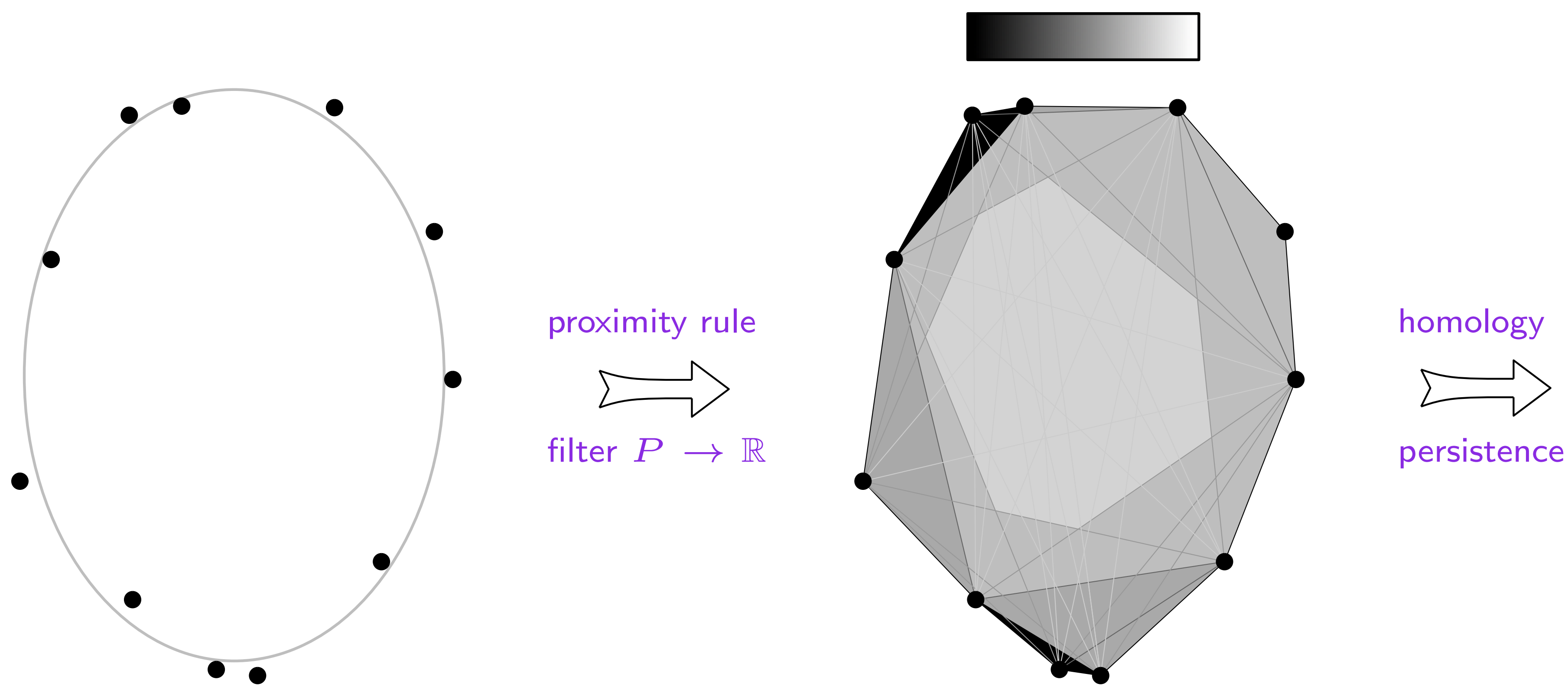
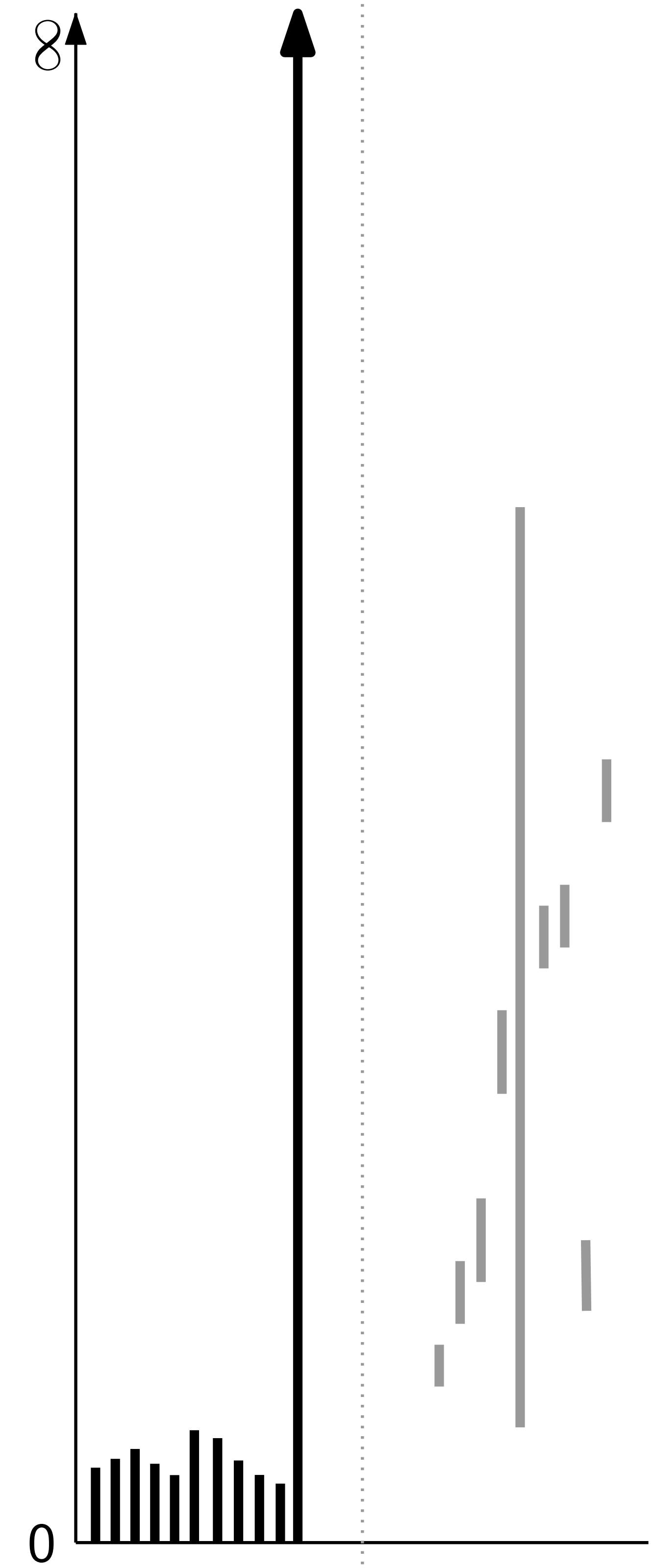
Recap' from yesterday: the TDA pipeline



point cloud P filtration $\mathcal{F}$



barcode (descriptor)

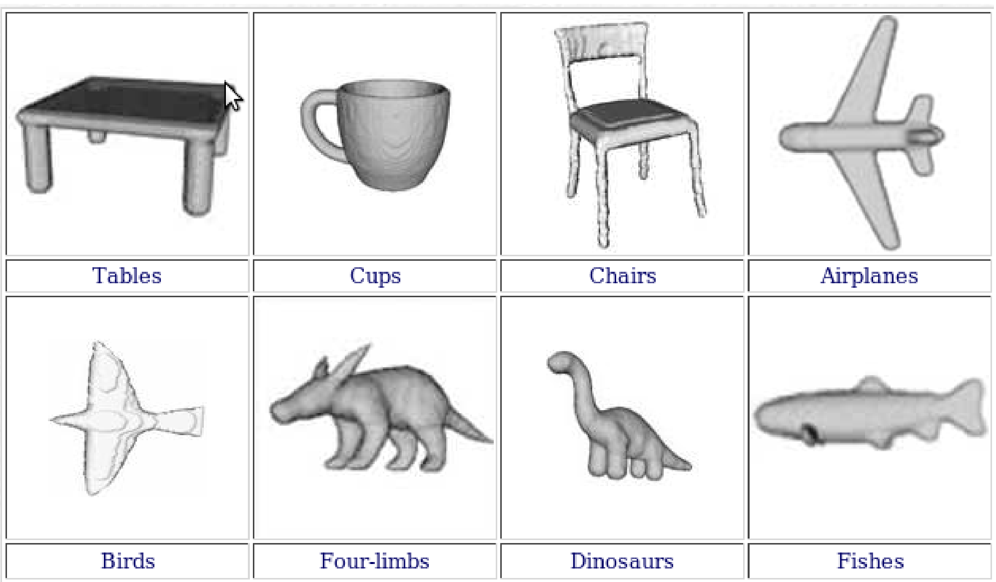
3 pillars to the theory (topological persistence):

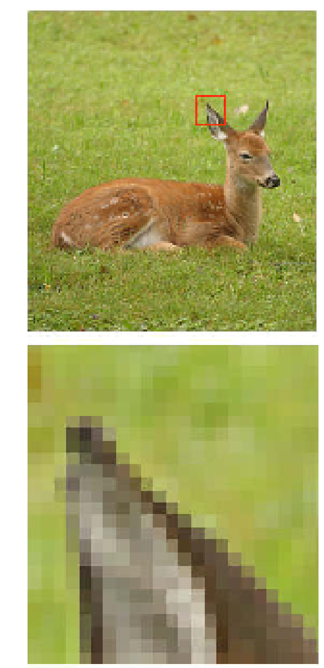
- decomposition theorems ($\exists$ barcodes)
- algorithms (computation of barcodes)
- stability theorems (barcodes as stable descriptors)

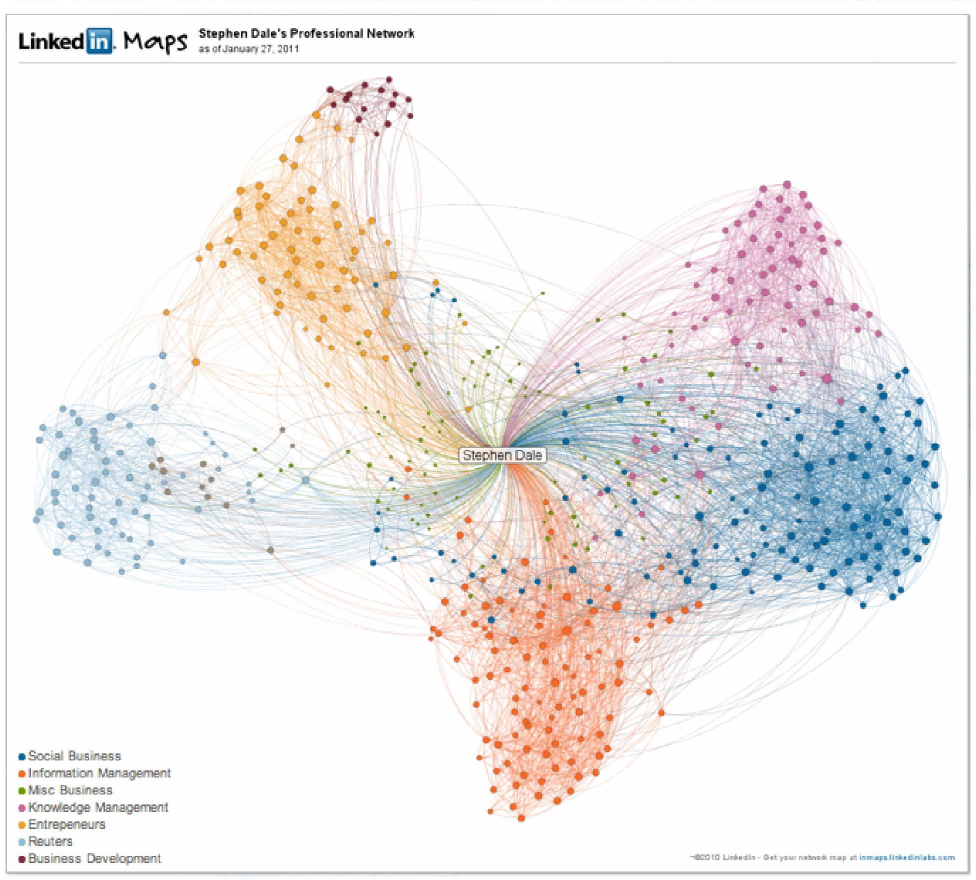
Geometric Data

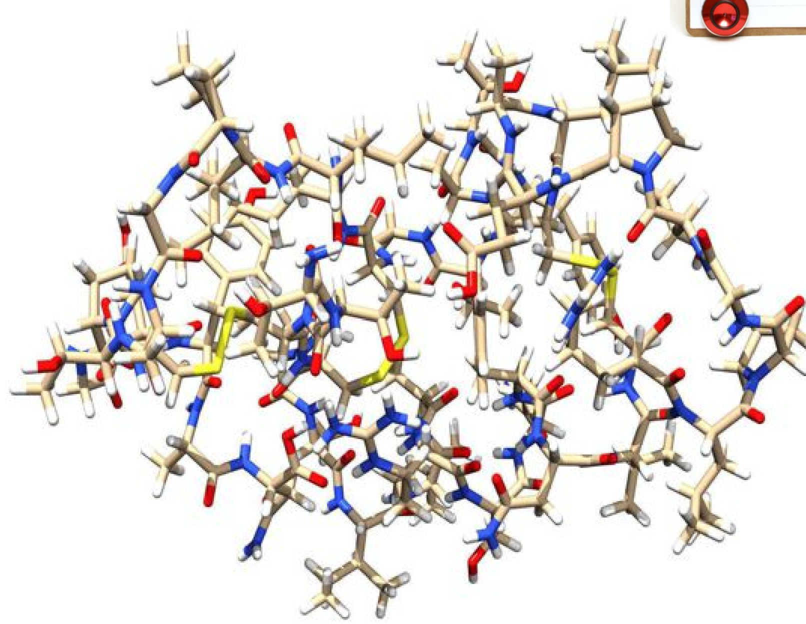
Input: point cloud equipped with a metric or (dis-)similarity measure

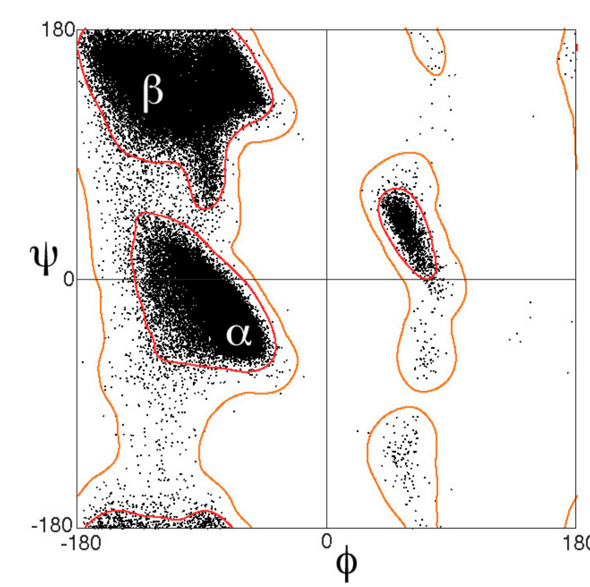
data point $\equiv$ image/patch, geometric shape, protein conformation, patient, LinkedIn user...











