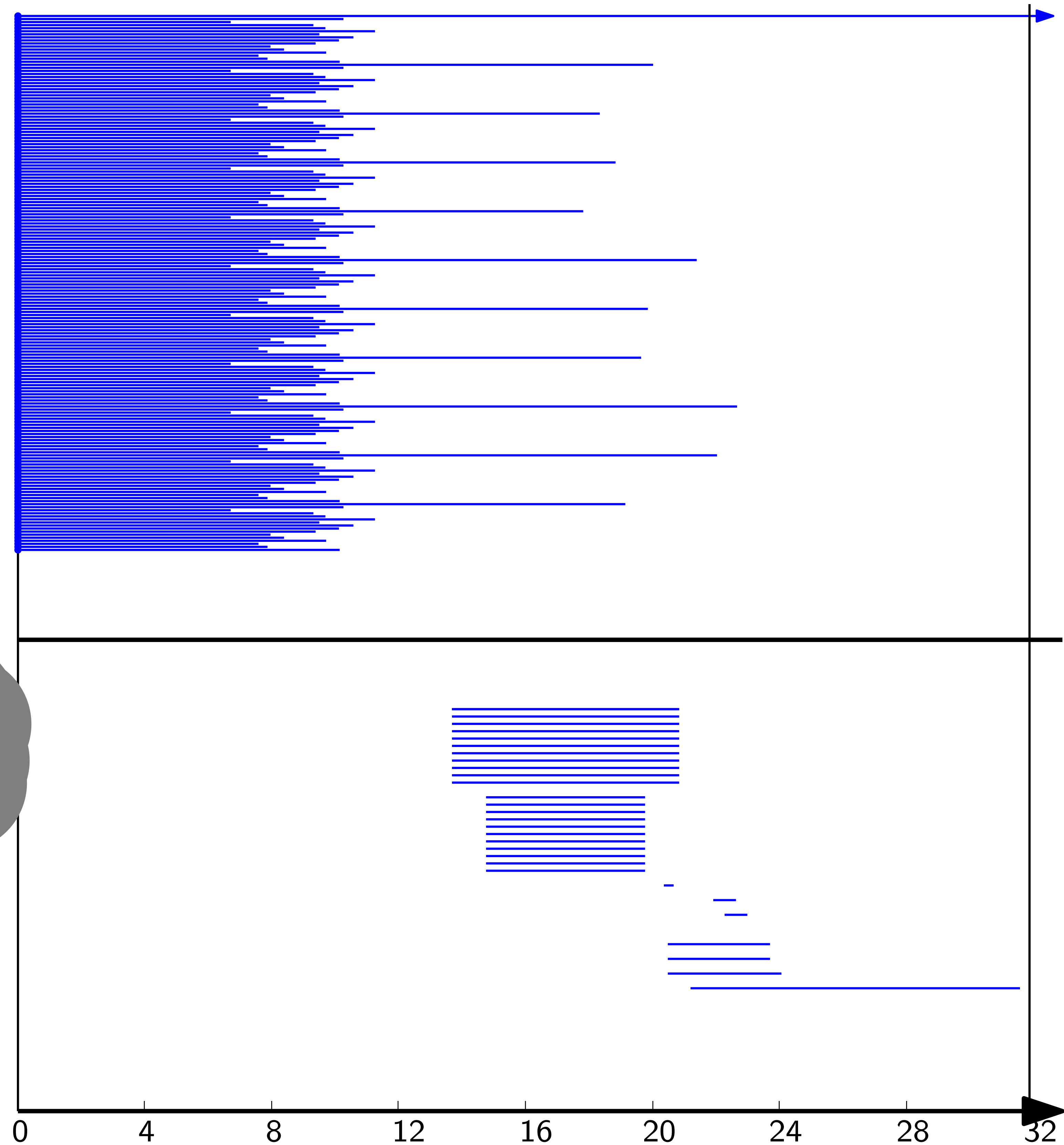
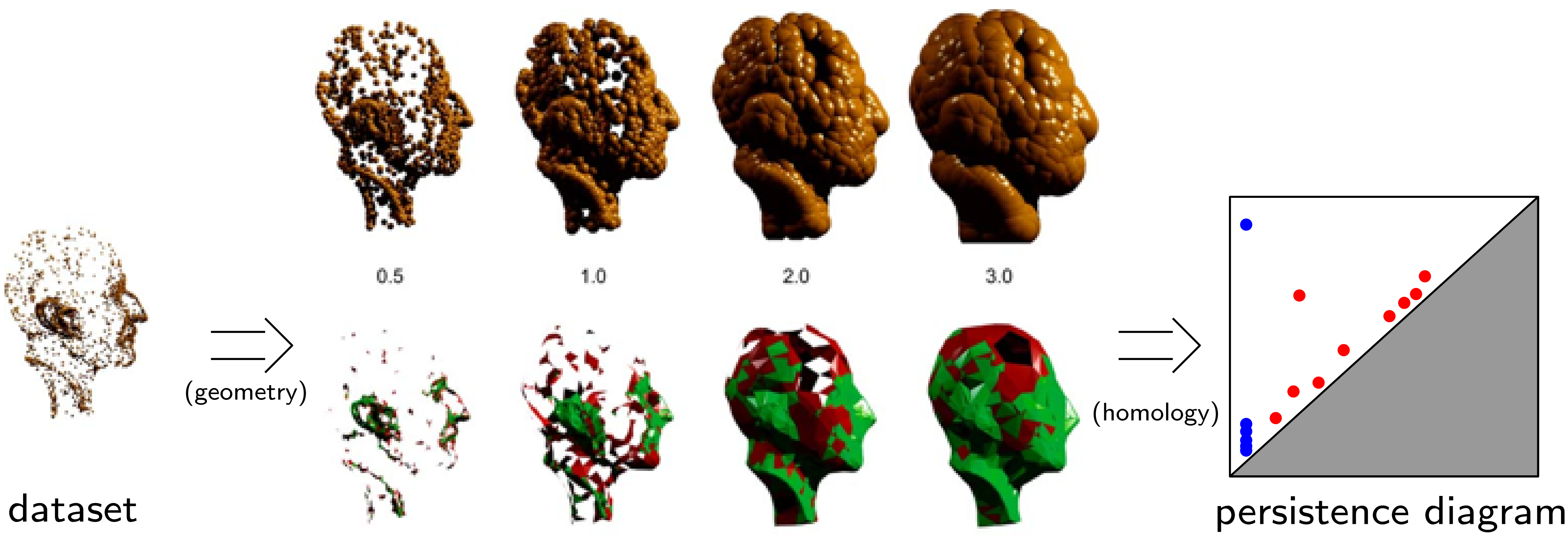




Global topological descriptors

Input: a compact metric space (X, d_X)

Descriptor: $\mathrm{dgm}\,\mathcal{F}(X, \mathrm{d}_X)$, where $\mathcal{F}(X, \mathrm{d}_X)$ is some simplicial filtration over X derived from d_X (proxy for union of balls)



Union of balls / Čech / Rips filtration

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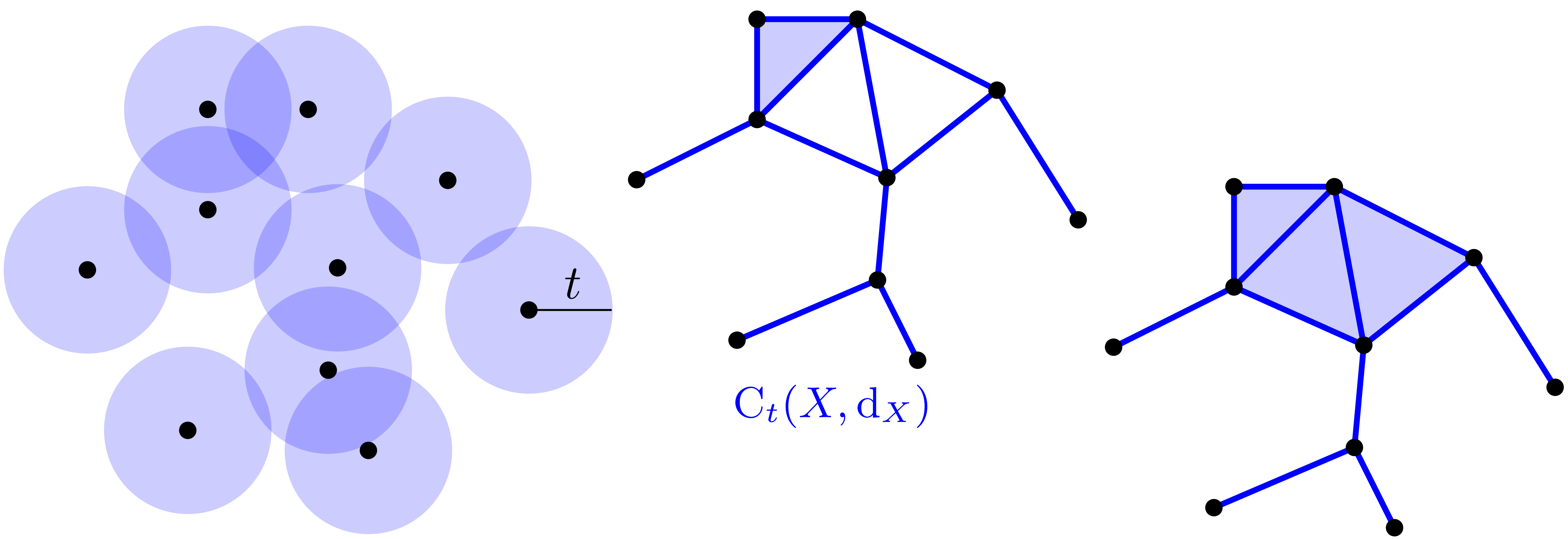
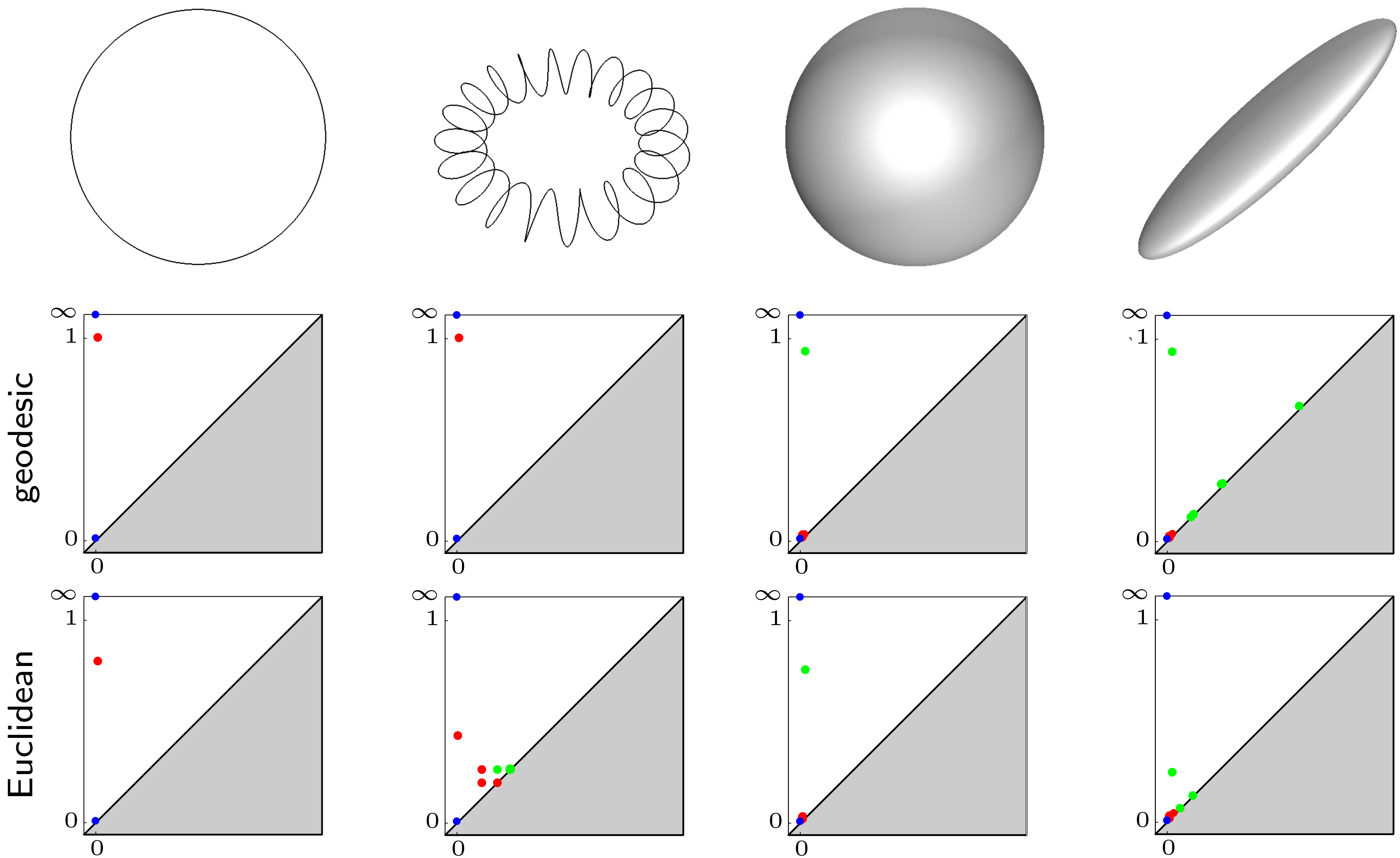


$\mathrm{C}_t(X, \mathrm{d}_X)$

$\mathrm{R}_{2t}(X, \mathrm{d}_X)$

Some examples

Descriptors of some elementary shapes (approximated from finite samples):



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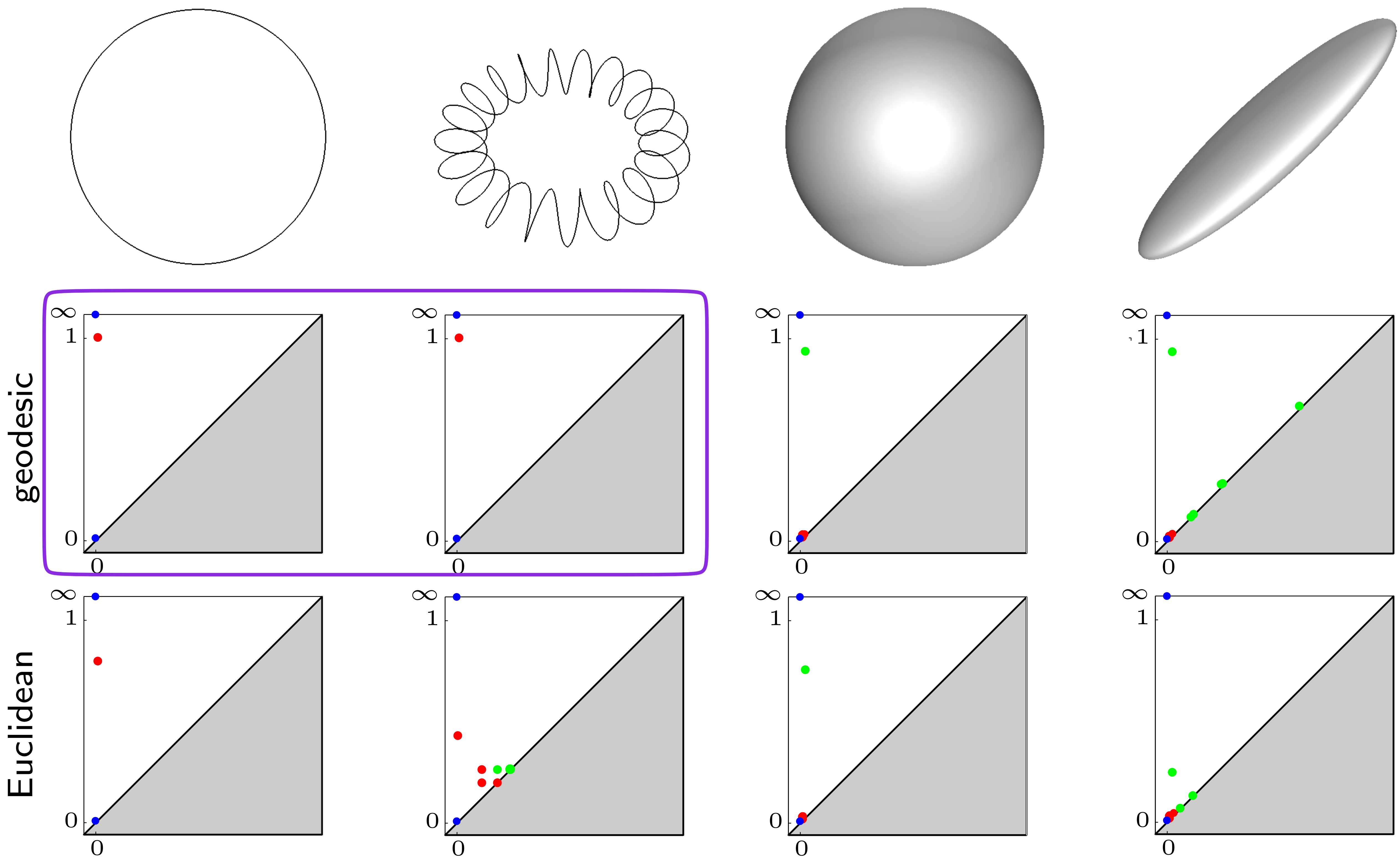

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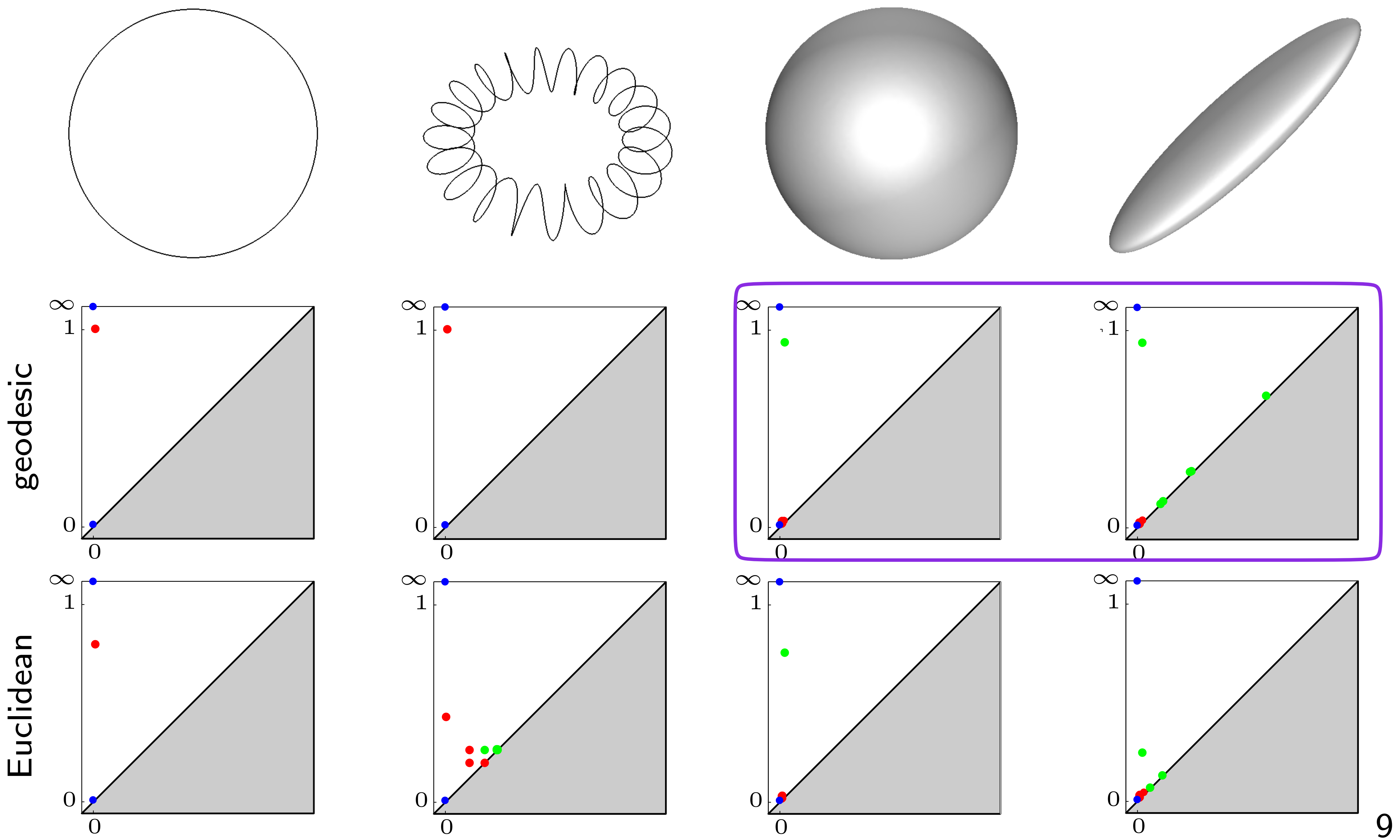
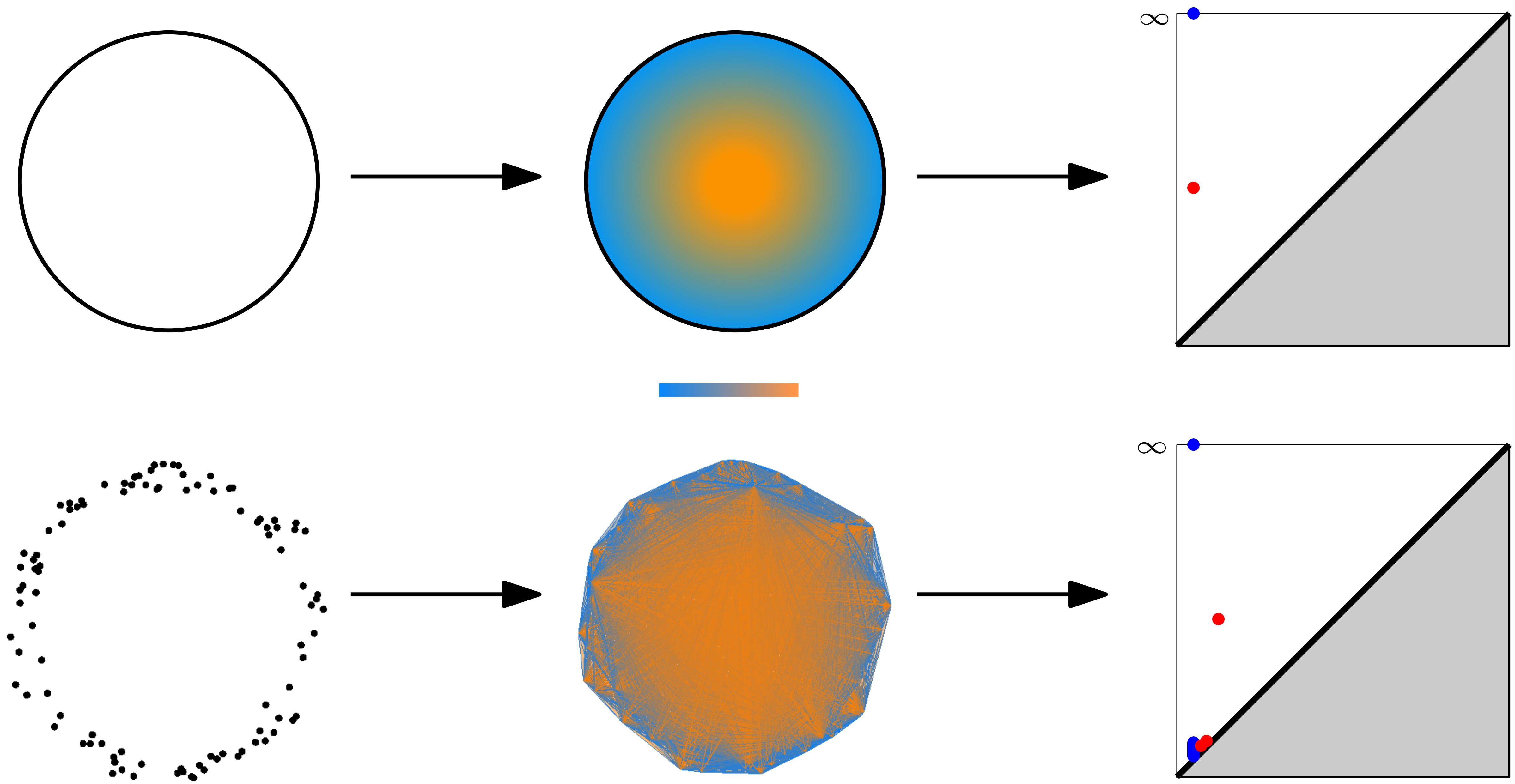