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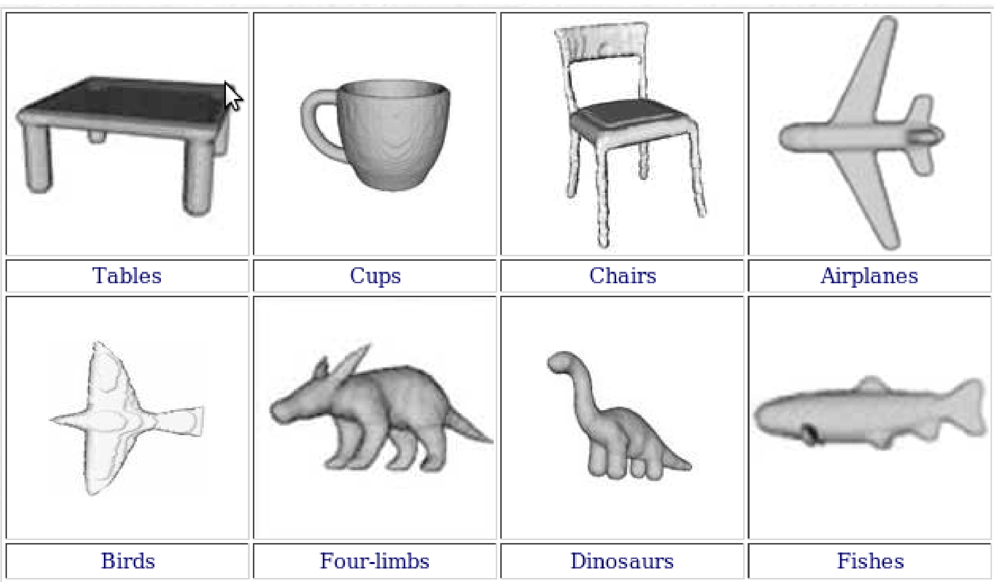
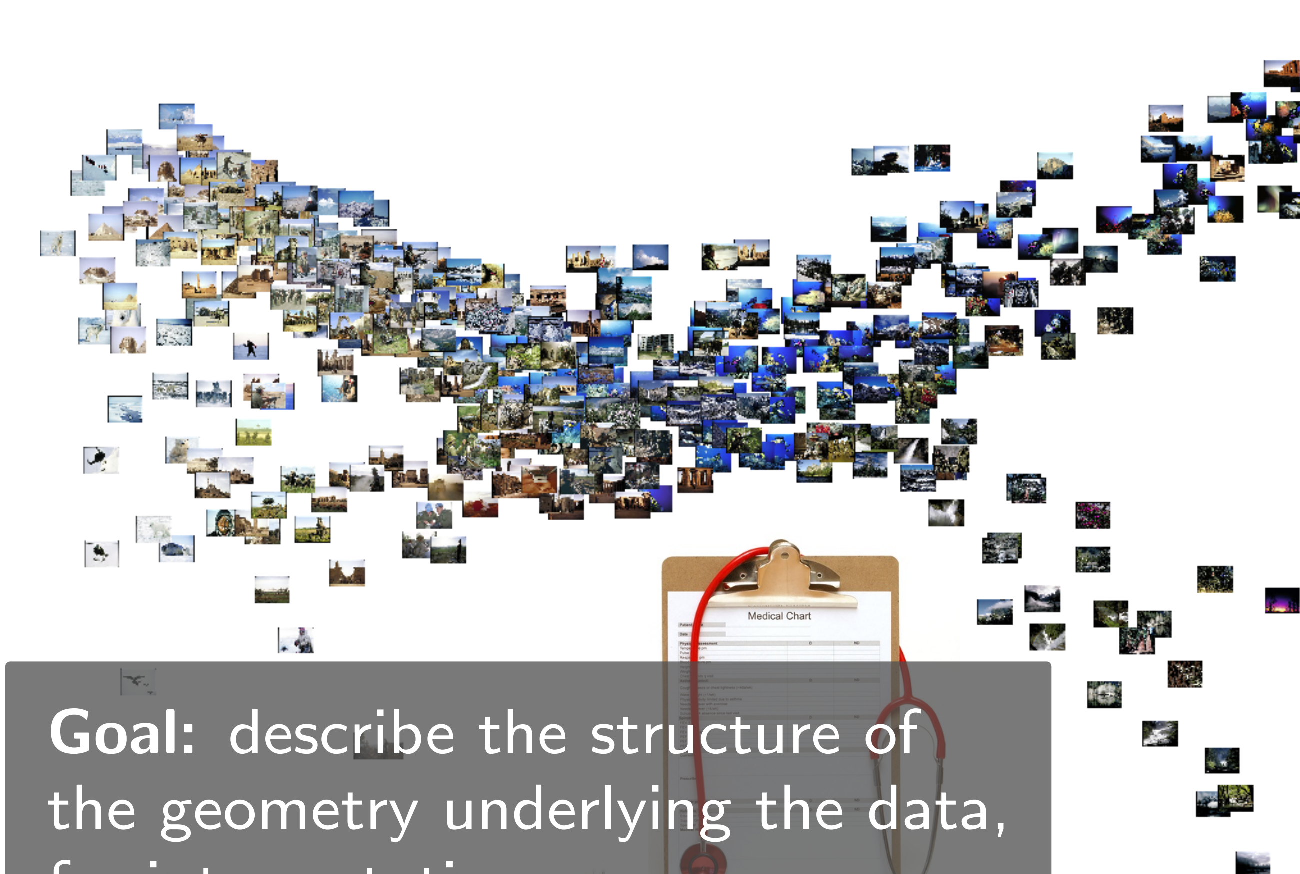
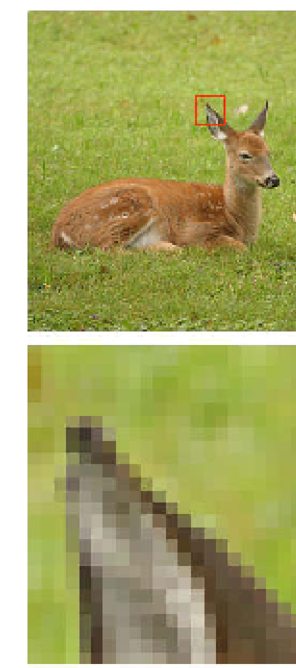
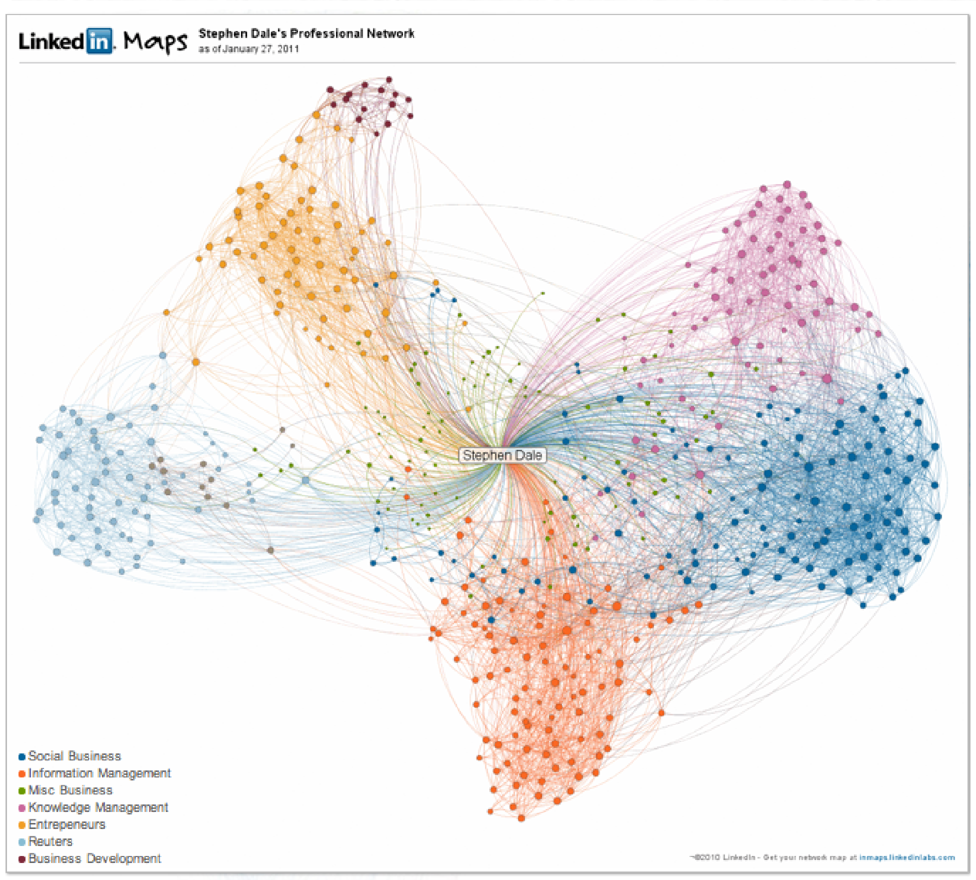
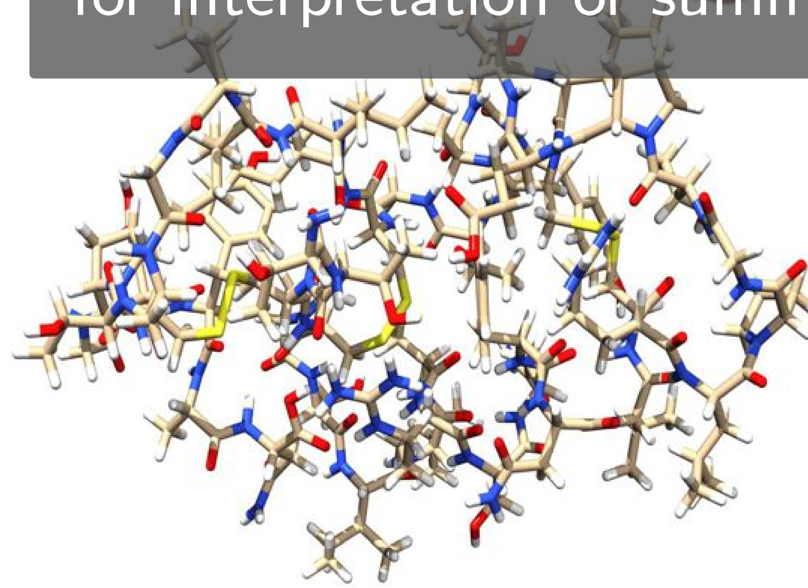


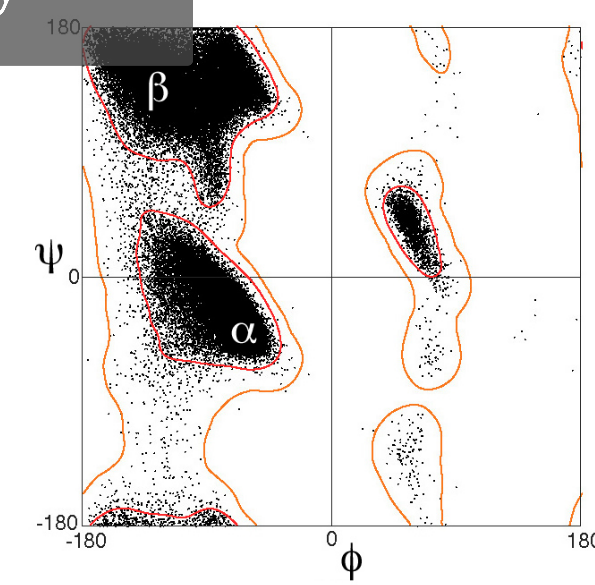






Goal: describe the structure of the geometry underlying the data, for interpretation or summary





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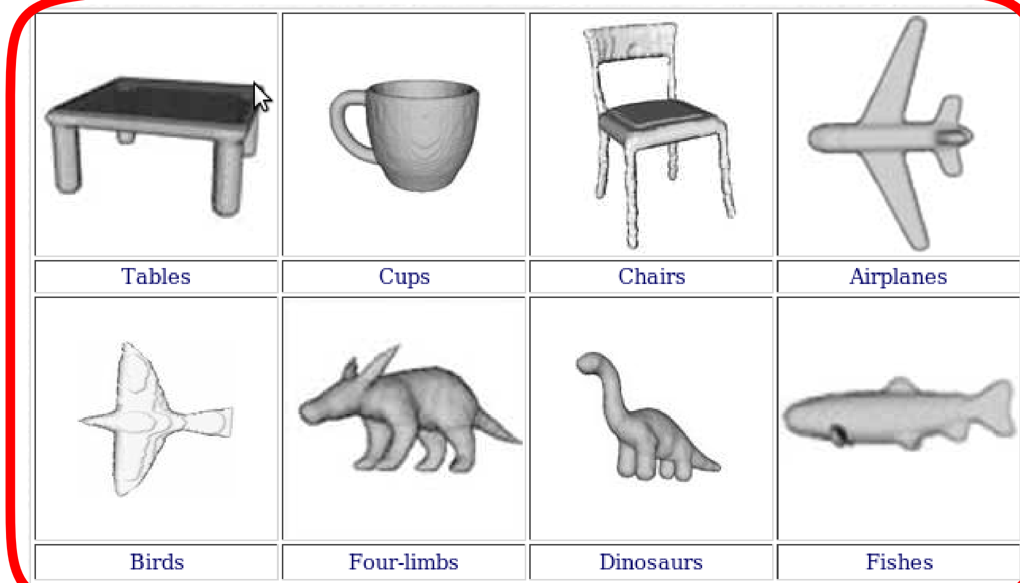

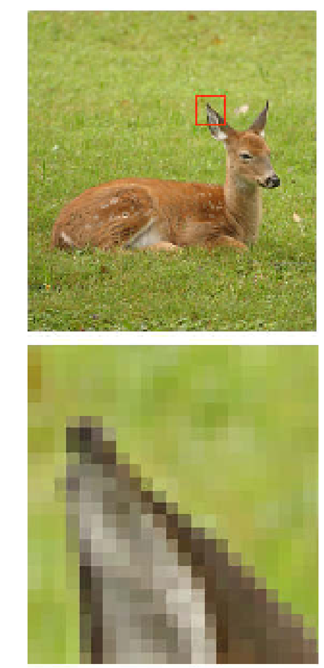

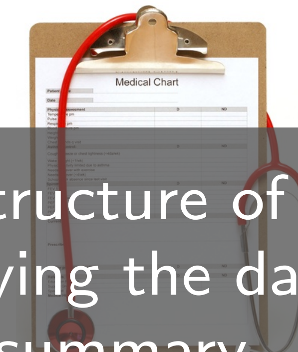

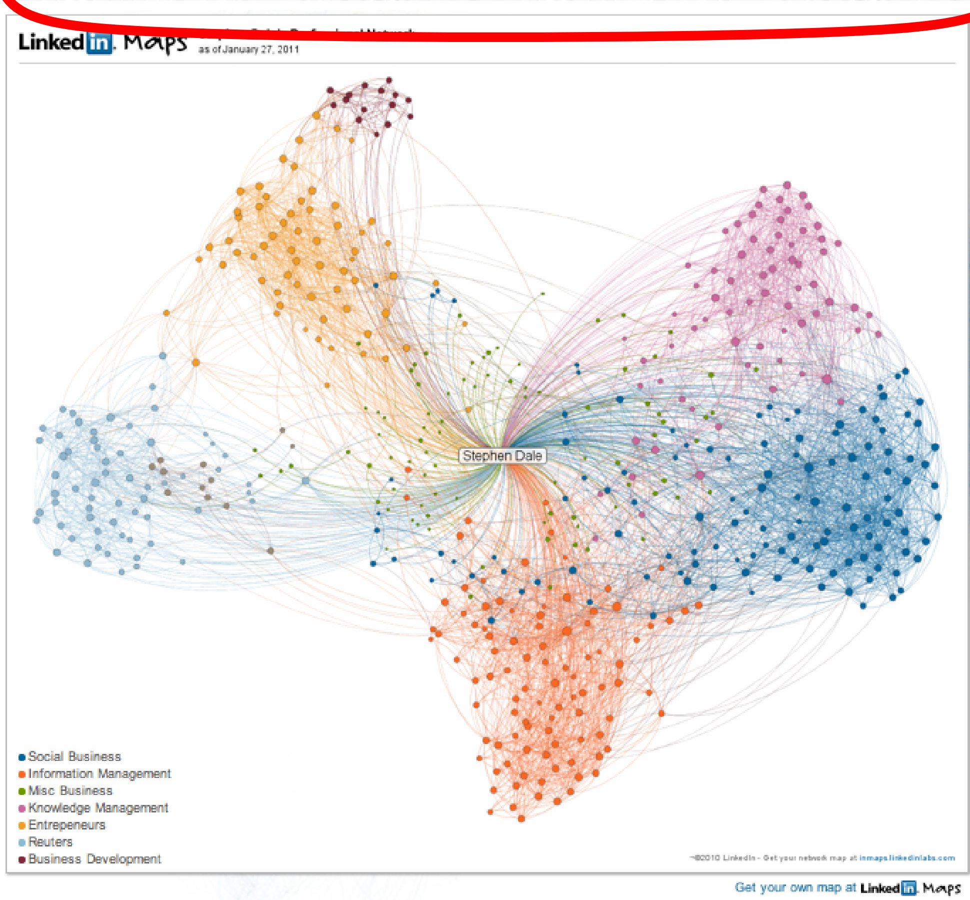

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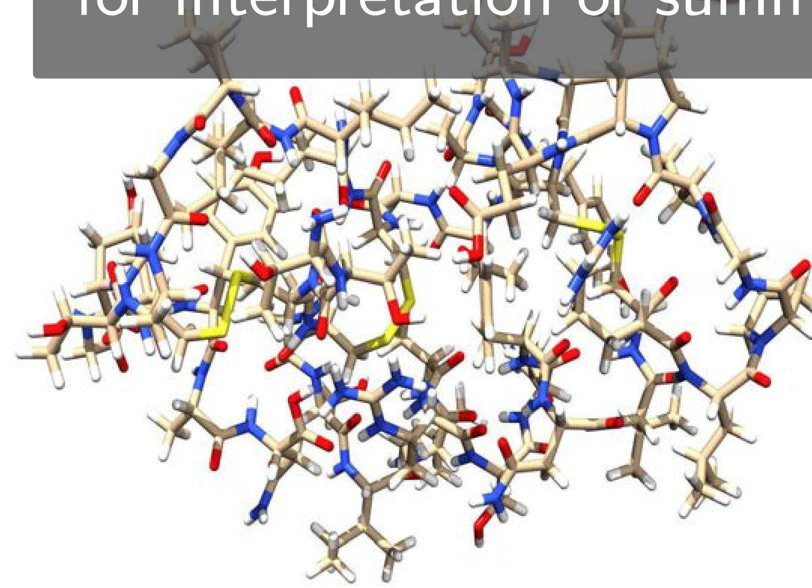
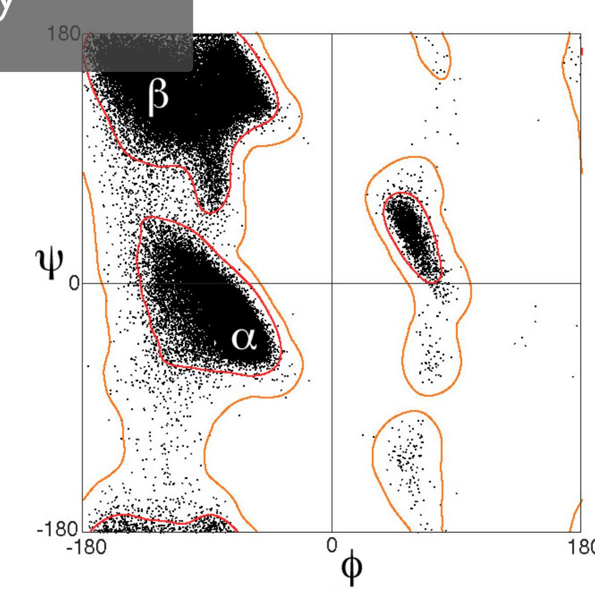
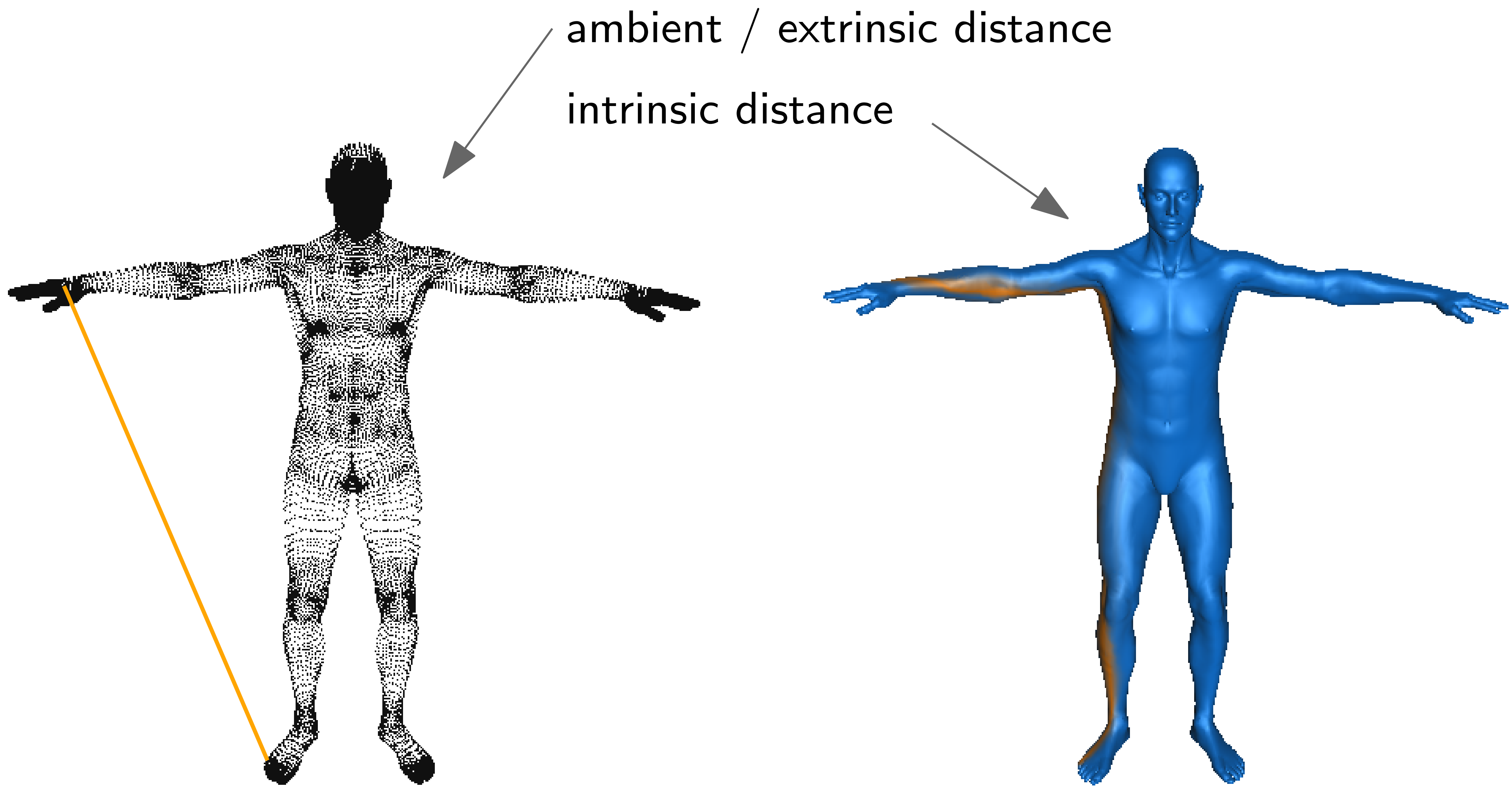