Stability

Theorem: [Chazal, de Silva, O. 2013]
For any compact metric spaces (X, d_X) and (Y, d_Y),
$\mathrm{d}_{\mathrm{B}}^{\infty}(\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X),\ \mathrm{dgm}\,\mathcal{R}(Y, \mathrm{d}_Y)) \leq 2\mathrm{d}_{\mathrm{GH}}(X, Y)$.



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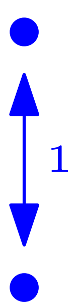
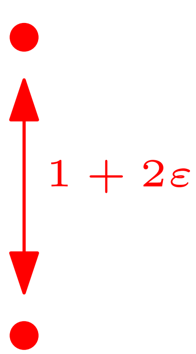
The bound is worst-case tight:

$X =$ 

$Y =$ 

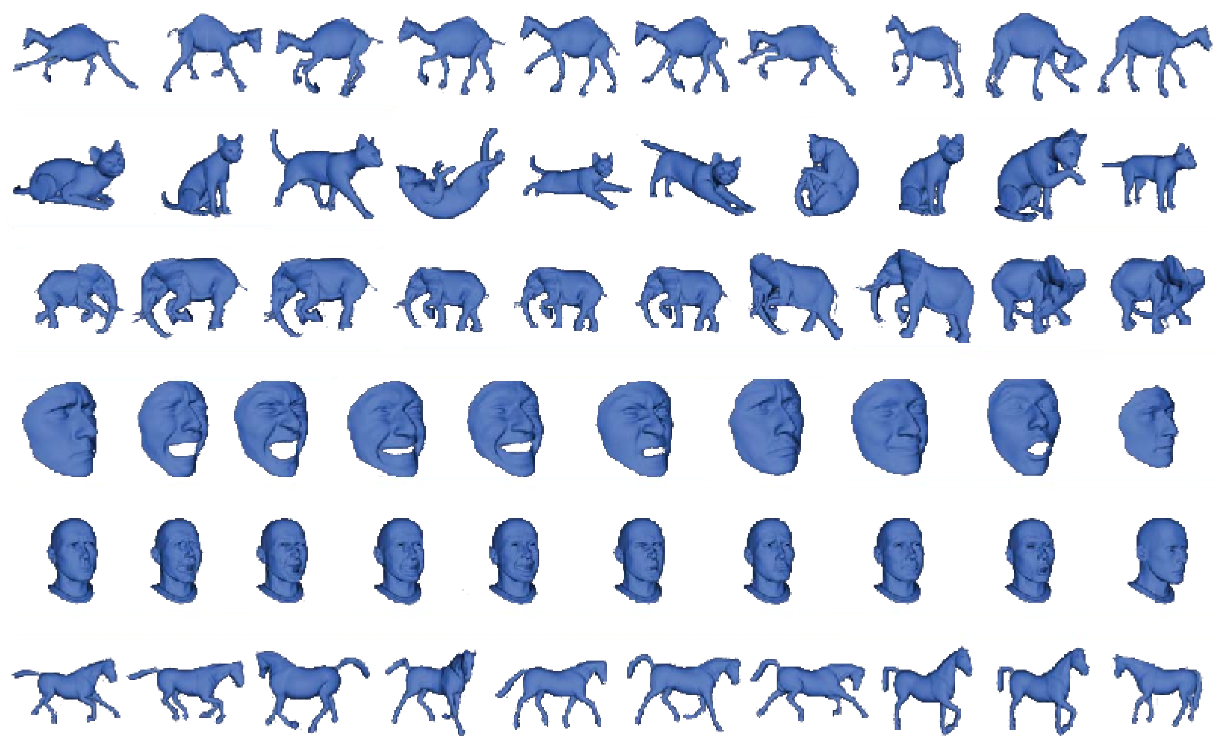
$$\mathrm{d}_\mathrm{GH}(X, Y) = \varepsilon$$

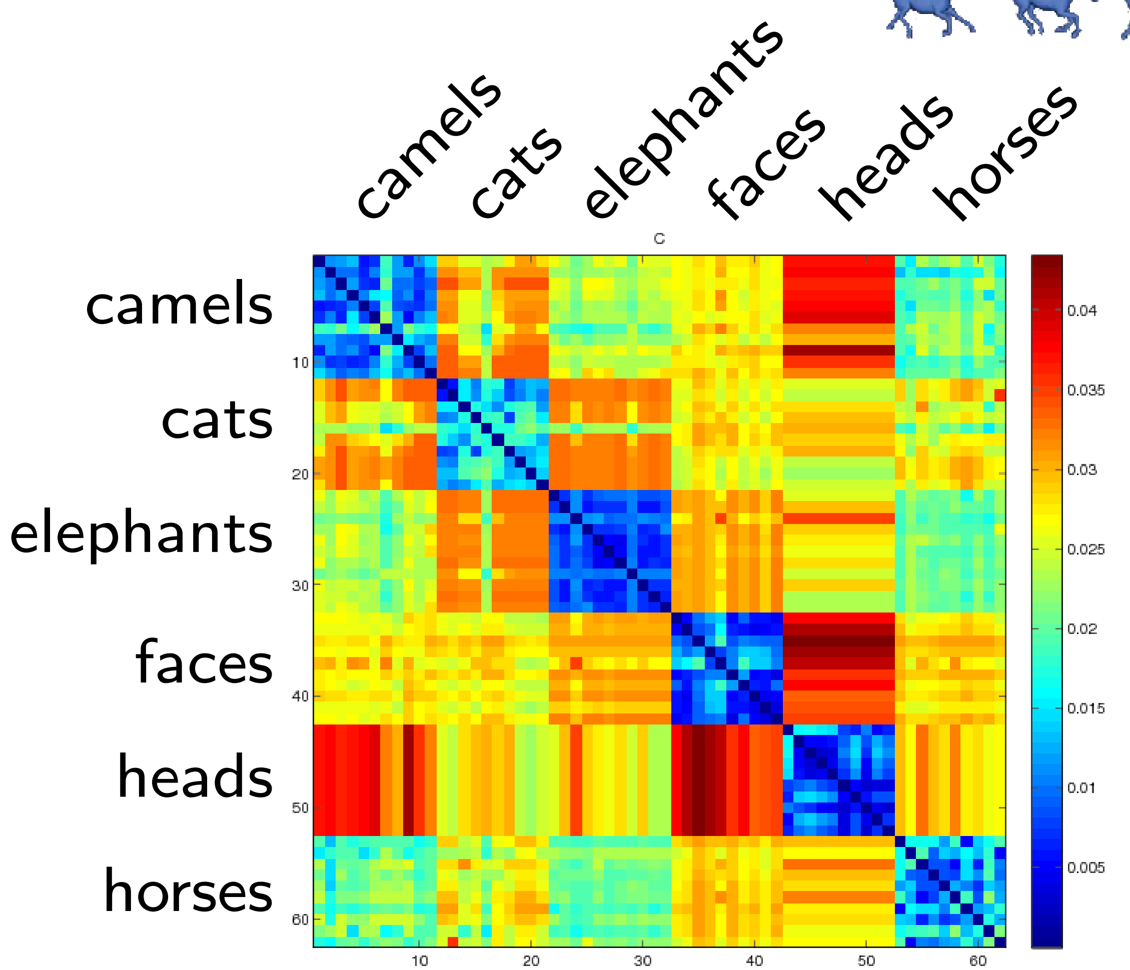
$$\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X) = \{(0, \infty),\ (0, 1)\}$$

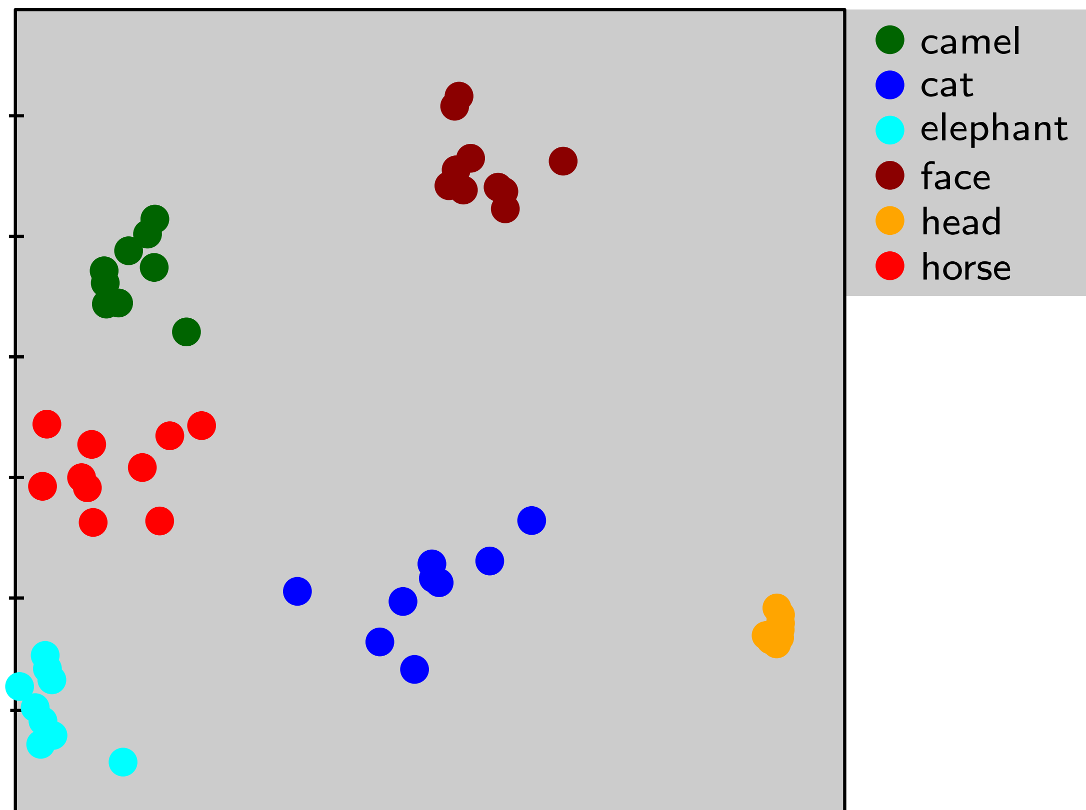
$$\mathrm{dgm}\,\mathcal{R}(Y, \mathrm{d}_Y) = \{(0, \infty),\ (0, 1 + 2\varepsilon)\}$$

$$\Rightarrow \mathrm{d}_\mathrm{B}^\infty(\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X),\ \mathrm{dgm}\,\mathcal{R}(Y, \mathrm{d}_Y)) = 2\varepsilon$$

Toy application (unsupervised shape classification)





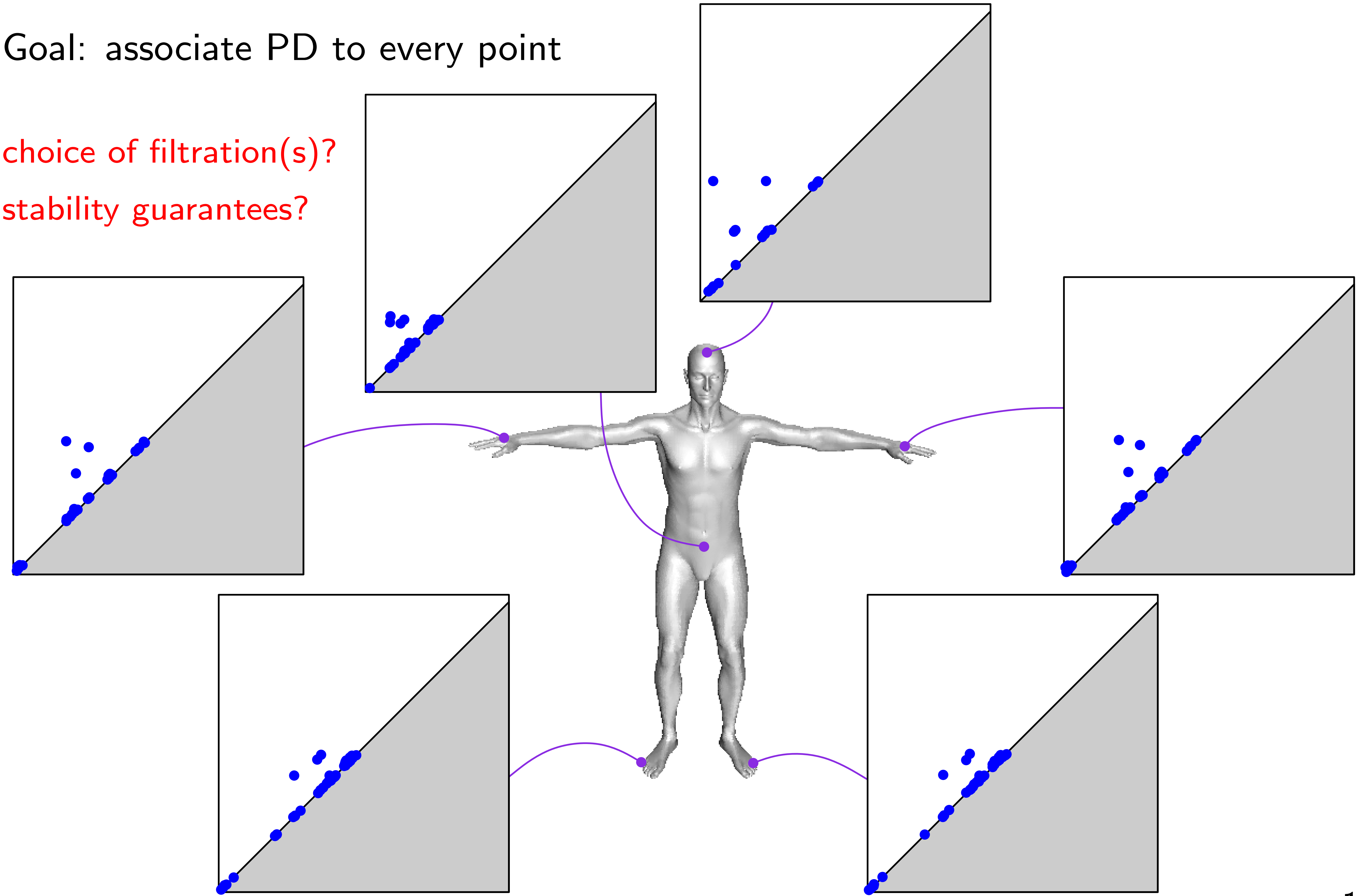


Local topological descriptors

Goal: associate PD to every point

choice of filtration(s)?

stability guarantees?



Local topological descriptors

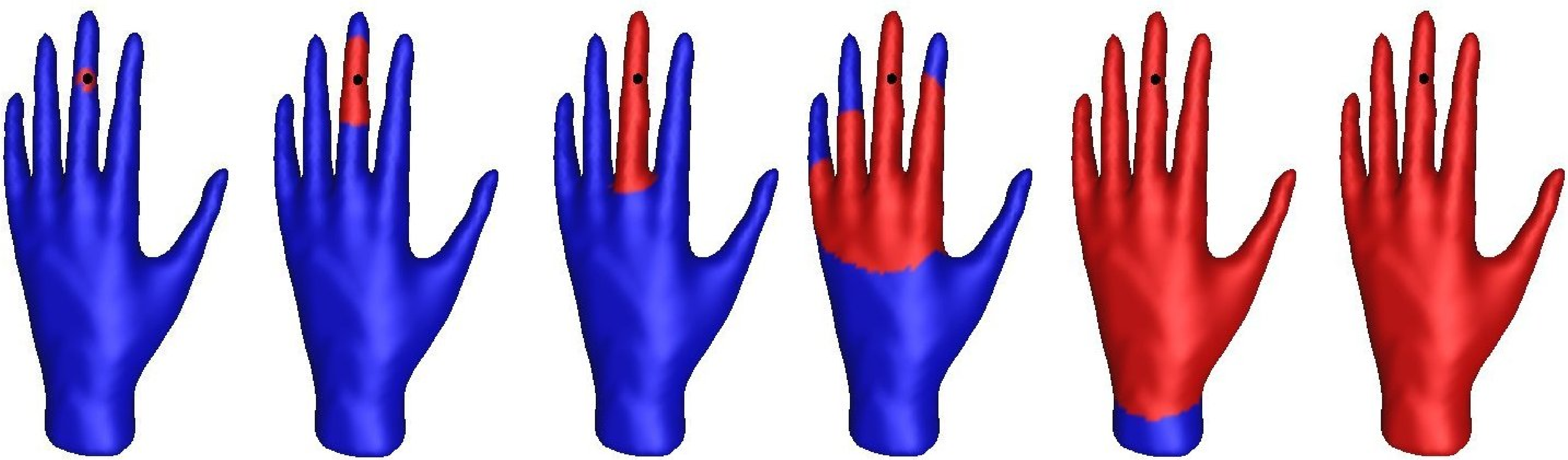
Input: a compact *length space* (X, d_X), a basepoint $x \in X$

Construction: filtration of the sublevel sets of $\mathrm{d}_X(x, \cdot)$

Descriptor: persistence diagram of the filtration

In practice: compute descriptor from point cloud using a pair of Rips complexes

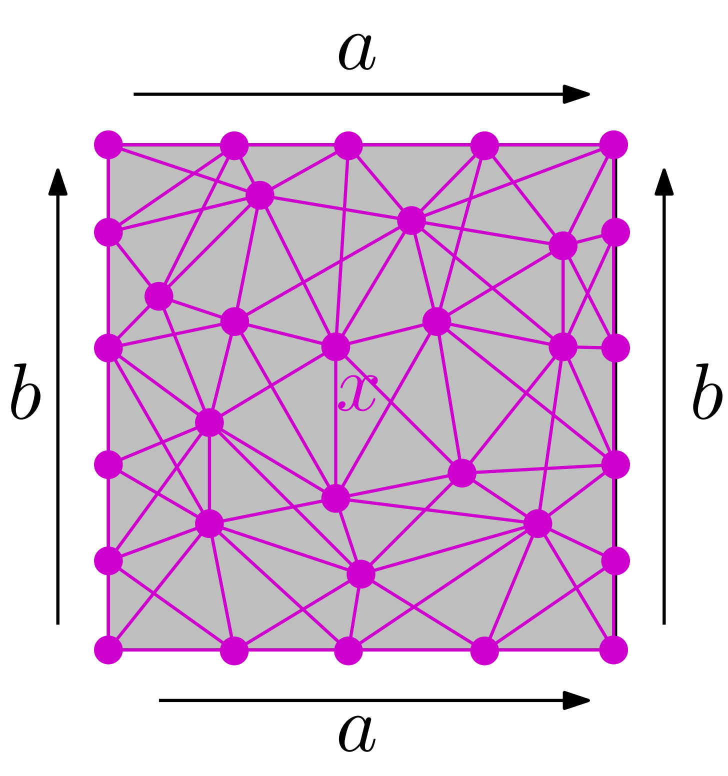
[Chazal et al. 2009]



Stability

Thm (local stability): [Carrière, O., Ovsjanikov 2015]
Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius ($\varrho(X), \varrho(Y) > 0$). Let $x \in X$ and $y \in Y$.
If $\mathrm{d}_{\mathrm{GH}}((X,x),(Y,y)) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

$$\mathrm{d}_{\mathrm{B}}(\mathrm{dgm}\, \mathrm{d}_X(\cdot, x), \mathrm{dgm}\, \mathrm{d}_Y(\cdot, y)) \leq 20\ \mathrm{d}_{\mathrm{GH}}((X,x),(Y,y)).$$



$$\mathrm{d}_{\mathrm{GH}}(T, X) \overset{\#X \to \infty}{\longrightarrow} 0$$

$$\mathrm{d}_{\mathrm{B}}(\mathrm{dgm}\, \mathrm{d}_T(\cdot, x),\ \mathrm{dgm}\, \mathrm{d}_X(\cdot, x)) > 0$$

Toy application (unsupervised shape segmentation)

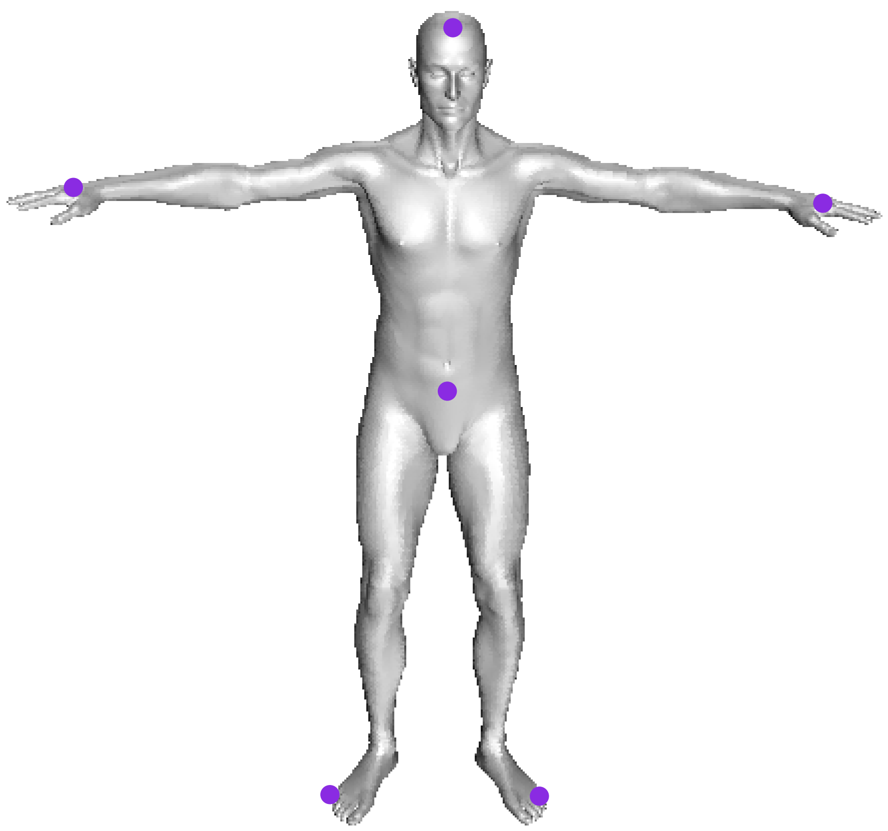
Experimental results:

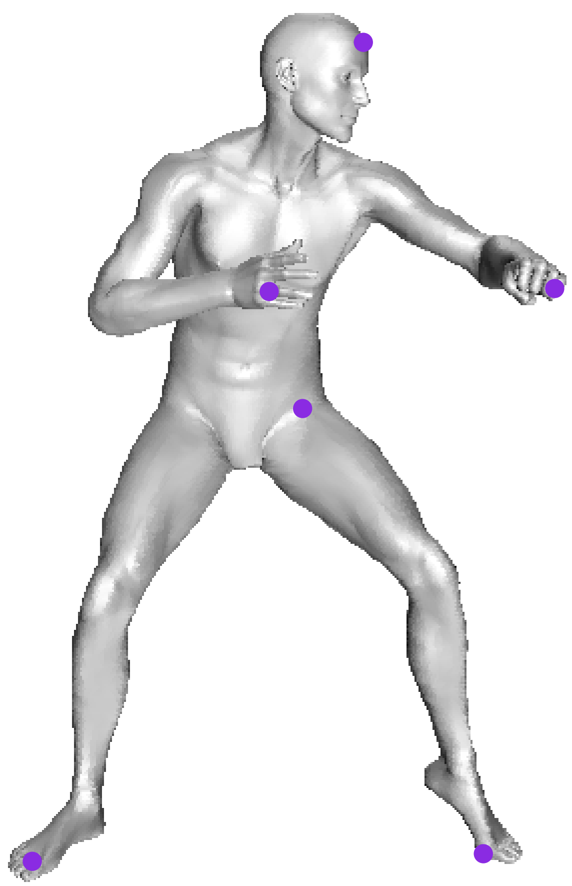
- input: shapes from the TOSCA database, in *mesh* form (triangulated)

- select a few base points by hand on each shape

- approximate geodesic distances to base points using the 1-skeleton graph

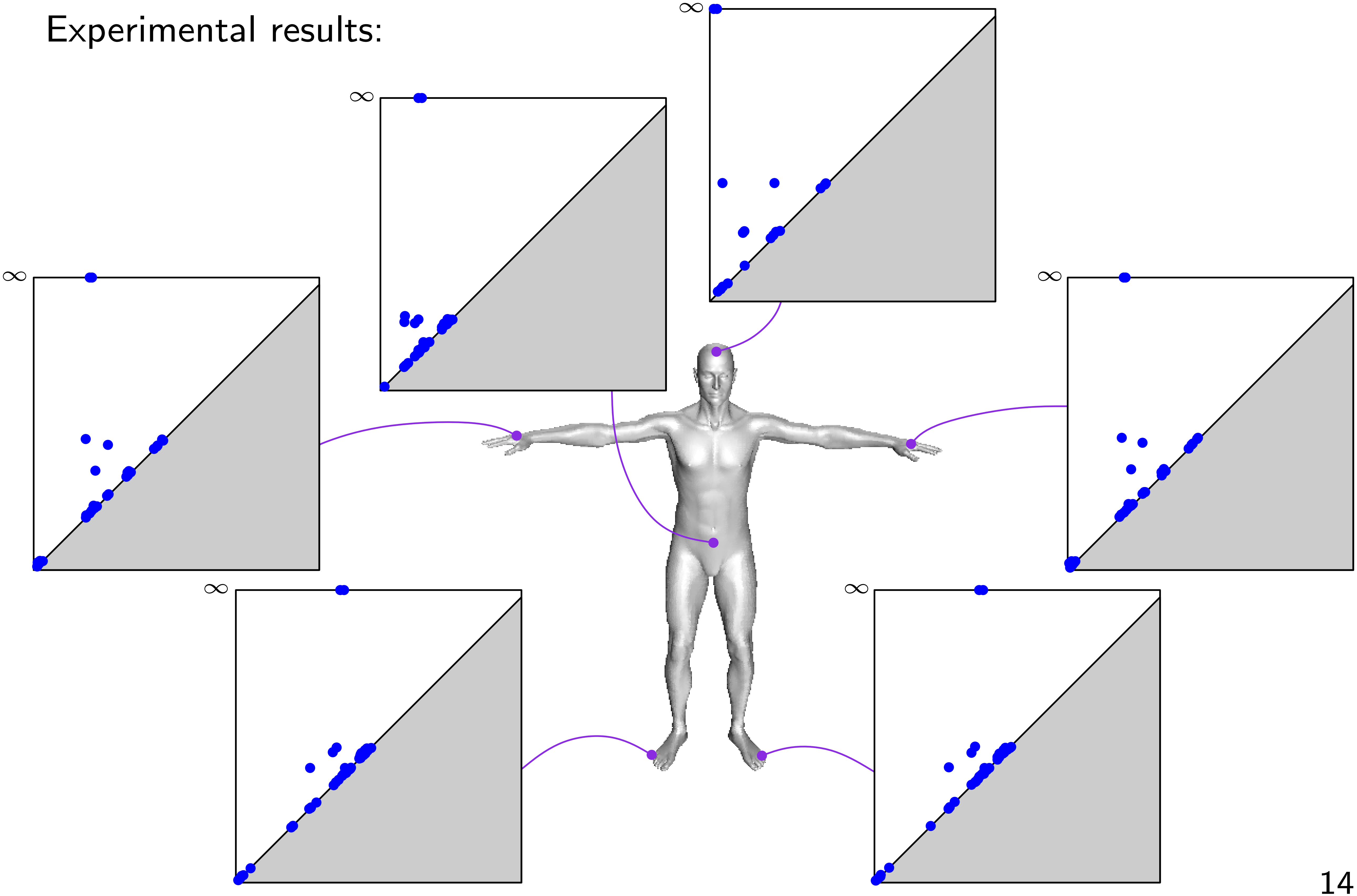
- use the PDs of the PL interpolations over the meshes as descriptors





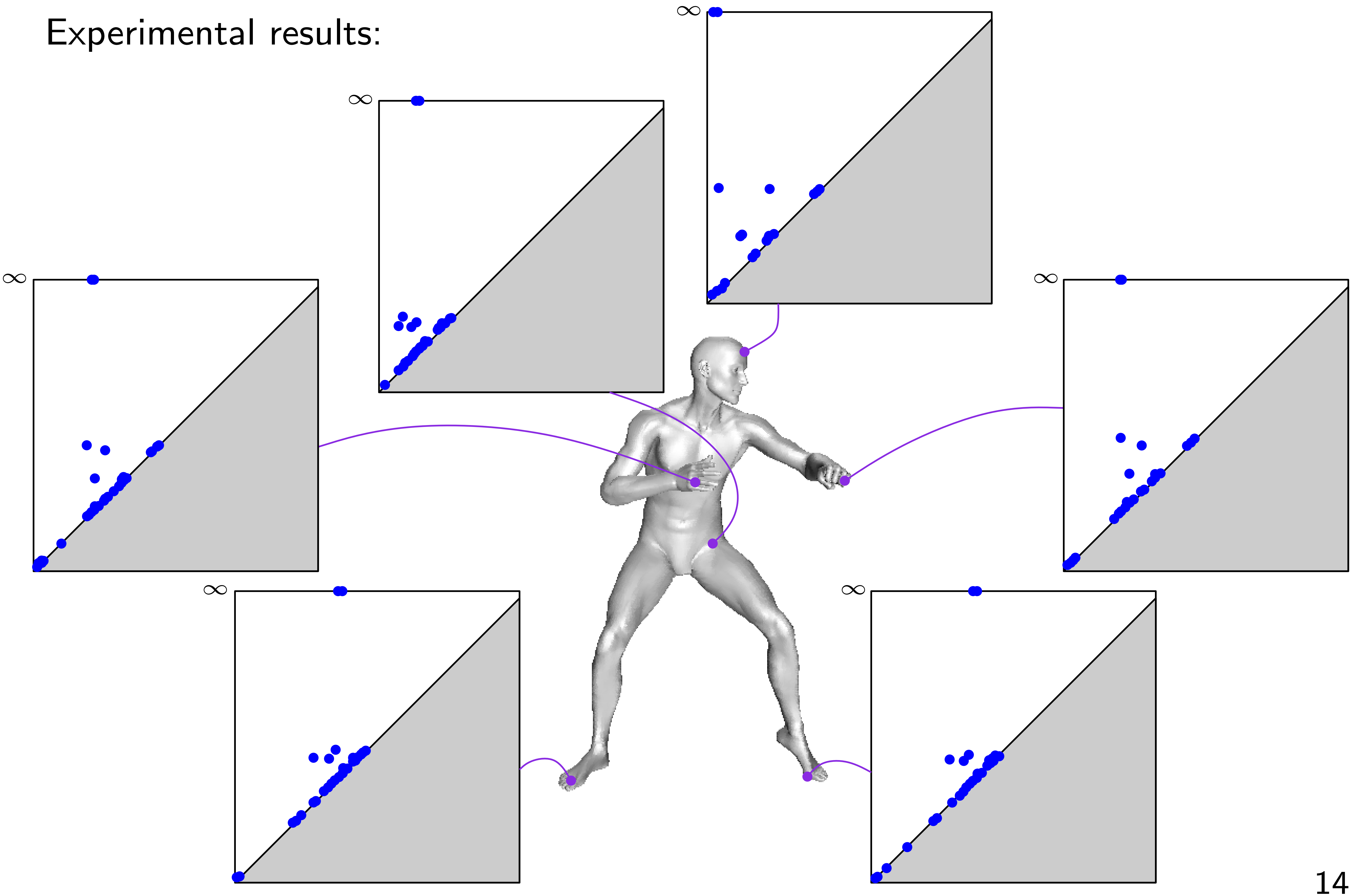
Toy application (unsupervised shape segmentation)

Experimental results:



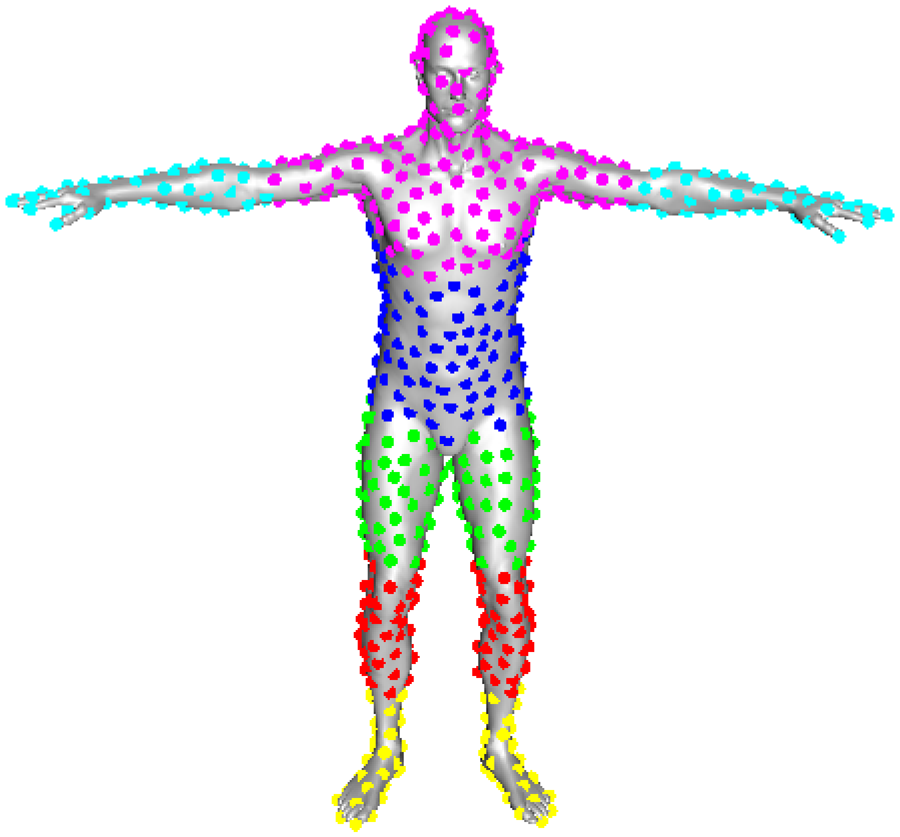
Toy application (unsupervised shape segmentation)

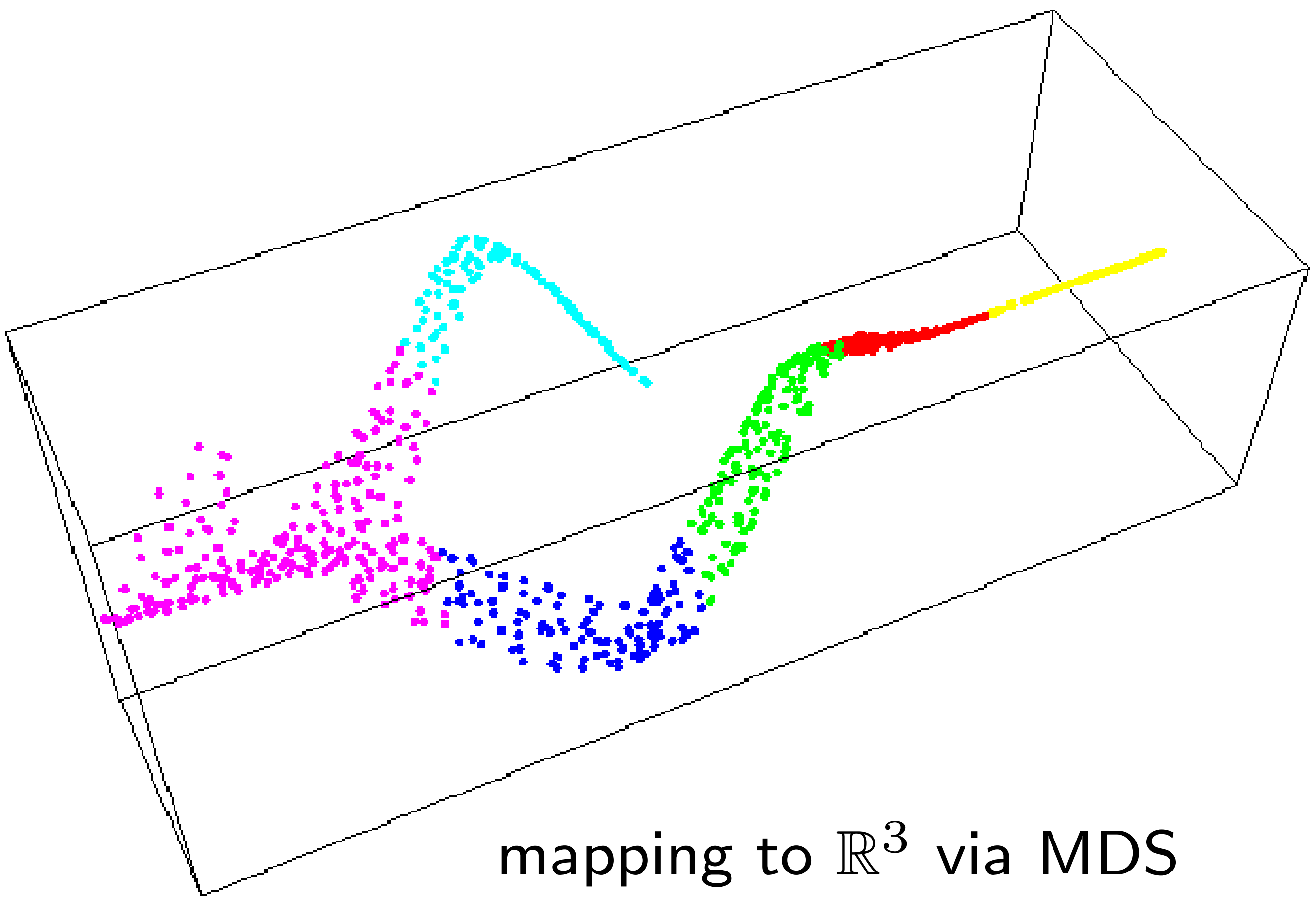
Experimental results:



Toy application (unsupervised shape segmentation)

Experimental results:



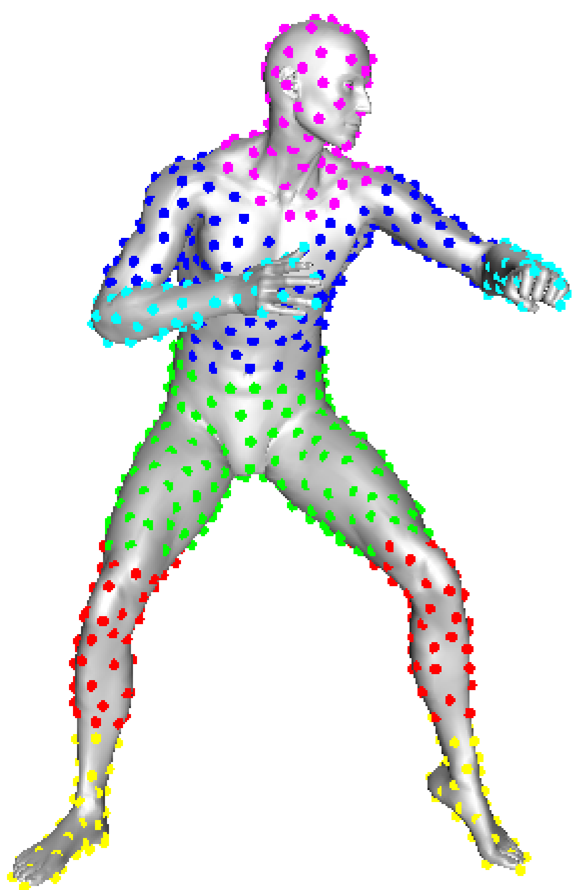


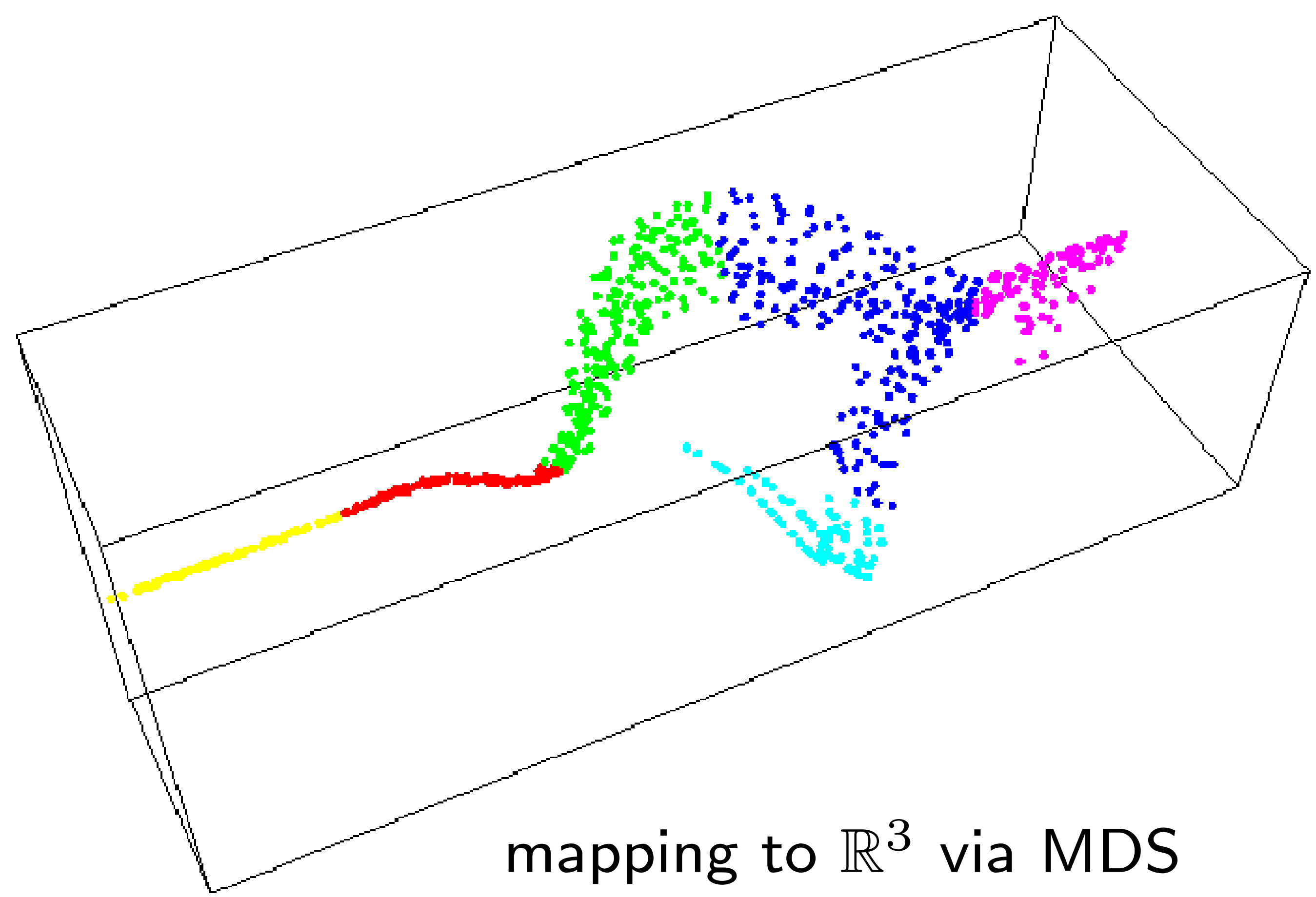
mapping to $\mathbb{R}^3$ via MDS

k-means in $\mathbb{R}^3$

Toy application (unsupervised shape segmentation)

Experimental results:





mapping to $\mathbb{R}^3$ via MDS

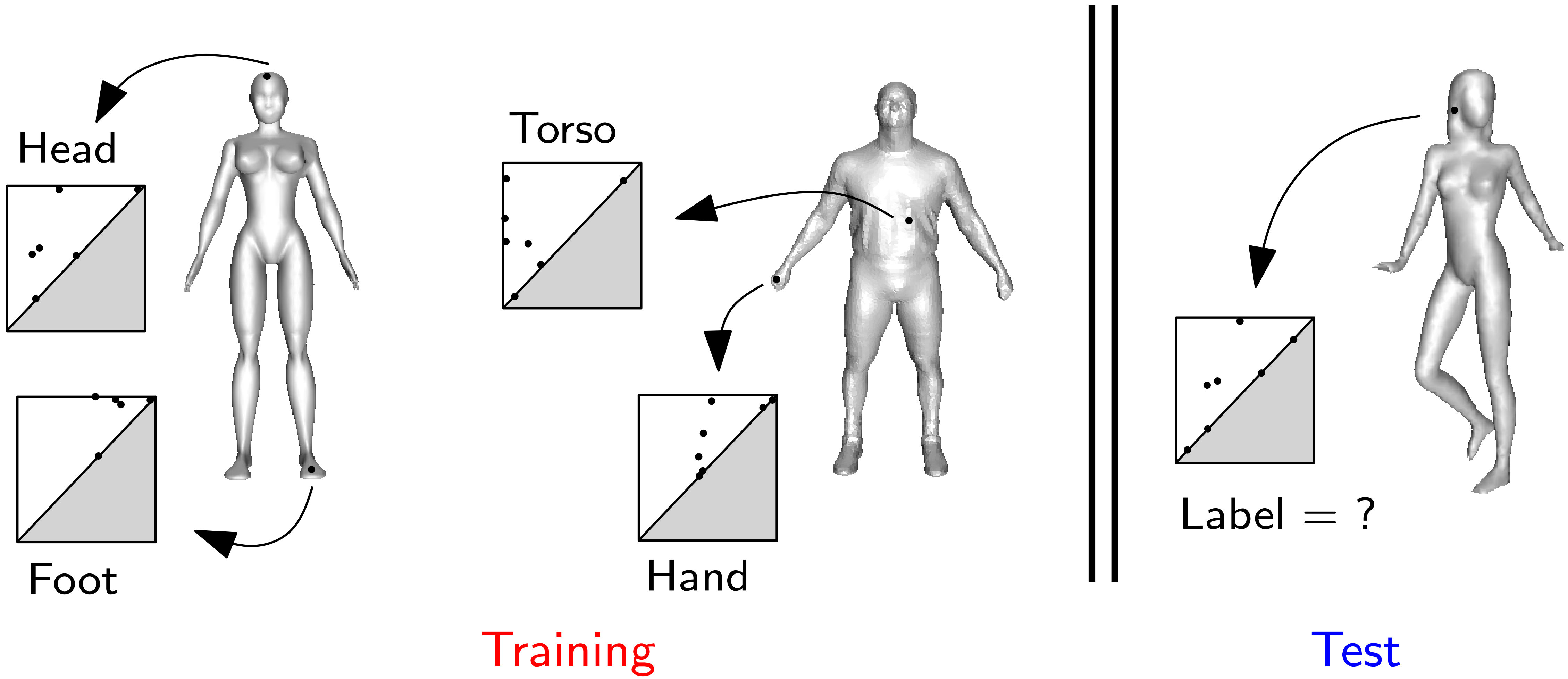
k-means in $\mathbb{R}^3$

Application to supervised shape segmentation

Goal: segment 3d shapes based on examples

Approach:

- train a (multiclass) classifier on PDs extracted from the training shapes
- apply classifier to PDs extracted from query shape



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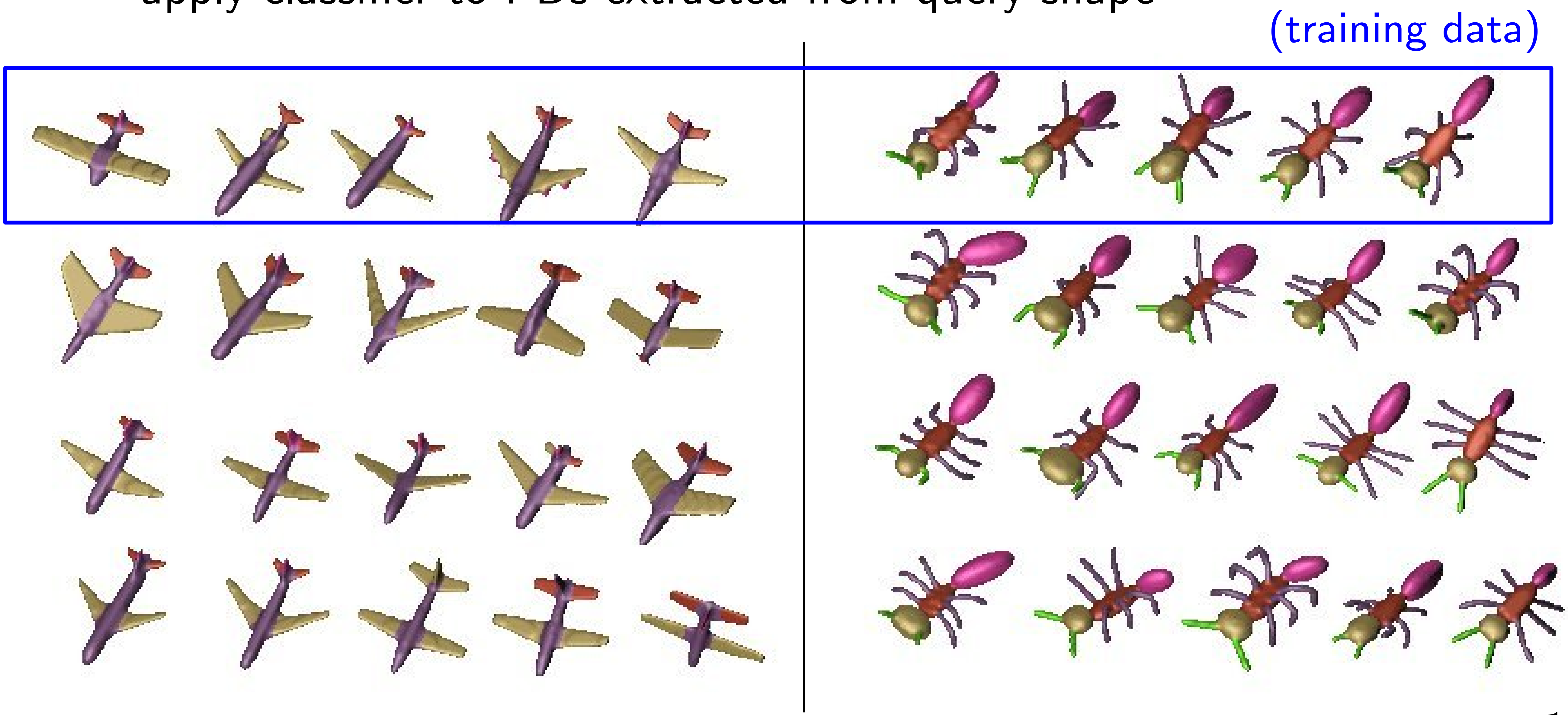

Application to supervised shape segmentation

Goal: segment 3d shapes based on examples

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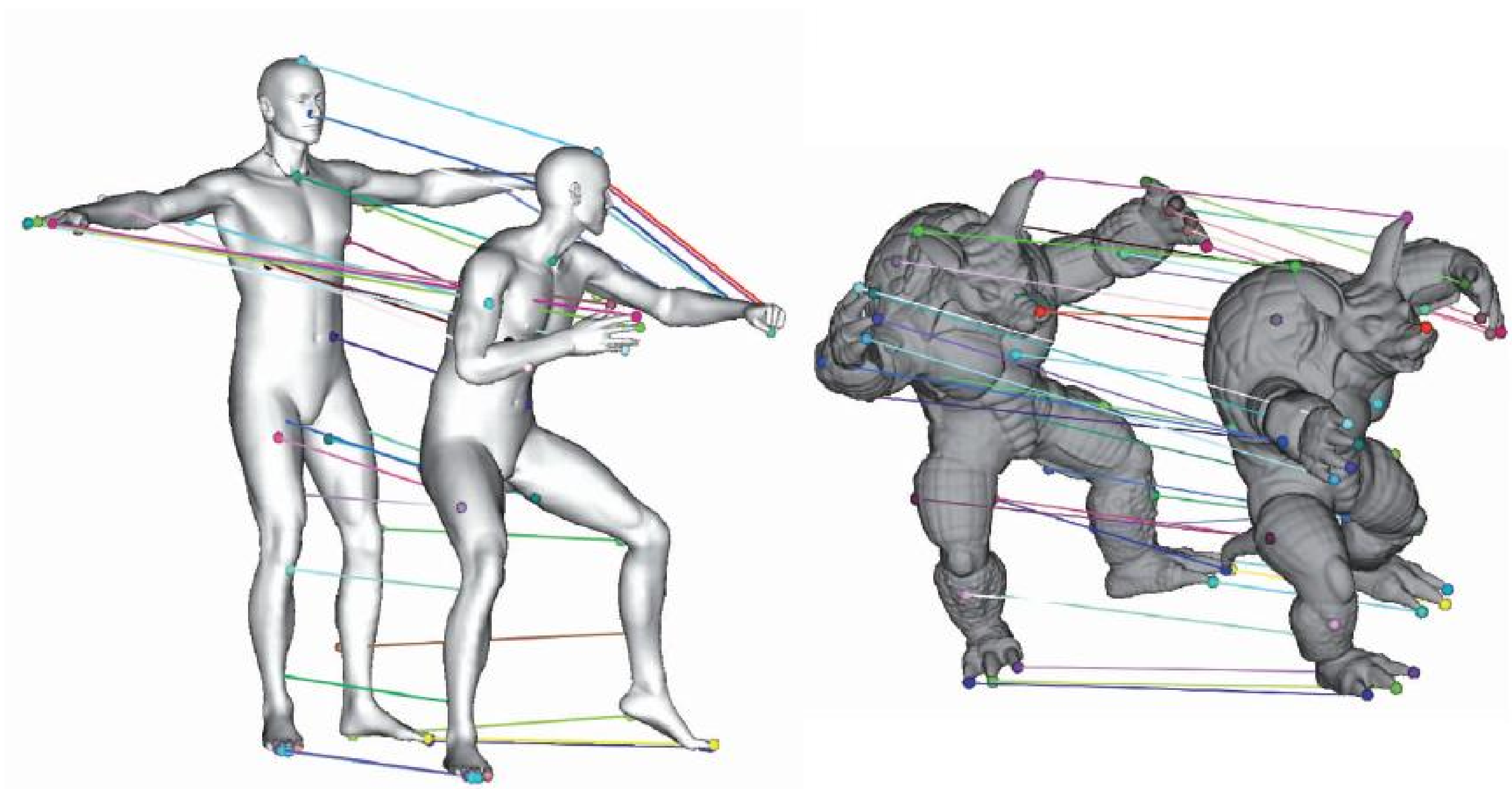
- train a (multiclass) classifier on PDs extracted from the training shapes
- apply classifier to PDs extracted from query shape

Accuracies (%) using TDA descriptors (kernels on barcodes):

	TDA	geometry	TDA + geometry
Human	74.0	78.7	**88.7**
Airplane	72.6	81.3	**90.7**
Ant	92.3	90.3	**98.5**
FourLeg	73.0	74.4	**84.2**
Octopus	85.2	94.5	**96.6**
Bird	72.0	75.2	**86.5**
Fish	79.6	79.1	**92.3**

Application to non-rigid shape matching



Application to non-rigid shape matching

Approach: use framework of *functional maps* [Ovsjanikov et al. 2012]

Given a point-to-point map $m : X \to Y$ (seen as measured spaces), consider

the **linear map** $m^* : L^2(Y) \to L^2(X)$ induced by pre-composition with m

- compute an optimal linear map that best preserves a set of signatures (vectors)

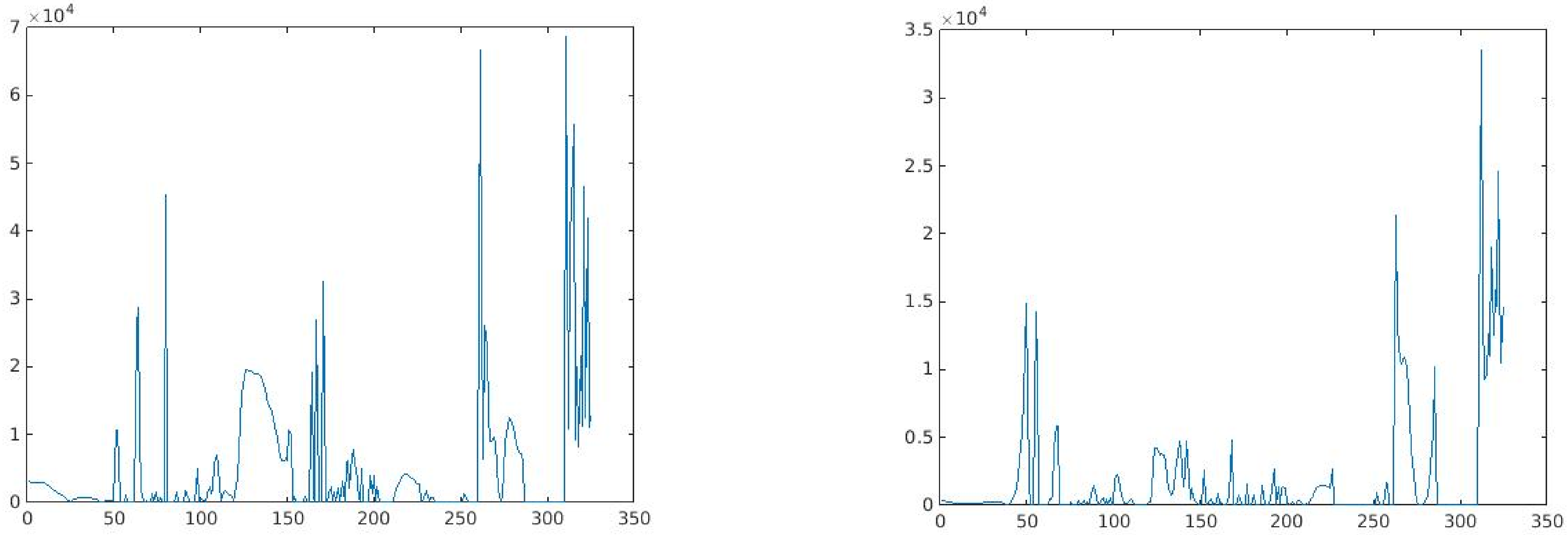
- derive a point-to-point correspondence from this map (via indicator functions)

- evaluate the quality of the correspondence

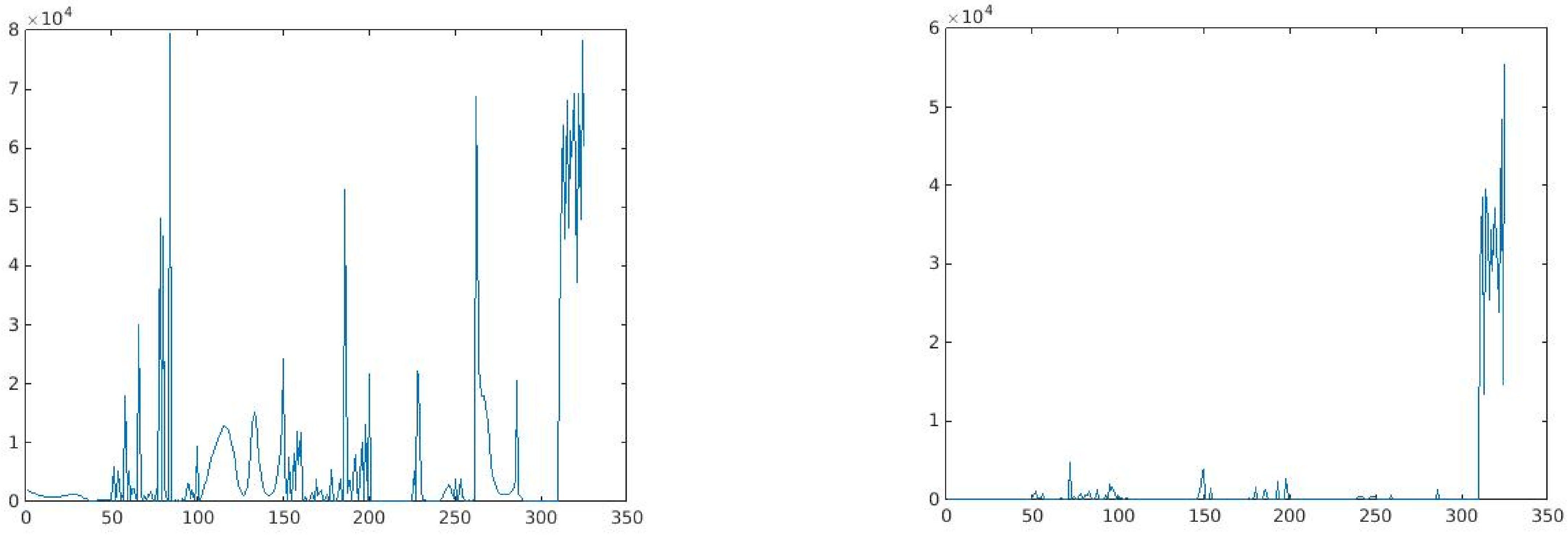
- reduce the dimensionality by taking the first k eigenfunctions
  of the Laplace-Beltrami operator

Application to non-rigid shape matching

Approach: use framework of *functional maps* [Ovsjanikov et al. 2012]



topological signatures (last 30 indices) have a high influence on the choice of optimal map