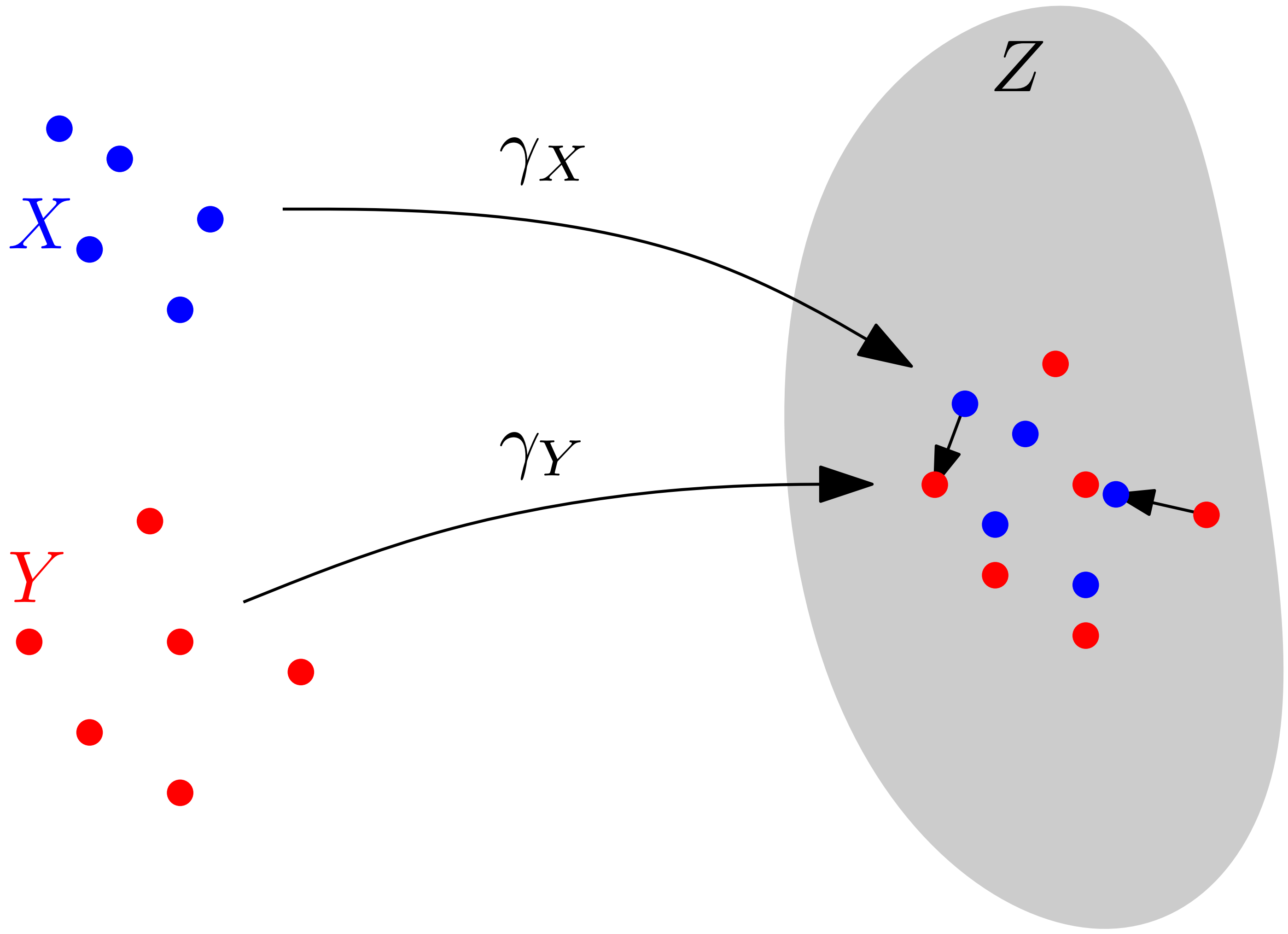
Mathematical framework

- geometric data set / underlying space $\equiv$ compact metric space



Mathematical framework

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



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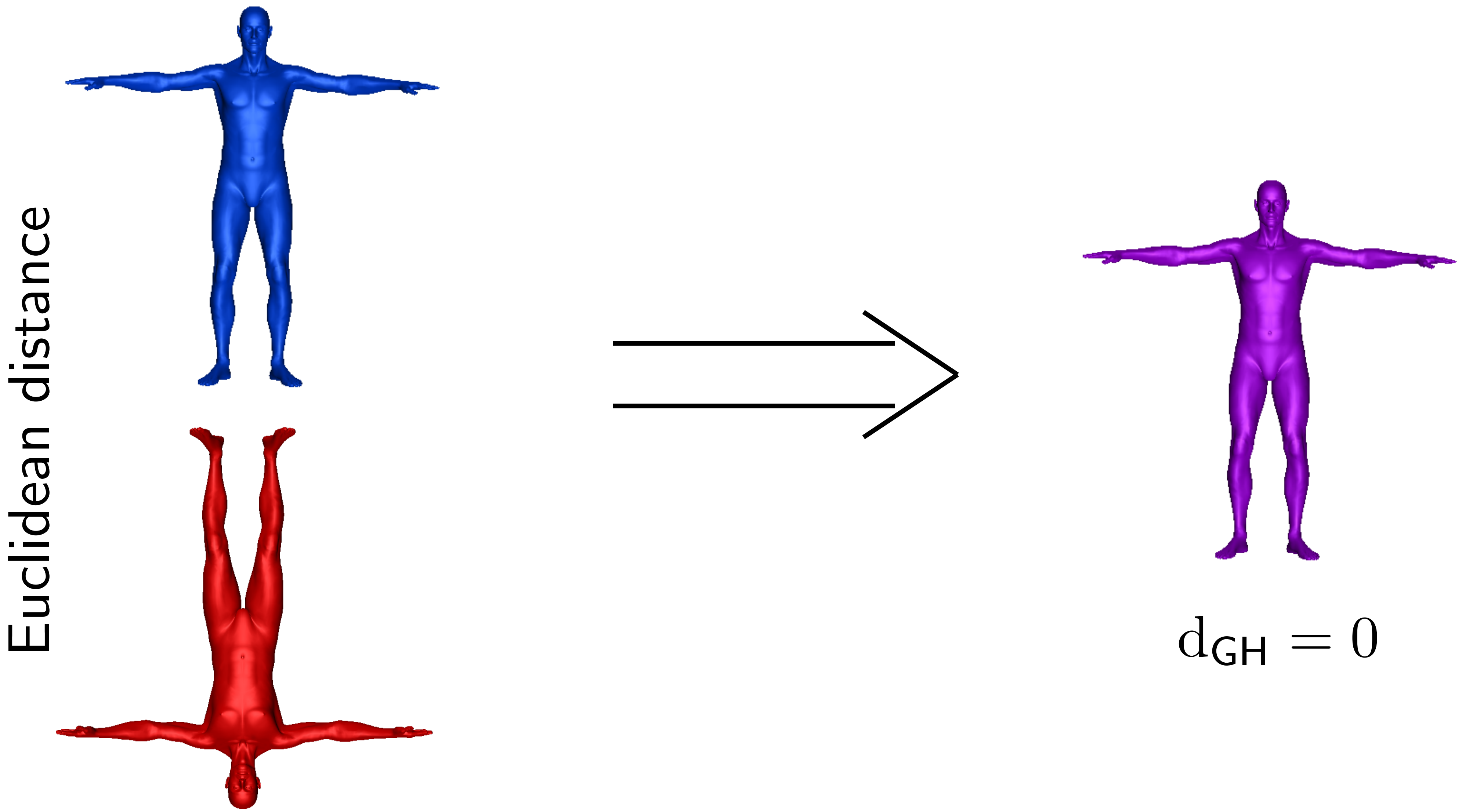

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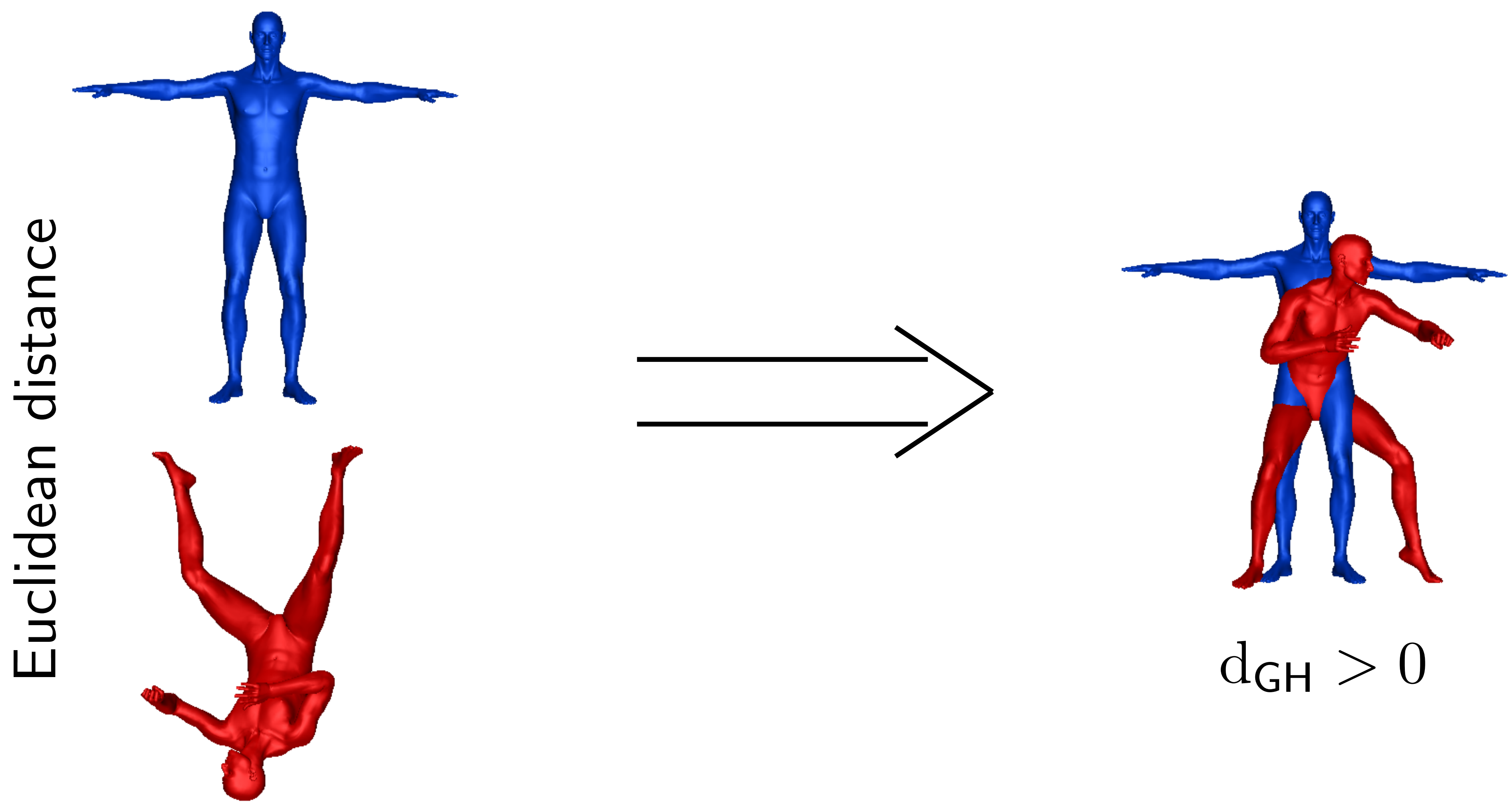

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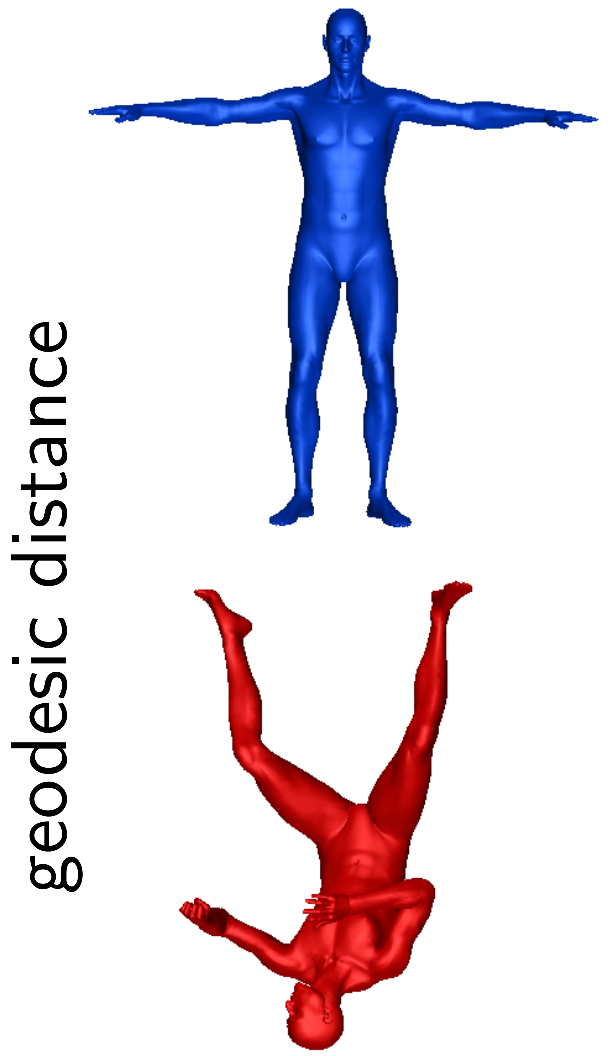


$\Longrightarrow$

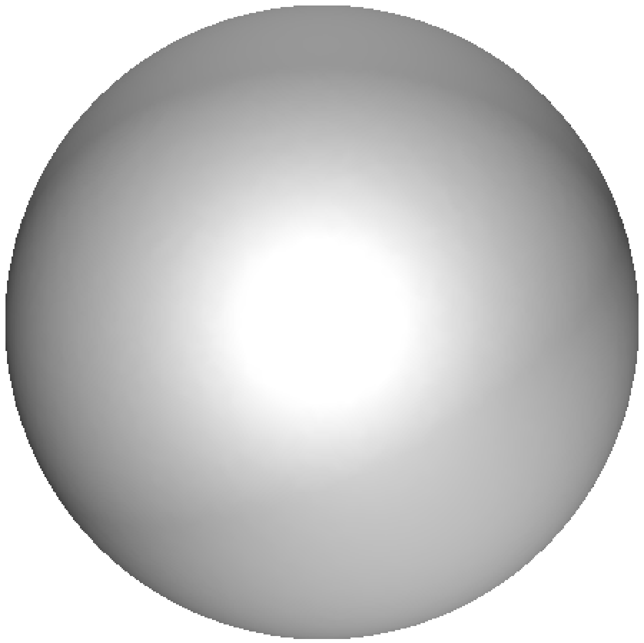
$d_{\mathsf{GH}} = 0$

Mathematical framework

- geometric data set / underlying space $\equiv$ compact metric space
- distance between compact metric spaces $\equiv$ Gromov-Hausdorff (GH) distance
- *descriptor* $\equiv$ persistence diagram (choose the filtration)

  - **multi-scale** $\equiv$ reflects the structure of the shape across scales
  - **global/local** $\equiv$ attached to the whole shape / to a base point(s)
  - **stable** $\equiv$ variations with GH-distance and base point location are controlled

Why use descriptors



isometries

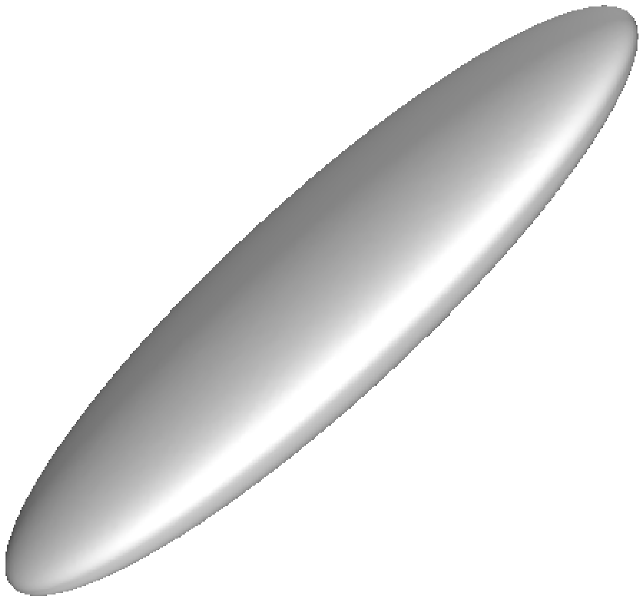
GH distance

hard to compute

[Bronstein^2, Kimmel 2006]

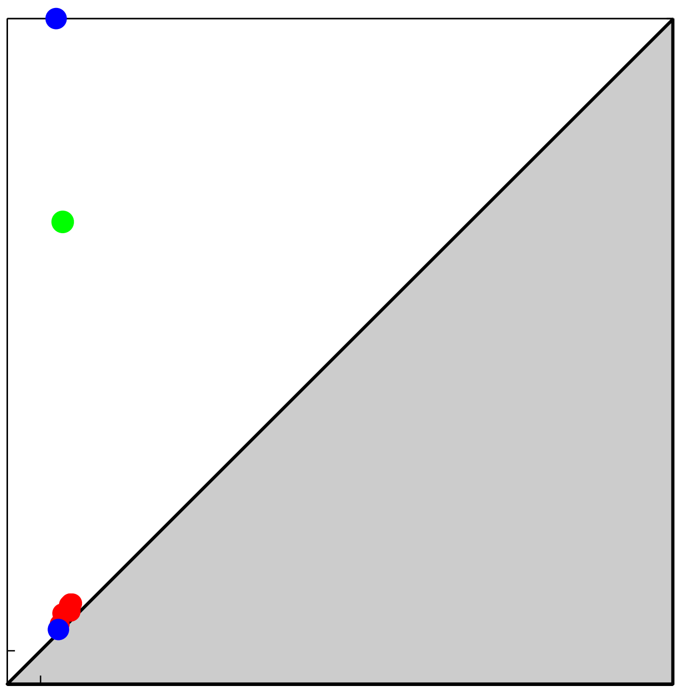
[Mémoli 2007]