Application to non-rigid shape matching

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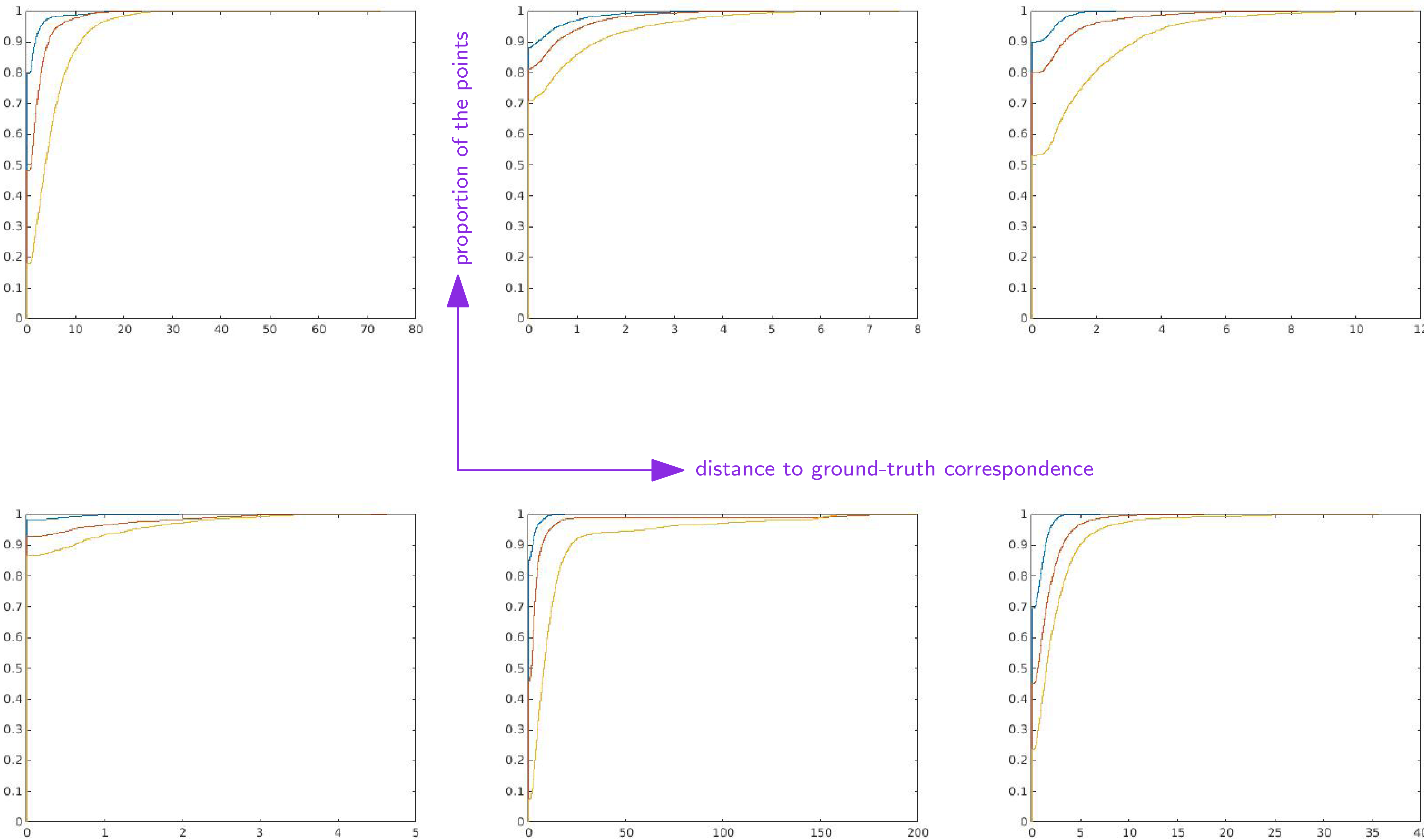

Application to non-rigid shape matching

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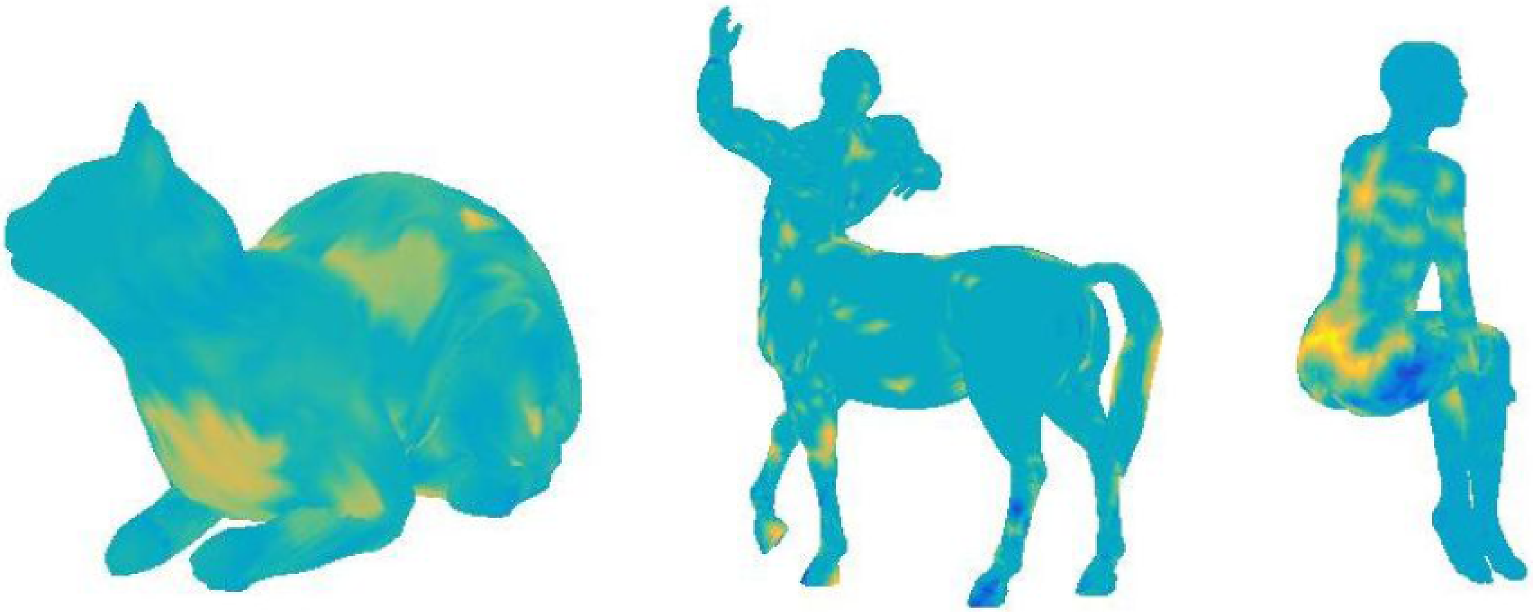
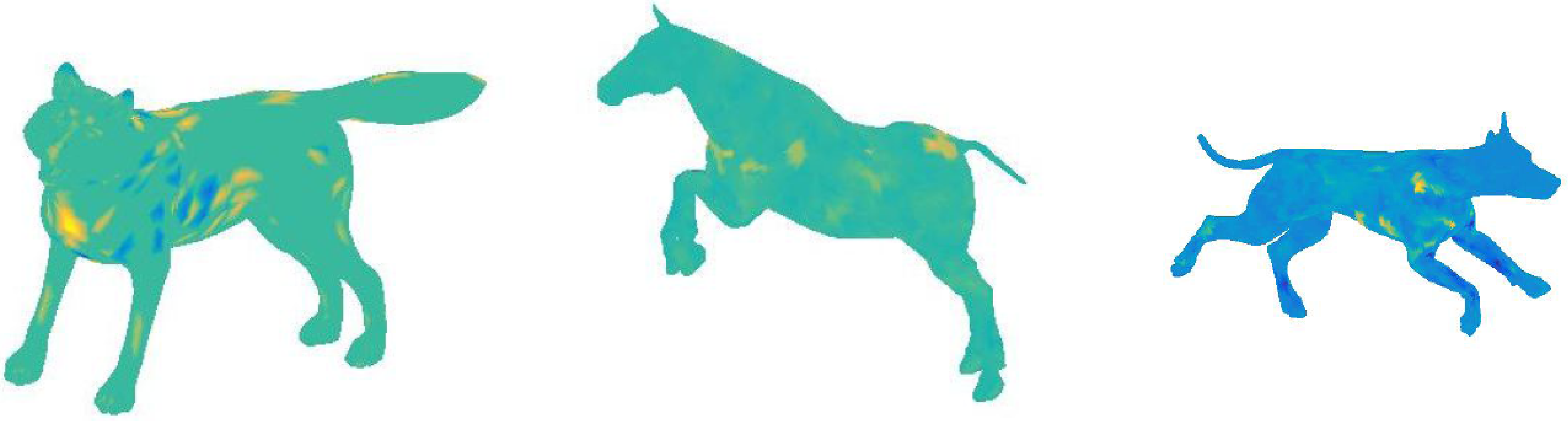
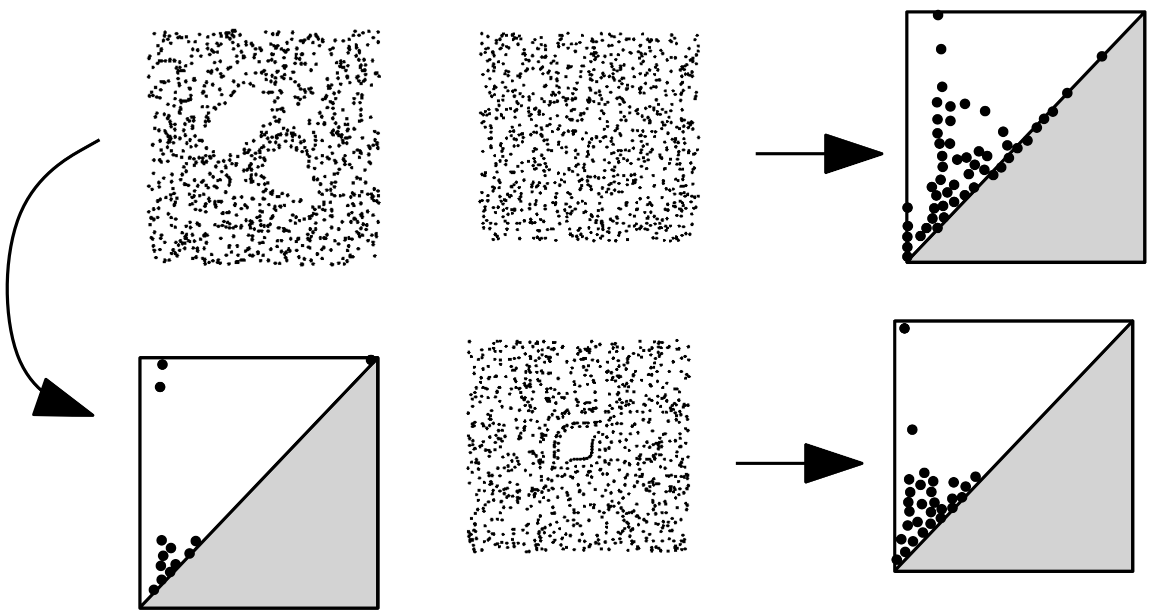


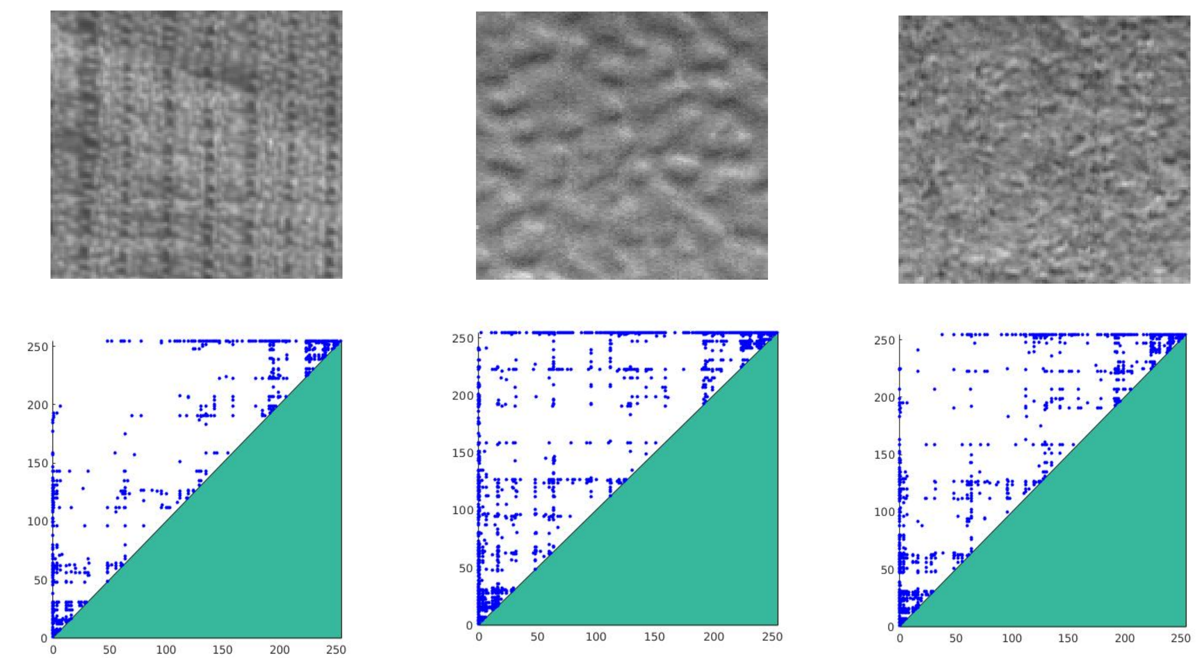
correspondences in flat regions are improved by topological signatures



Applications on other types of data

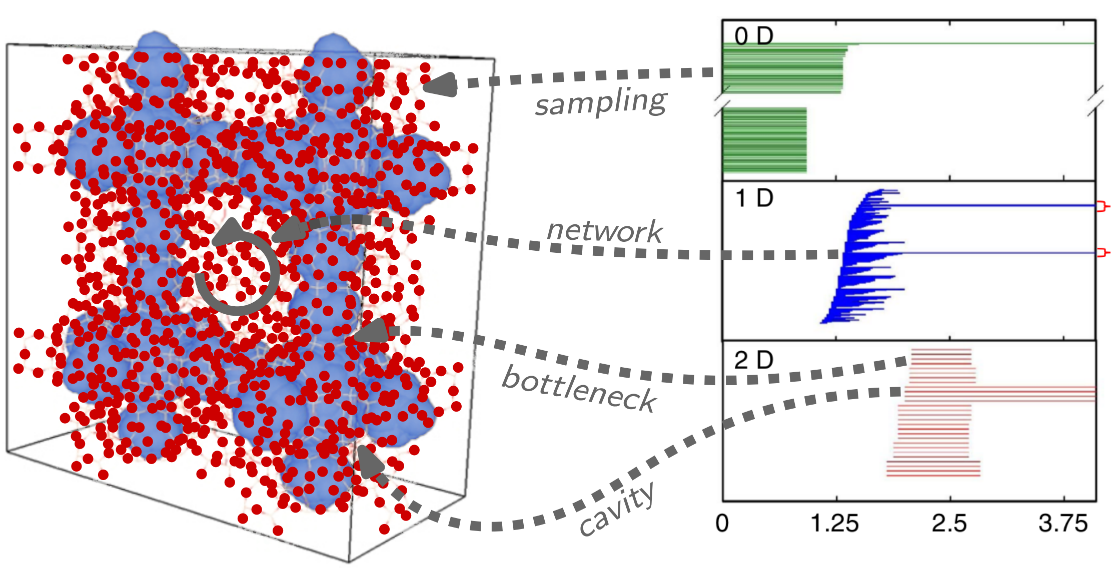
parameter inference
in dynamical systems



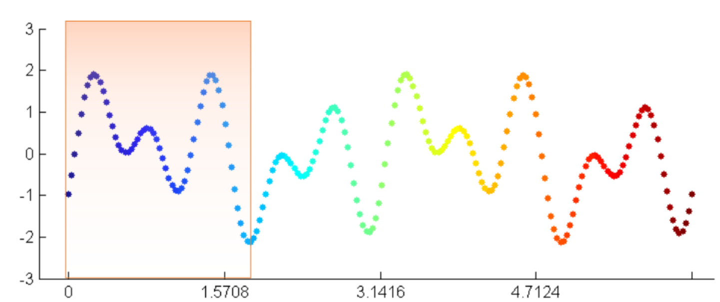


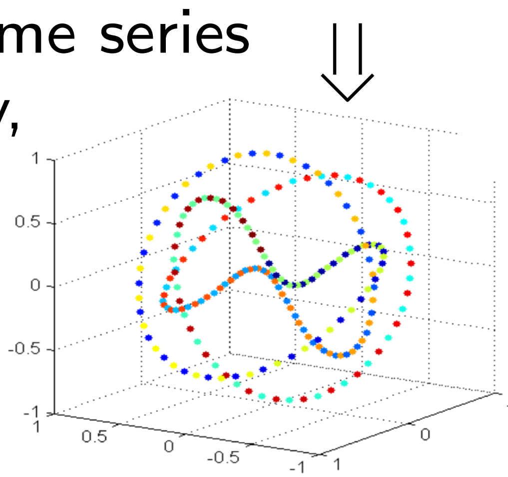
texture classification

classification/retrieval of
zeolites conformations

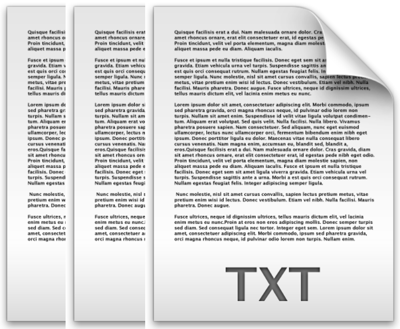


uni-/multivariate time series
analysis (periodicity,
anomaly detection)

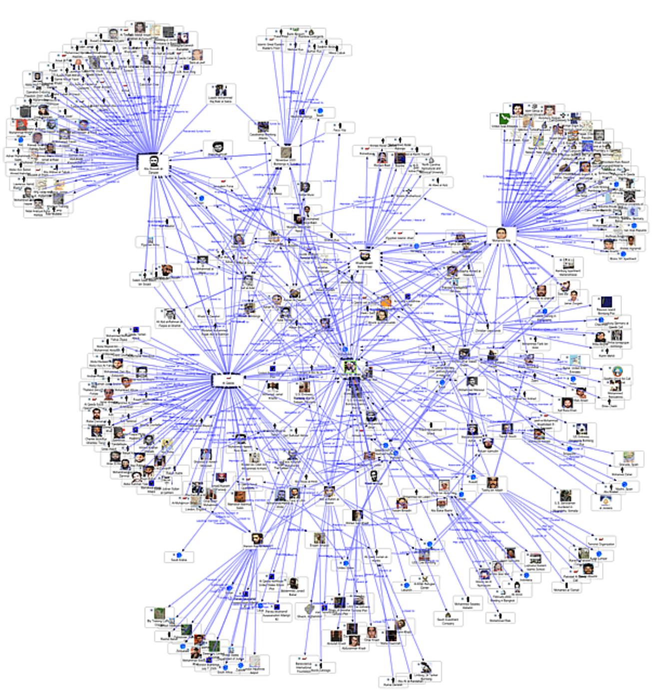


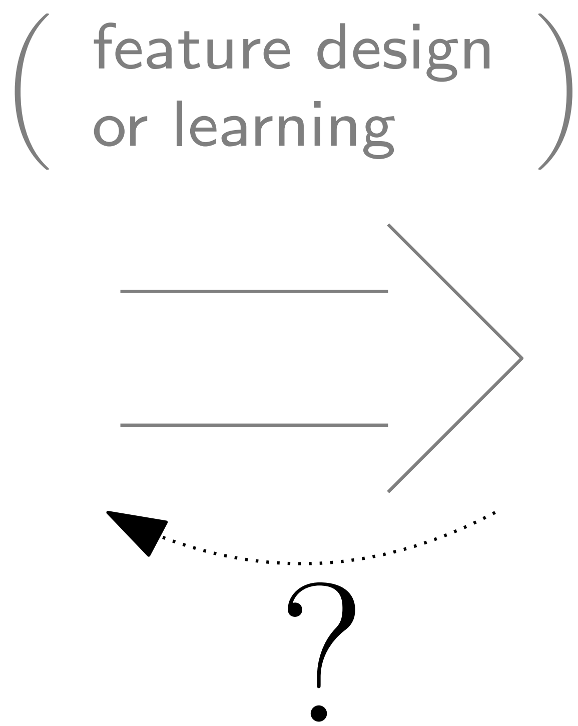


The preimage problem in the data Sciences

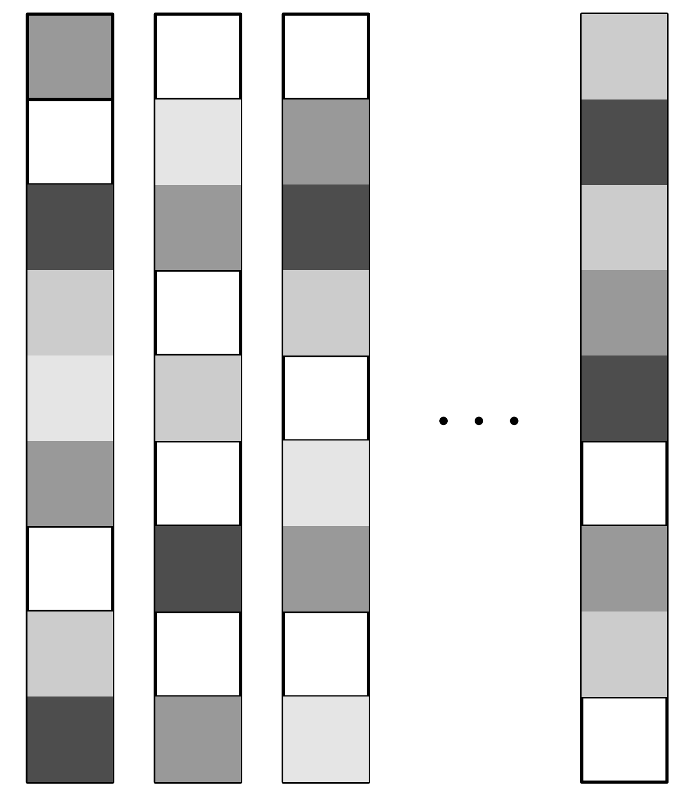


Data



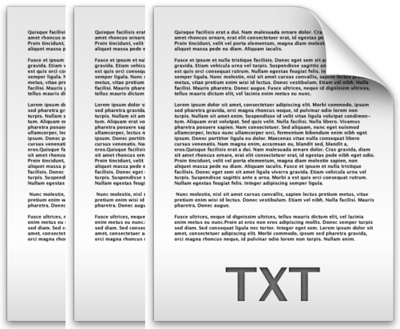


Features $\in \mathbb{R}^n$

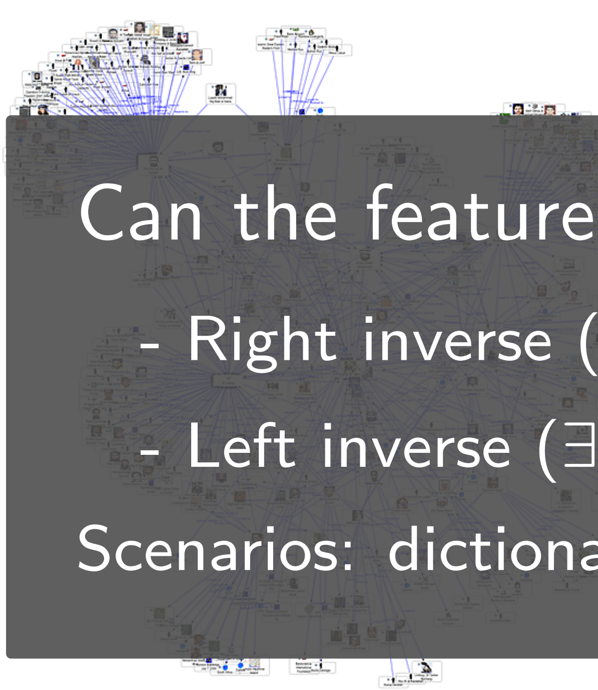


- bag of words, word2vec
- shape contexts, heat kernels
- node2vec, Laplacian fact., rand. walks
- dim. reduction, auto-encoders, etc.

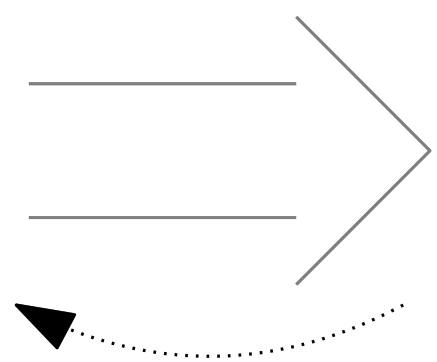
The preimage problem in the data Sciences



Data

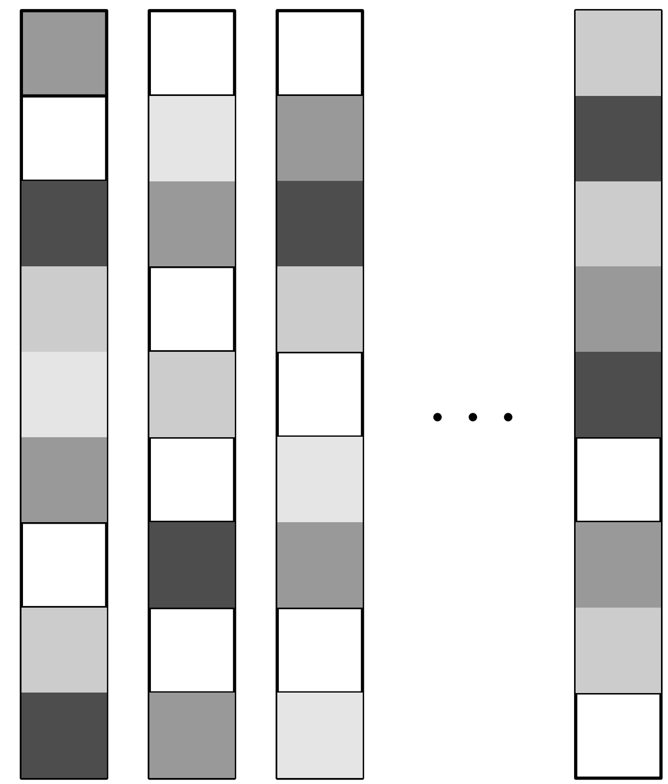


(feature design or learning)



?

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



Can the feature map be inverted?

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

Scenarios: dictionaries, deep layers, stats, etc.

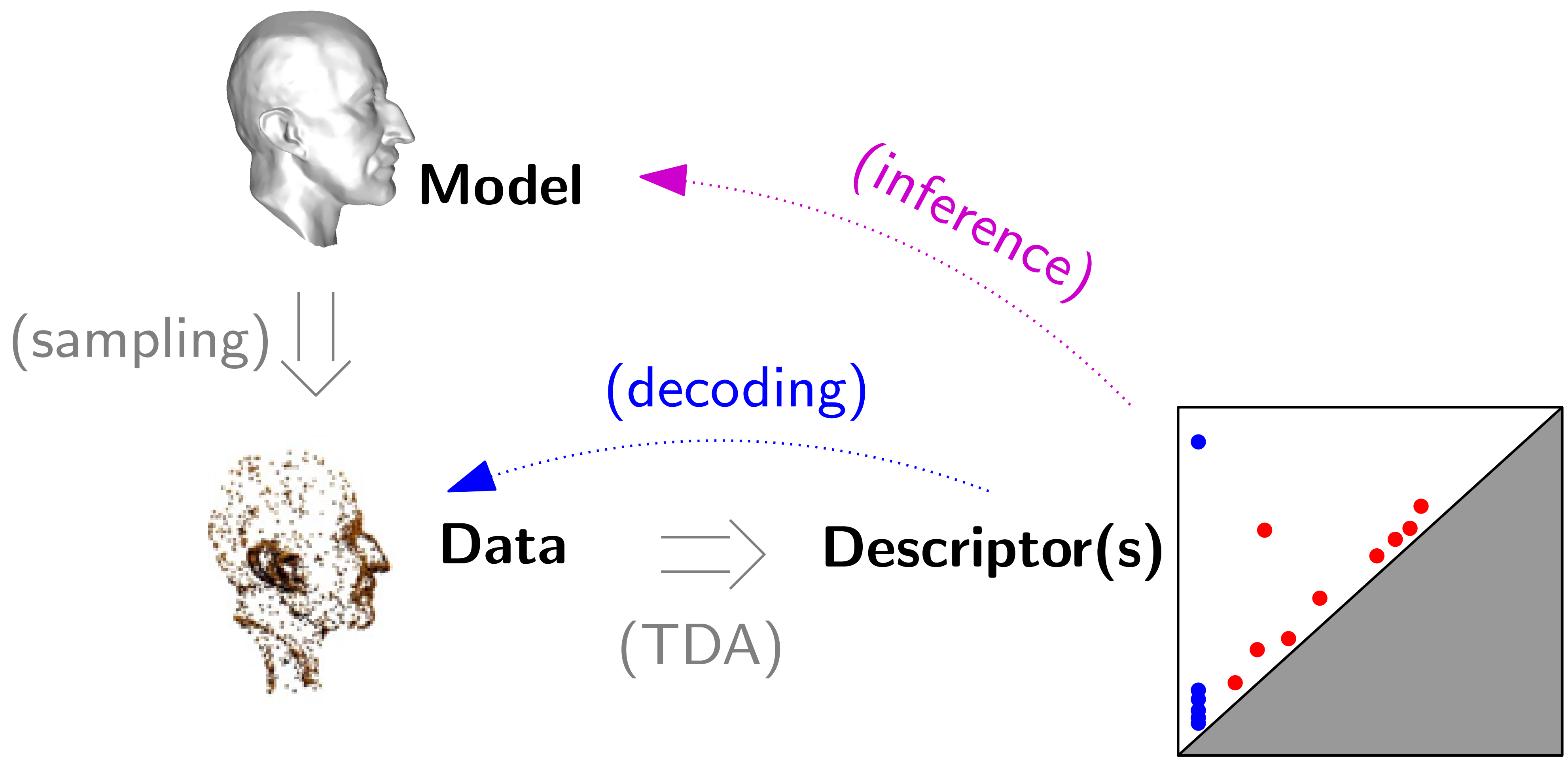
bag of words, word2vec

shape contexts, heat kernels

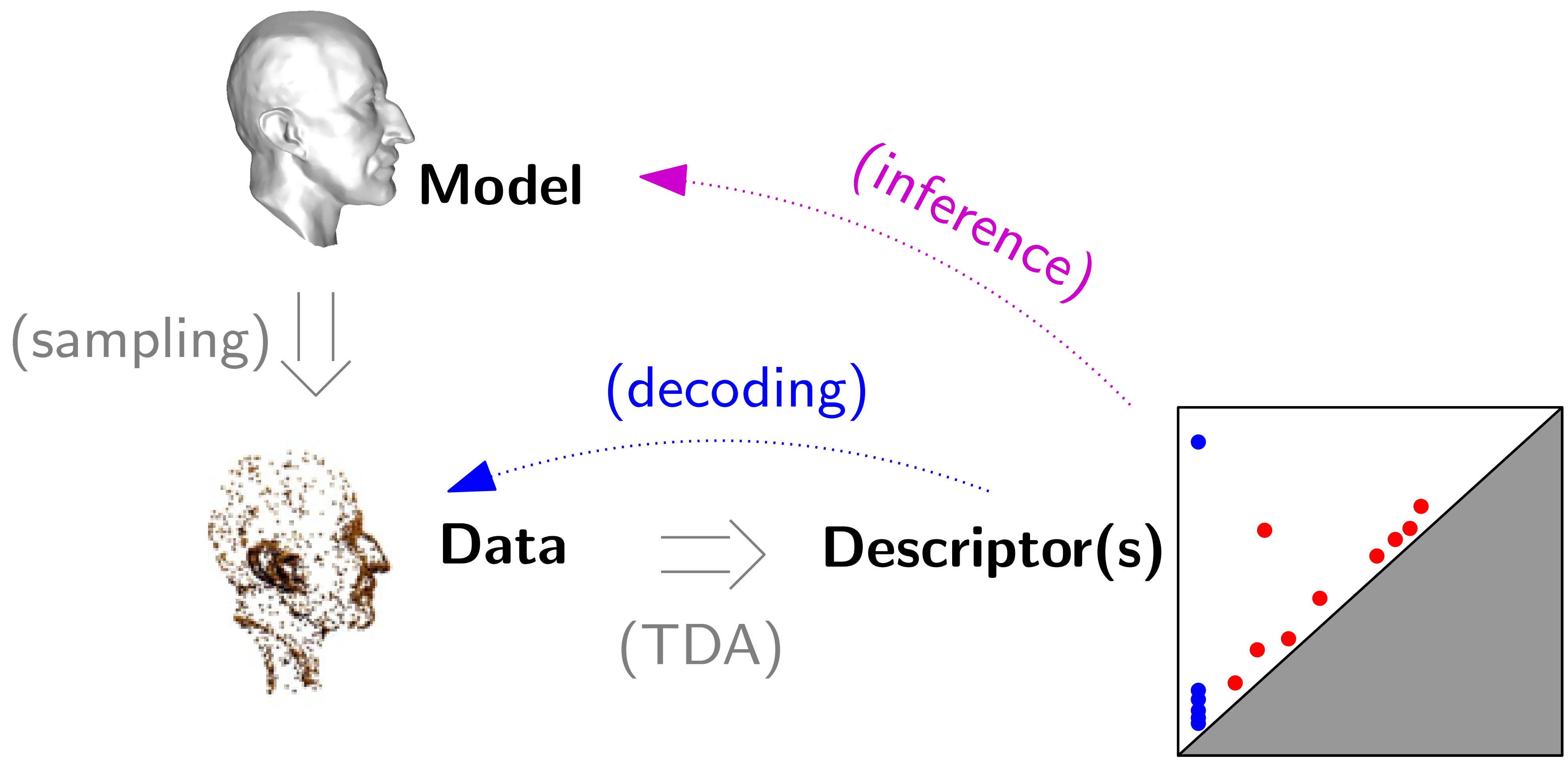
node2vec, Laplacian fact., rand. walks

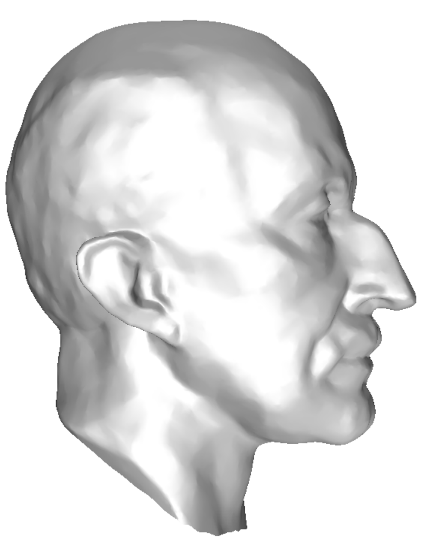
dim. reduction, auto-encoders, etc.

TDA and the preimage problem

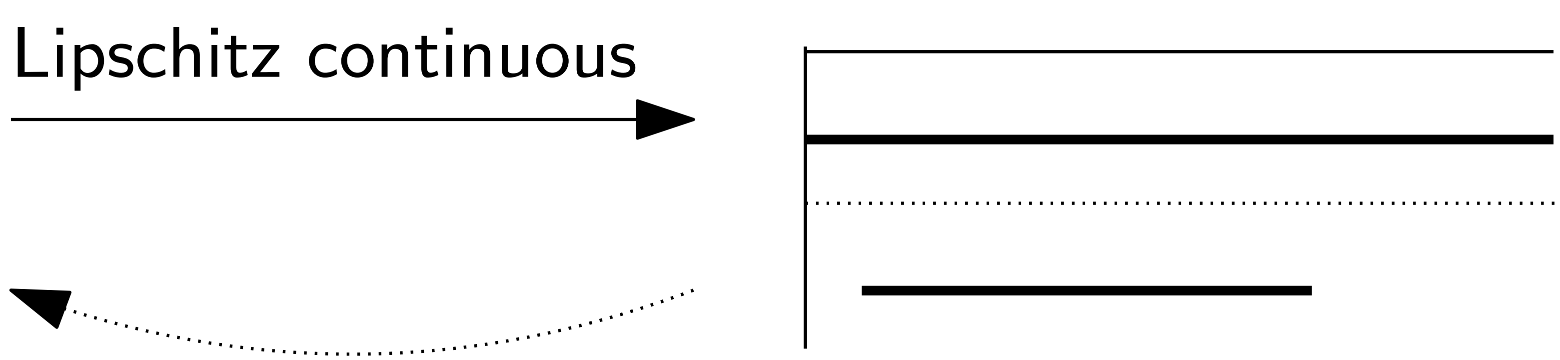


TDA and the preimage problem





compact metric space

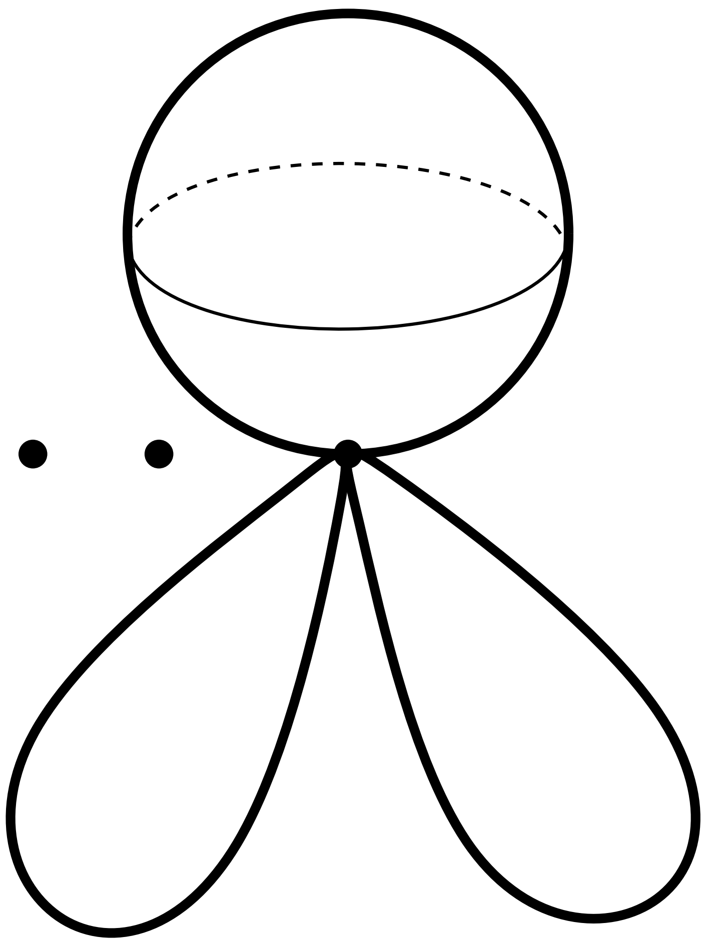


right inverse: realize barcode as the PH of some isom. class

left inverse: characterize isom. class uniquely

Right inverses for TDA

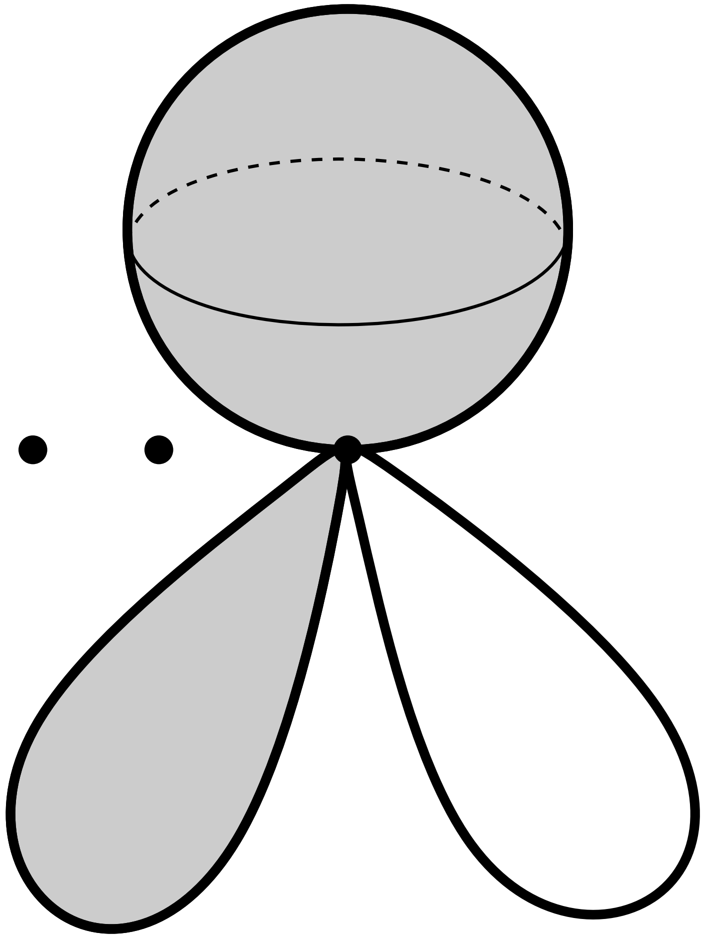
Fact: [Folklore] Any (graded) finite-dim. vector space (f.g. abelian group) can be realized as the (graded) $\tilde{H}$ of a CW-complex



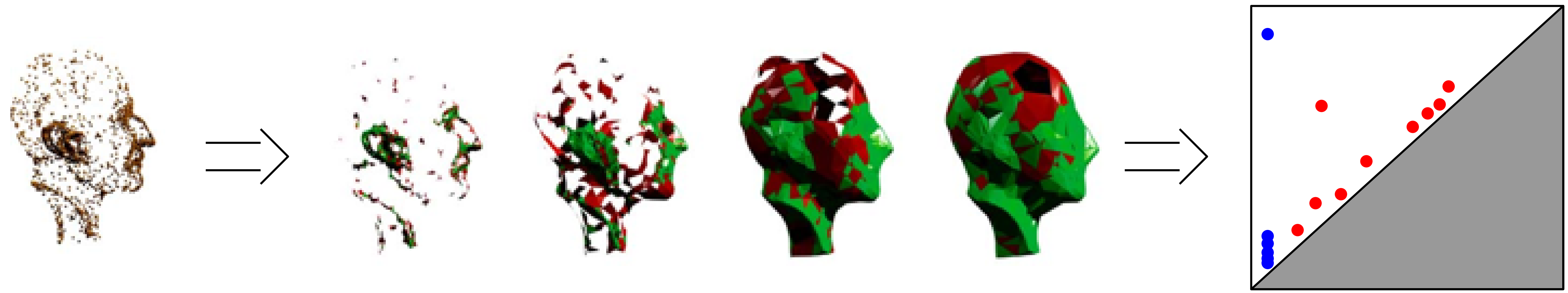
Right inverses for TDA

Fact: [Folklore] Any (graded) finite-dim. vector space (f.g. abelian group) can be realized as the (graded) $\tilde{\mathrm{H}}$ of a CW-complex

Fact: [Folklore] Any (graded) persistence barcode/diagram can be realized as the (graded) $\mathrm{P}\tilde{\mathrm{H}}$ of a piecewise-constant function on a bouquet of spheres.