[Agarwal et al. 2015]



shape space

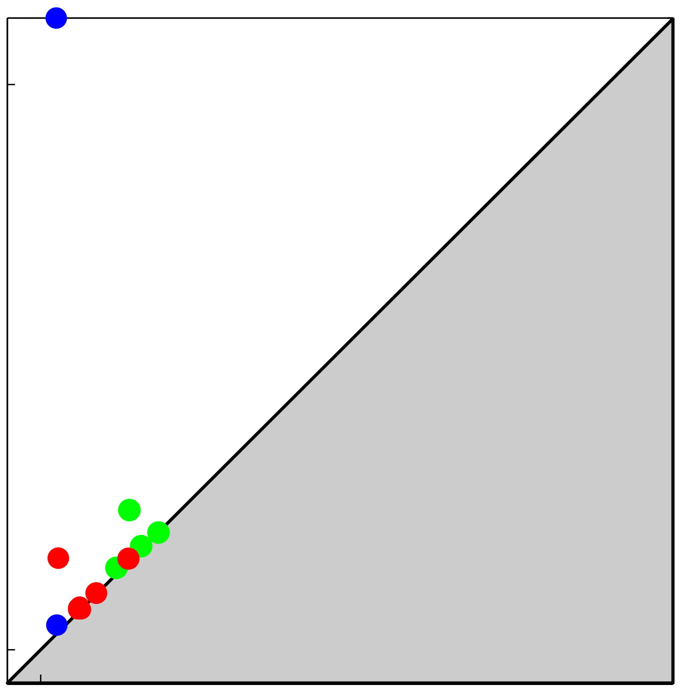
descriptors space



equality

distance

easy to compute



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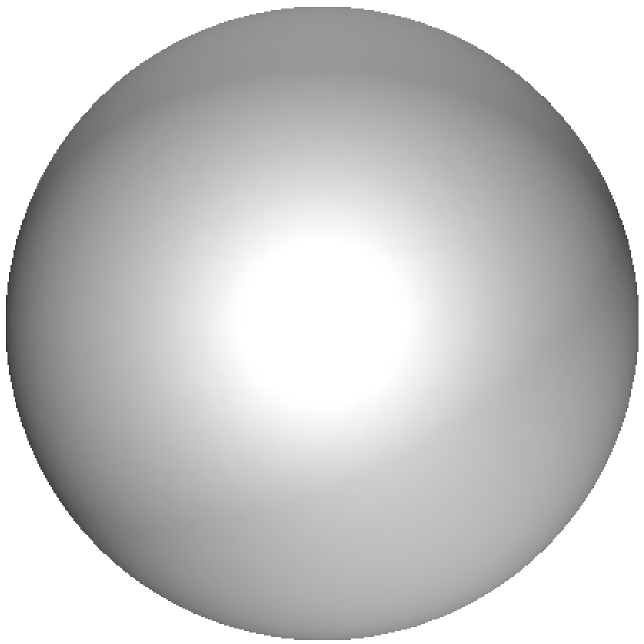

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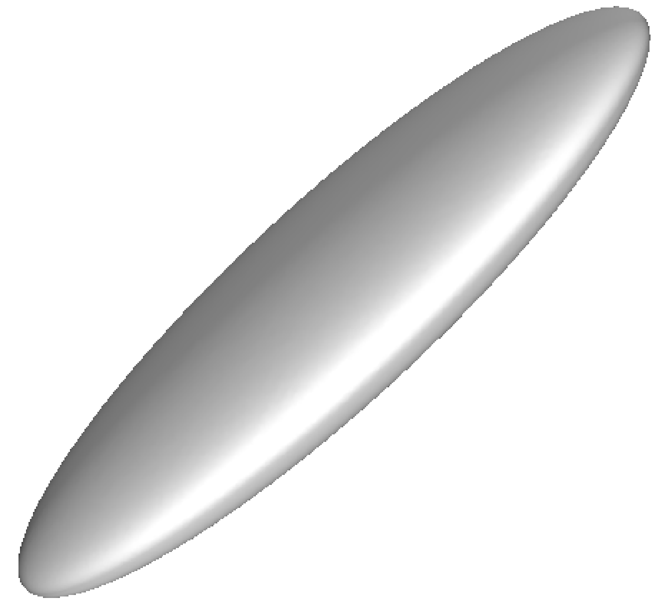
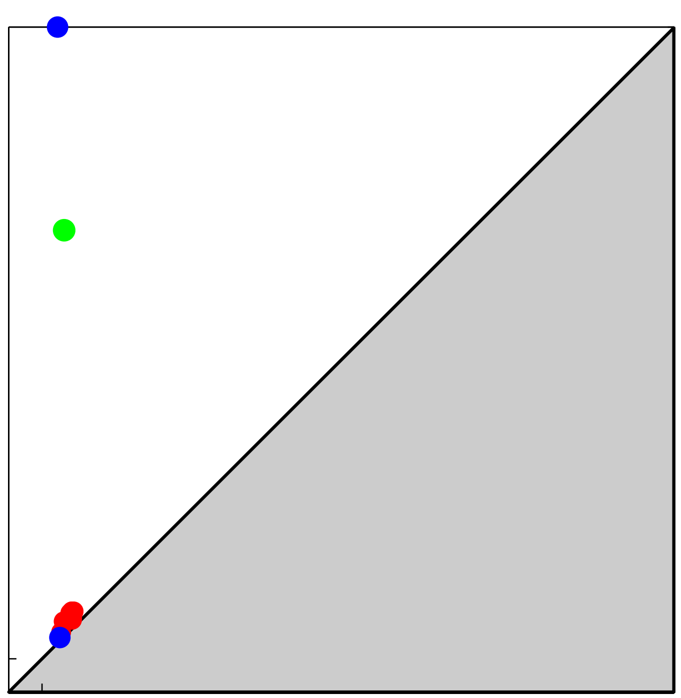


shape space

Ideally, descriptors distance = GH distance

descriptors space



equality

distance

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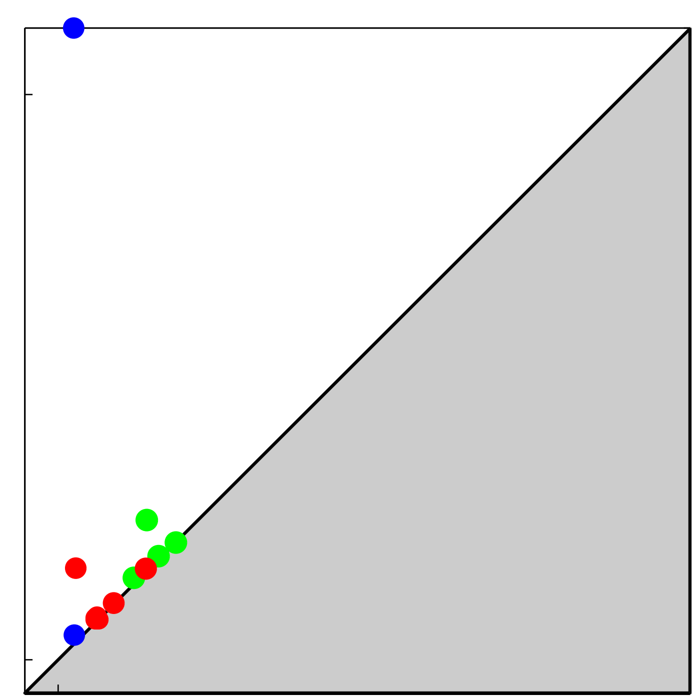
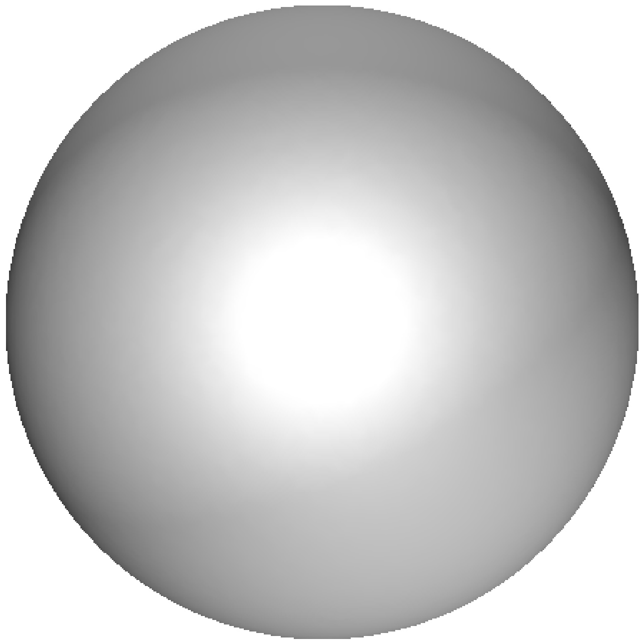


Why use descriptors



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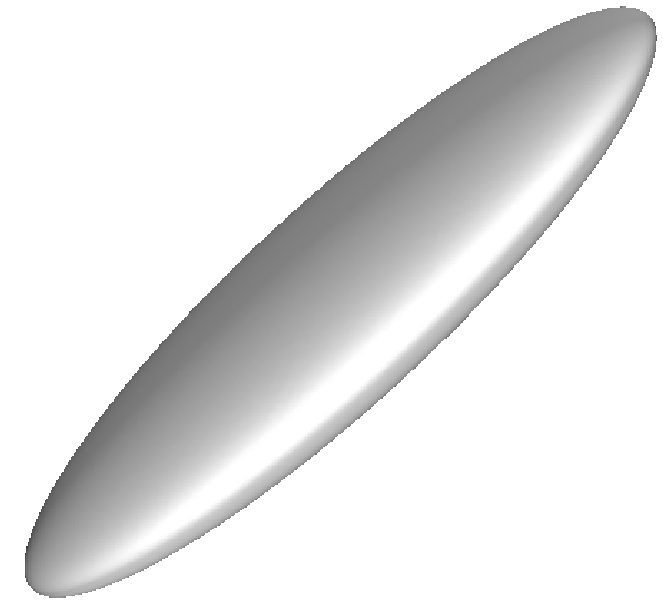
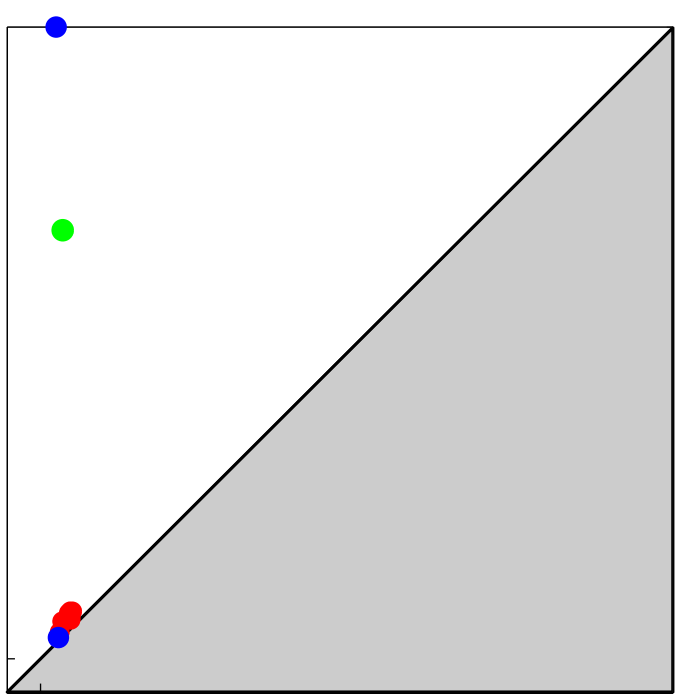


shape space

descriptors space

Ideally, descriptors distance $=$ GH distance

In reality, $\leq$



equality
distance
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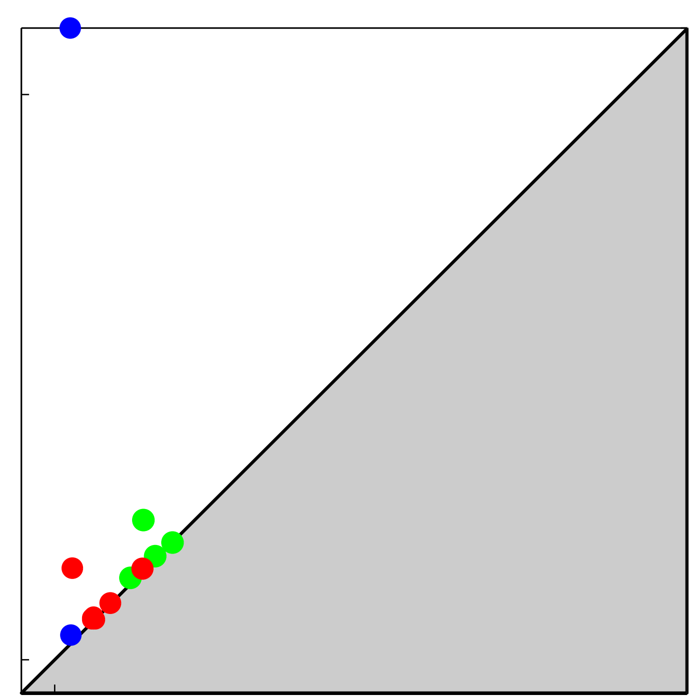

Why use descriptors

Some descriptors for images / 3d shapes / metric spaces:

- diameter
- curvature (mean, Gaussian, sectional)
- shape context (distribution of distances)
- heat kernel signature (heat diffusion)
- wave kernel signature (Maxwell's equations)
- spin image (local neighborhood parametrization)
- SIFT features (local distribution of gradient orientations)
- etc.

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geometry

statistics

Menu

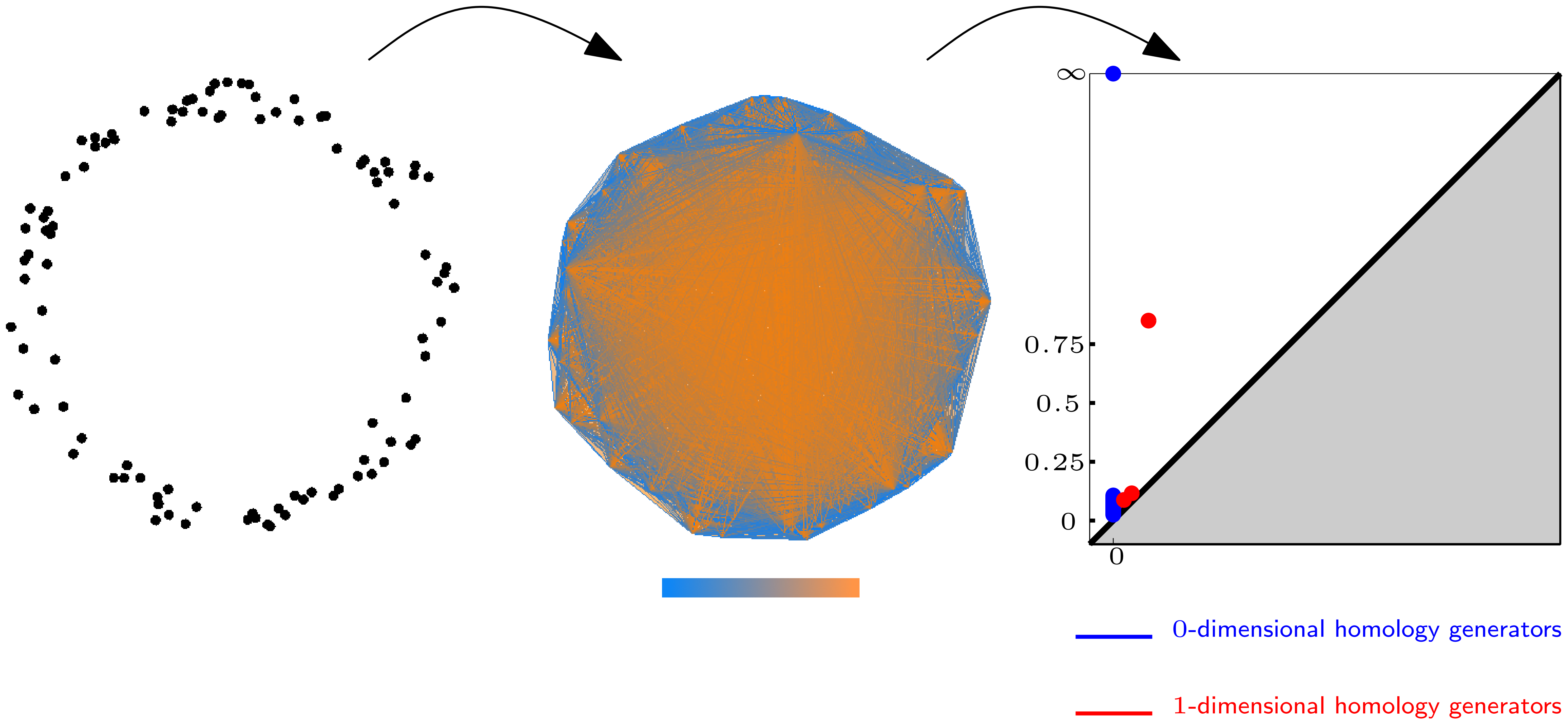
1. Global topological descriptors

2. Local topological descriptors

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)