Right inverses (local) for TDA



point cloud — Čech / Rips filtration — diagram

$$u \in \mathbb{R}^{nd} \longmapsto v \in \mathbb{R}^{2^n-1}$$

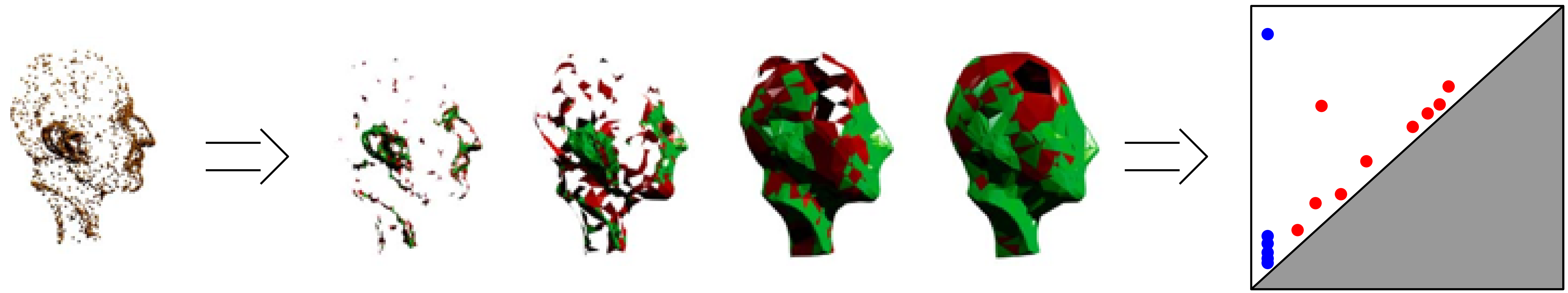
Thm: [Gameiro, Hiraoka, Obayashi]

(i) *Generic* point cloud $\Rightarrow \exists \Omega \ni u$ in $\mathbb{R}^{nd}$ over which the correspondence $u \mapsto v$ can be extended to a map $f : \Omega \to \mathbb{R}^{2^n-1}$ computing persistence barcodes.

(ii) For Ω small enough, f is of class C^∞.

Observation: pairing given by order of distances is constant in small enough O.

Right inverses (local) for TDA



point cloud Čech / Rips filtration diagram

$u \in \mathbb{R}^{nd}$ $\longmapsto$ $v \in \mathbb{R}^{2^n-1}$

Thm: [Gameiro, Hiraoka, Obayashi]

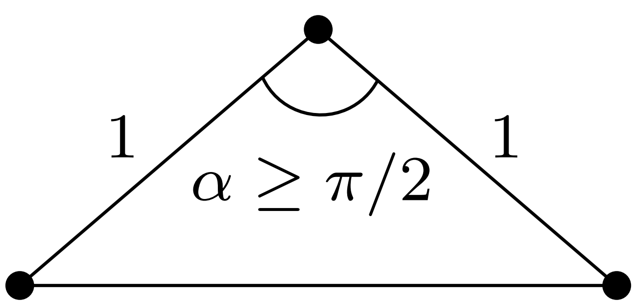
(i) *Generic* point cloud $\Rightarrow \exists \Omega \ni u$ in $\mathbb{R}^{nd}$ over which the correspondence $u \mapsto v$ can be extended to a map $f : \Omega \to \mathbb{R}^{2^n-1}$ computing persistence barcodes.

(ii) For Ω small enough, f is of class C^∞.

$\rightarrow$ adapt Newton-Raphson continuation method to build right inverse of f in $f(\Omega)$
(Jacobian matrix of f can be singular $\rightsquigarrow$ use pseudo-inverse)

Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations



$$\operatorname{dgm} \mathcal{C}(P, \ell_2) = \{(0, +\infty)\} \sqcup \{(0, \tfrac{1}{2})\} \sqcup \{(0, \tfrac{1}{2})\}$$

$$\operatorname{dgm} \mathcal{R}(P, \ell_2) = \{(0, +\infty)\} \sqcup \{(0, 1)\} \sqcup \{(0, 1)\}$$

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

Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations

Prop: [Folklore]
For any *metric tree* (X, d_X):

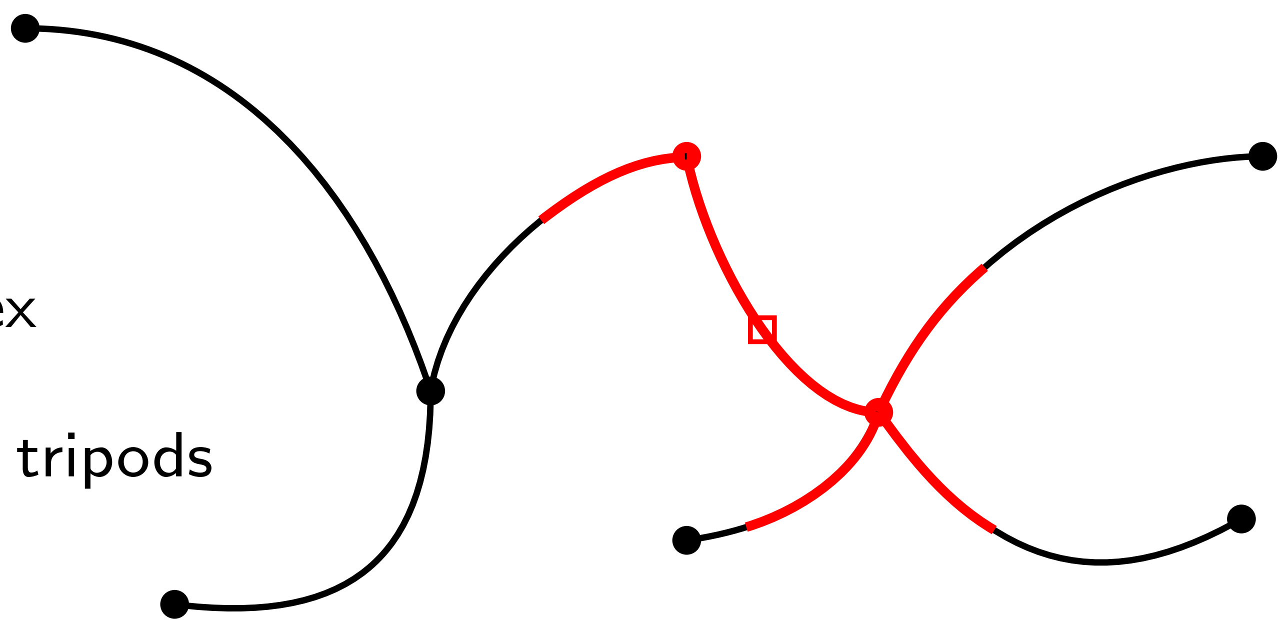
$$\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X) = \mathrm{dgm}\,\mathcal{C}(X, \mathrm{d}_X) = \{(0, +\infty)\}$$

$\Rightarrow$ no information on the metric

X is 0-hyperbolic

$\Rightarrow$ metric balls are convex

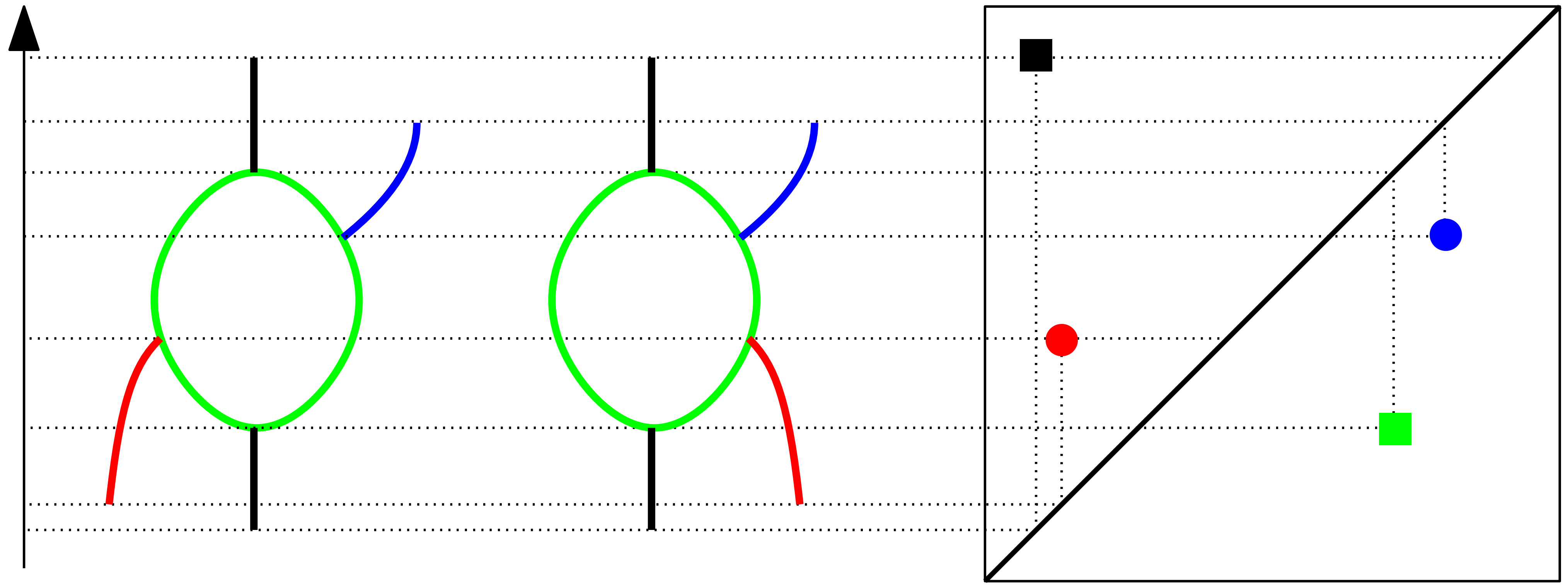
$\Rightarrow$ geodesic triangles are tripods



Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations

- Reeb graphs



⇒ Reeb graphs are indistinguishable from their diagrams

Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations
- Reeb graphs
- Real-valued functions

Prop: [Folklore]
Given $f : X \to \mathbb{R}$ and $h : Y \to X$ homeomorphism,

$$\operatorname{dgm} f \circ h = \operatorname{dgm} f$$

Too large a group of transformations...

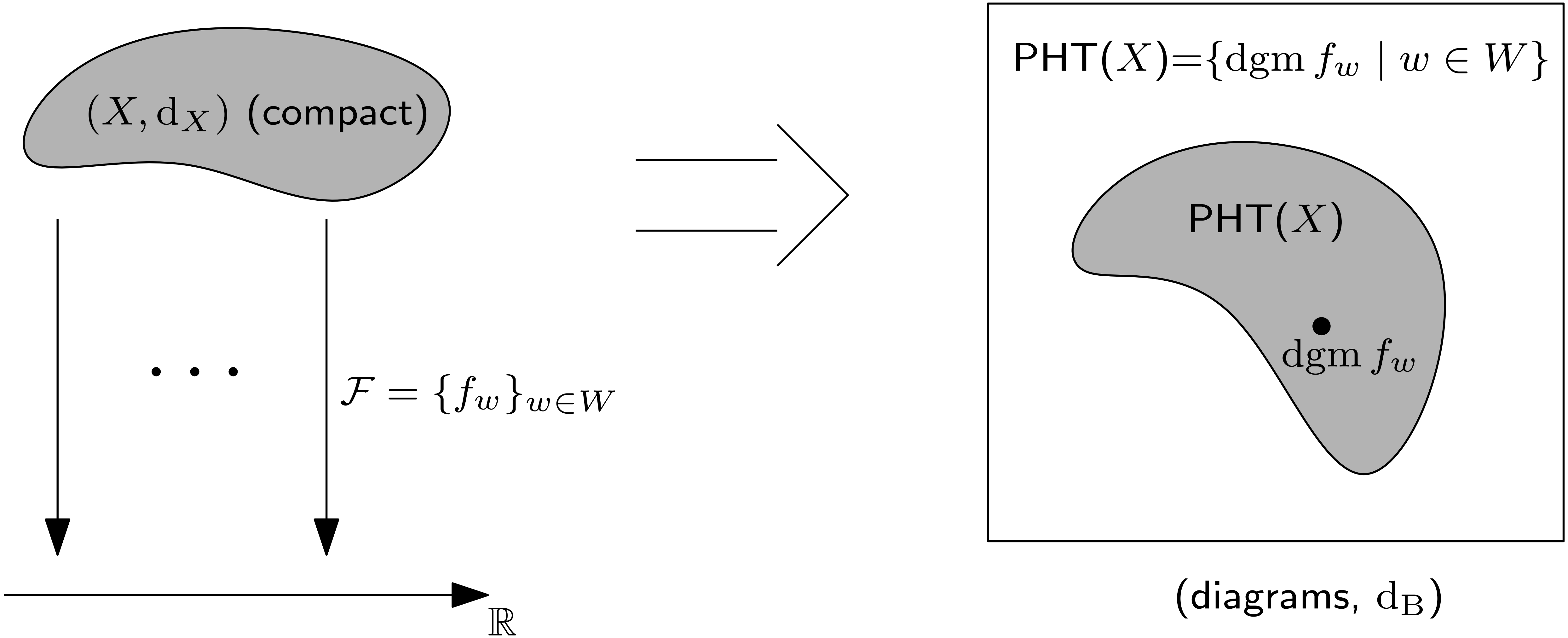
Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations
- Reeb graphs
- Real-valued functions

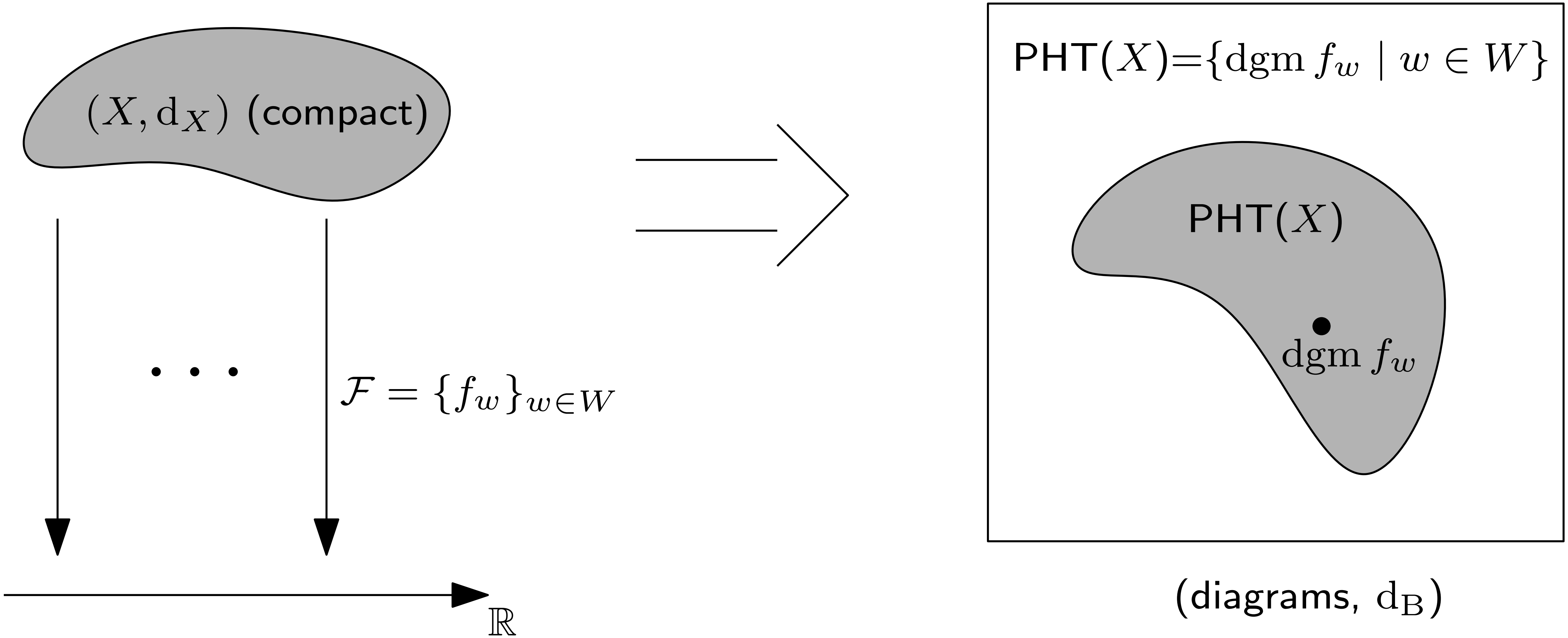
possible solutions:

- richer topological invariants (e.g. persistent homotopy)
- use multiple filter functions (**aggregation** vs multipersistence)

Persistent Homology Transform (PHT)



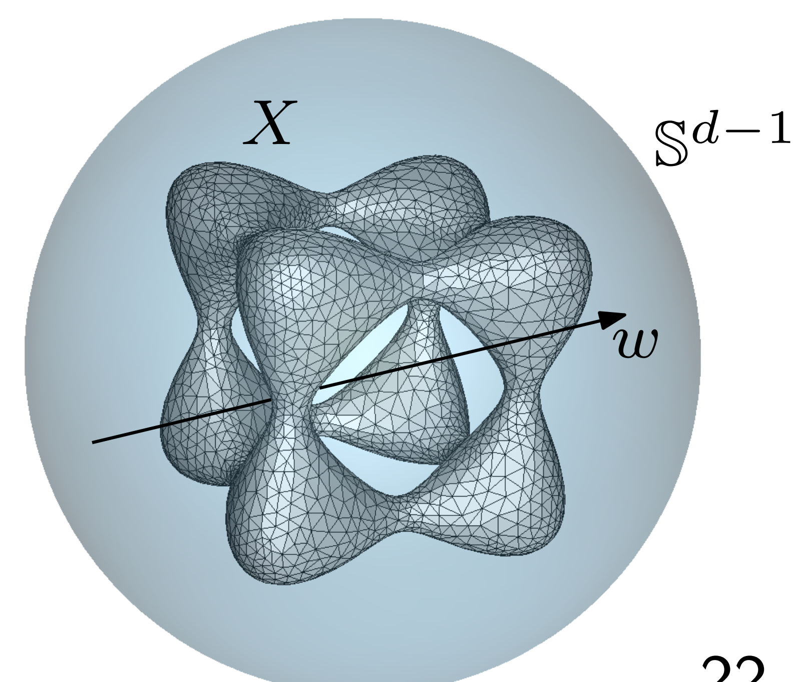
Persistent Homology Transform (PHT)



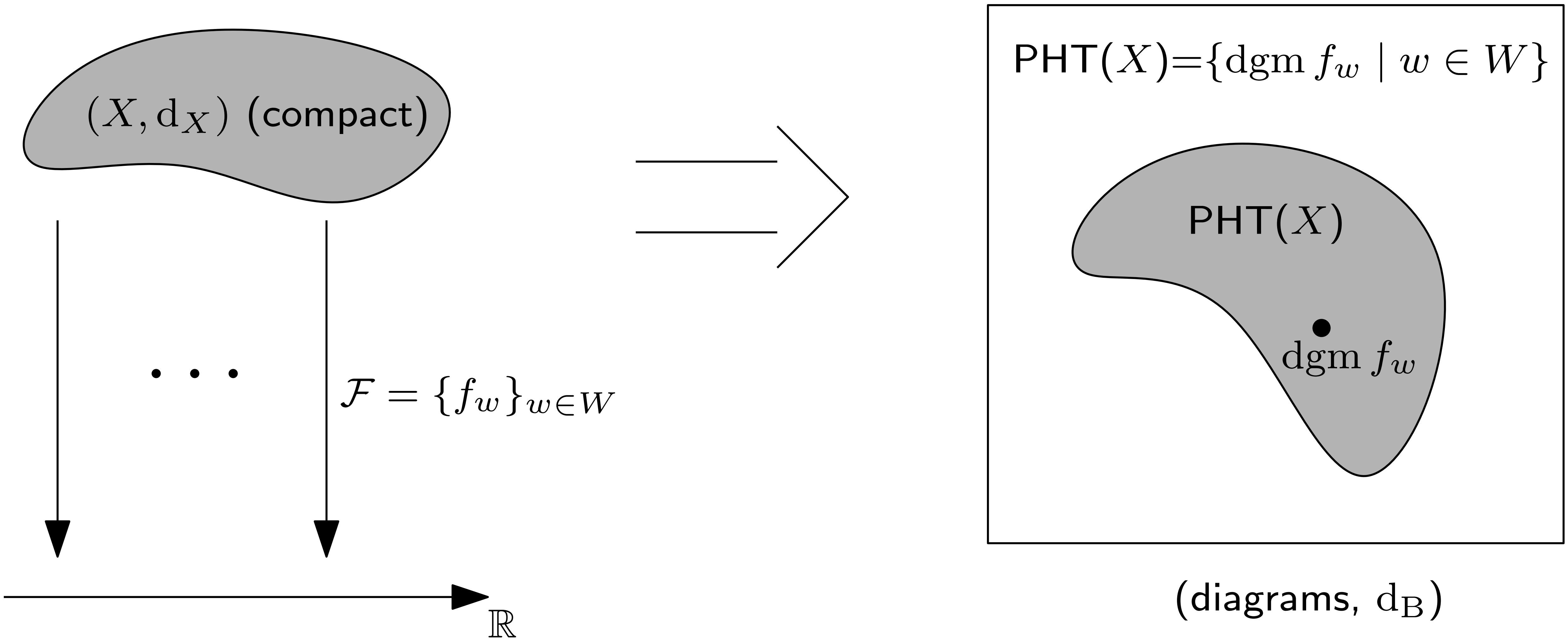
Thm: [Boyer, Curry, Mukherjee, Turner 2014, 2018]
[Ghrist, Levanger, Mai 2018]

Let $\mathcal{F} = \{\langle \cdot, w \rangle\}_{w \in \mathbb{S}^{d-1}}$, where d is fixed. Then, PHT is injective on the class of semialgebraic sets in $\mathbb{R}^d$.

Still true for a fixed finite set of directions (of size exponential in d). [Curry, Mukherjee, Turner]



Persistent Homology Transform (PHT)



Thm: [Boyer, Curry, Mukherjee, Turner 2014, 2018]
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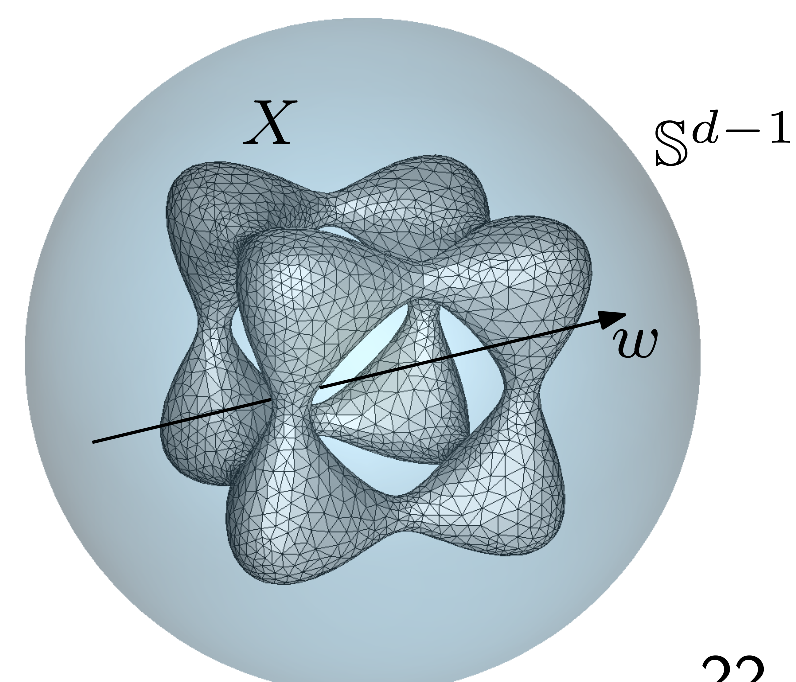
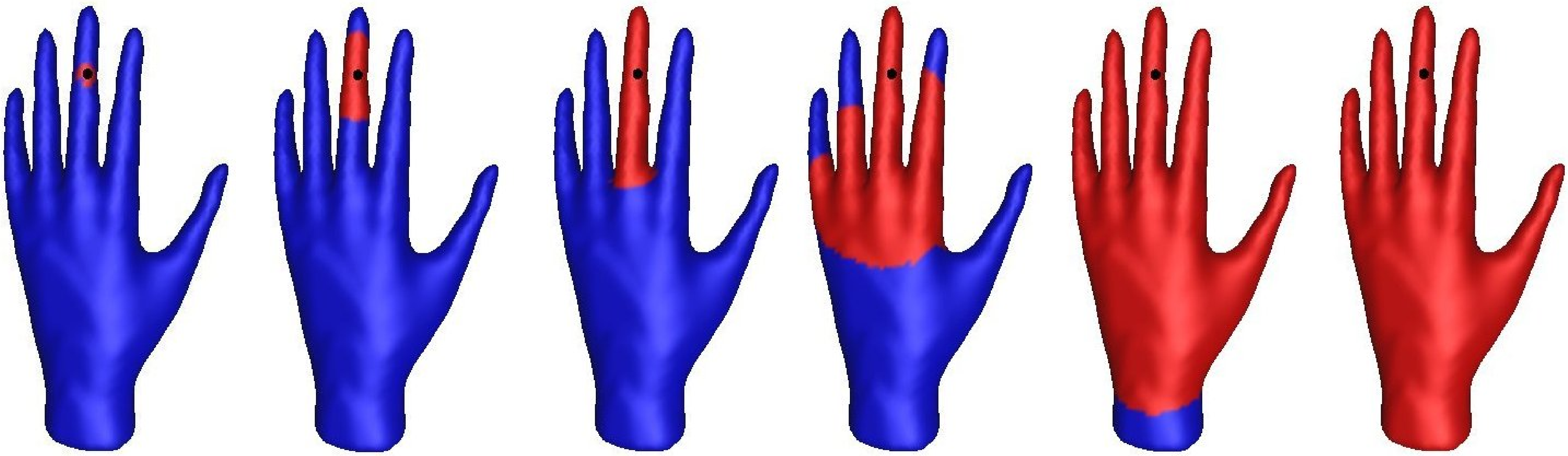
Let $\mathcal{F} = \{\langle \cdot, w \rangle\}_{w \in \mathbb{S}^{d-1}}$, where d is fixed. Then, PHT is injective on the class of semialgebraic sets in $\mathbb{R}^d$.

Corollary: PHT is a sufficient statistic for such sets
$\Rightarrow$ parametric inference



PHT for length spaces

Given a compact length space (X, d_X), take $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$



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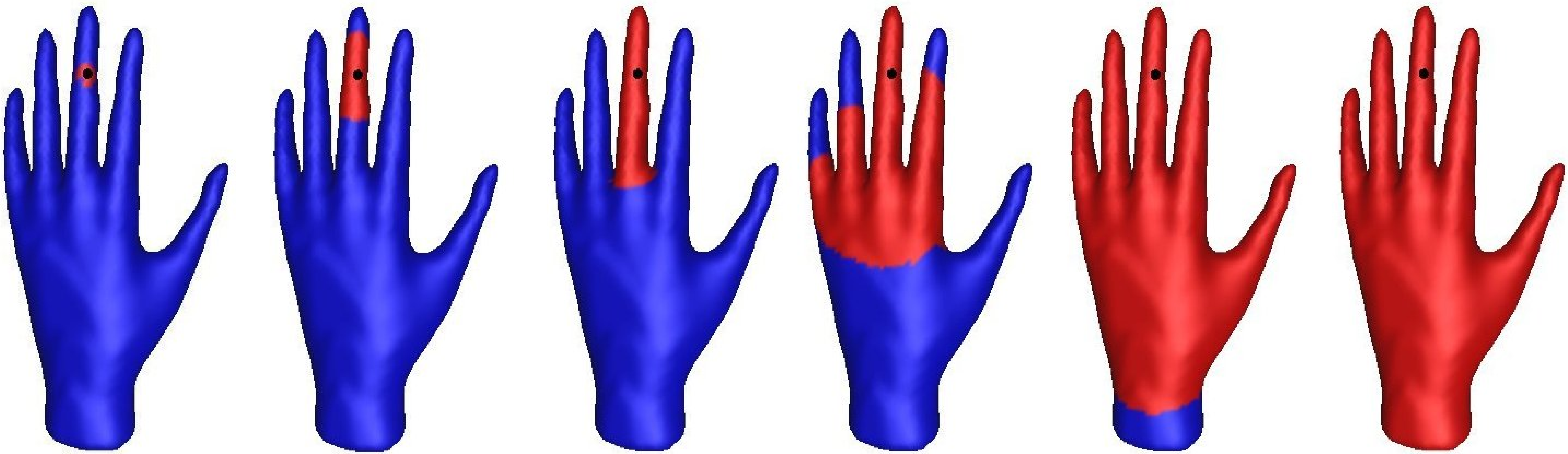

Thm (local stability): [Carrière, O., Ovsjanikov 2015]

Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius ($\varrho(X), \varrho(Y) > 0$). Let $x \in X$ and $y \in Y$. If $\mathrm{d}_{\mathrm{GH}}((X, x), (Y, y)) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

$$\mathrm{d}_{\mathrm{B}}(\mathrm{dgm}\, \mathrm{d}_X(\cdot, x), \mathrm{dgm}\, \mathrm{d}_Y(\cdot, y)) \leq 20\ \mathrm{d}_{\mathrm{GH}}((X, x), (Y, y)).$$

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Corollary (local stability of PHT):
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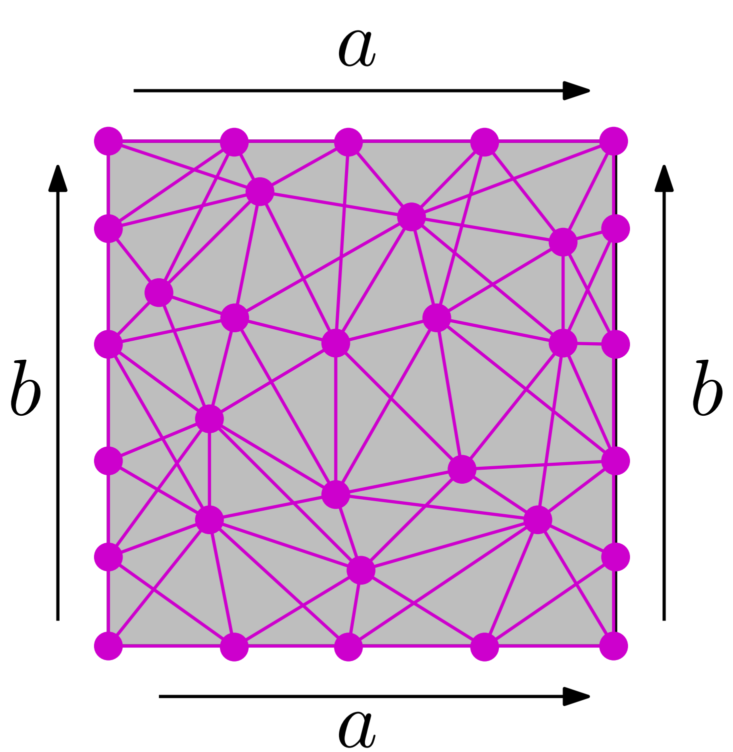

$$\mathrm{d}_{\mathrm{GH}}(T, X) \overset{\#X \to \infty}{\longrightarrow} 0$$

$\mathrm{d}_{\mathrm{H}}(\mathrm{PHT}_2(T), \mathrm{PHT}_2(X))$ is bounded away from 0

PHT for metric graphs

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

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

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

$$\mathrm{d_H}(\mathsf{PHT}(X), \mathsf{PHT}(Y)) \leq 18\, \mathrm{d_{GH}}(X, Y).$$

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

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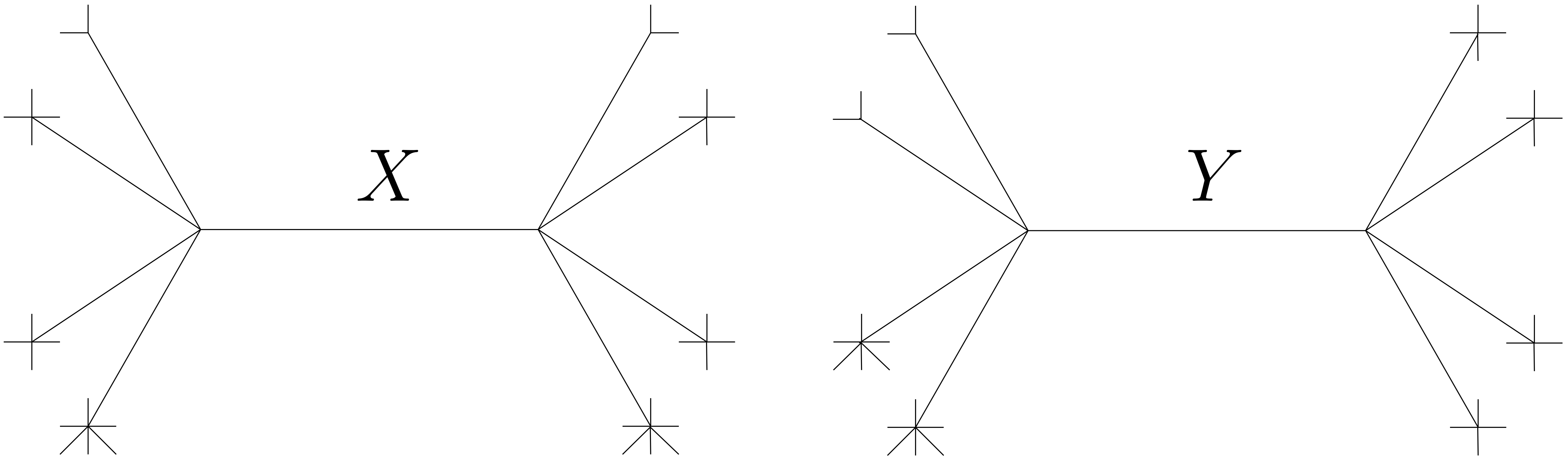
Q: injectivity of PHT on metric graphs? [O., Solomon 2017]

PHT for metric graphs

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



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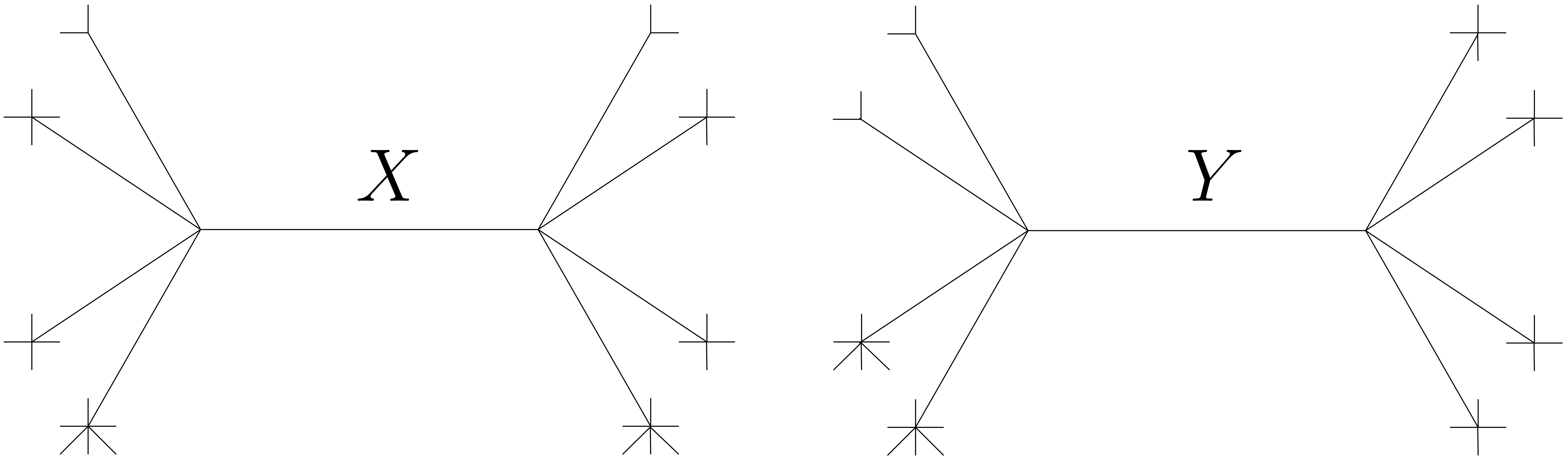


$\mathsf{PHT}(X) = \mathsf{PHT}(Y)$ while $X \not\simeq Y$

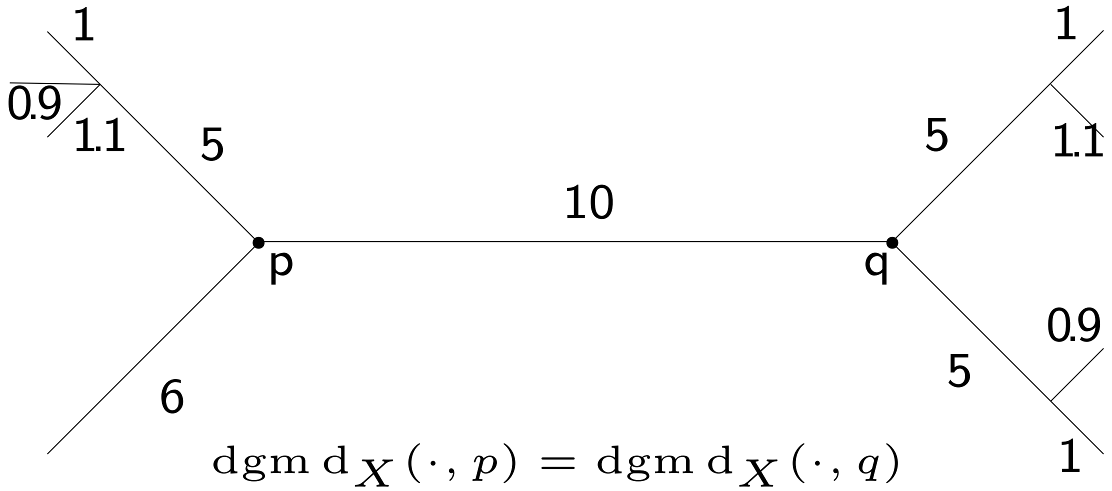
Note: $\mathrm{Aut}(X)$ is non-trivial, hence $\Psi_X : x \mapsto \mathrm{dgm}\,\mathrm{d}_X(\cdot, x)$ is not injective

PHT for metric graphs

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

Thm 1:
PHT is injective on Inj_Ψ.

Thm 2:
Inj_Ψ is GH-dense among the compact metric graphs.



Note: Ψ_X injective $\underset{\not\Leftarrow}{\Rightarrow}$ $\mathrm{Aut}(X)$ trivial

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PHT is injective on Inj_Ψ.

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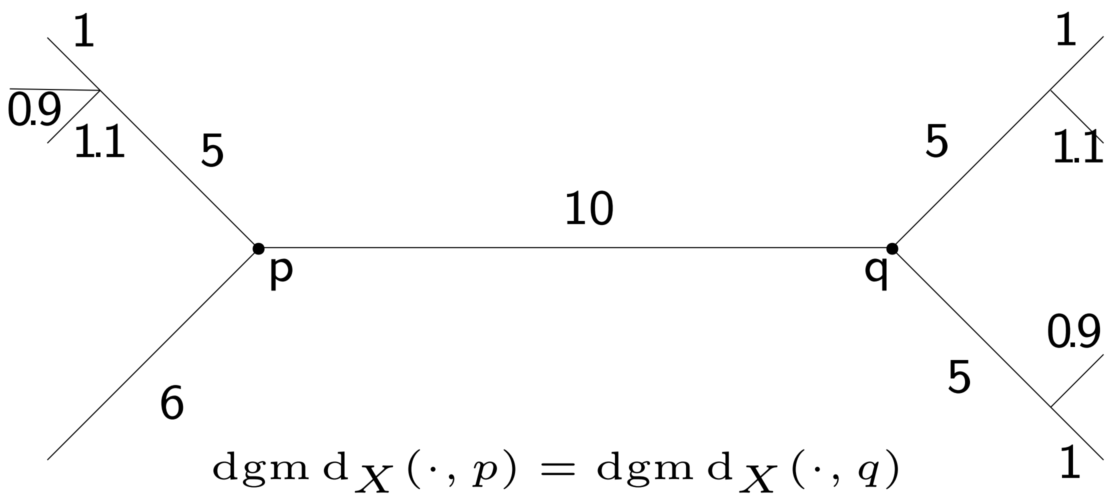
+ Gromov's density result

Corollary:

There is a GH-dense subset of the compact length spaces on which PHT is injective.



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PHT is injective on Inj_Ψ.

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Inj_Ψ is GH-dense among the compact metric graphs.

Corollary:

There is a GH-dense subset of the compact length spaces on which PHT is injective.

Thm 3:

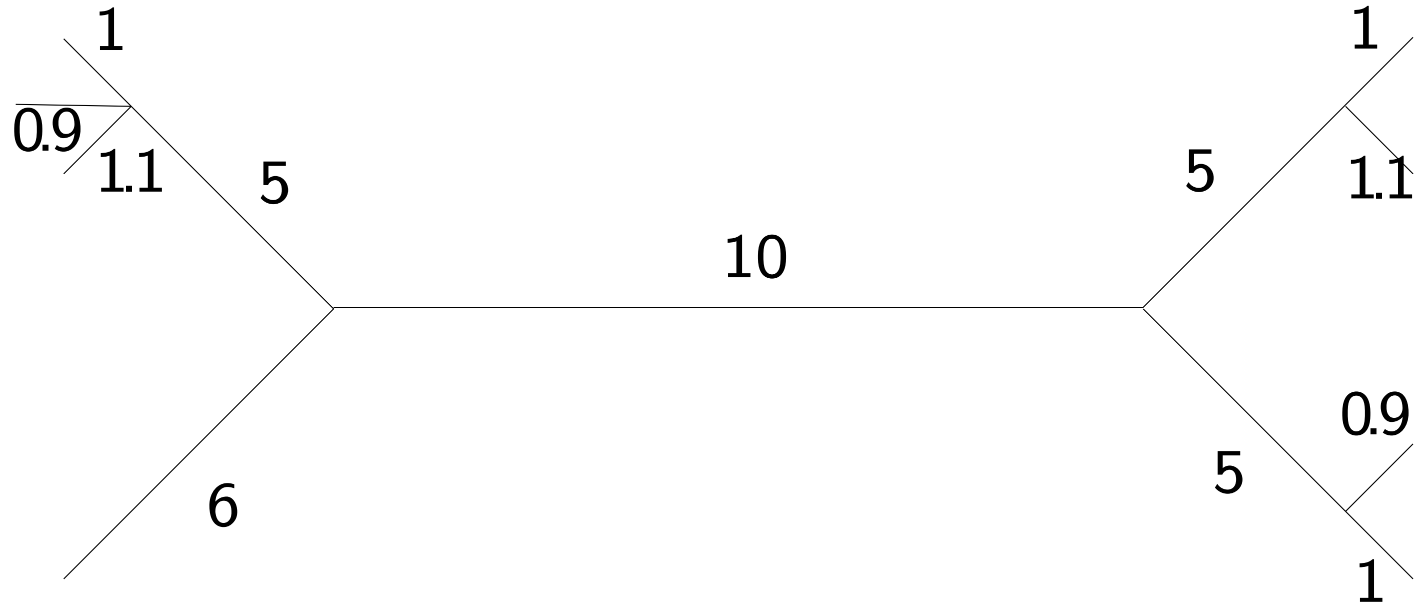
PHT is GH-*locally* injective on compact metric graphs.

Generic injectivity

Generative model:

metric graph $\equiv$ combinatorial graph (V, E) + edge weights $E \to \mathbb{R}_+$

mixture (proba. mass function , proba. measure **with density** on $\mathbb{R}_+^{|E|}$)



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Thm 4:

Under this model, there is a full-measure subset of the metric graphs on which PHT is injective.

Thank you