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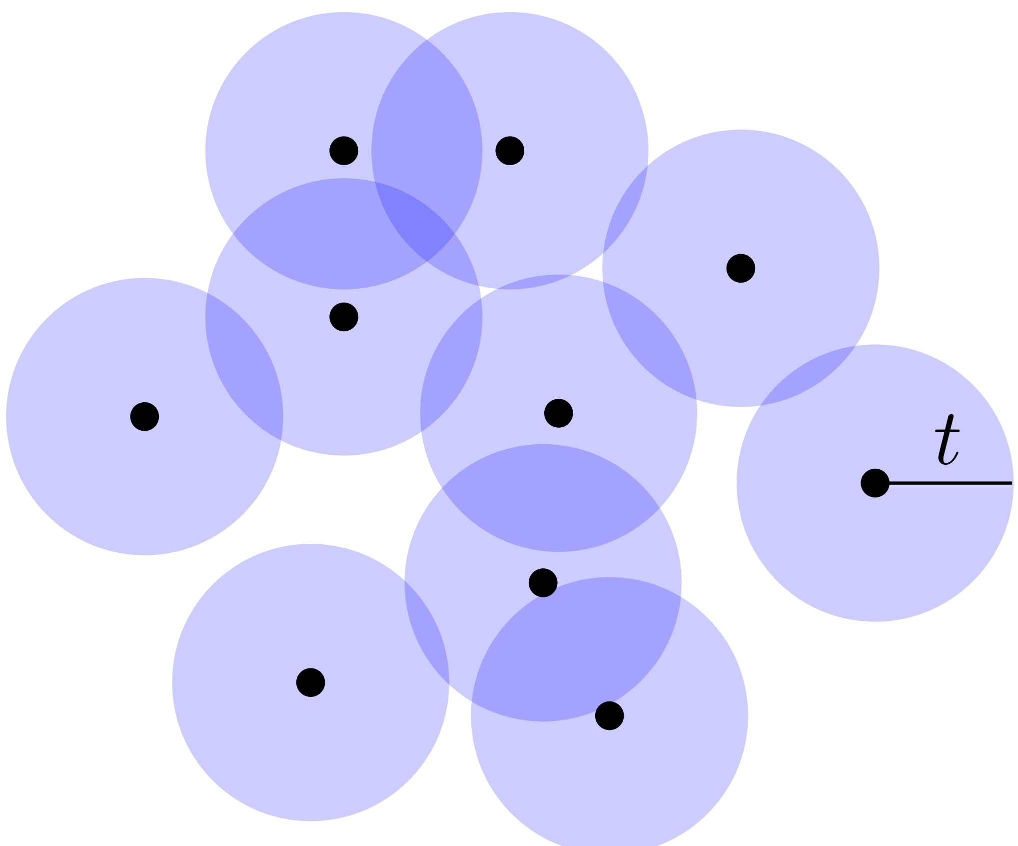
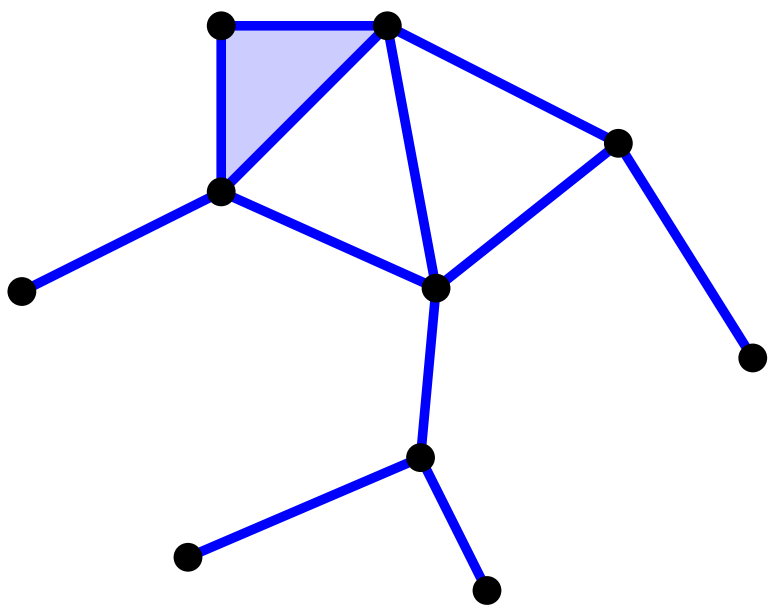
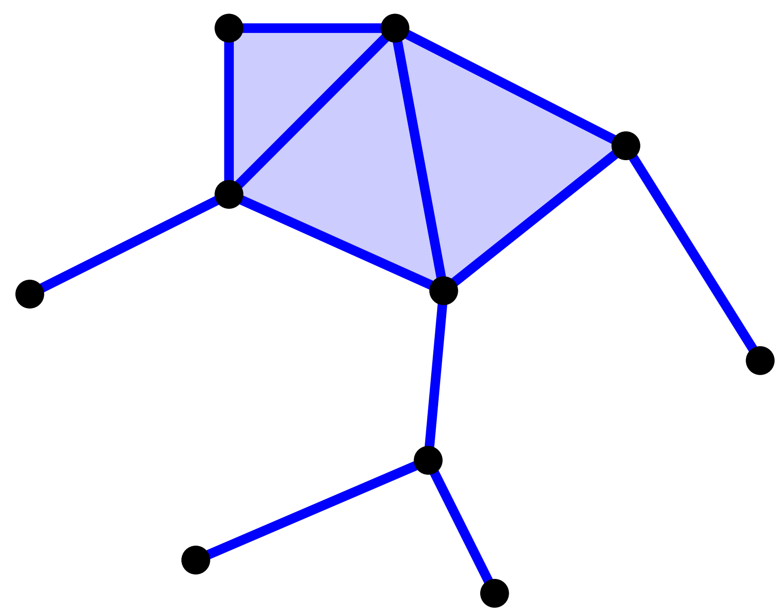




$\mathrm{C}_t(X, \mathrm{d}_X)$



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

$\rightarrow$ popular choices:
- Čech/Nerve filtration $\mathcal{C}(X, \mathrm{d}_X)$
- (Vietoris)-Rips filtration $\mathcal{R}(X, \mathrm{d}_X)$

Global topological descriptors

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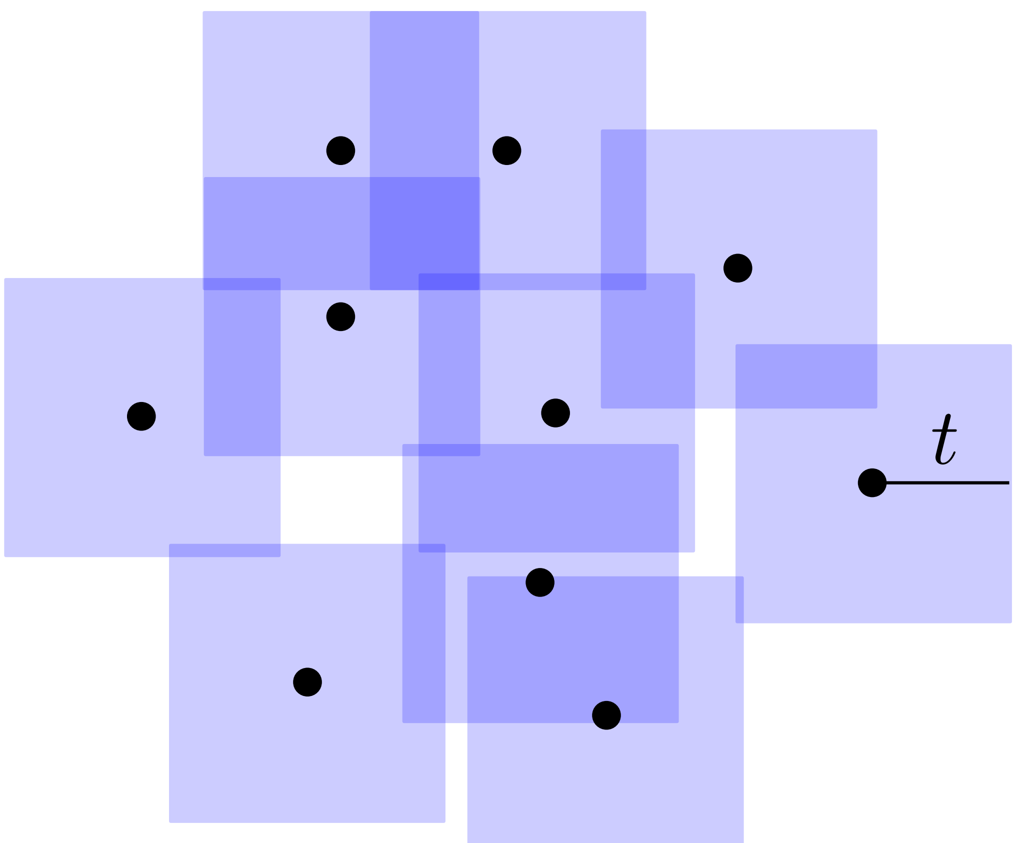

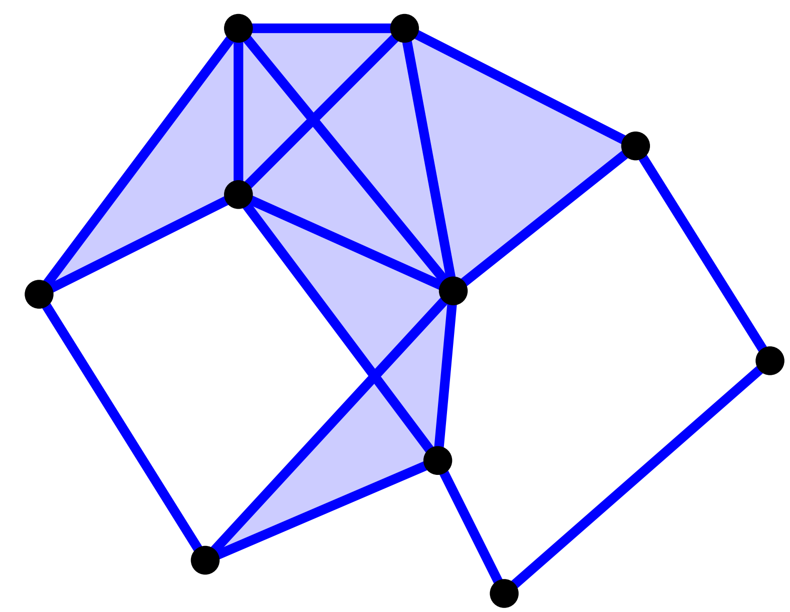

$\mathrm{C}_t(X, \mathrm{d}_X) = \mathrm{R}_{2t}(X, \mathrm{d}_X)$

→ popular choices:
- Čech/Nerve filtration $\mathcal{C}(X, \mathrm{d}_X)$
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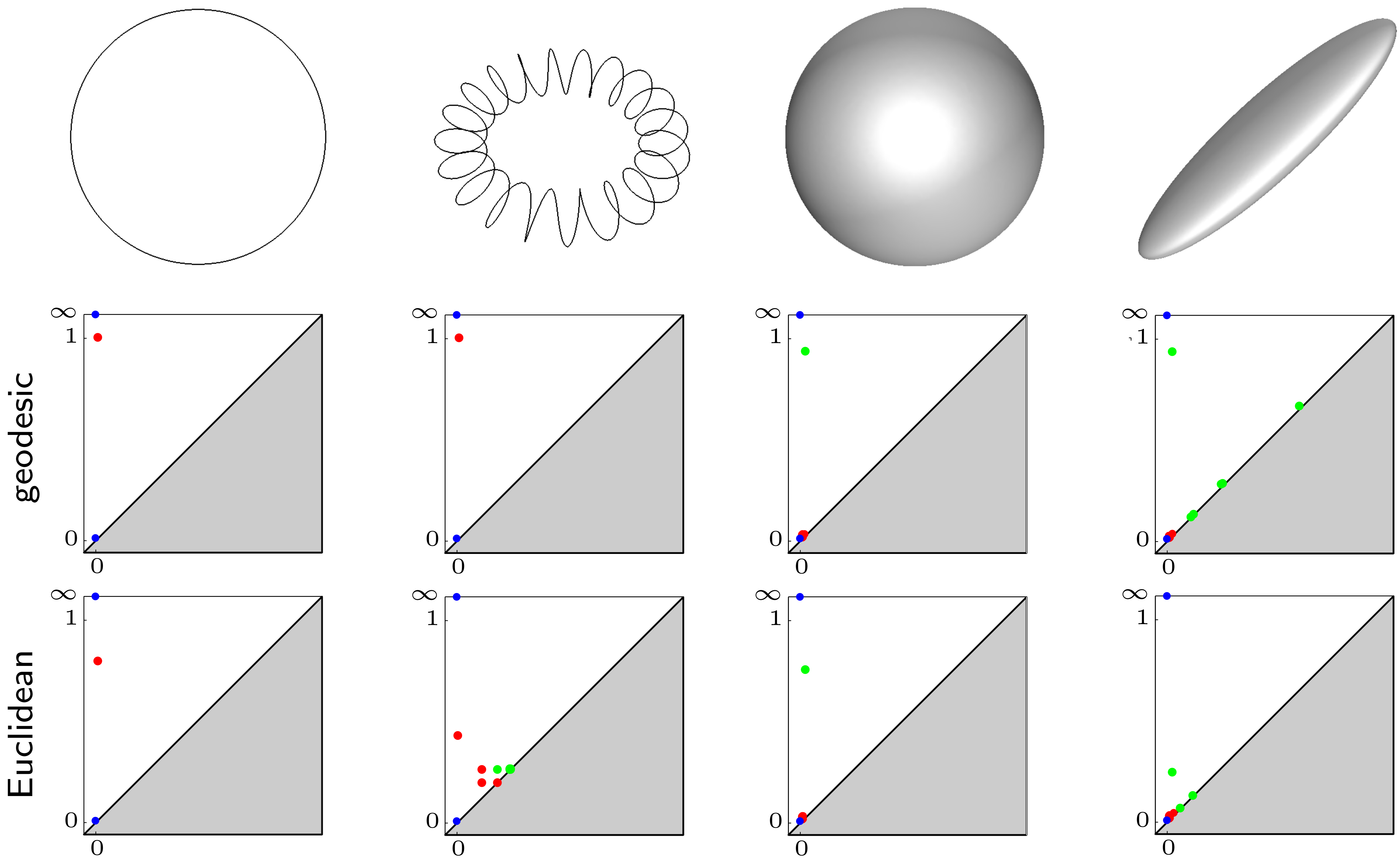
Some examples

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



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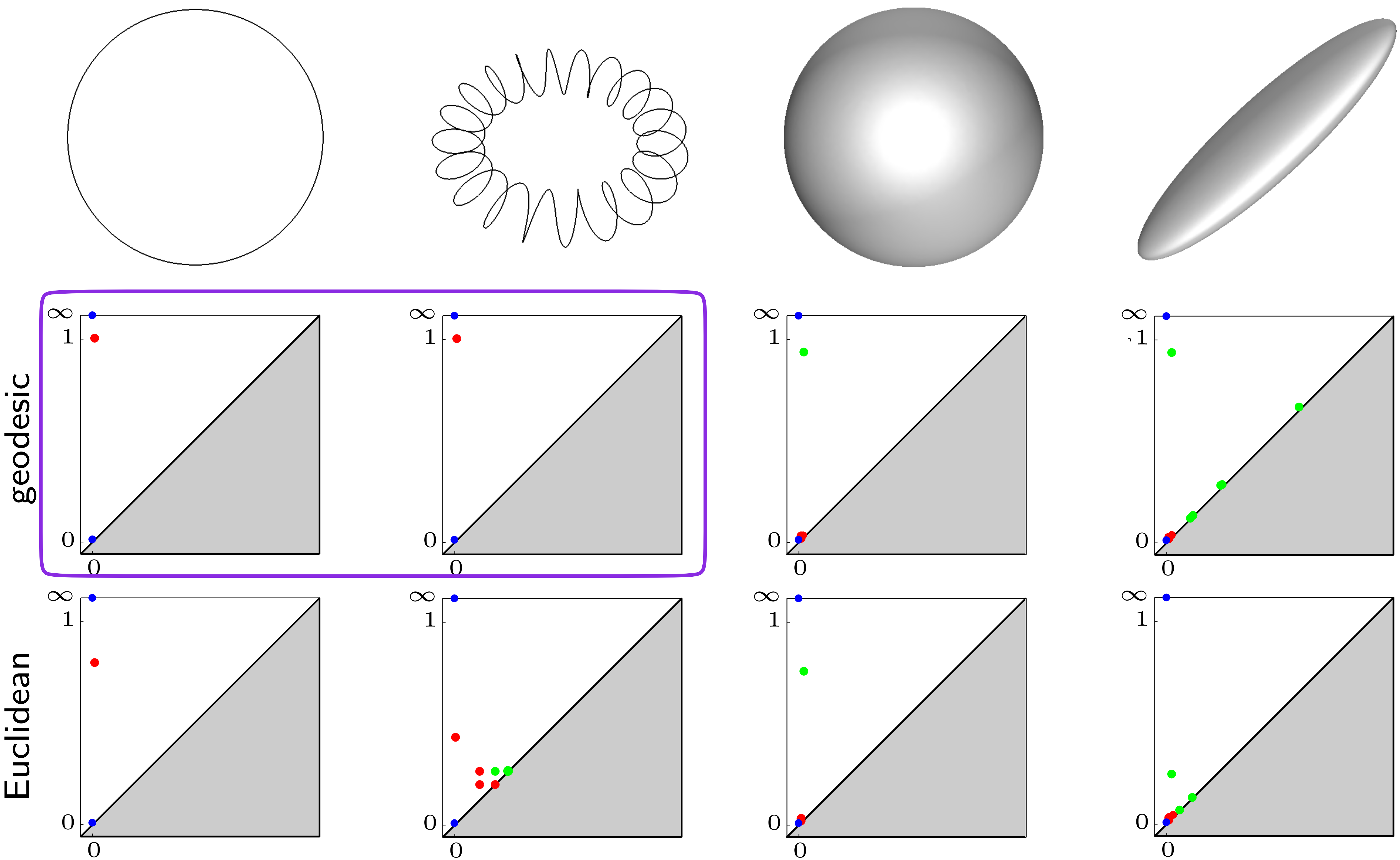

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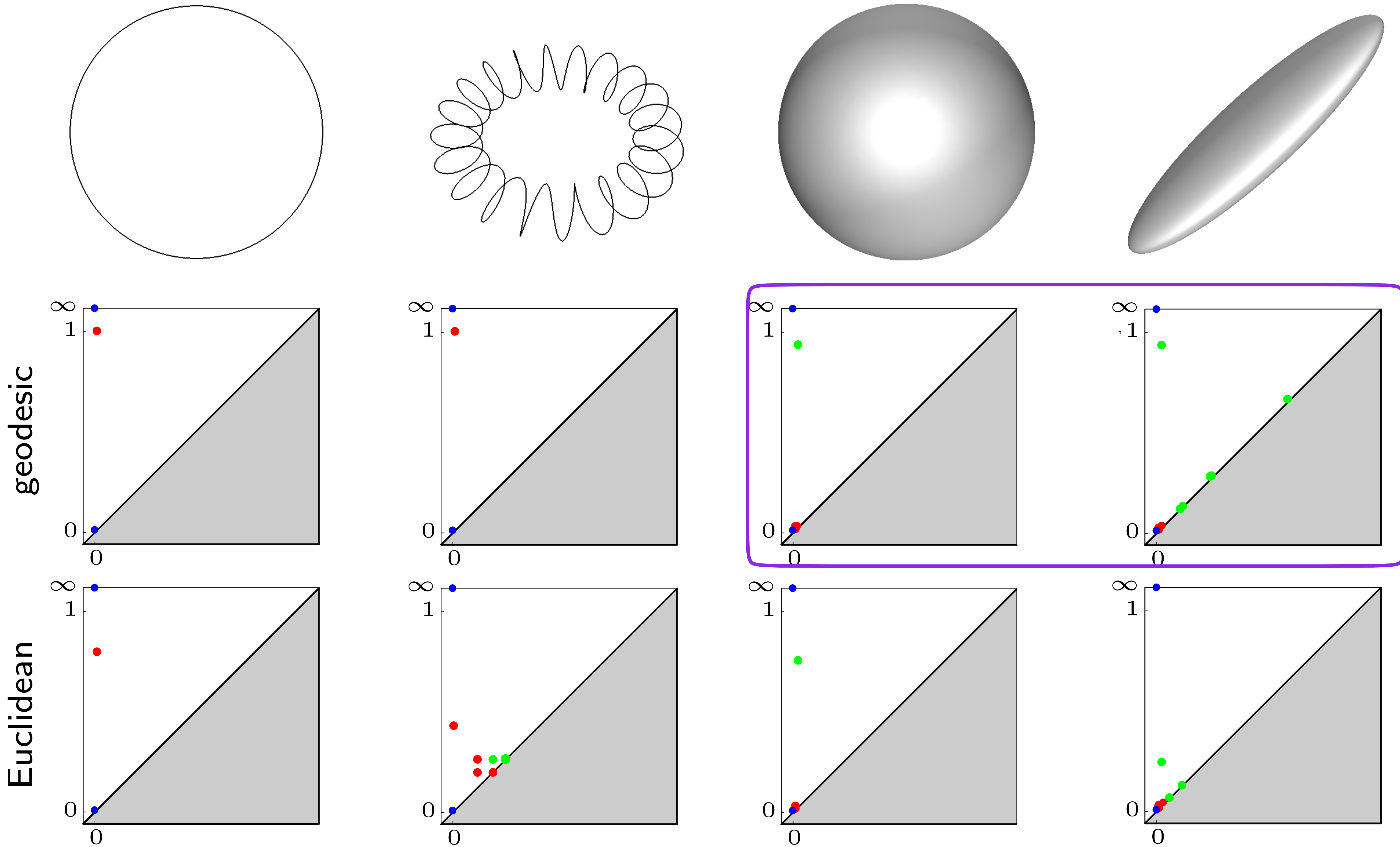
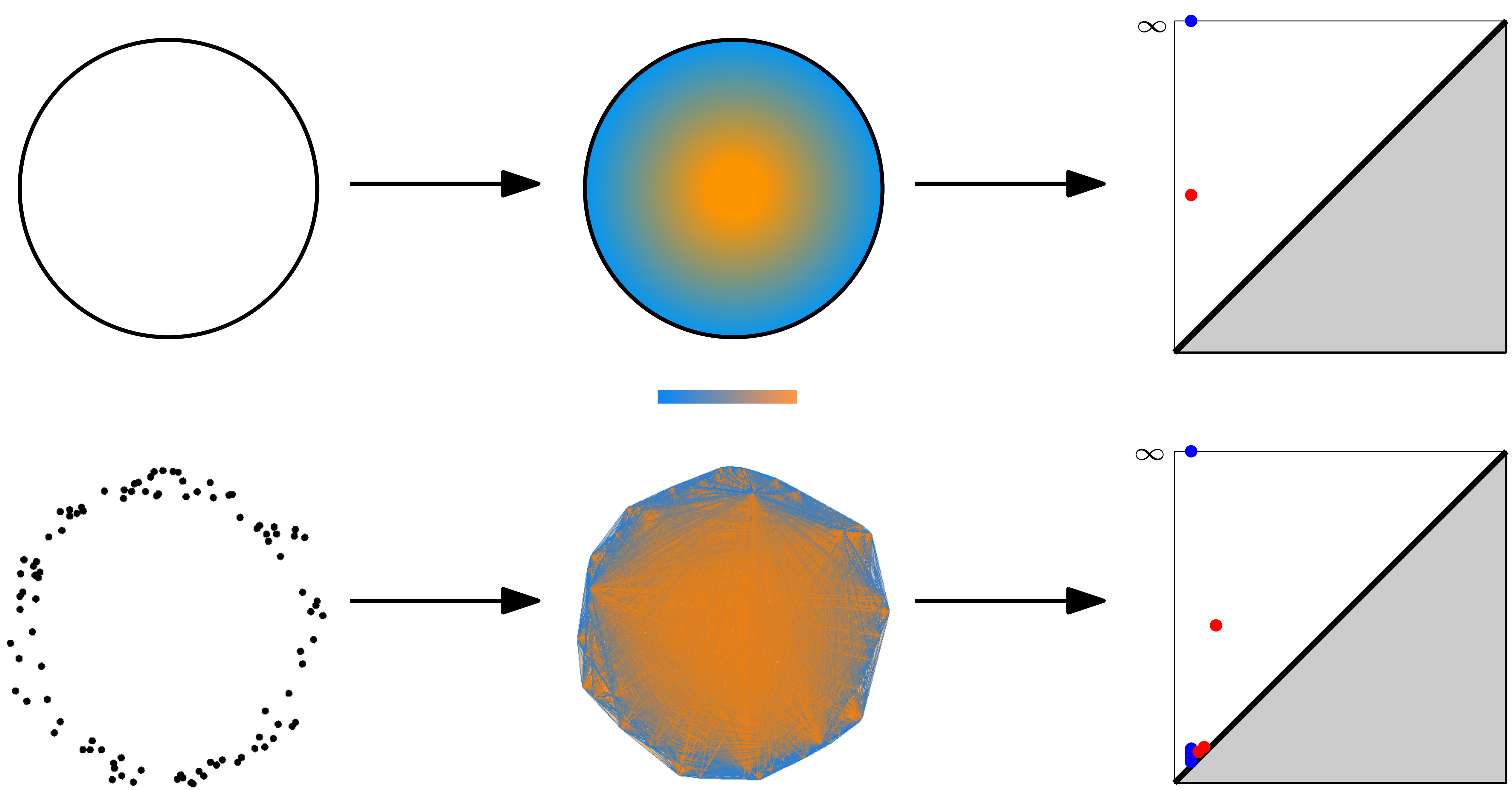


Stability

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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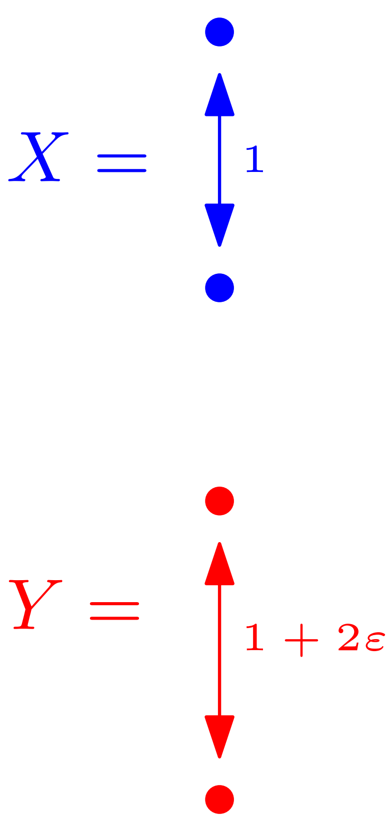
The bound is worst-case tight...



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

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

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

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

Stability

Theorem: [Chazal, de Silva, O. 2013]
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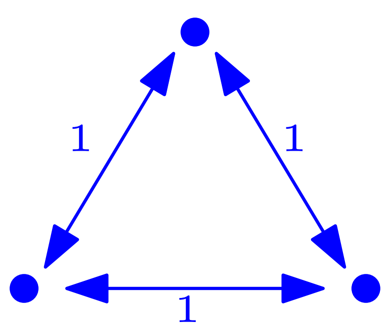
The bound is worst-case tight... but it is still only an upper bound

$X =$

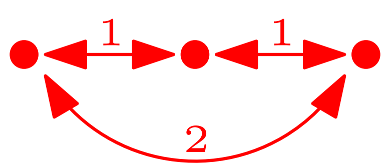


$$\mathrm{d}_{\mathrm{GH}}(X, Y) = \frac{1}{2}$$

$$\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X) = \{(0, \infty),\ (0, 1),\ (0.1)\}$$

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

$Y =$



$$\Rightarrow \mathrm{d}_\mathrm{B}^\infty(\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X),\ \mathrm{dgm}\,\mathcal{R}(Y, \mathrm{d}_Y)) = 0$$

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Theorem: [Chazal, de Silva, O. 2013]
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Variants and extensions:

- other filtrations: v Cech / Nerve, witness complex, etc.

- larger classes of metric spaces: precompact, totally bounded, etc.

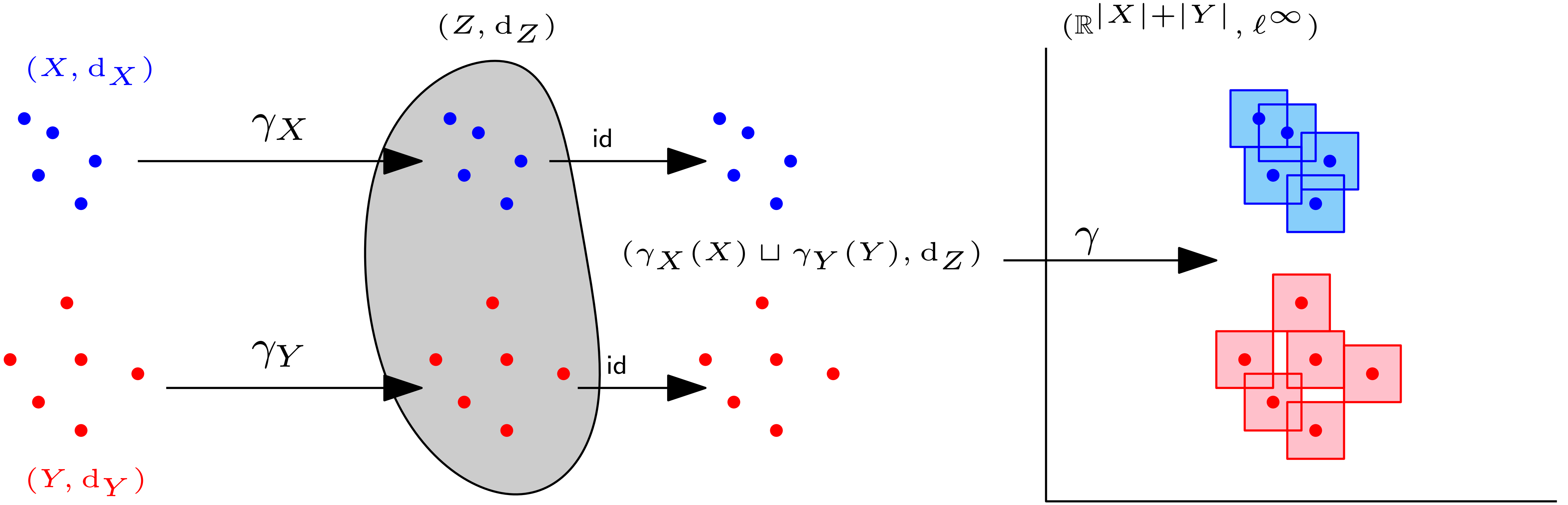
- (dis-)similarity measures

Stability

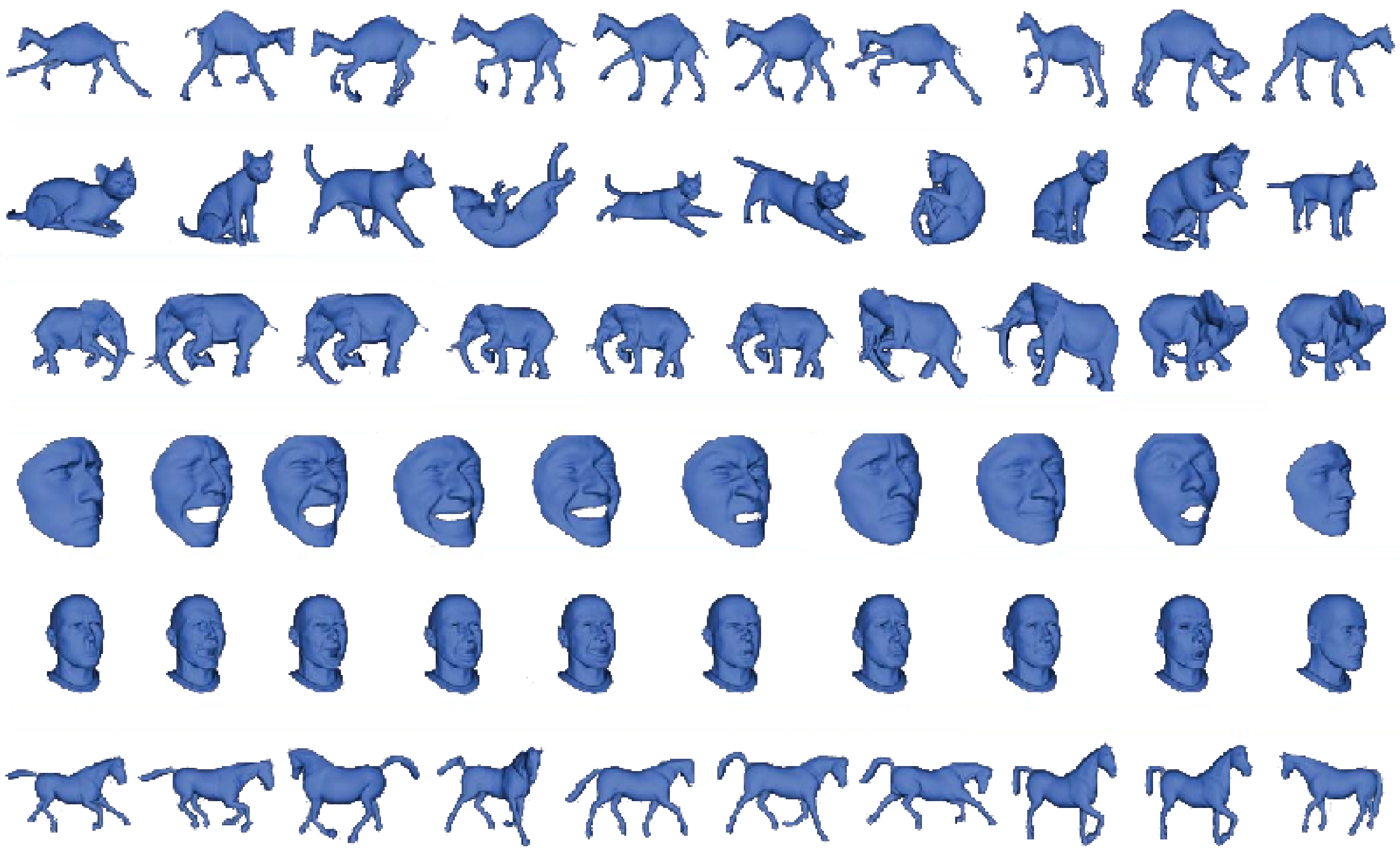
finite

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

Proof outline:



Toy application (unsupervised shape classification)



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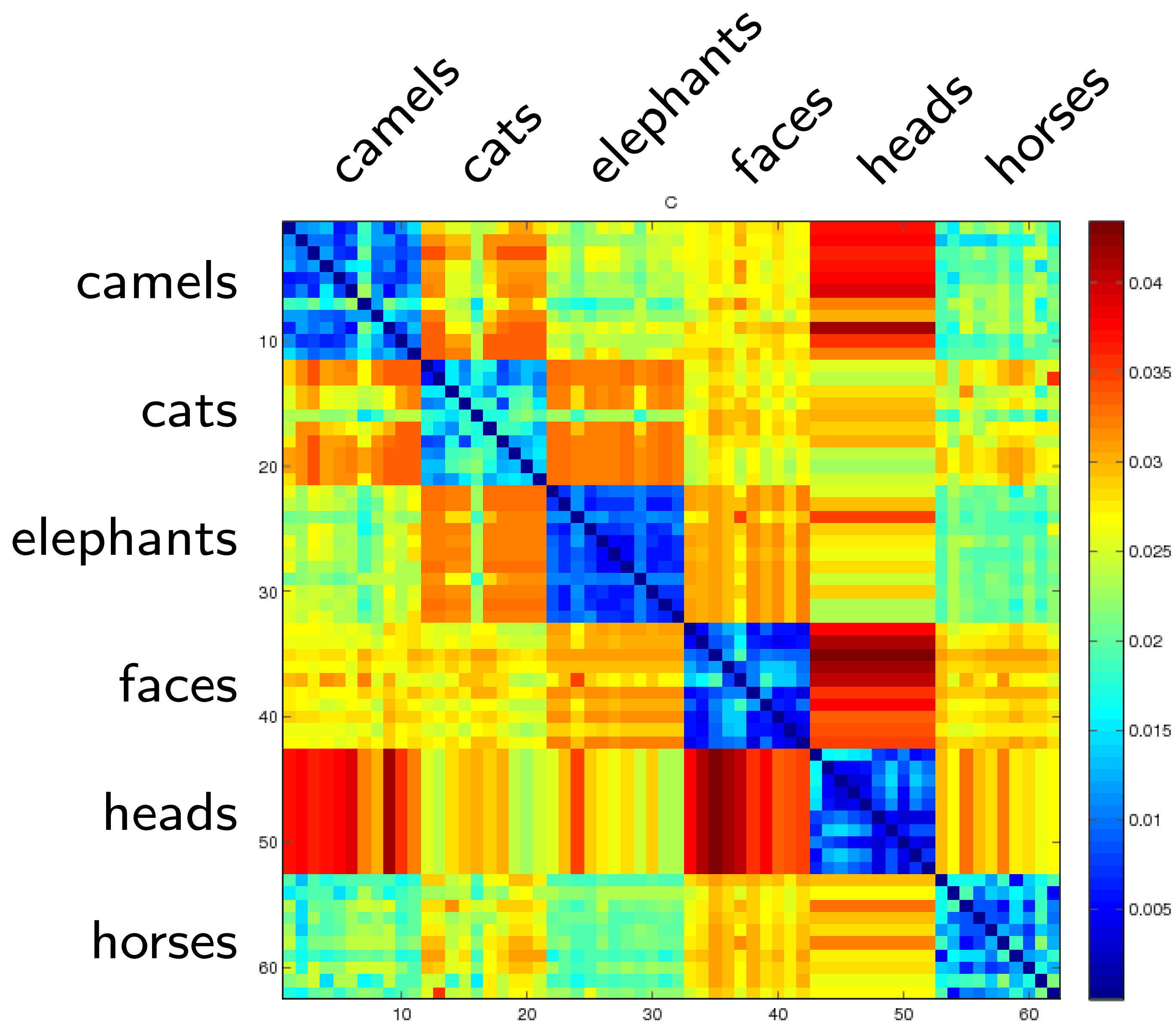

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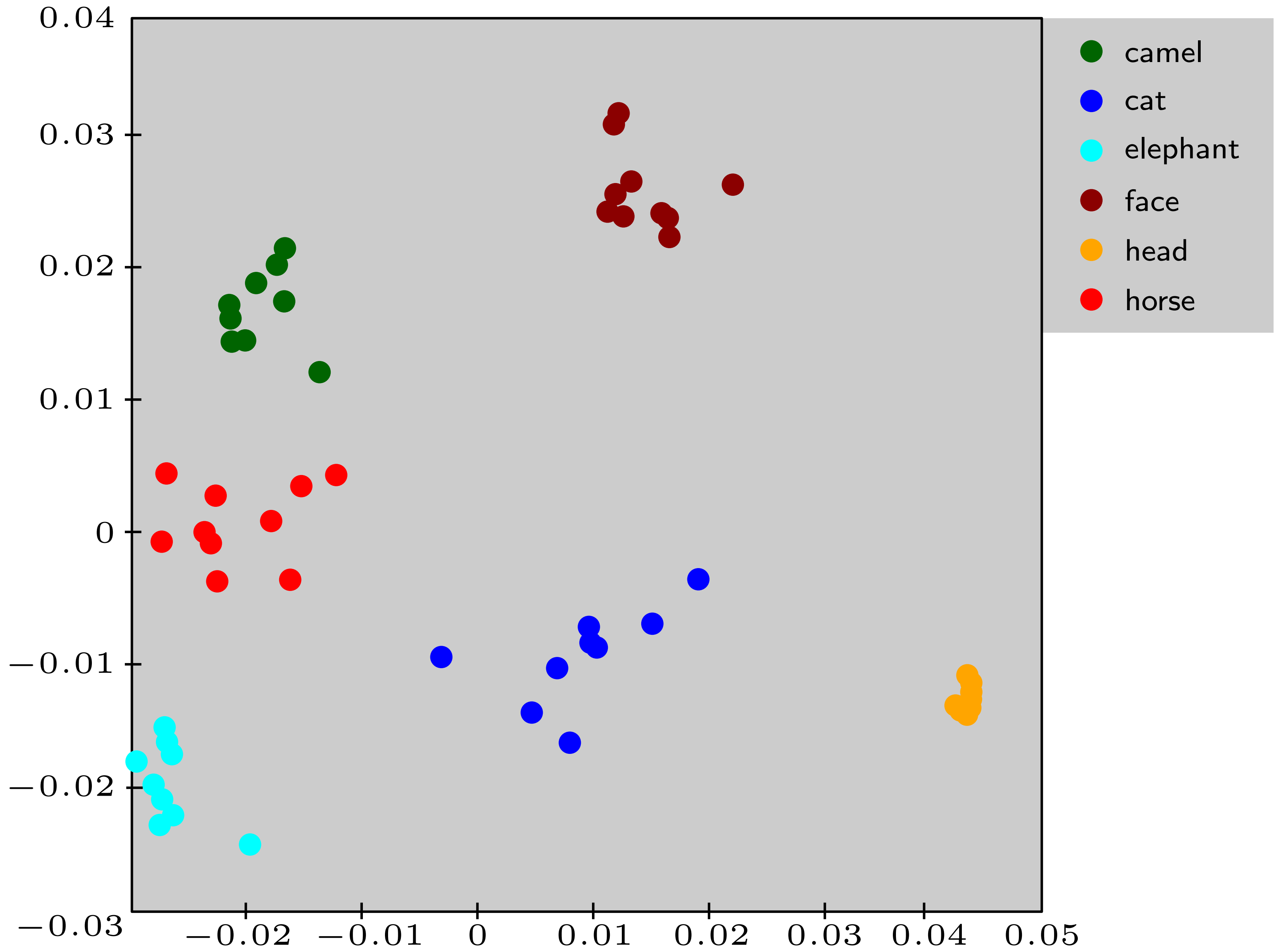
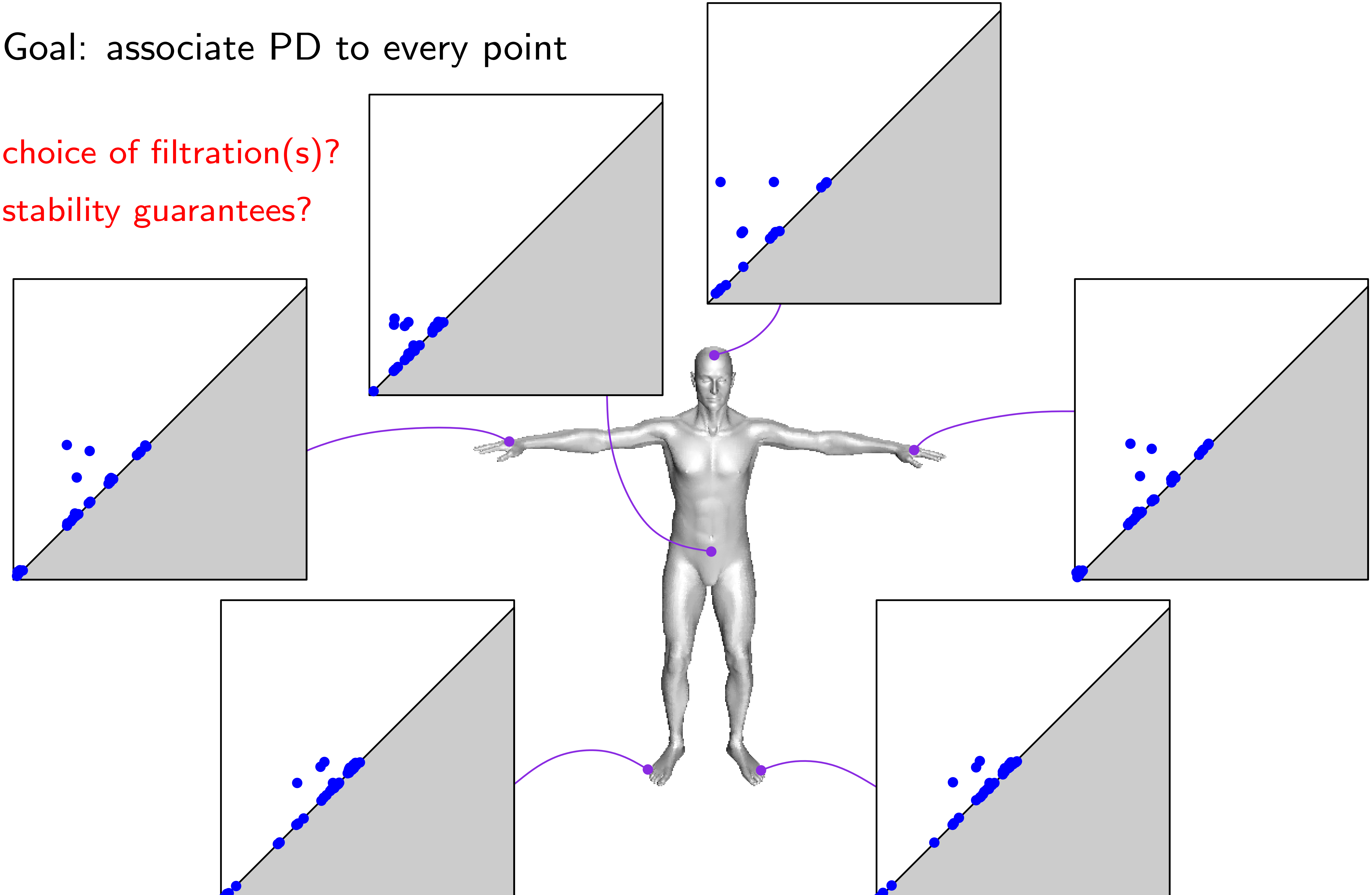


Local topological descriptors

Goal: associate PD to every point

choice of filtration(s)?

stability guarantees?



Local topological descriptors

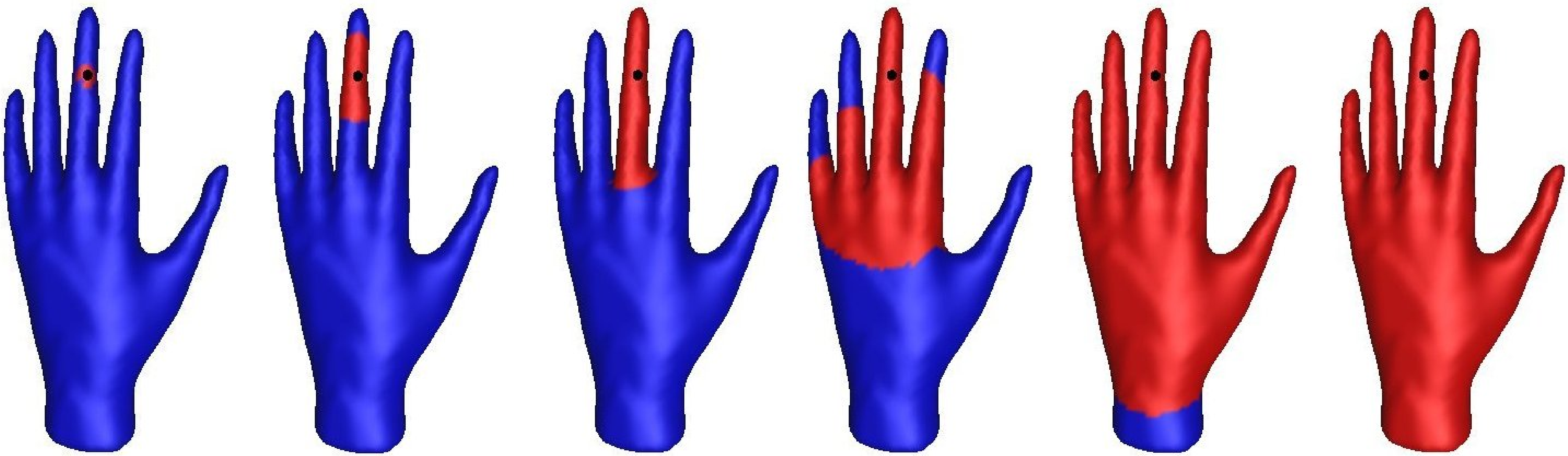
Input: a compact *intrinsic* metric space (X, d_X), a basepoint $x_0 \in X$

Construction: filtration of the sublevel sets of $\mathrm{d}_{x_0}(\cdot) = \mathrm{d}_X(x_0, \cdot)$

Descriptor: persistence diagram of the filtration, denoted $\mathrm{dgm}\,\mathrm{d}_{x_0}$

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

[Chazal et al. 2009]



Stability

Theorem: [Carrière, O., Ovsjanikov 2015]
Let (X, d_X) and (Y, d_Y) be compact intrinsic metric spaces with positive *convexity radius* ($\varrho(X), \varrho(Y) > 0$). Let $x_0 \in X$ and $y_0 \in Y$.
If $\mathrm{d}_{\mathrm{GH}}((X, x_0), (Y, y_0)) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then
$\mathrm{d}_{\mathrm{B}}^{\infty}(\mathrm{dgm}\, \mathrm{d}_{x_0}, \mathrm{dgm}\, \mathrm{d}_{y_0}) \leq 20\ \mathrm{d}_{\mathrm{GH}}((X, x_0), (Y, y_0))$.

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Definitions:

- convexity radius
- Gromov-Hausdorff distance between pointed spaces

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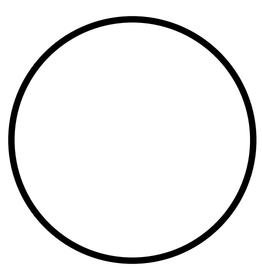
Prerequisite: $\mathrm{d}_{\mathrm{GH}}(X, Y) < \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$

$X =$ 

$$\mathrm{d}_{\mathrm{GH}}(X, Y) < \infty = \varrho(Y)$$

$Y =$ 

$$\mathrm{d}_{\mathrm{B}}^{\infty}(\mathrm{dgm}\, f, \mathrm{dgm}\, g) = \infty$$

Toy application (unsupervised shape segmentation)

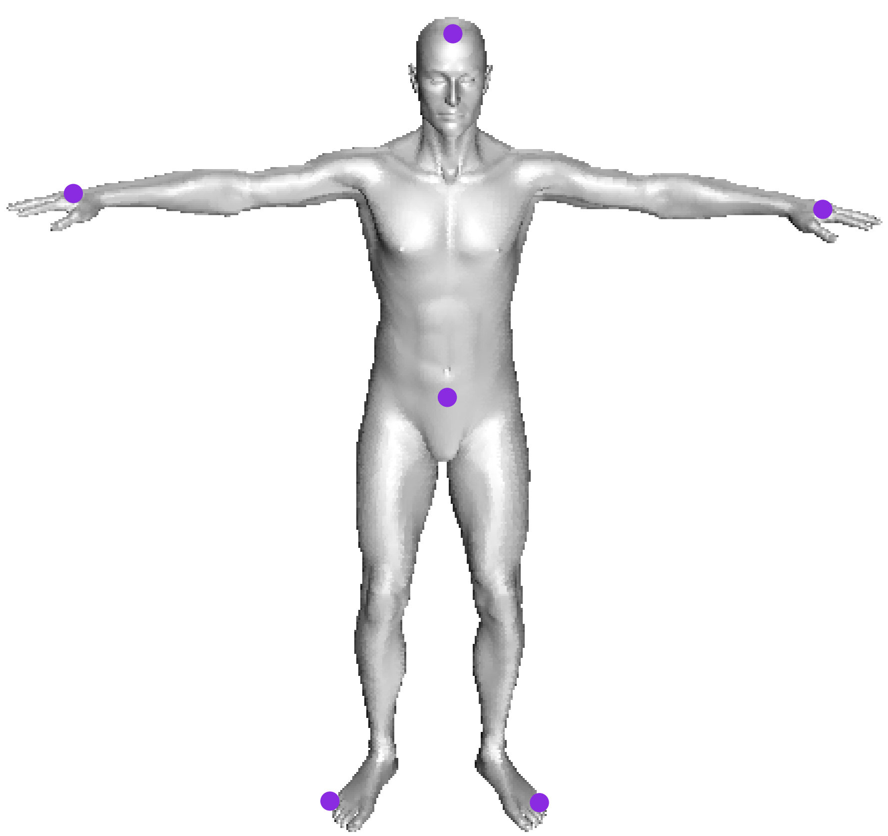
Experimental results:

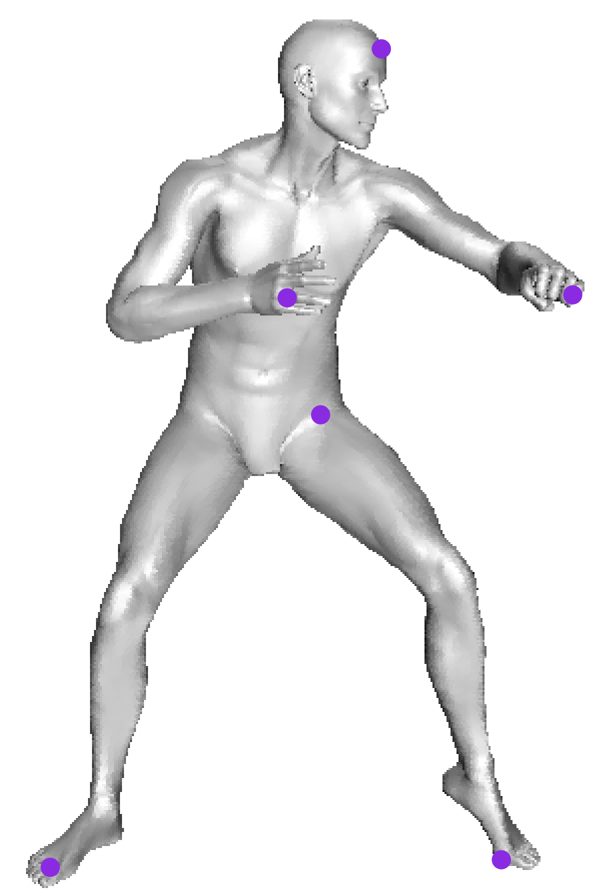
- input: shapes from the TOSCA database, in *mesh* form (triangulated)

- 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





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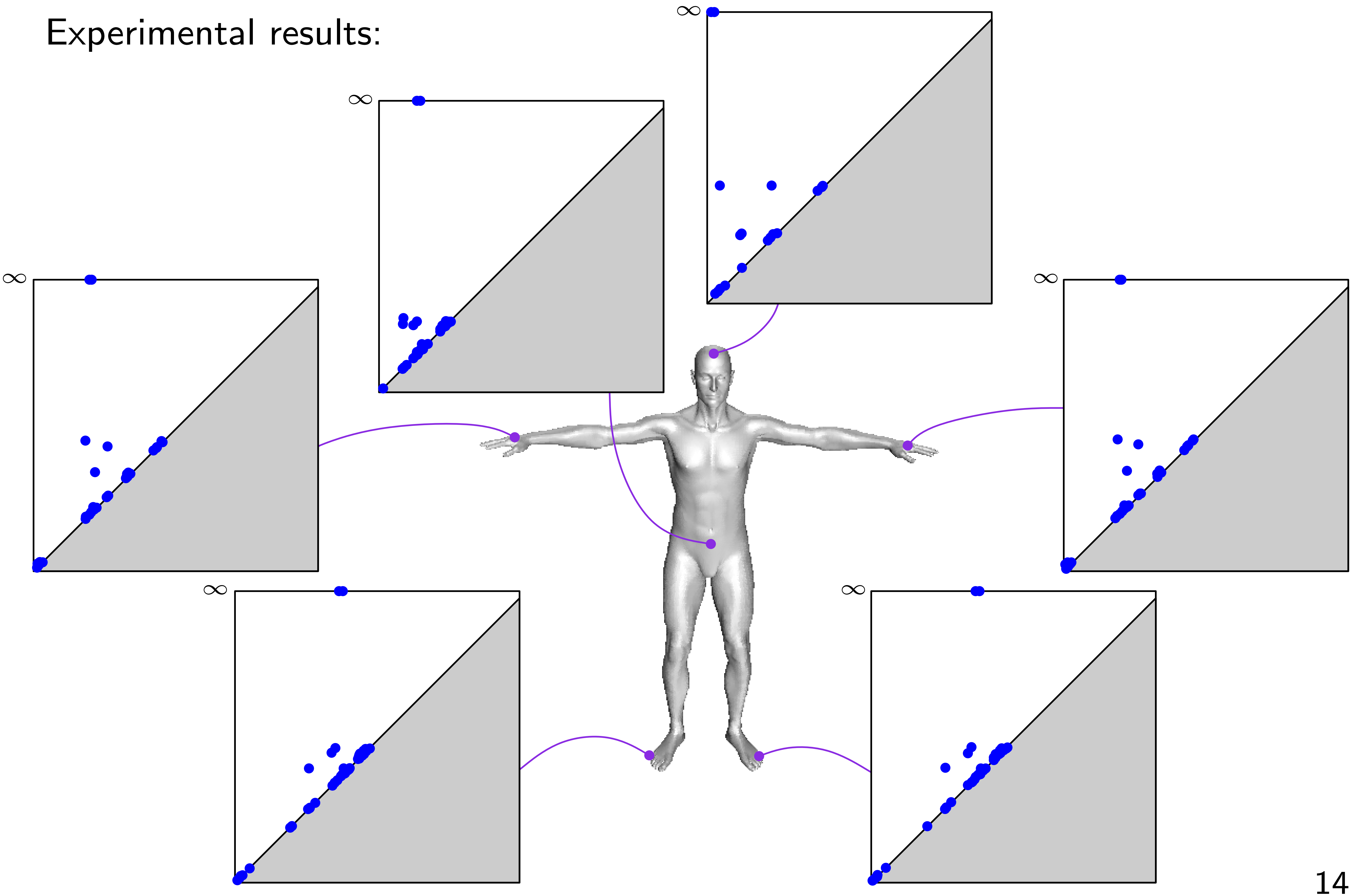

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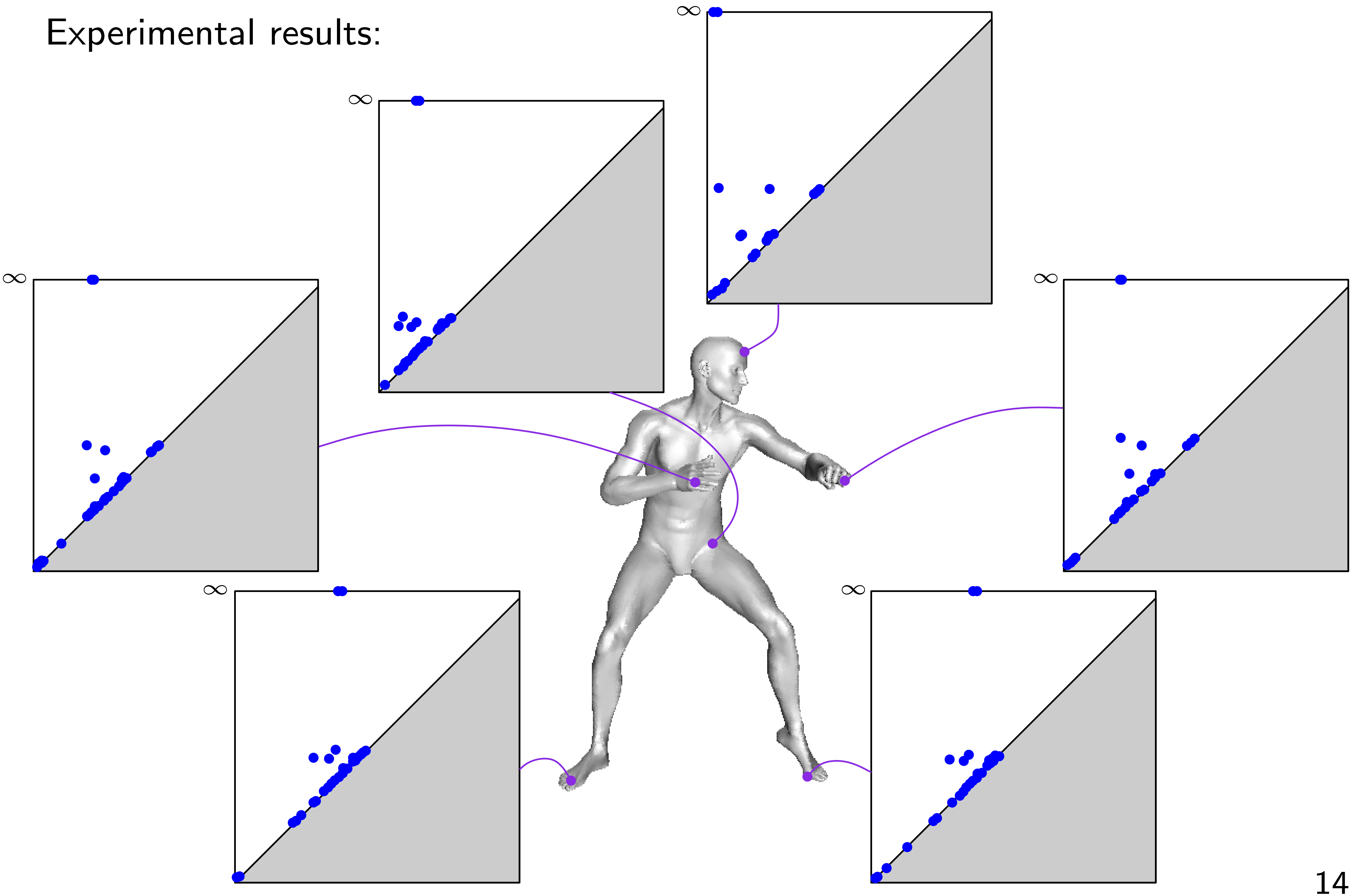

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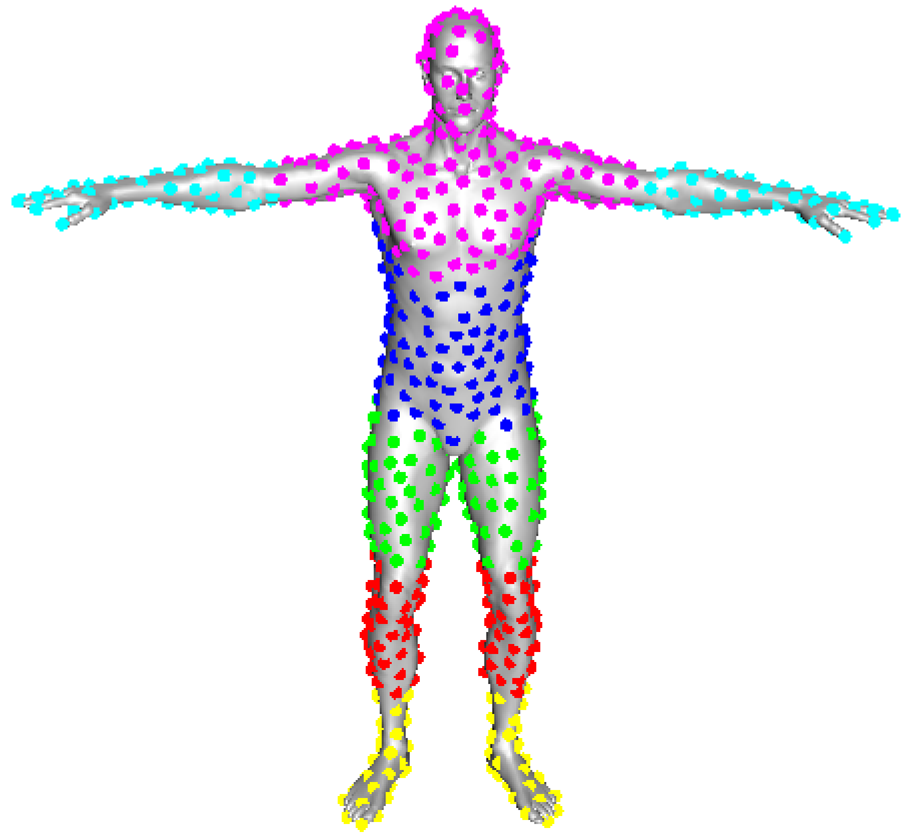
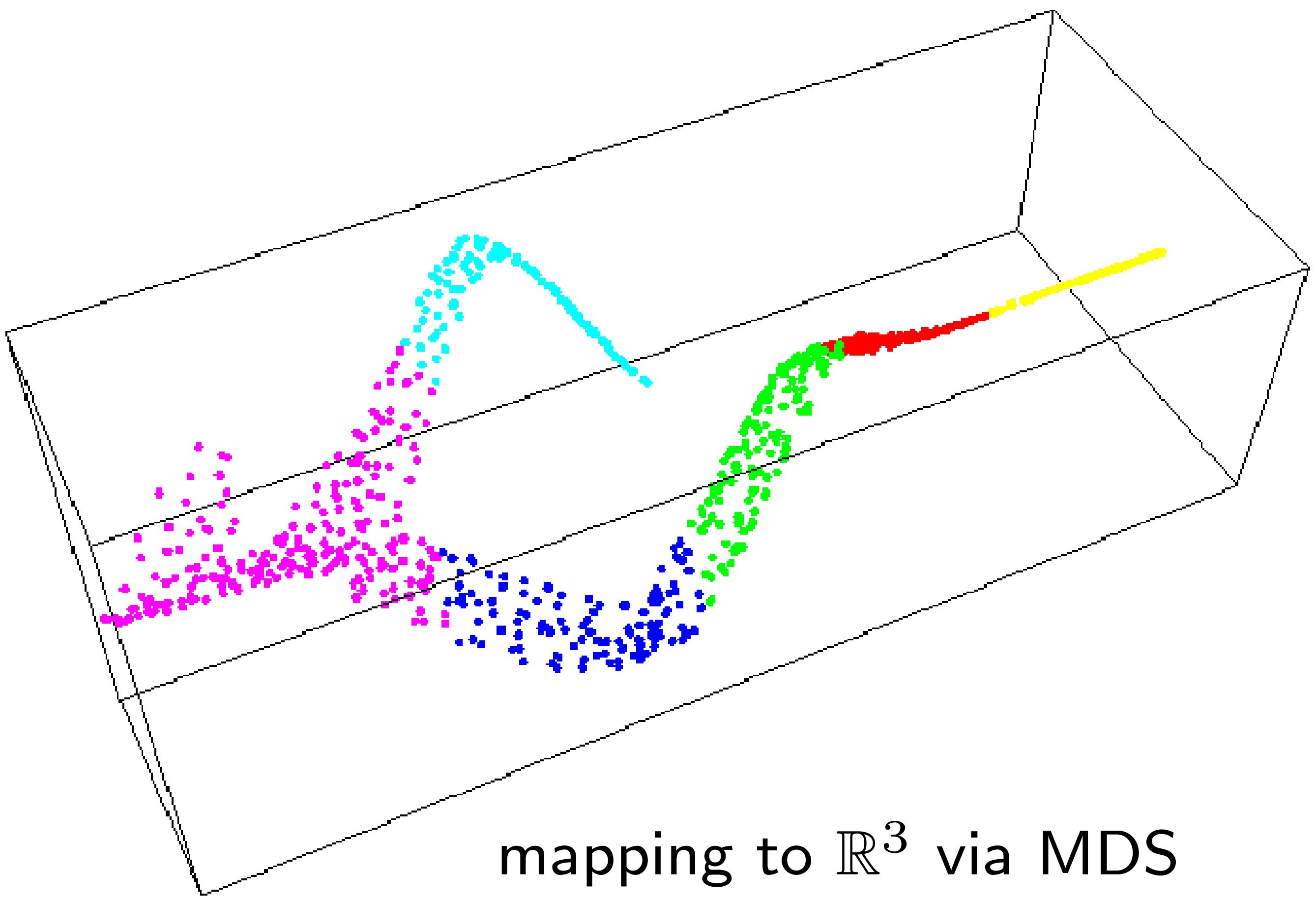
Experimental results:





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

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

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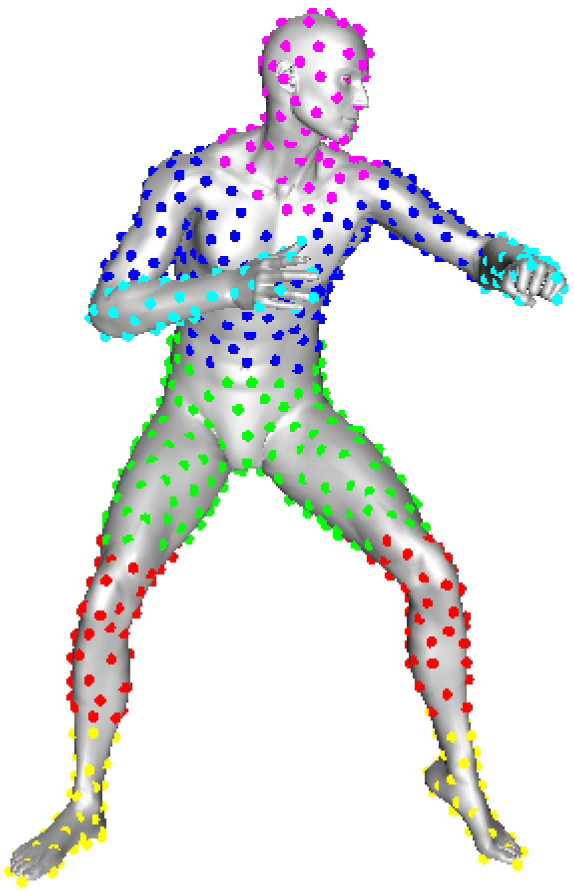

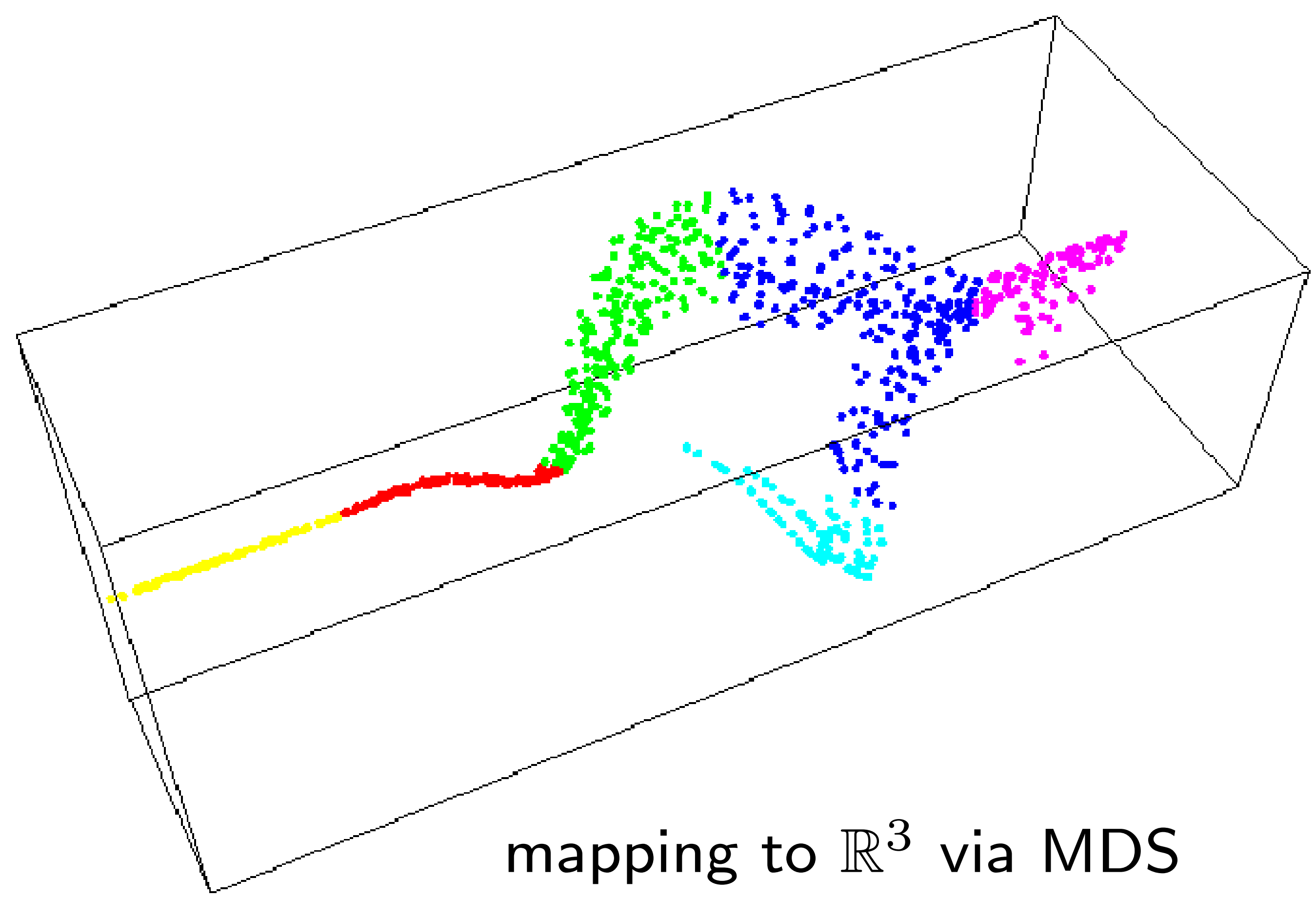

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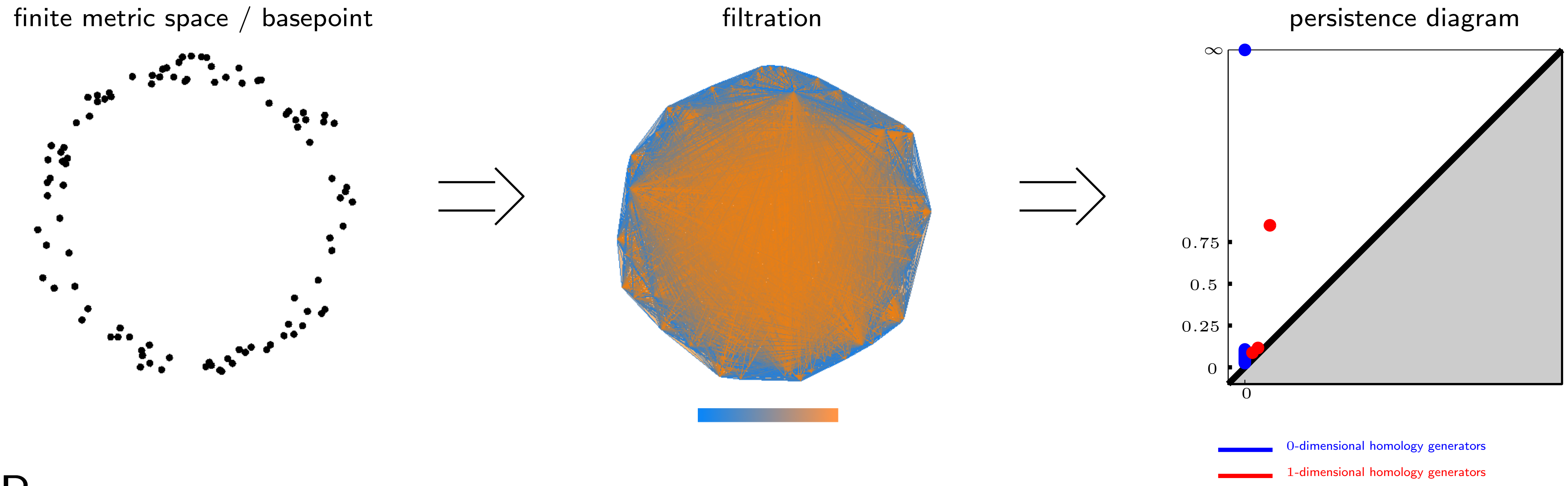
Recap'



Pros:

- topological descriptors carry information of a different nature

- they enjoy stability properties, e.g. $\mathrm{d}_{\mathrm{B}}^{\infty}(\mathcal{R}(X), \mathcal{R}(Y)) \leq 2\mathrm{d}_{\mathrm{GH}}(X, Y)$

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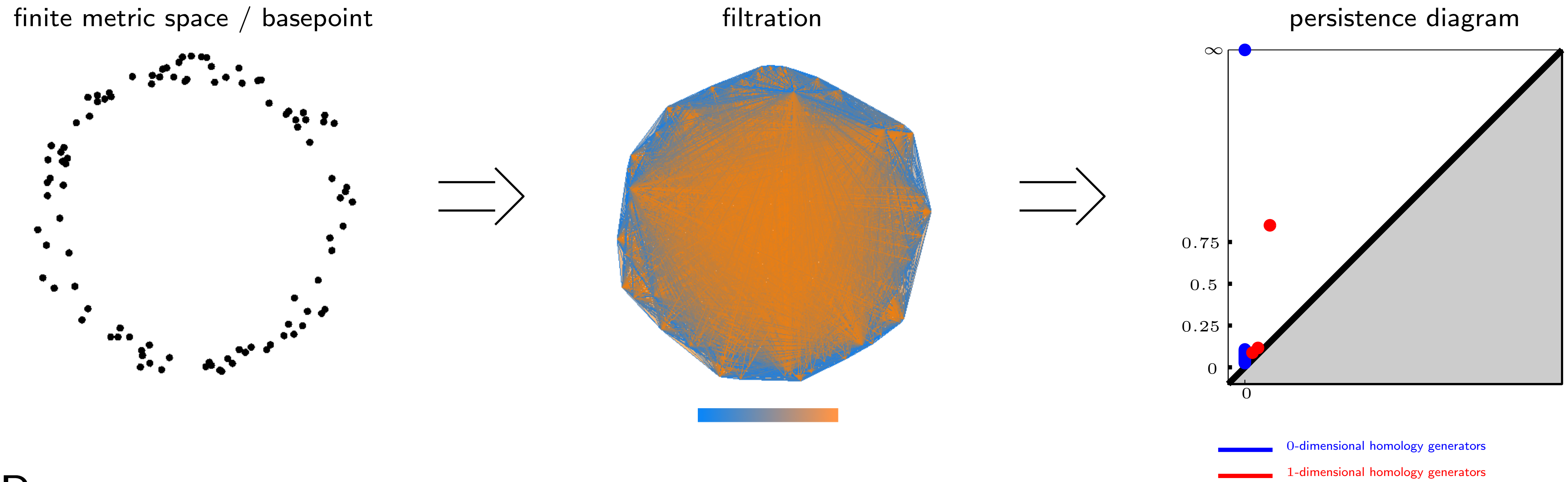

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Cons:

- the space of persistence diagrams is not a vector/Hilbert space
  $\rightarrow$ bad for supervised learning and statistics
- descriptors can be slow to compute and (more importantly) to compare
  $\rightarrow$ bad for applications

Addendum: proof of stability

finite

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

Proof outline: