Geometric Sciences in Action
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Centre International de Rencontres Mathématiques

Topological Data Analysis with the Gudhi library

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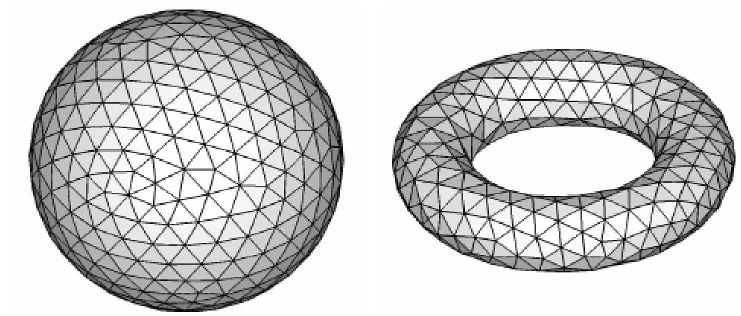
Inria informatics mathematics

What is Topological Data Analysis?

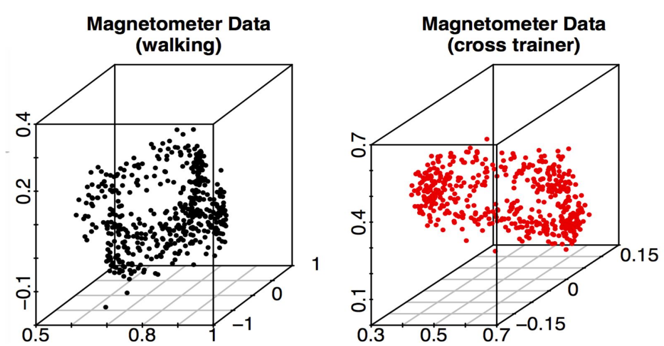
Topological Data Analysis is:

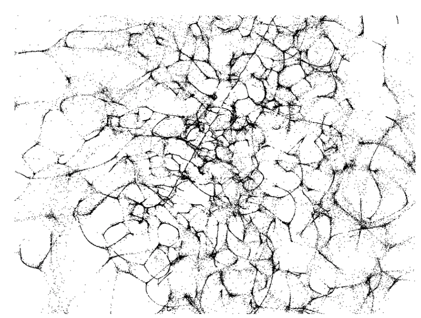
a mathematically grounded framework...

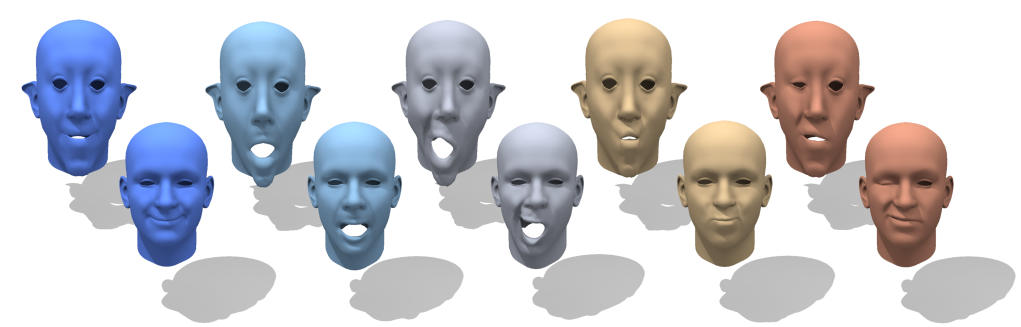
$$H_k = Z_k / B_k$$



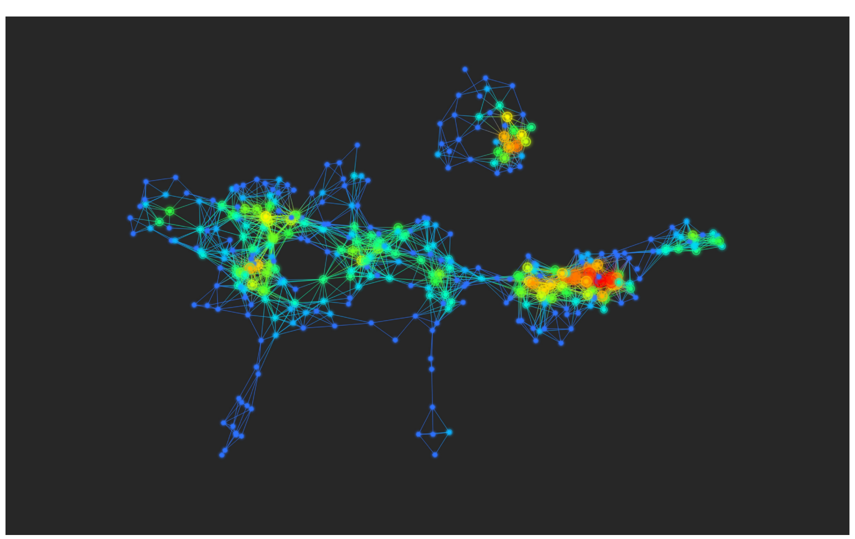
...that applies to a wide variety of data sets...



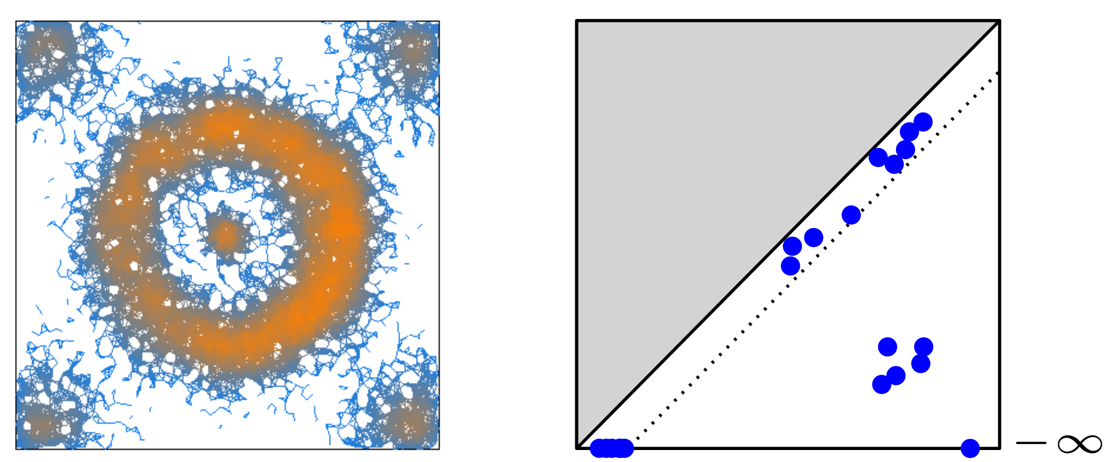




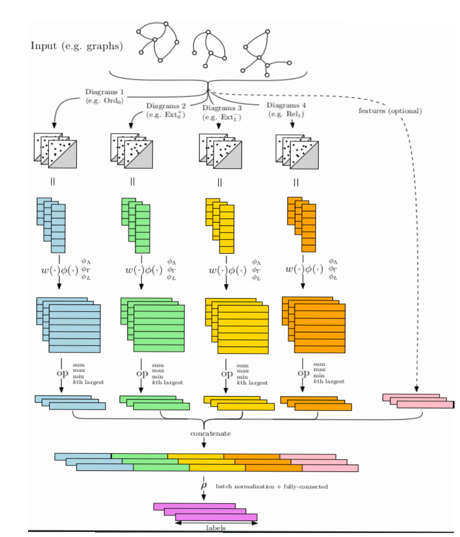
...for a wide variety of tasks.



Mapper: exploratory data analysis



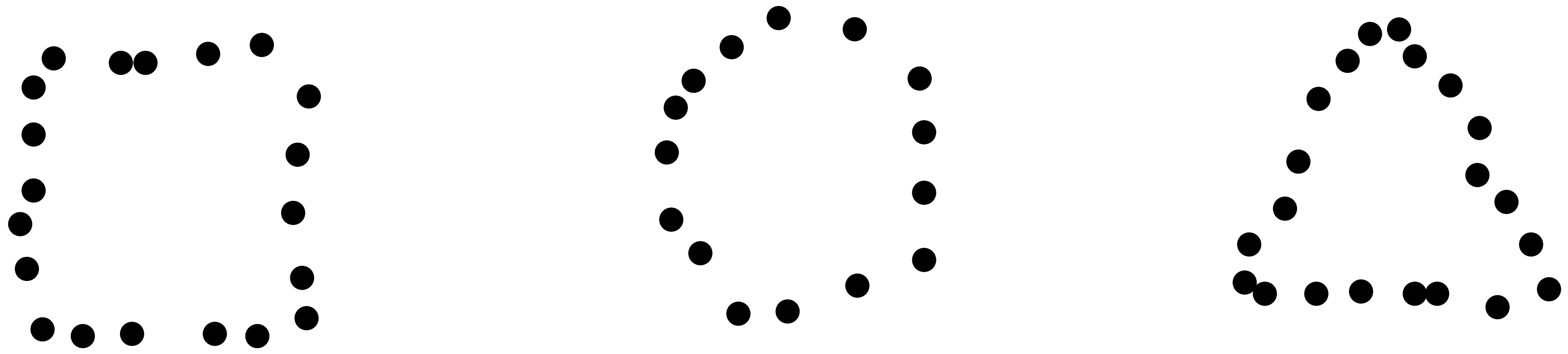
ToMATo: clustering



Persistence diagrams: machine learning

What is Topological Data Analysis?

Its main goal is to compute the topology of spaces (number and sizes of connected components, loops, cavities, etc) from samplings...



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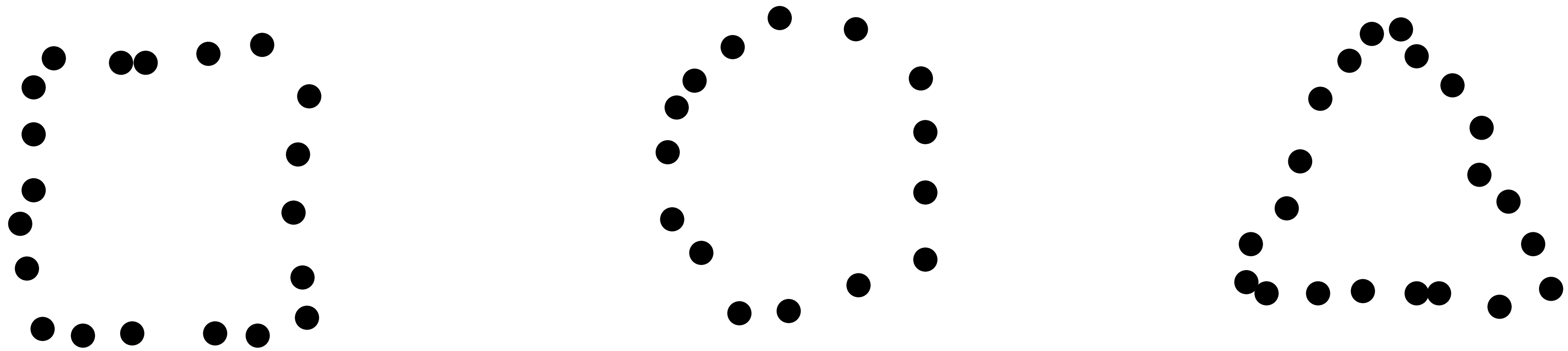

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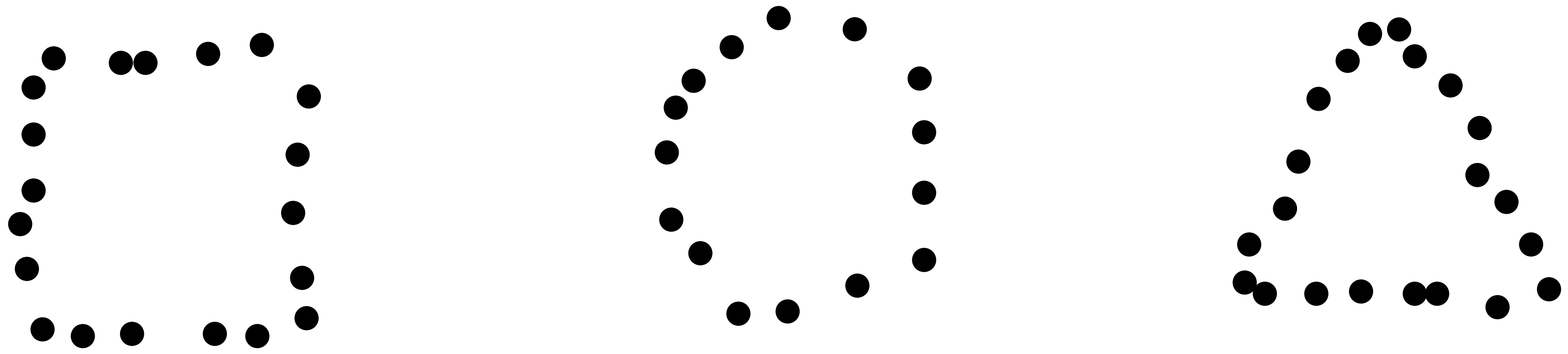
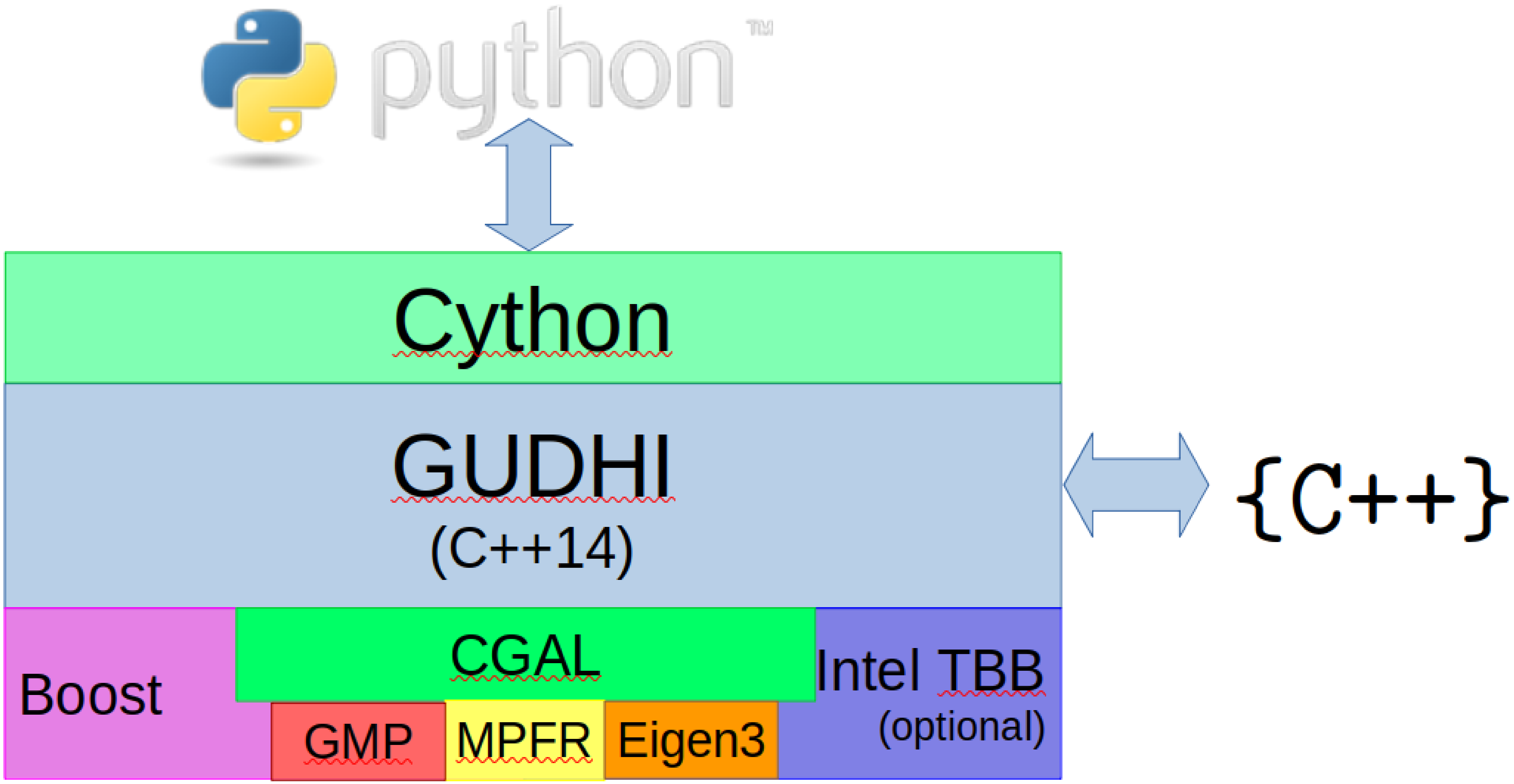


...and to summarize this info into descriptors suitable for data science

The Gudhi library



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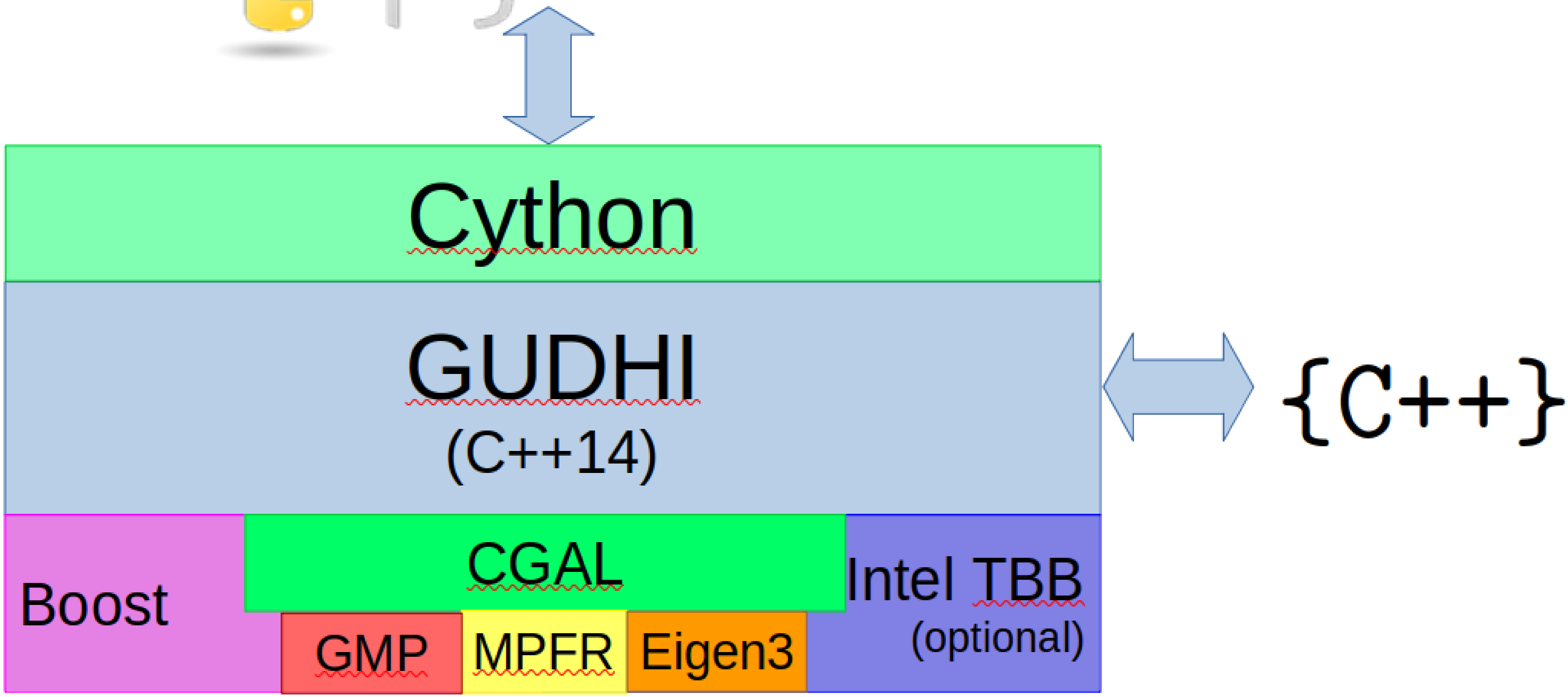
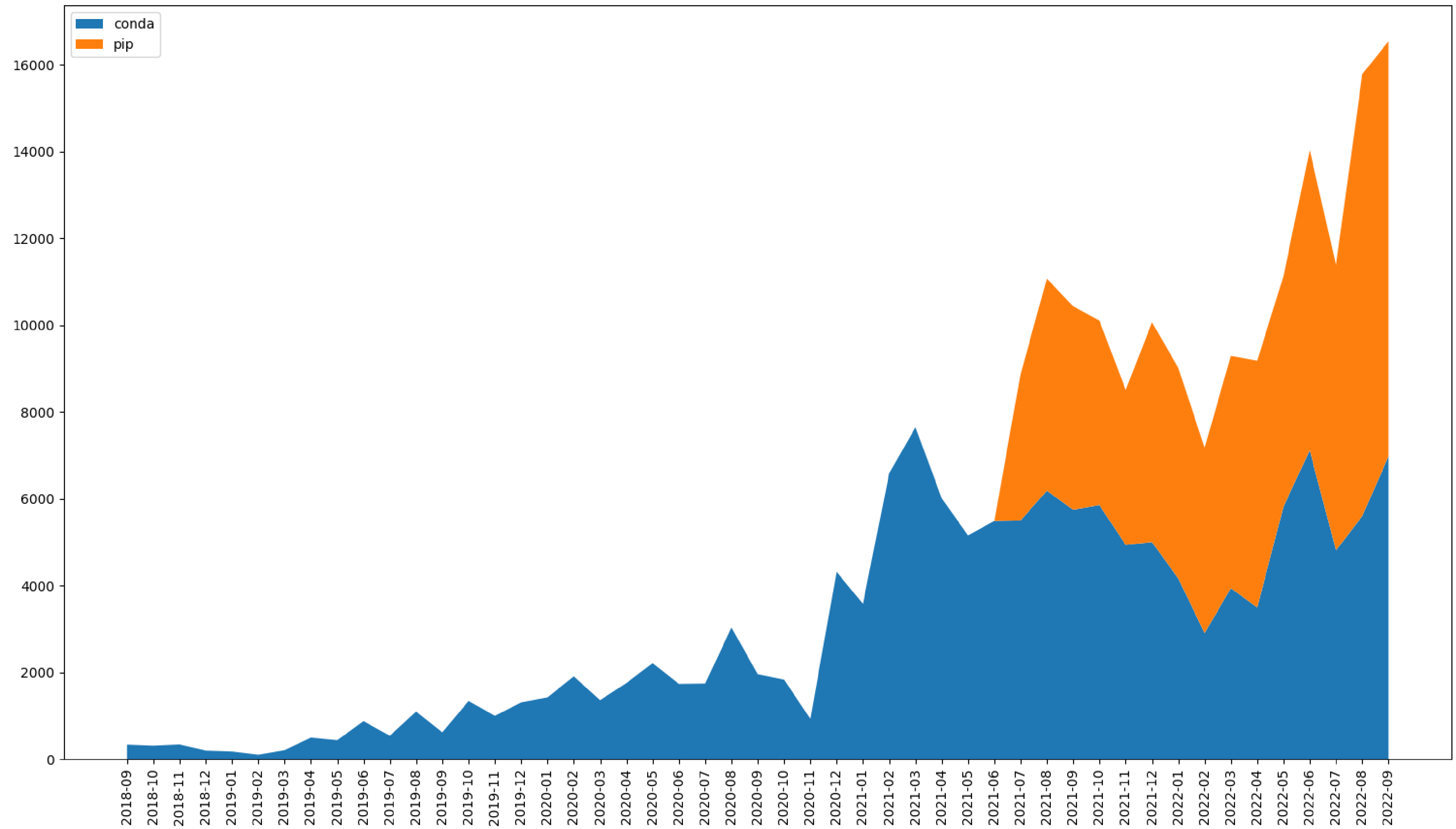


The Gudhi library

conda: ∼250 000 total downloads
pip: ∼34 000 downloads over the last 6 months



I. Turn datasets into simplicial complexes

II. Compute and compare persistence diagrams

III. Feed / regularize ML models w/ topology

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II. Compute and compare persistence diagrams

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Čech/Alpha complexes

Def: Given a point cloud $P = \{P_1, \ldots, P_n\} \subset \mathbb{R}^d$, its Čech complex of radius $r > 0$ is the abstract simplicial complex $C(P, r)$ s.t. $\mathrm{vert}(C(P, r)) = P$ and

$$\sigma = [P_{i_0}, P_{i_1}, \ldots, P_{i_k}] \in C(P, r) \quad \text{iif} \quad \cap_{j=0}^{k} B(P_{i_j}, r) \neq \emptyset.$$

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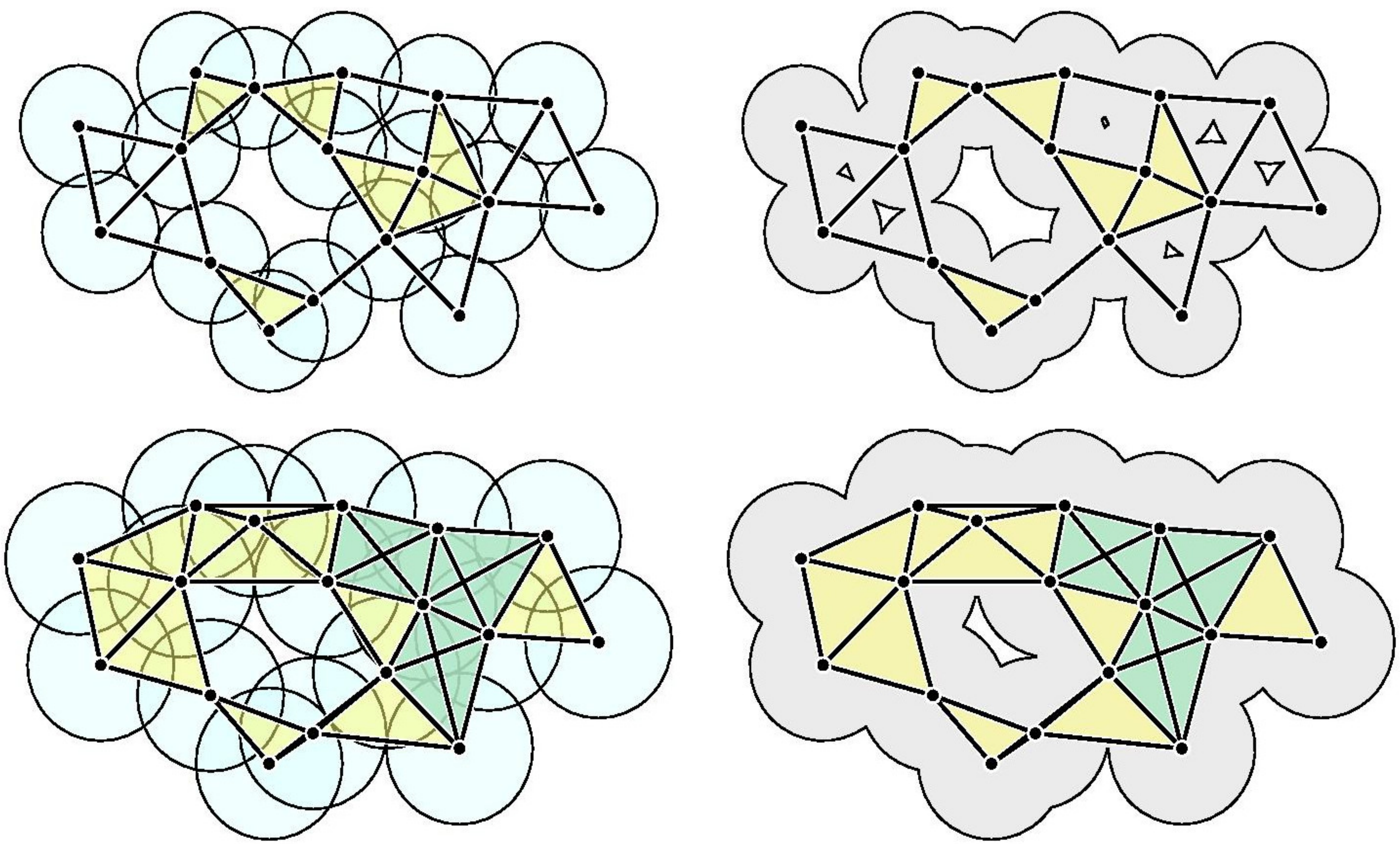

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In [ ]:
```
torus = gudhi.read_points_from_off_file(off_file='datasets/tore3D_1307.off')
ac = gudhi.AlphaComplex(points=torus)
st = ac.create_simplex_tree()
```

Čech/Alpha complexes

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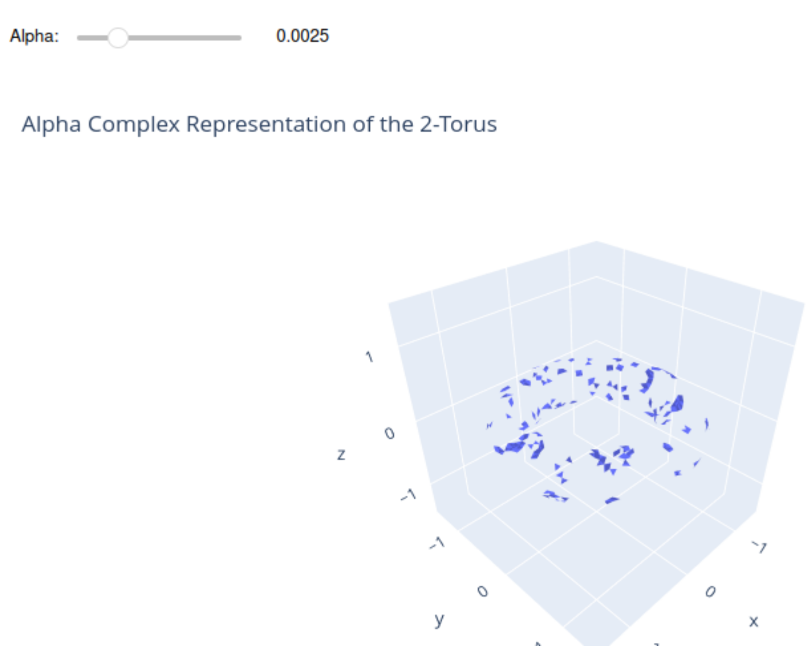
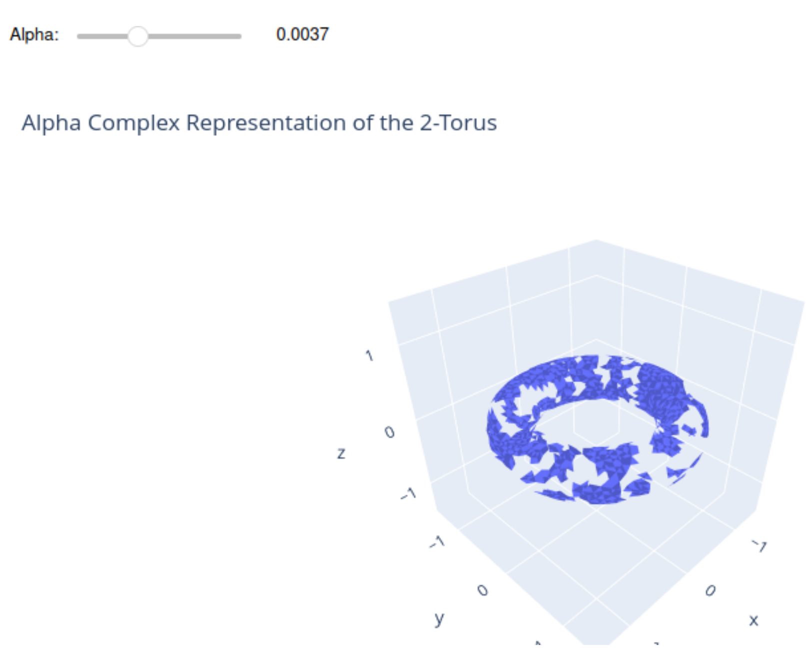
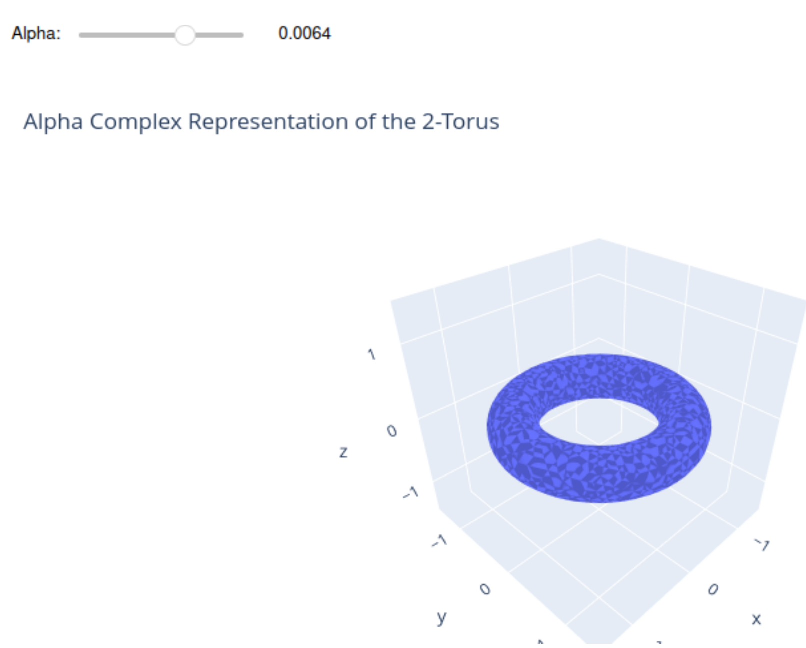
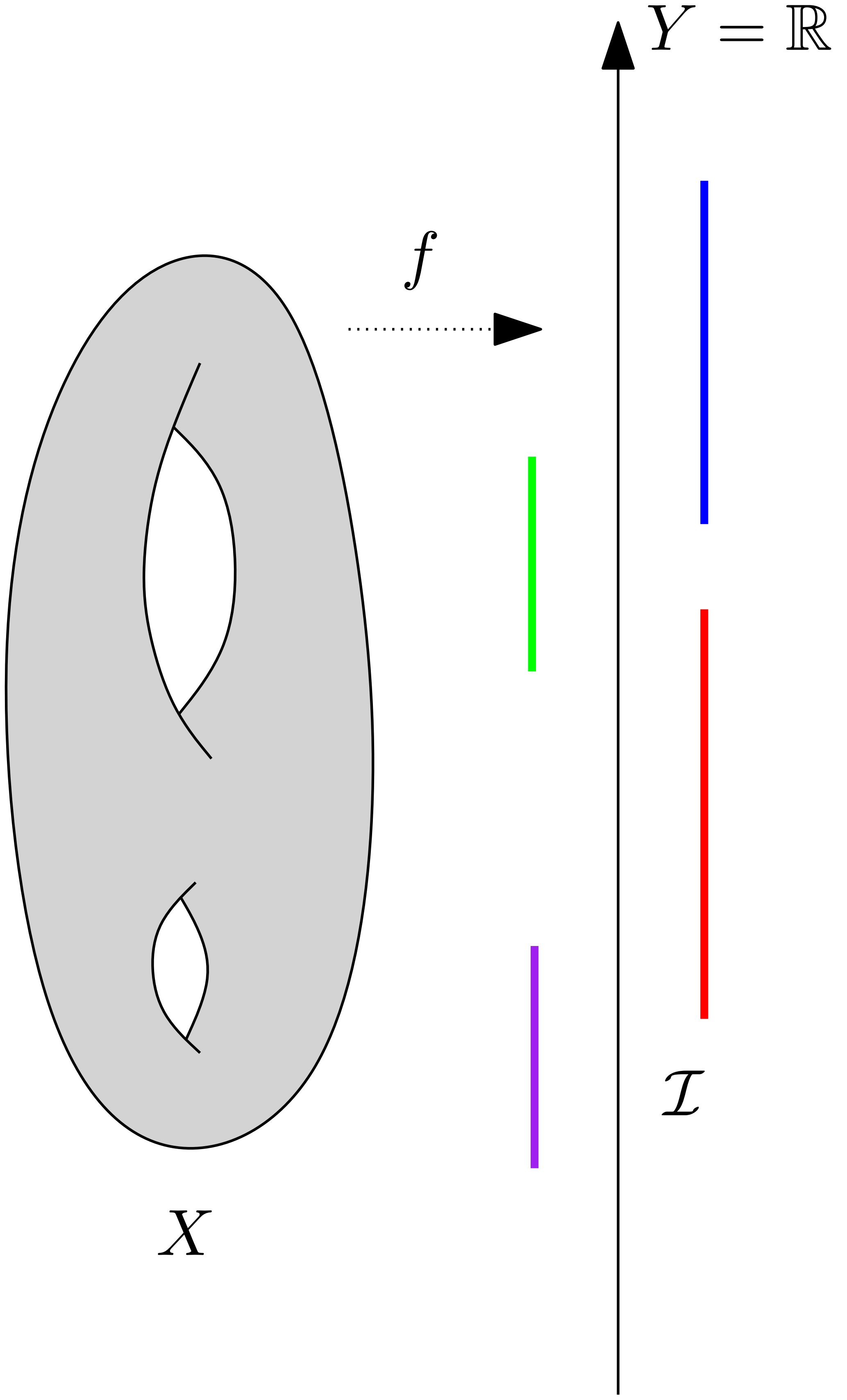






Mapper complexes



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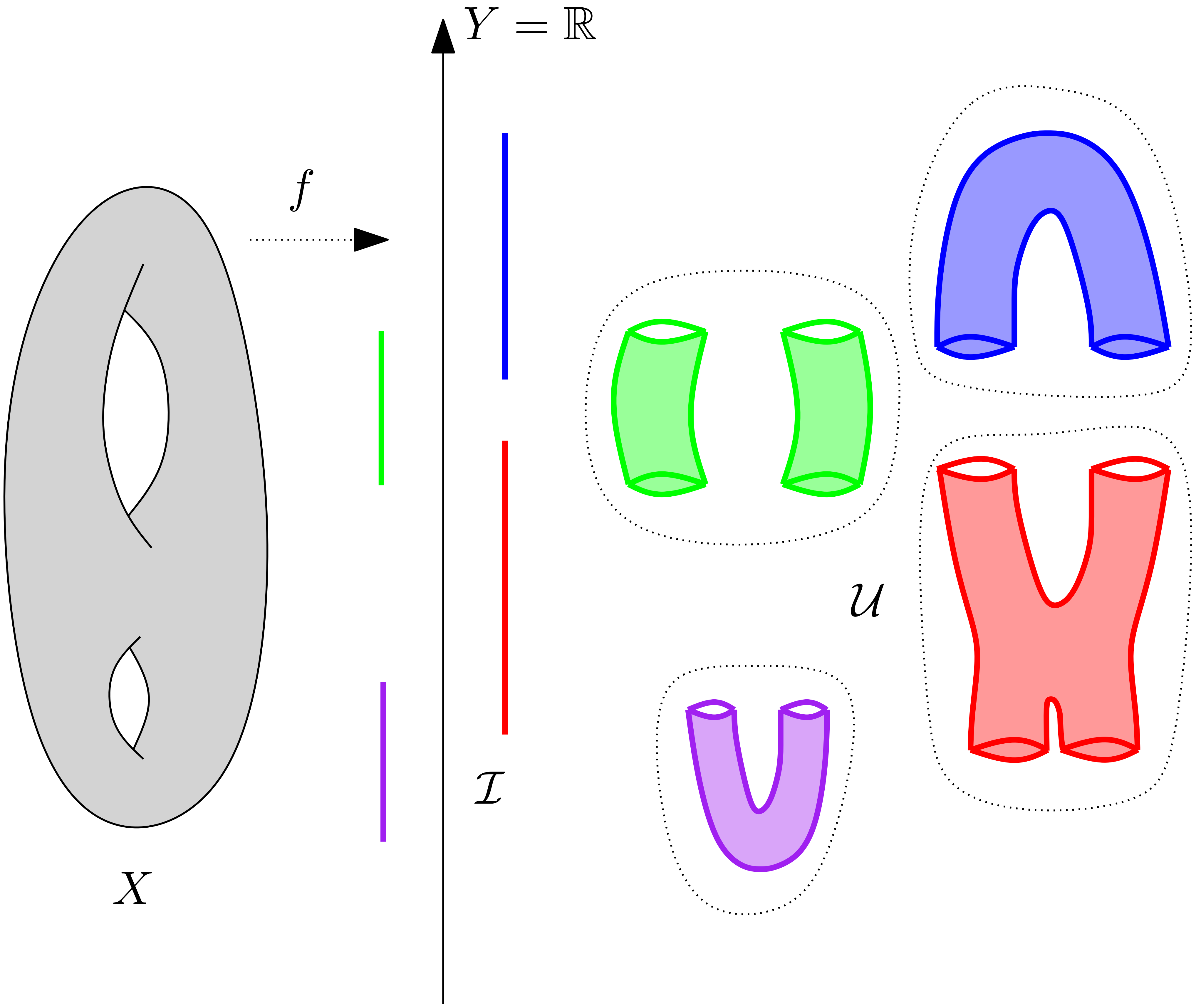

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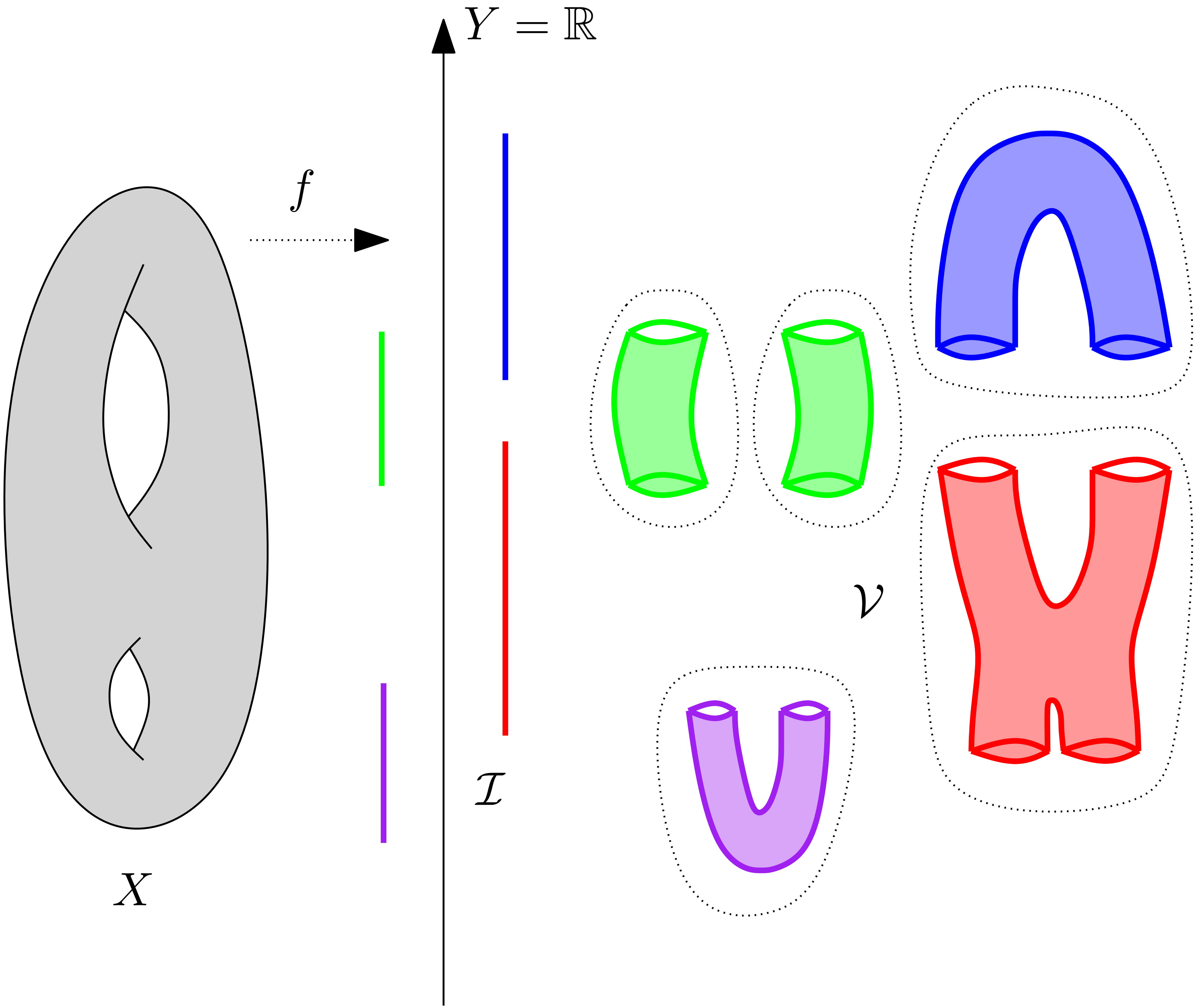

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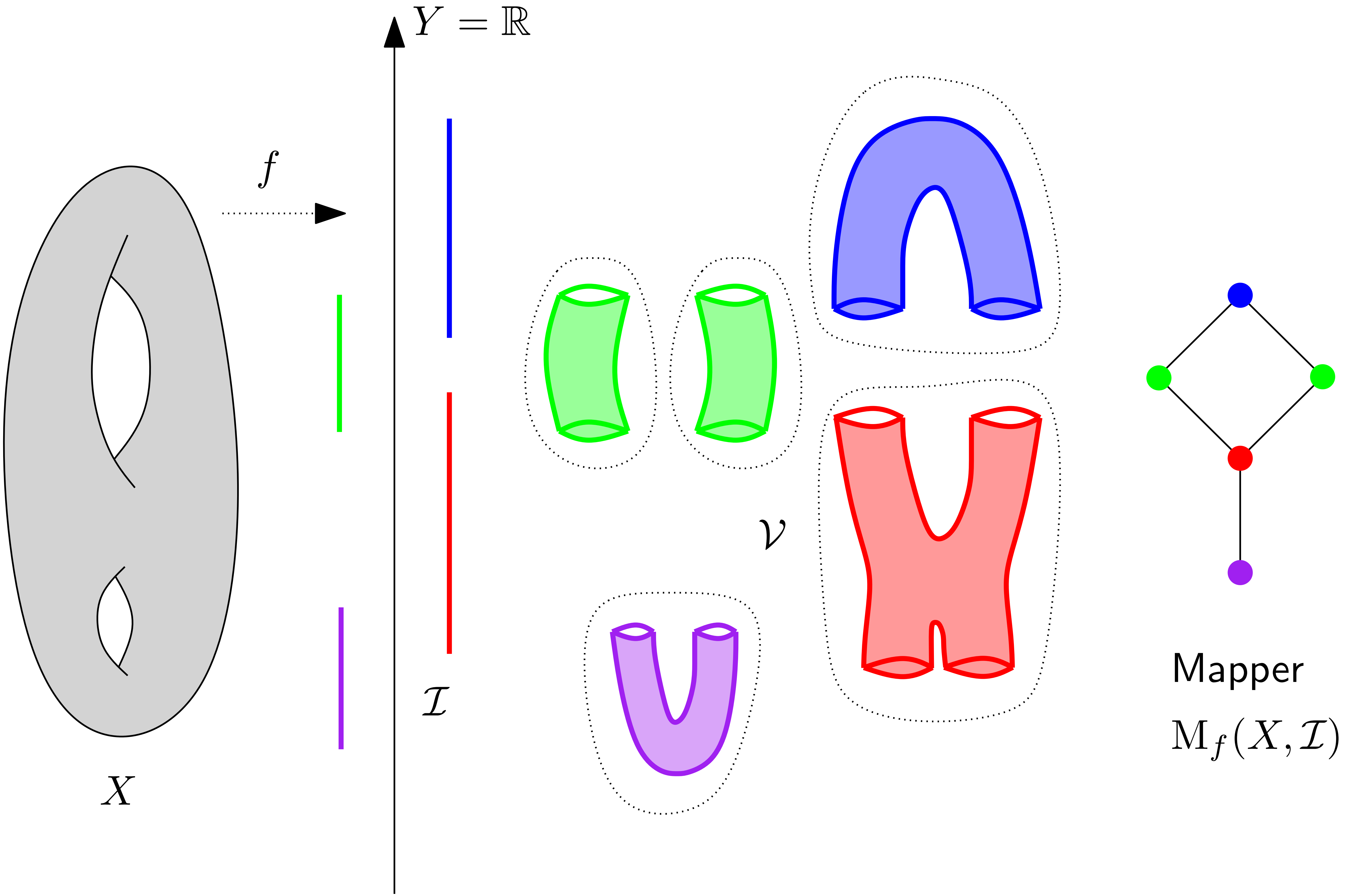

Mapper complexes

Input:

- topological space X
- continuous function $f : X \to Y$ (99% of the time $Y = \mathbb{R}^D$)
- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals: $\mathrm{im}(f) \subseteq \bigcup_{I \in \mathcal{I}} I$

Method:

- Compute *pullback cover* $\mathcal{U}$ of X: $\mathcal{U} = \{f^{-1}(I)\}_{I \in \mathcal{I}}$
- Refine $\mathcal{U}$ by separating each of its elements into its various connected components in X $\to$ connected cover $\mathcal{V}$
- The Mapper is the *nerve* of $\mathcal{V}$:
  - 1 vertex per element $V \in \mathcal{V}$
  - 1 edge per intersection $V \cap V' \neq \emptyset$, $V, V' \in \mathcal{V}$
  - 1 k-simplex per $(k+1)$-fold intersection $\bigcap_{i=0}^{k} V_i \neq \emptyset$, $V_0, \cdots, V_k \in \mathcal{V}$

Mapper complexes

Input:

- point cloud $P \subseteq X$ with metric d_P
- continuous function $f : P \to \mathbb{R}$
- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals: $\mathrm{im} f \subseteq \bigcup_{I \in \mathcal{I}} I$

Method:

- Compute *pullback cover* $\mathcal{U}$ of P: $\mathcal{U} = \{f^{-1}(I)\}_{I \in \mathcal{I}}$
- Refine $\mathcal{U}$ by separating each of its elements into its various clusters, as identified by a clustering algorithm $\to$ connected cover $\mathcal{V}$
- The Mapper is the *nerve* of $\mathcal{V}$:
  - 1 vertex per element $V \in \mathcal{V}$
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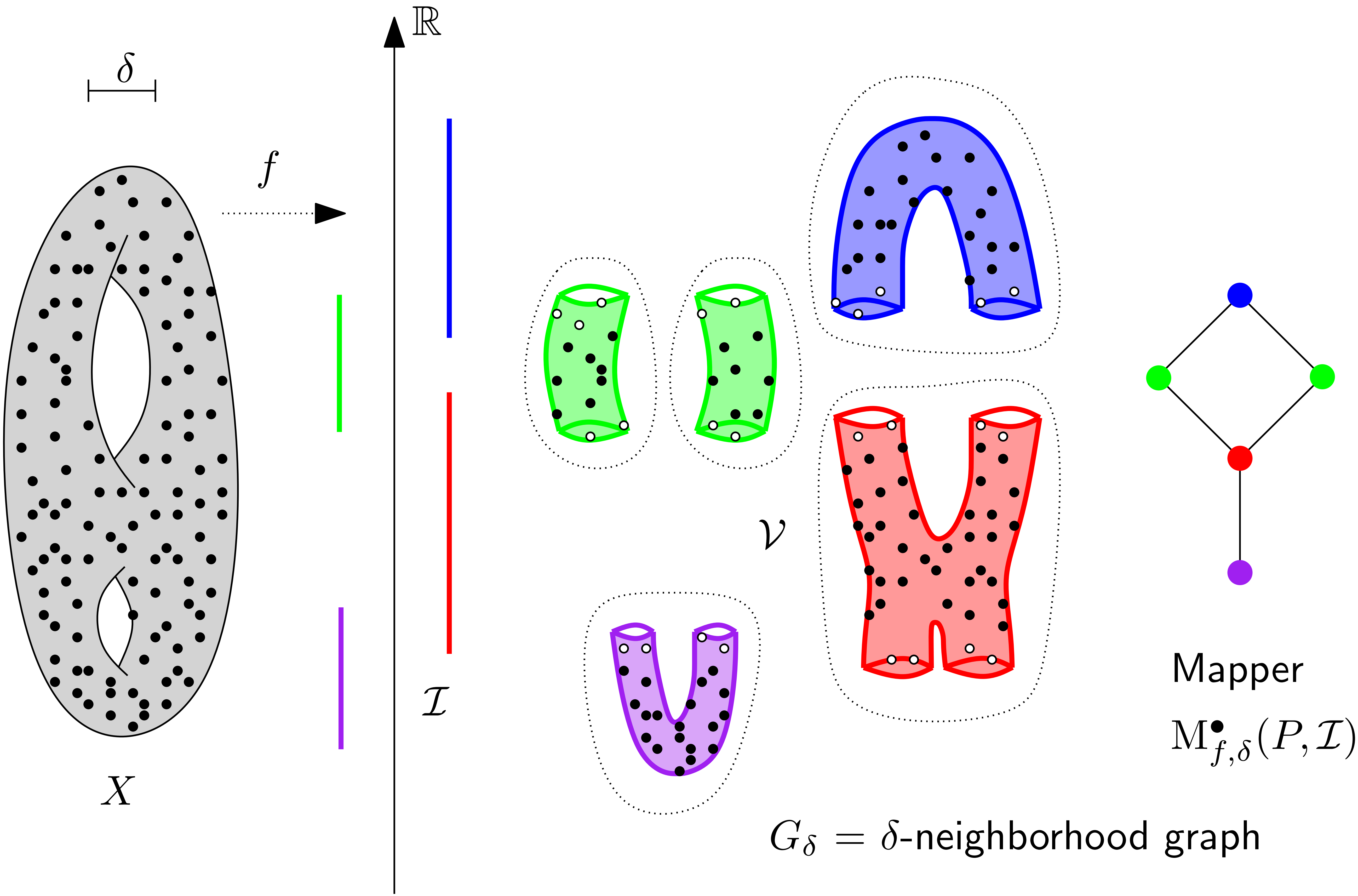
intersections are assessed by the presence of common data points

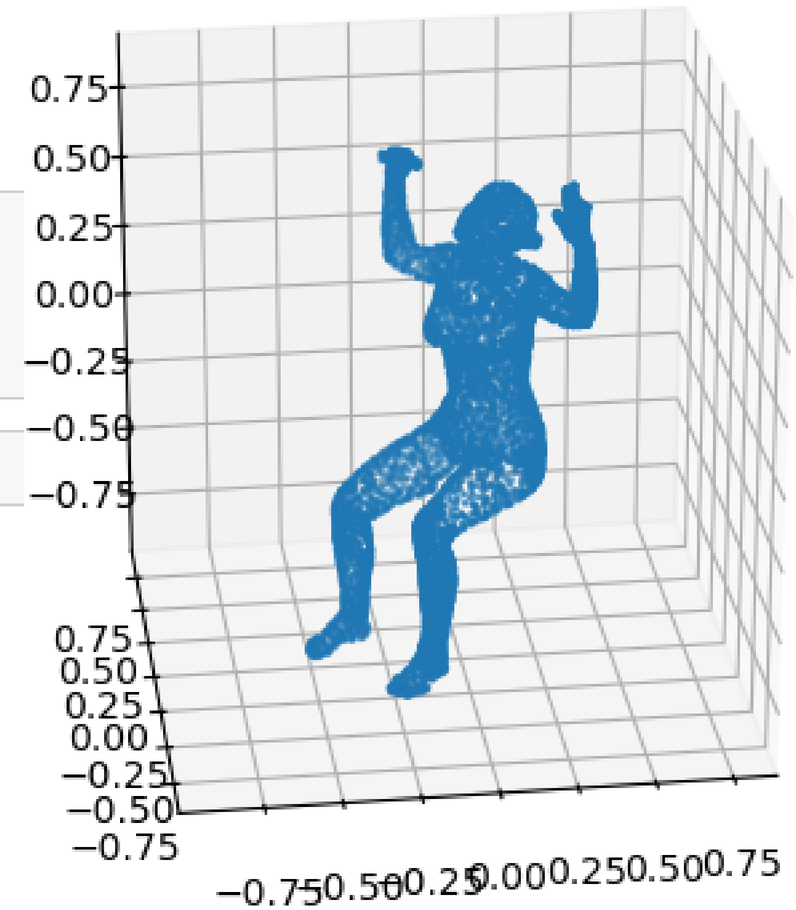
Mapper complexes



Mapper complexes

In [22]:
```
cover_complex = MapperComplex(
    input_type='point cloud', min_points_per_node=0,
    clustering=None, N=100, beta=0., C=10,
    filter_bnds=None, resolutions=[20,2], gains=None, verbose=verbose)
```

In [23]:
```
_ = cover_complex.fit(X, filters=filt2d, colors=filt2d)
```



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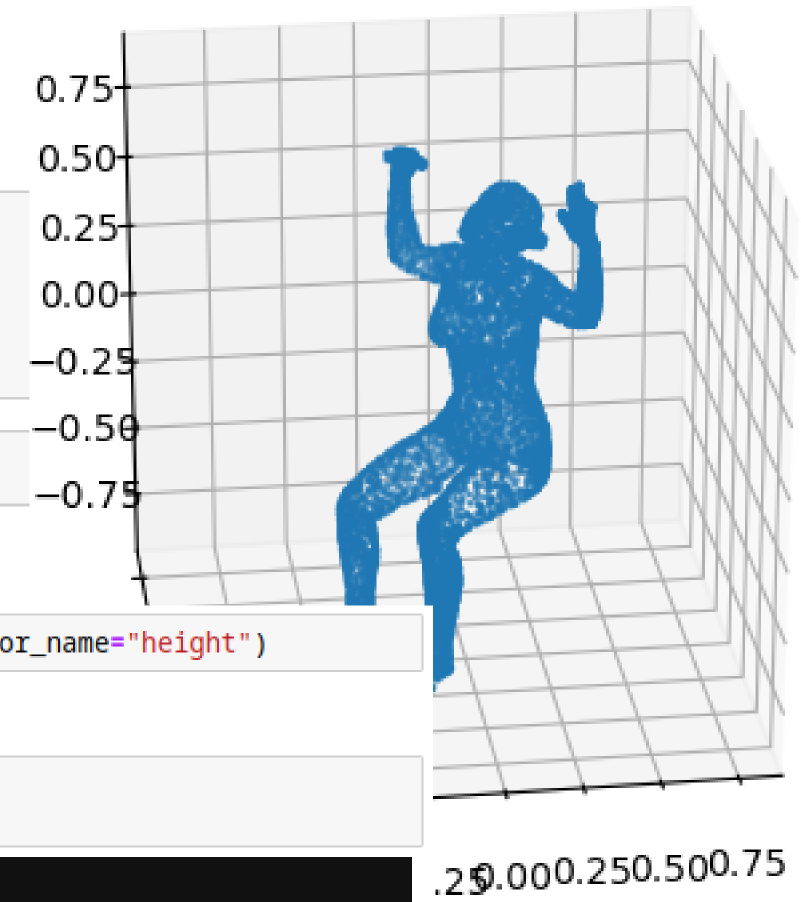

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```

In [23]:
```
_ = cover_complex.fit(X, filters=filt2d, colors=filt2d)
```

In [24]:
```
cover_complex.save_to_html(file_name="human", data_name="human", cover_name="uniform", color_name="height")
```

'human.html' is generated. You can now use your favorite web browser to visualize it.

In [25]:
```
from IPython.display import IFrame
IFrame(src="human.html", width='100%', height='500px')
```

Out[25]:

I. Turn datasets into simplicial complexes

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Computation with filtrations and matrix reduction

Algorithms for computing the homology groups of a simplicial complex work by *decomposing* it with a so-called *filtration*.

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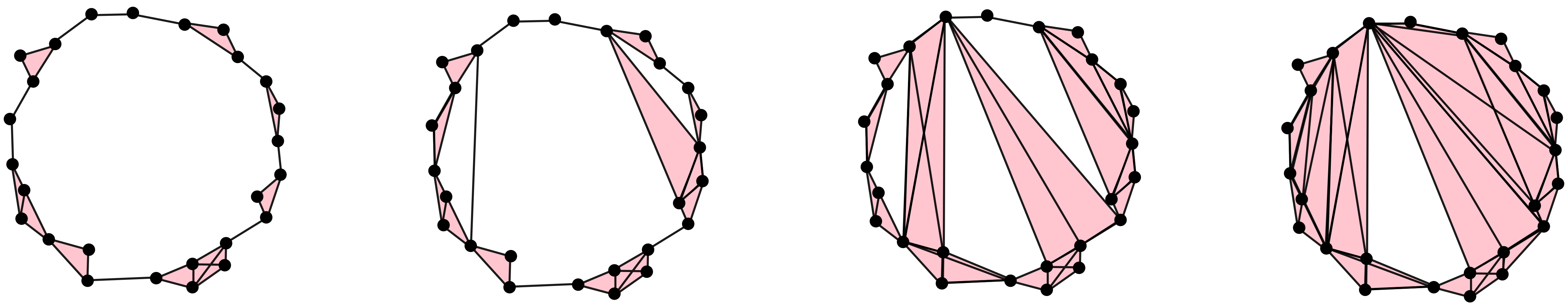

Def: A filtered simplicial complex S is a family $\{S_u\}_{u \in \mathbb{R}}$ of subcomplexes of some fixed simplicial complex S s.t. $S_a \subseteq S_b$ for any $a \leq b$.

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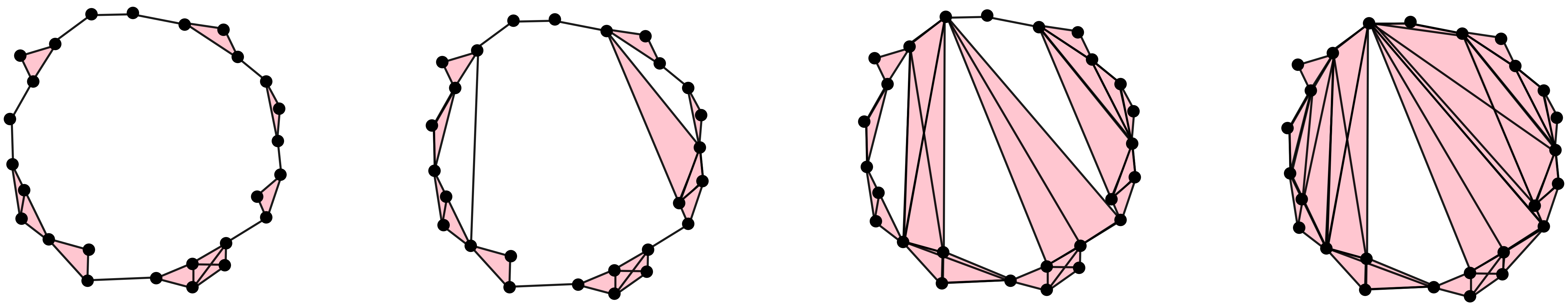

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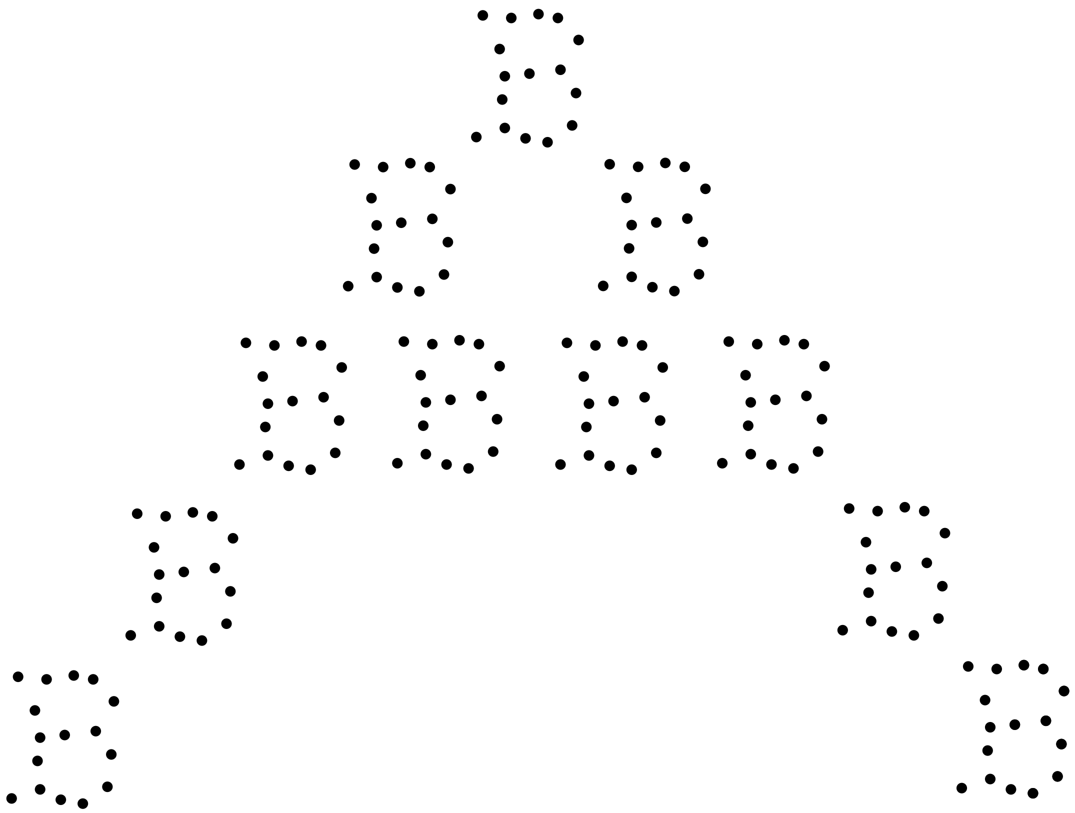
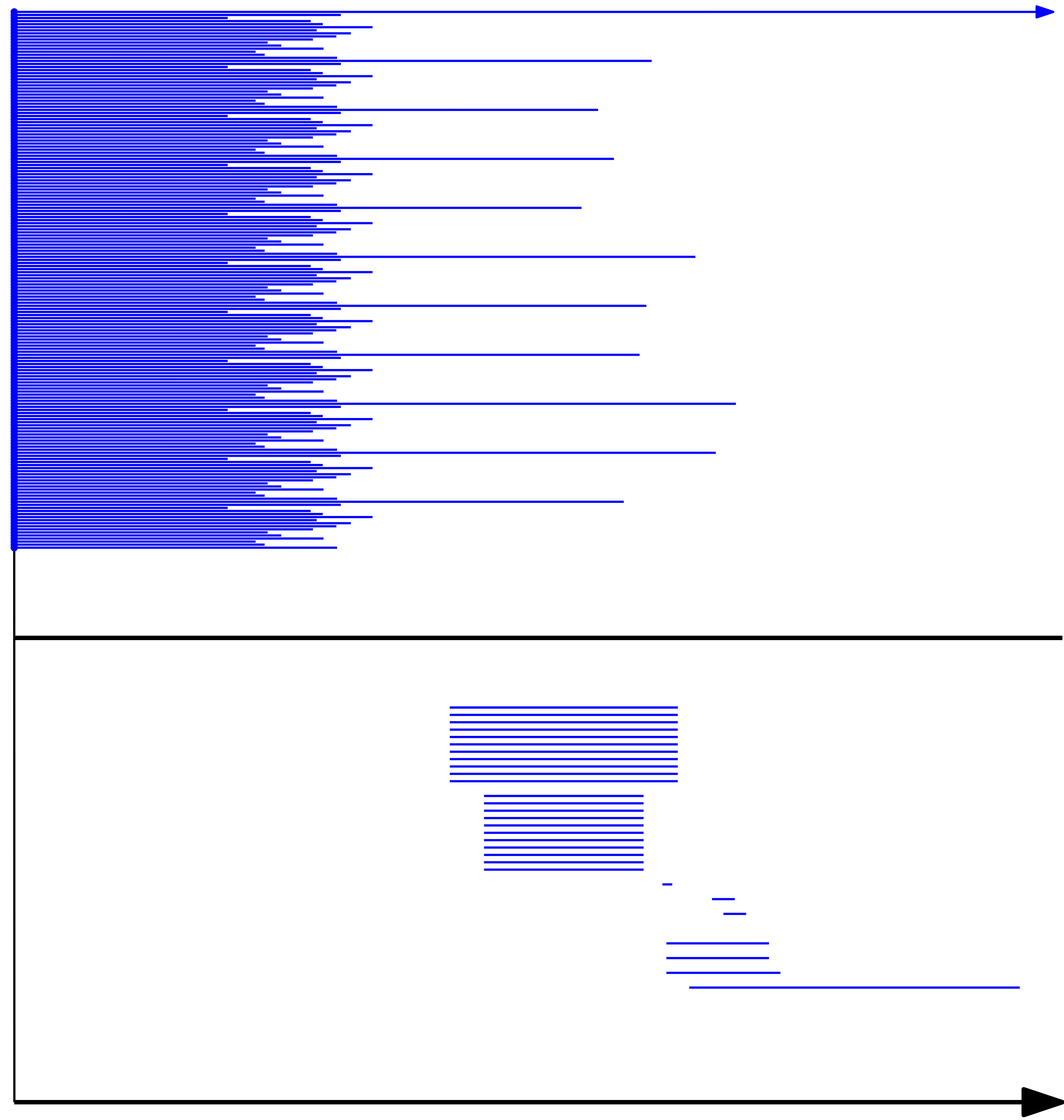
Def: The persistence barcode (resp. diagram) D is a set of points in the plane (resp. intervals) encoding the topological features that appeared and disappeared in the filtration.

Persistence of Čech complexes





H_0 (connected components) + H_1 (loops)

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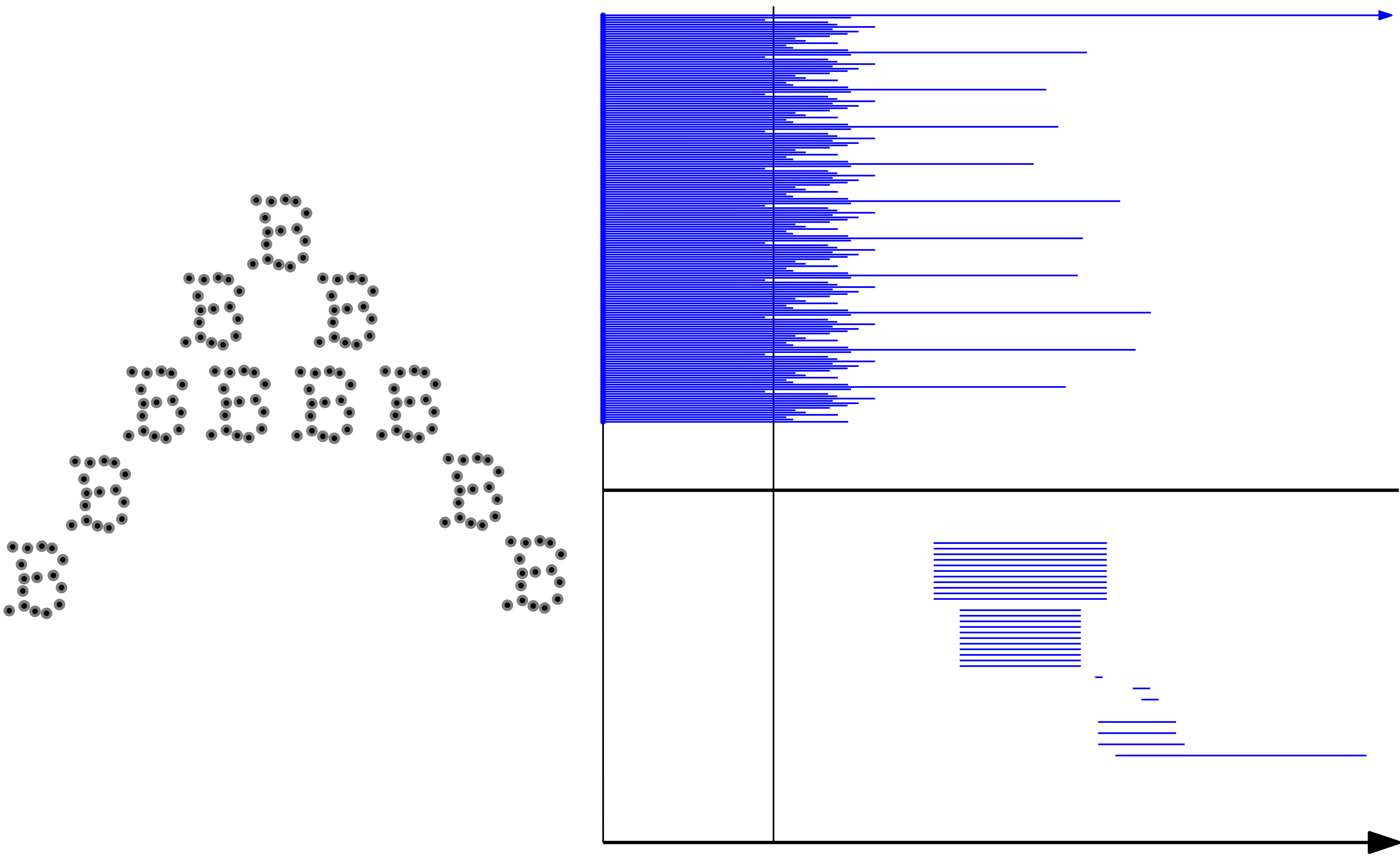

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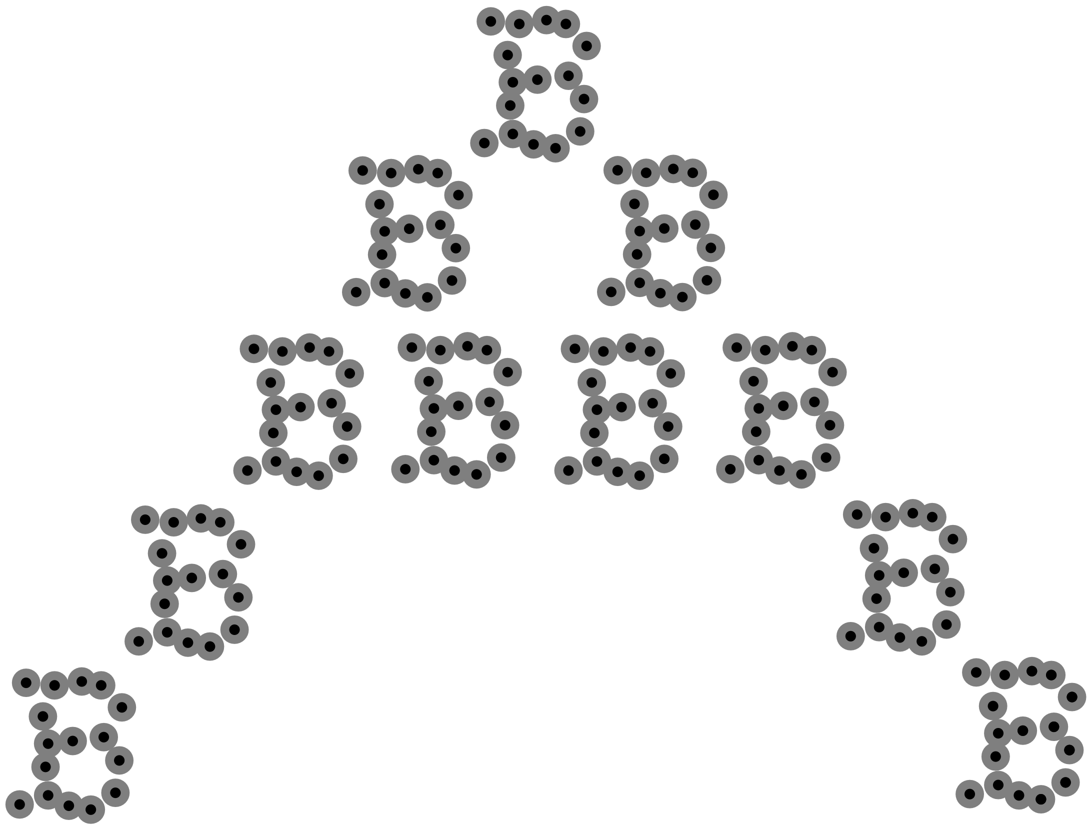

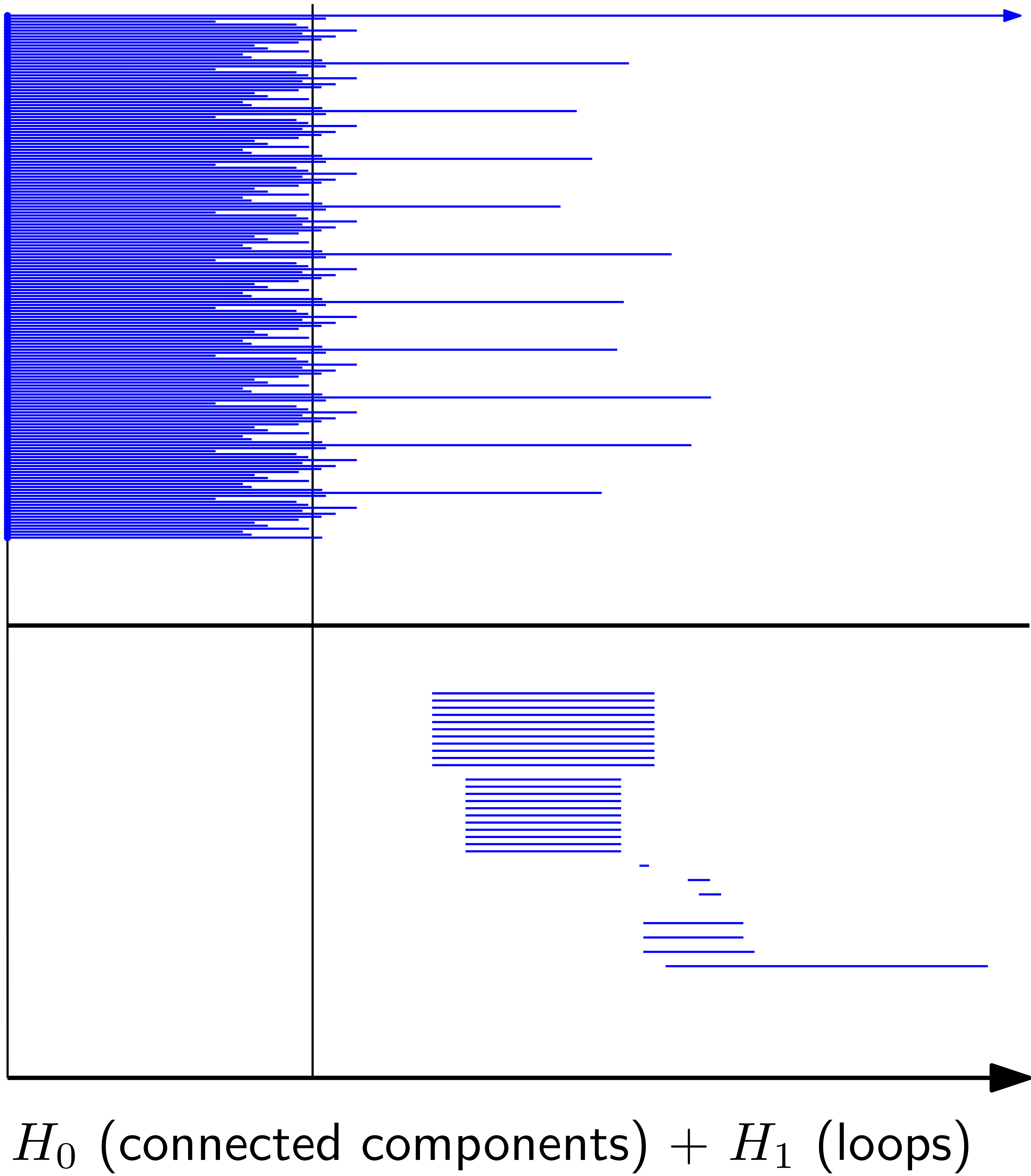

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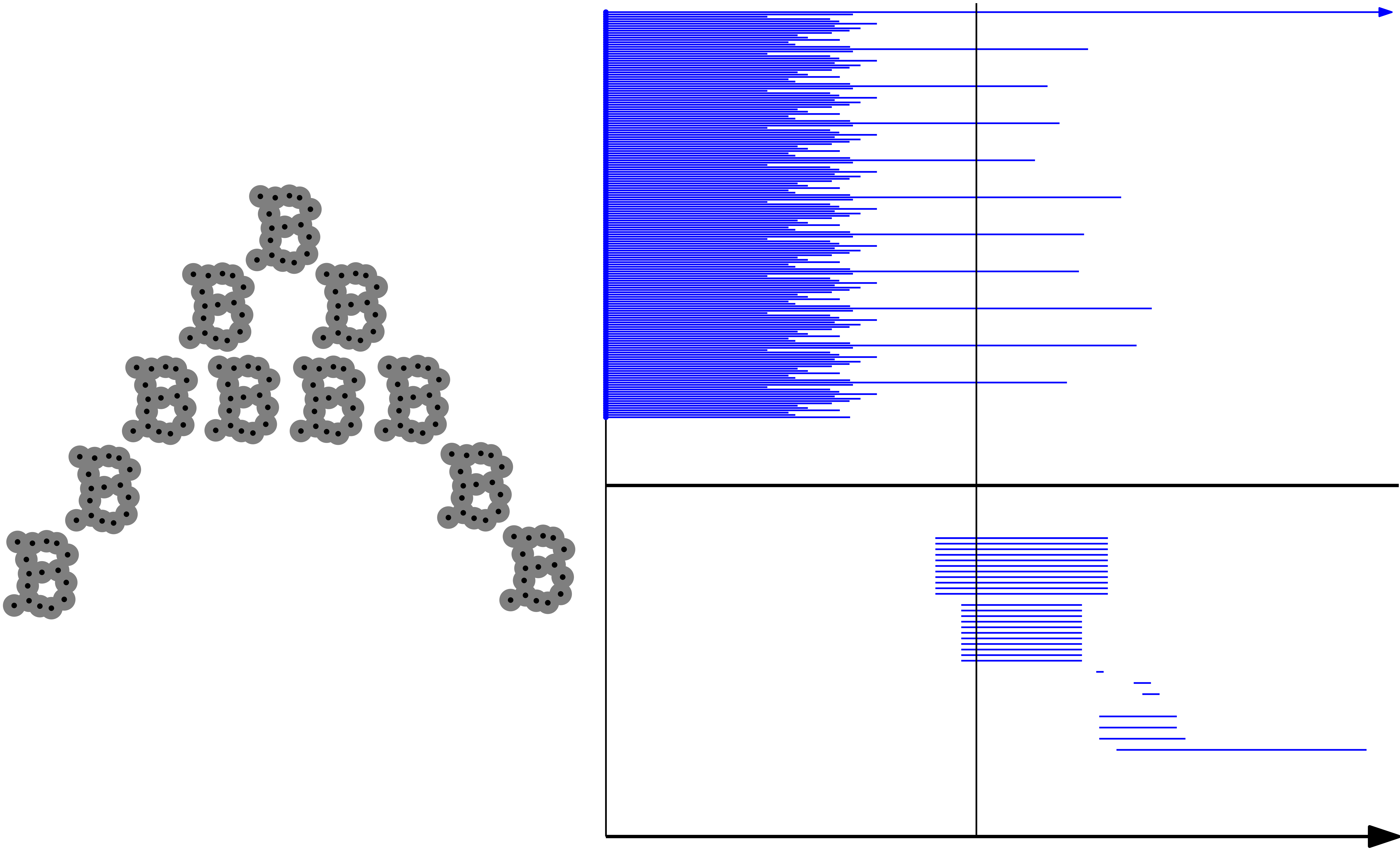

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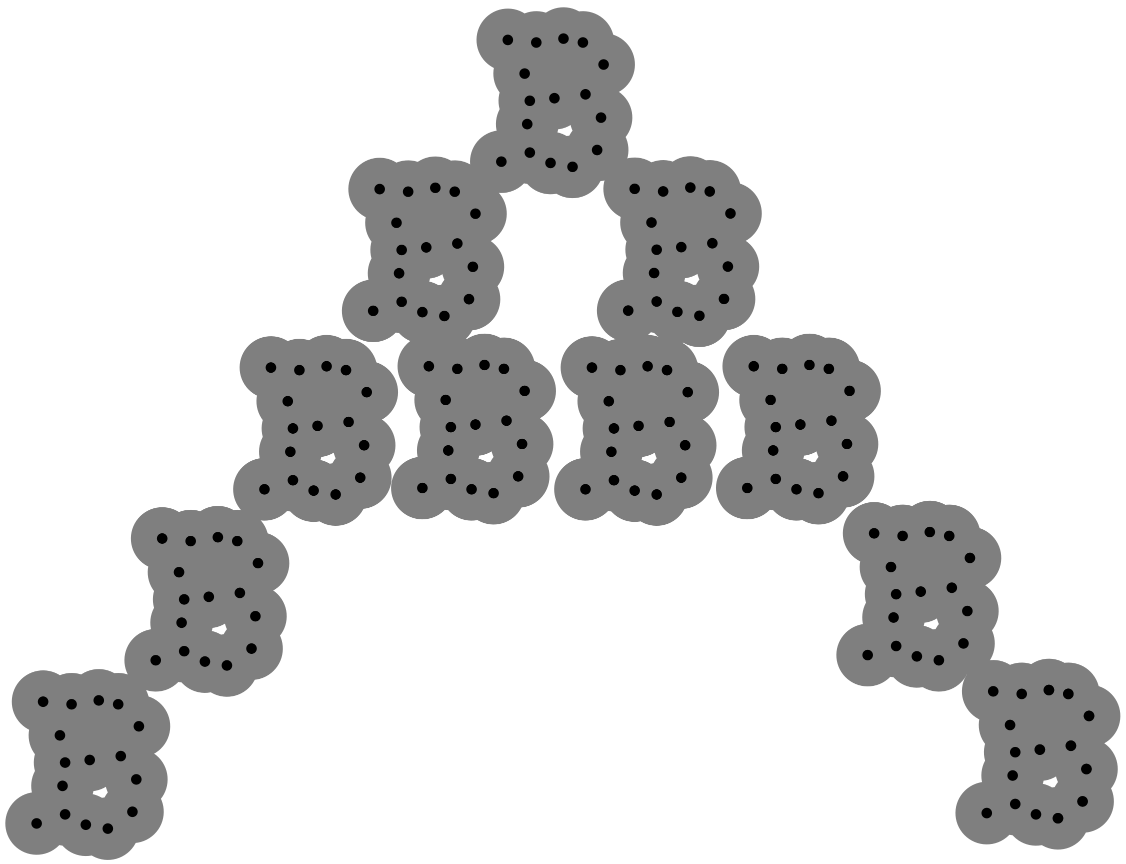

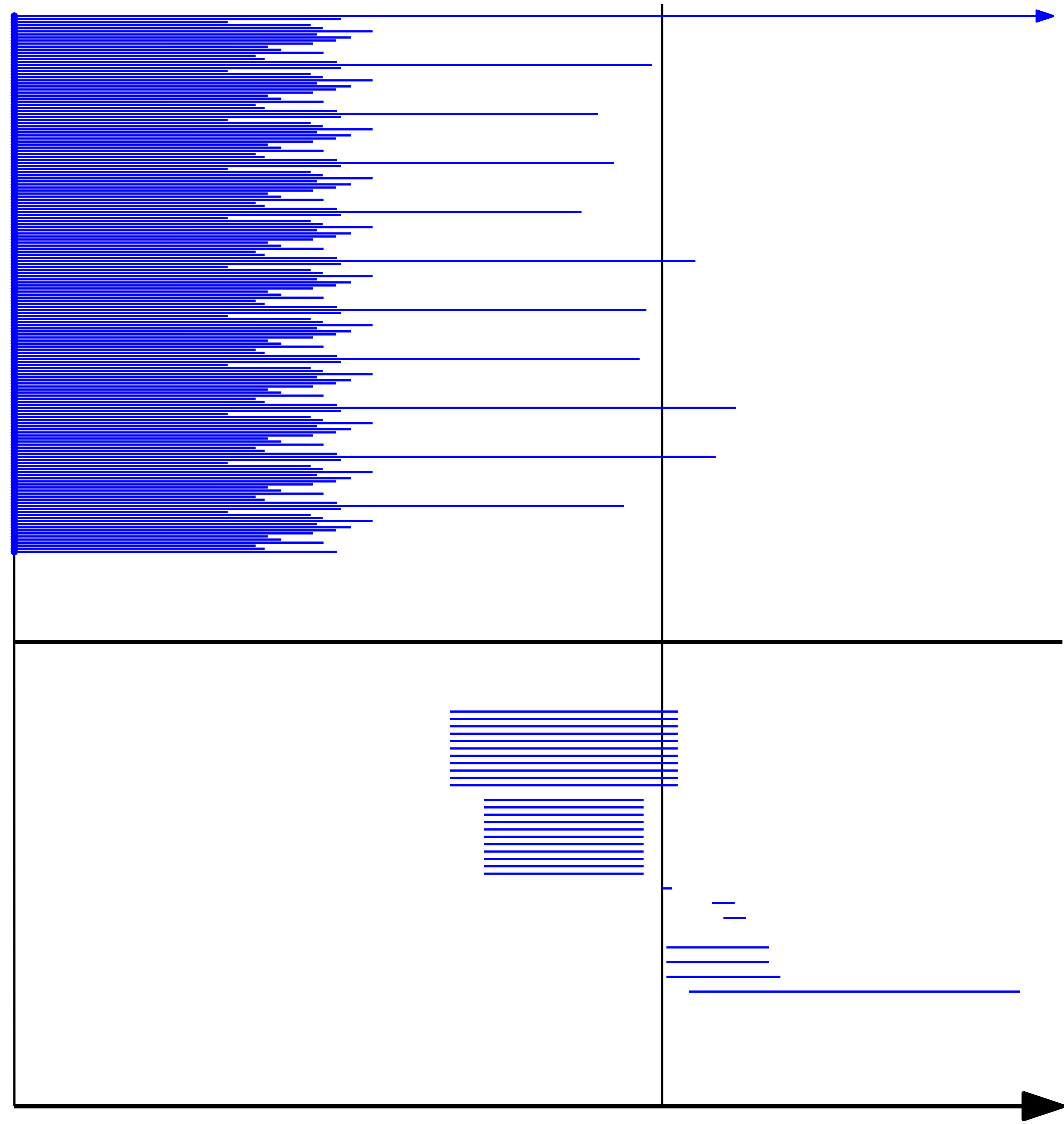

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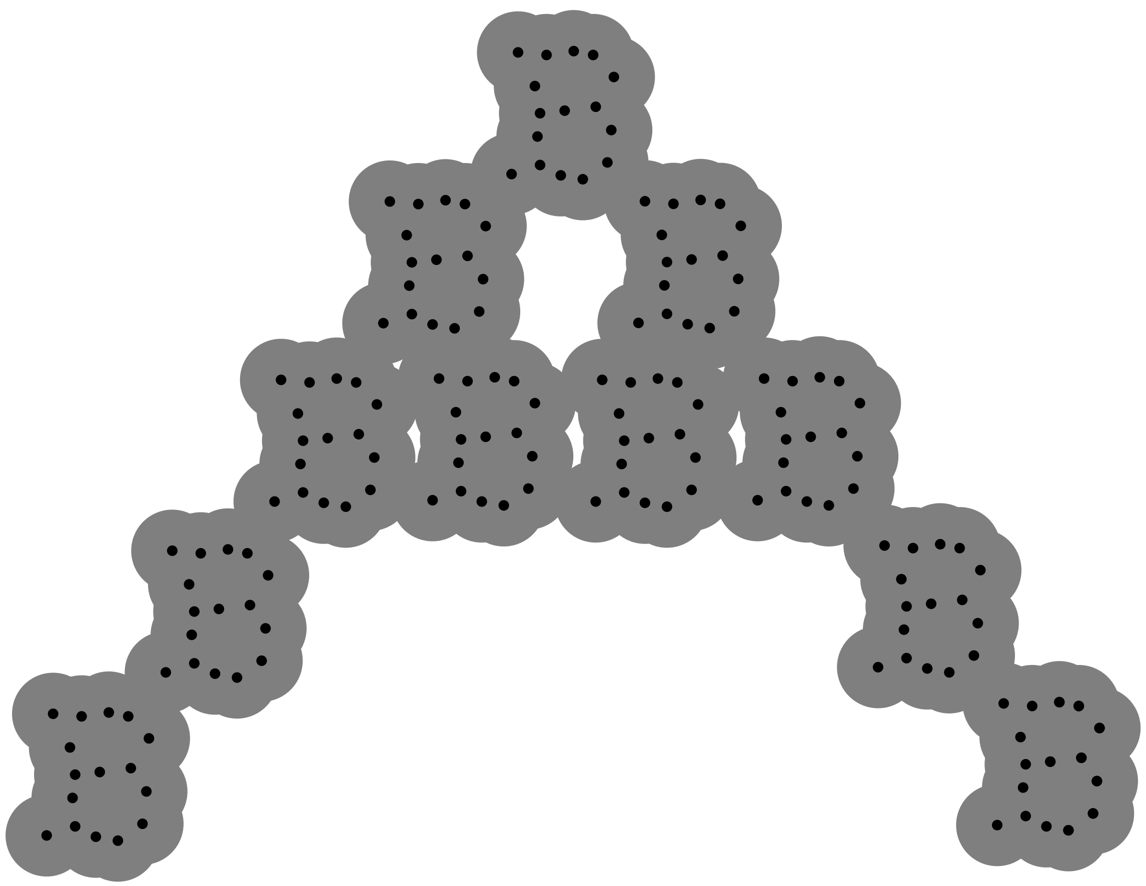

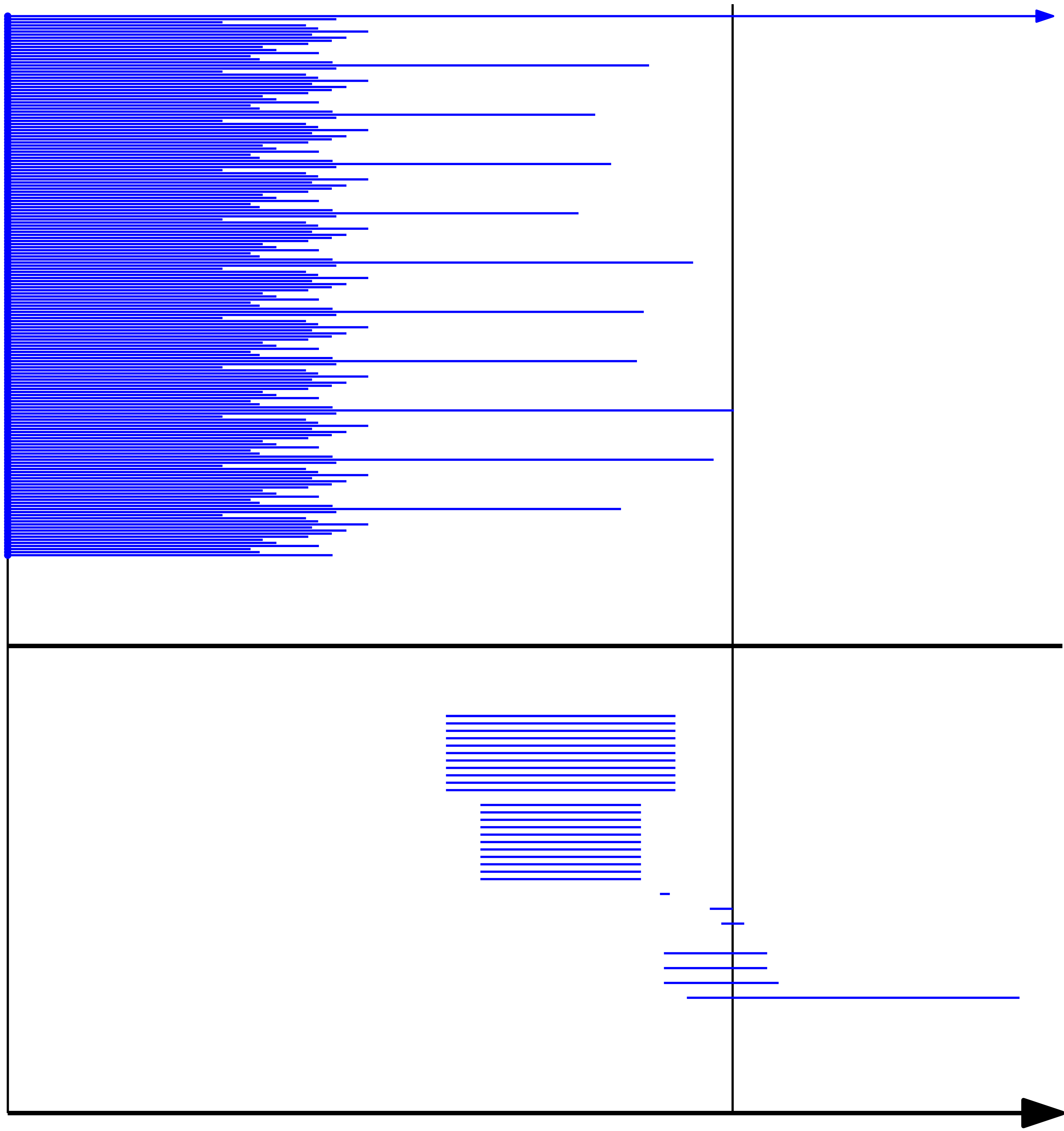

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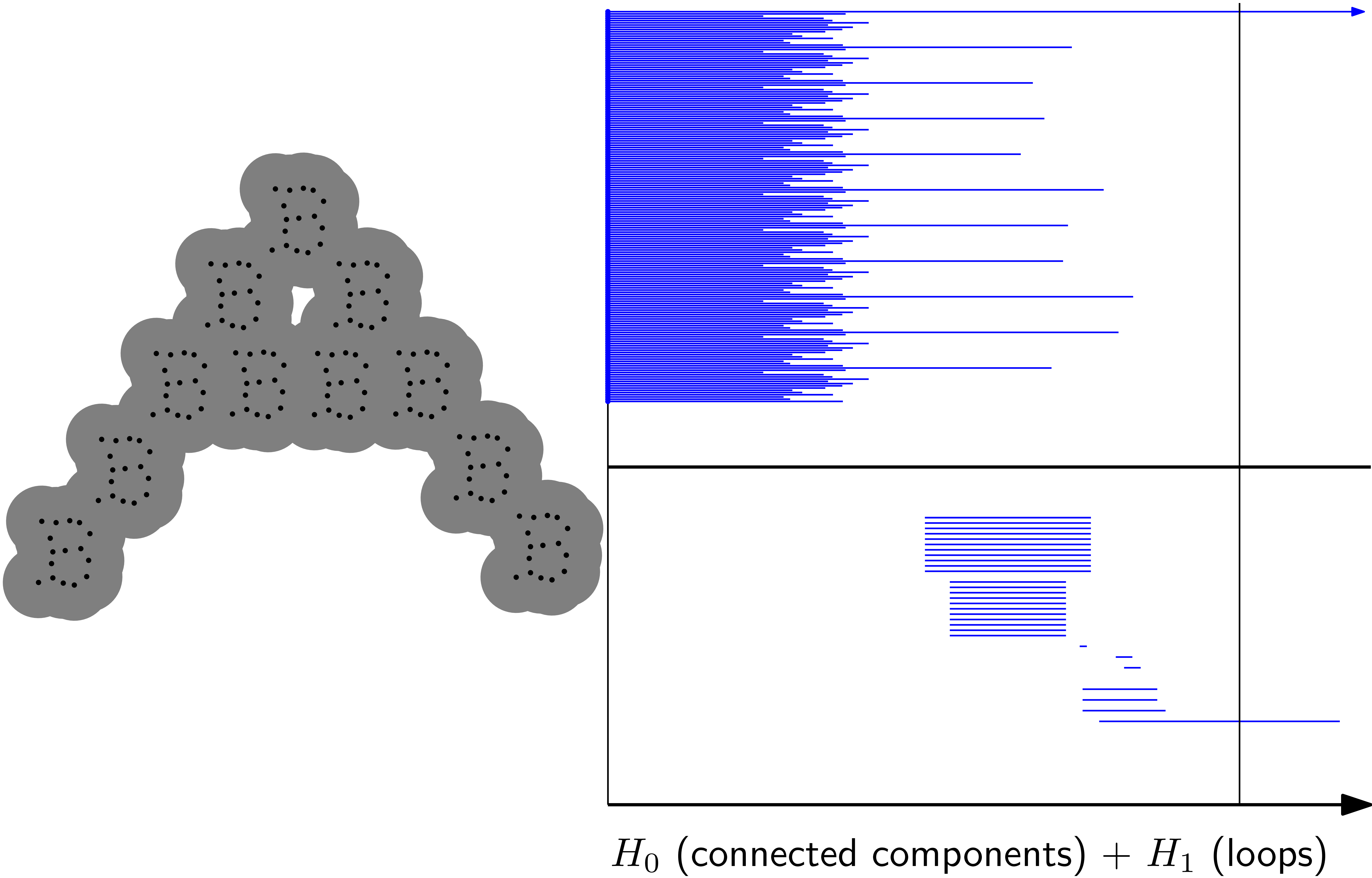

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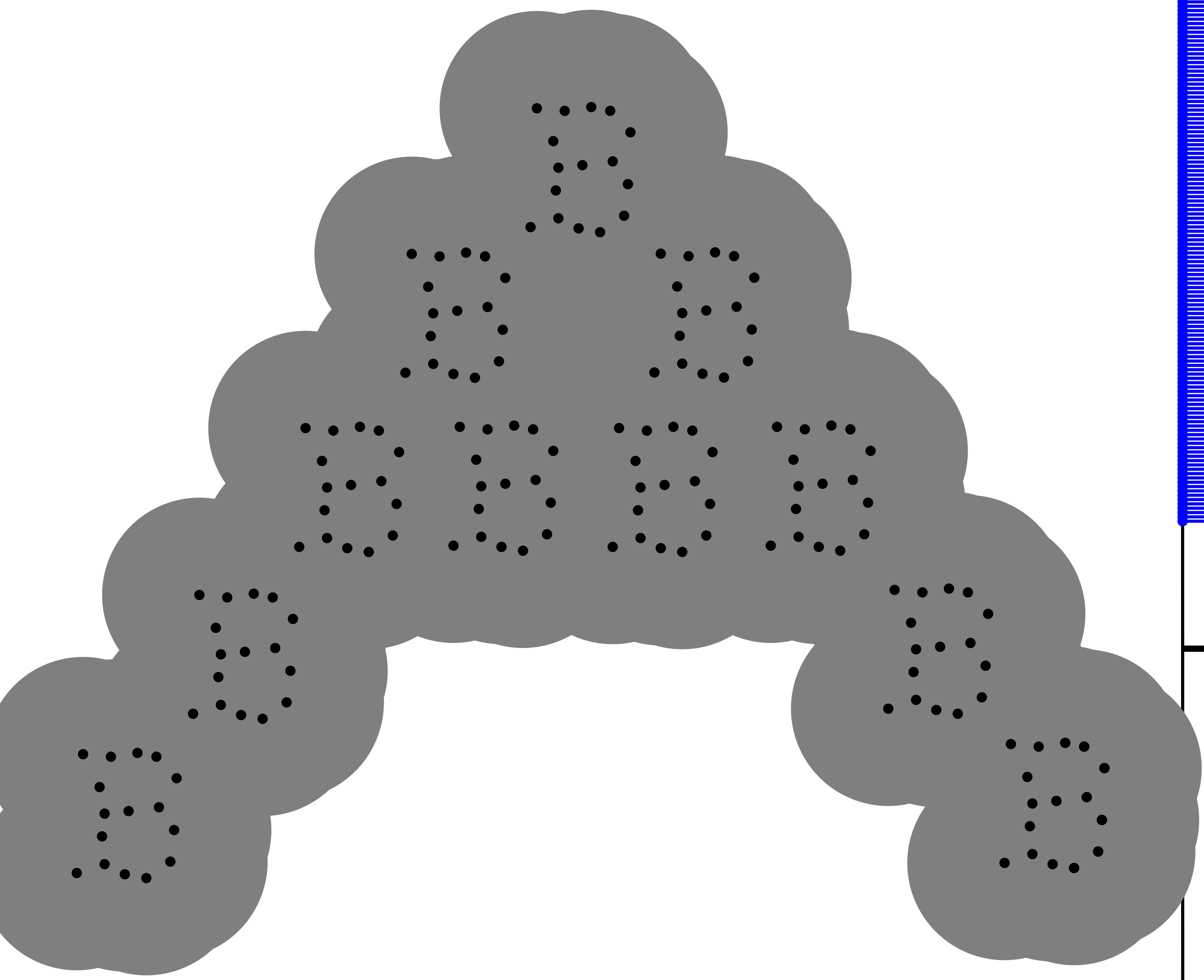
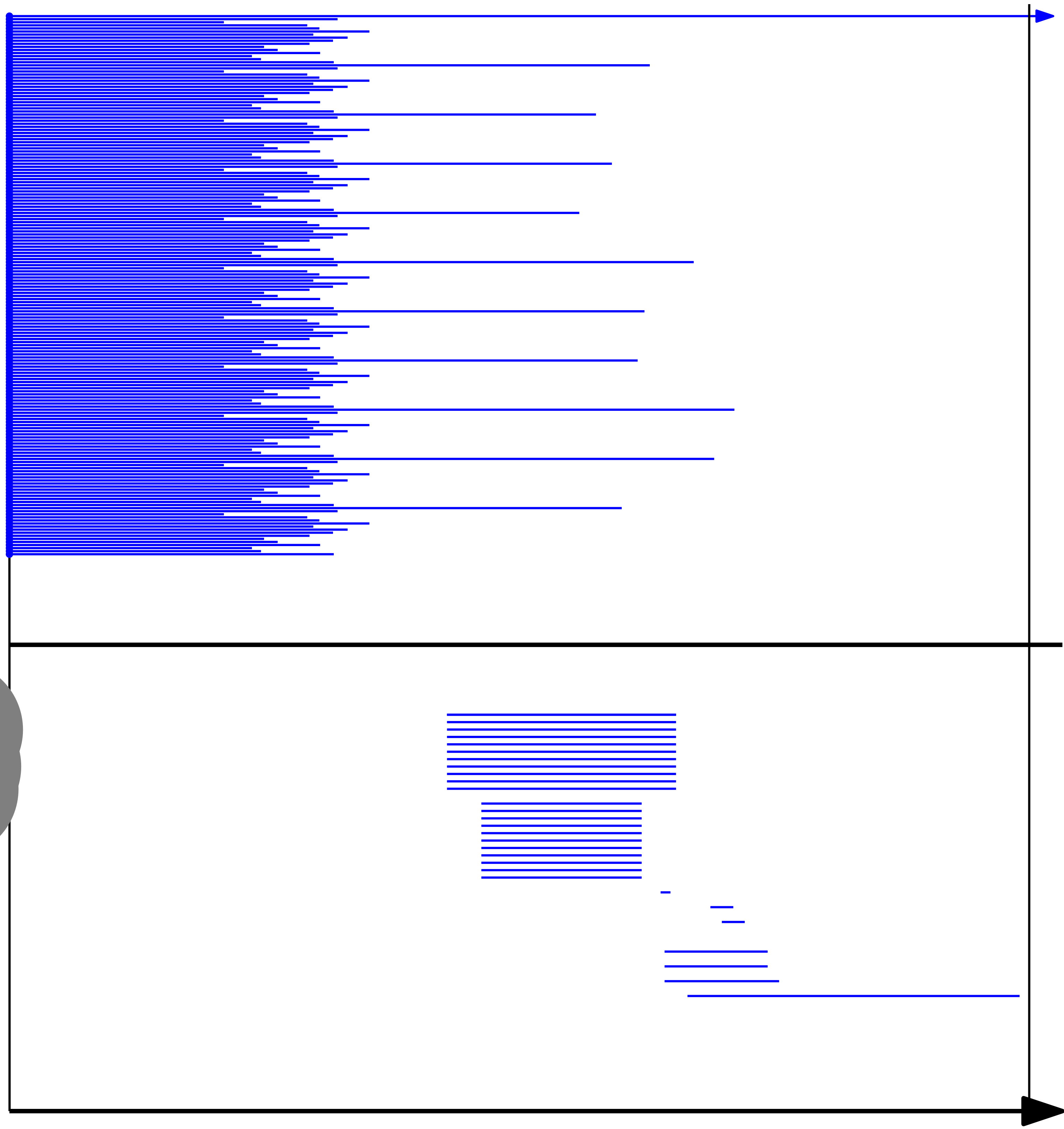
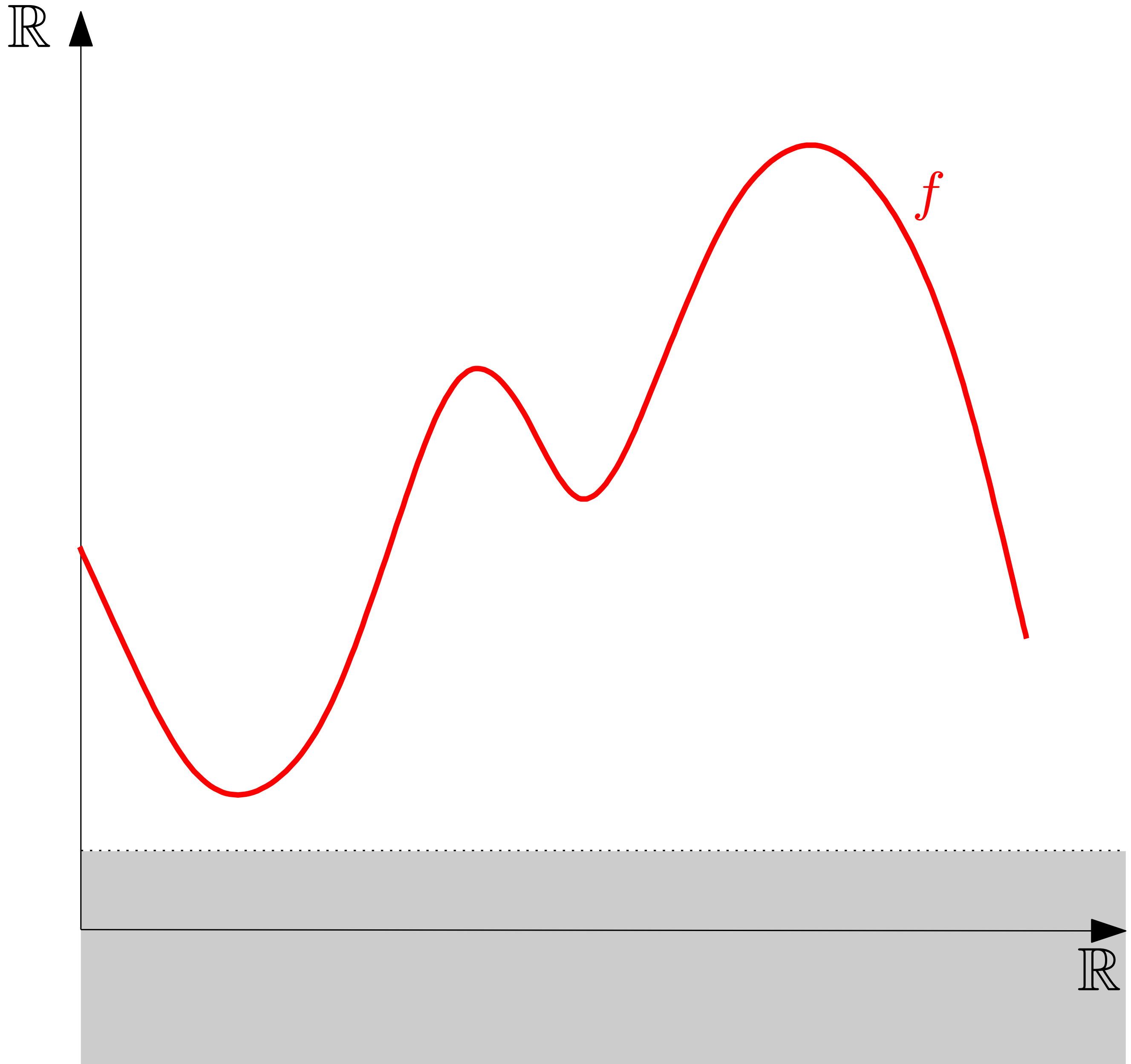




H_0 (connected components) + H_1 (loops)

Persistence of sublevel sets of function

H_0 (connected components)



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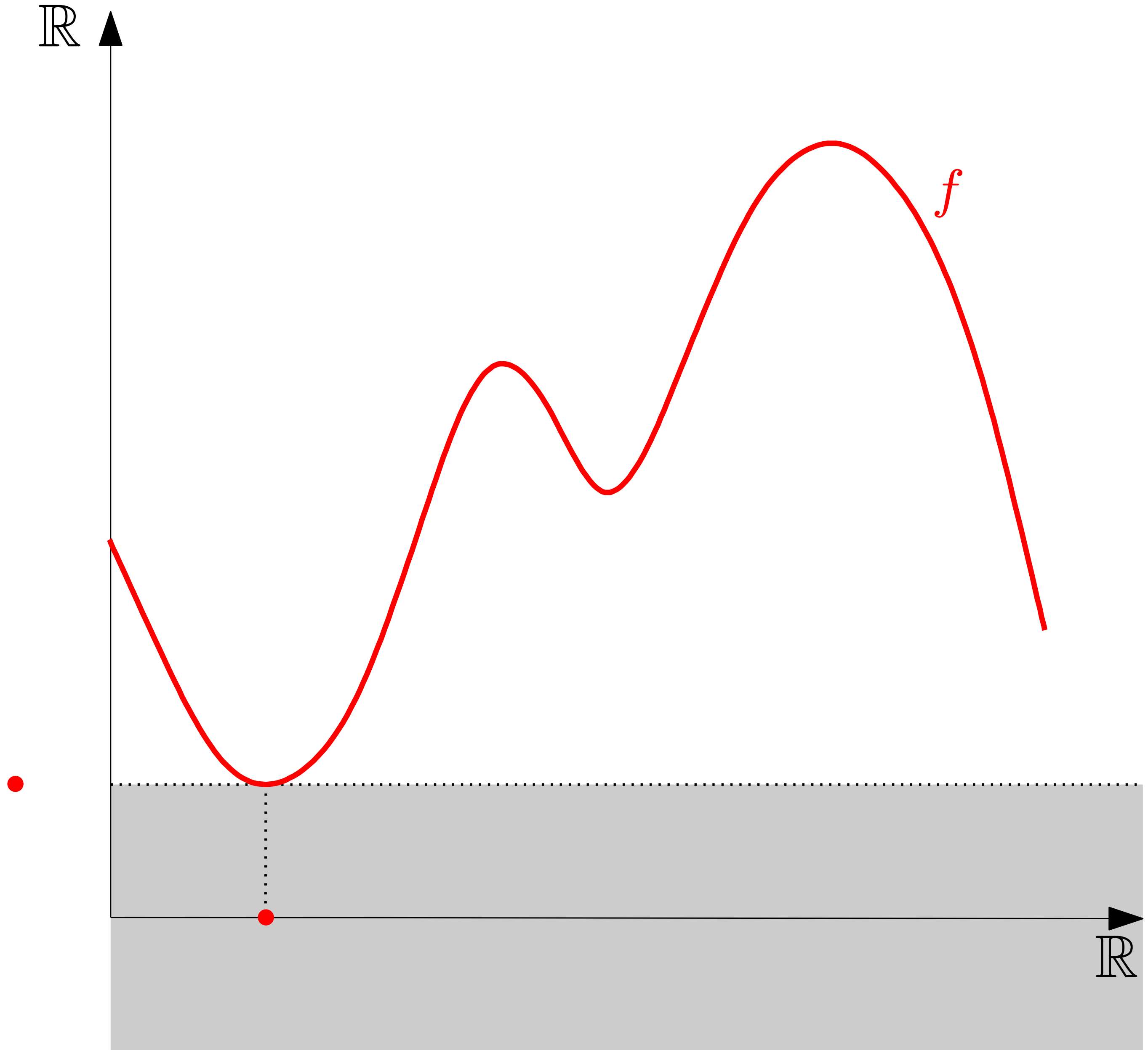

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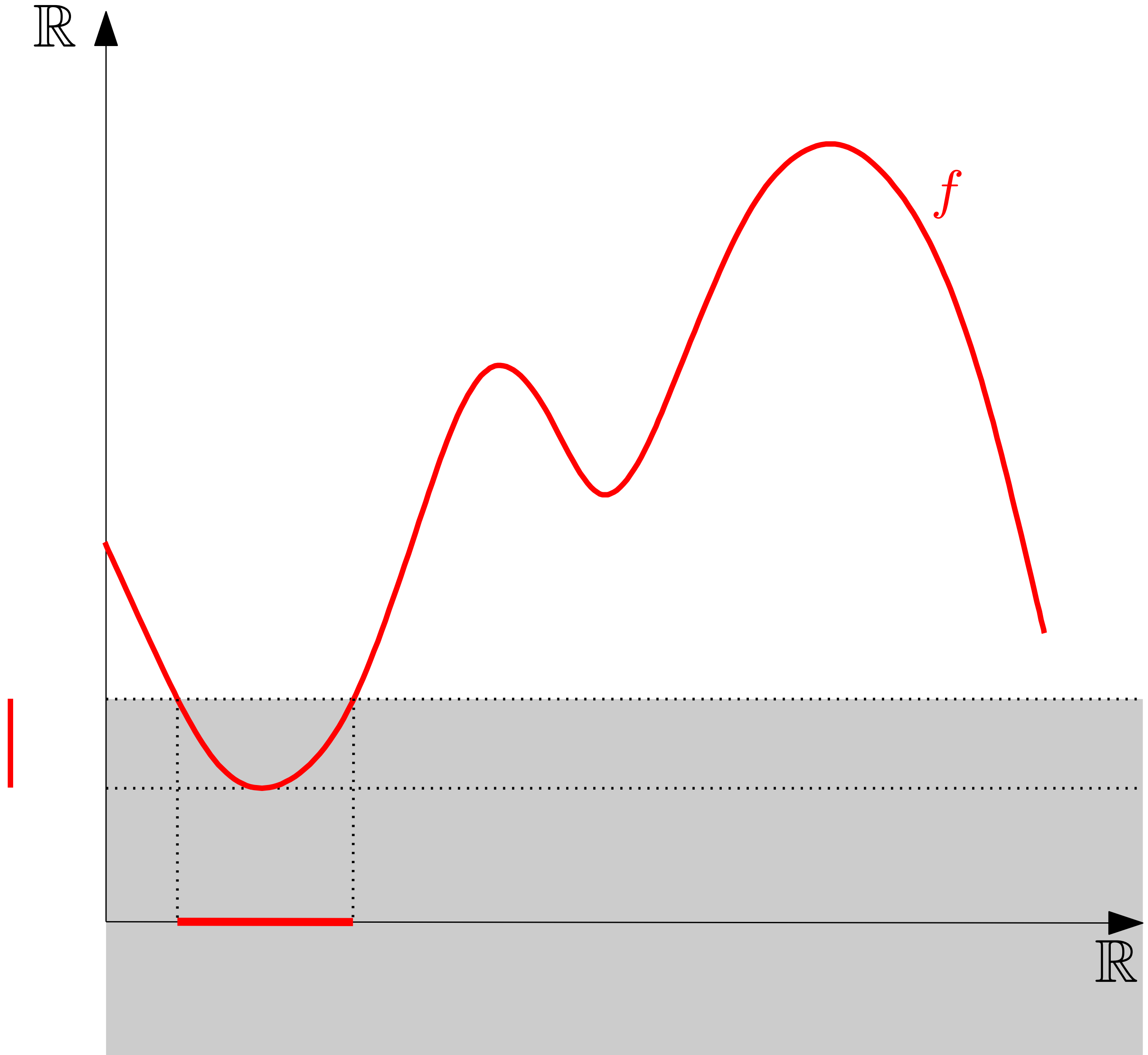

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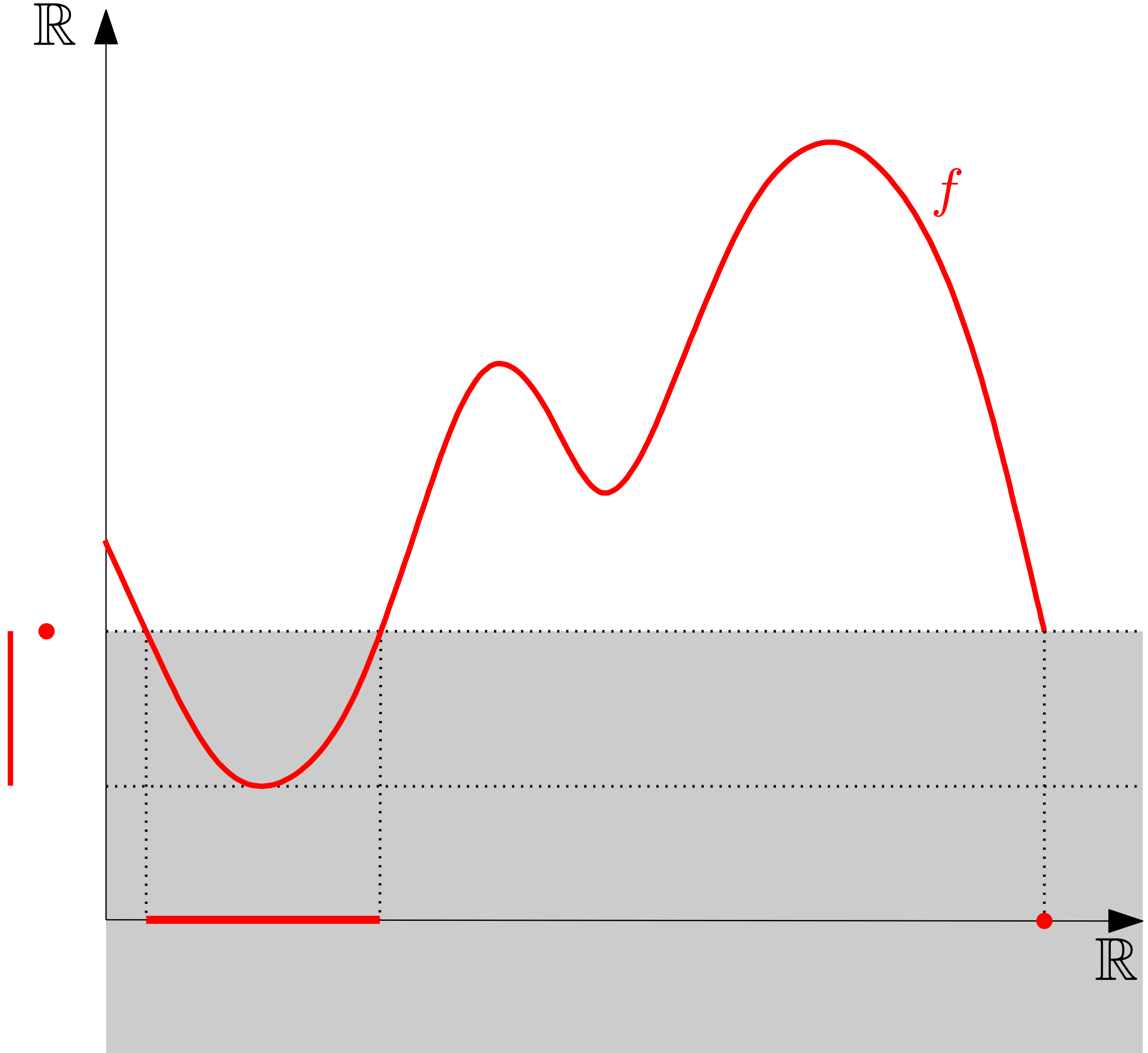

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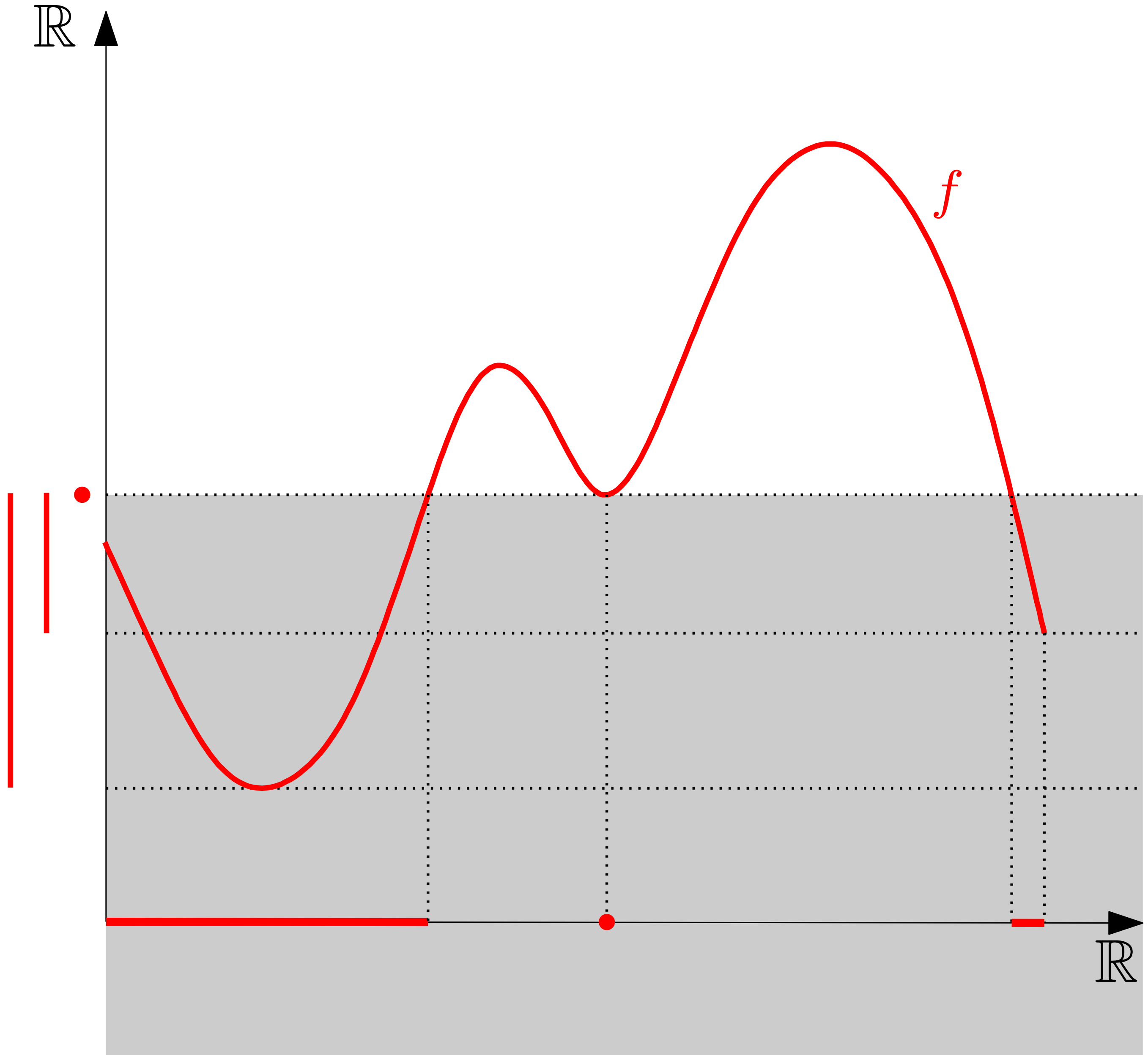
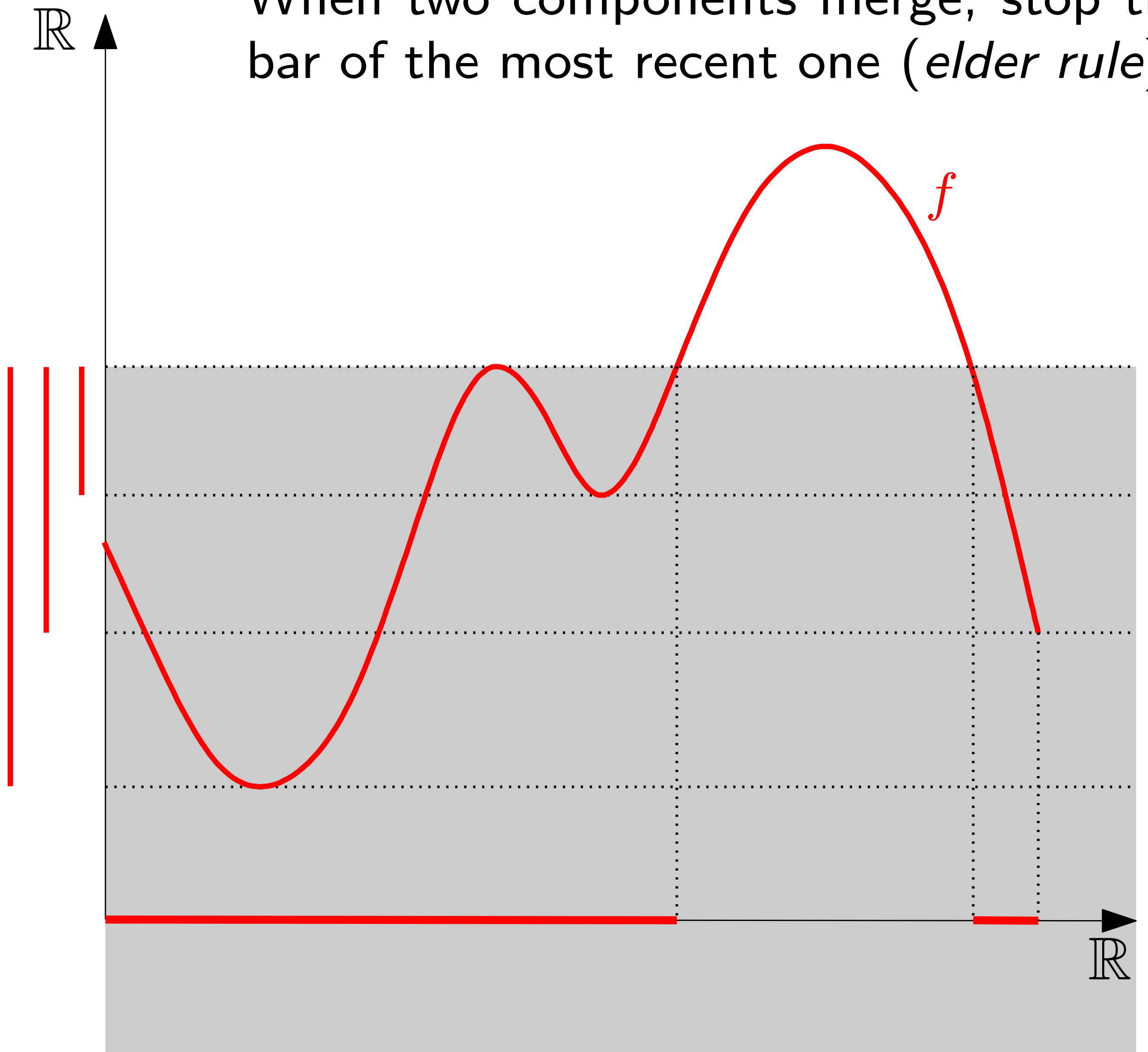


Persistence of sublevel sets of function

H_0 (connected components)

When two components merge, stop the bar of the most recent one (*elder rule*).



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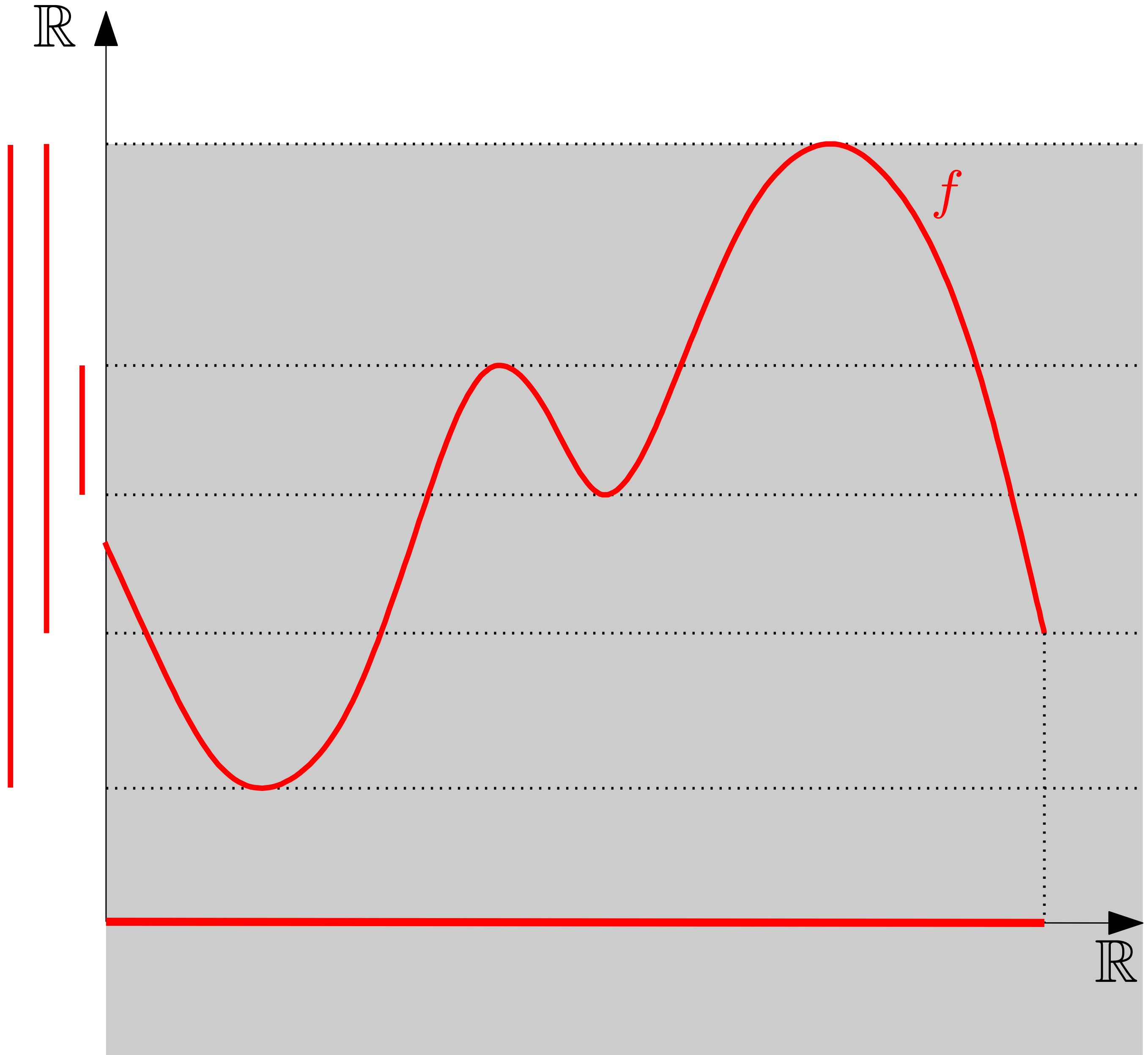

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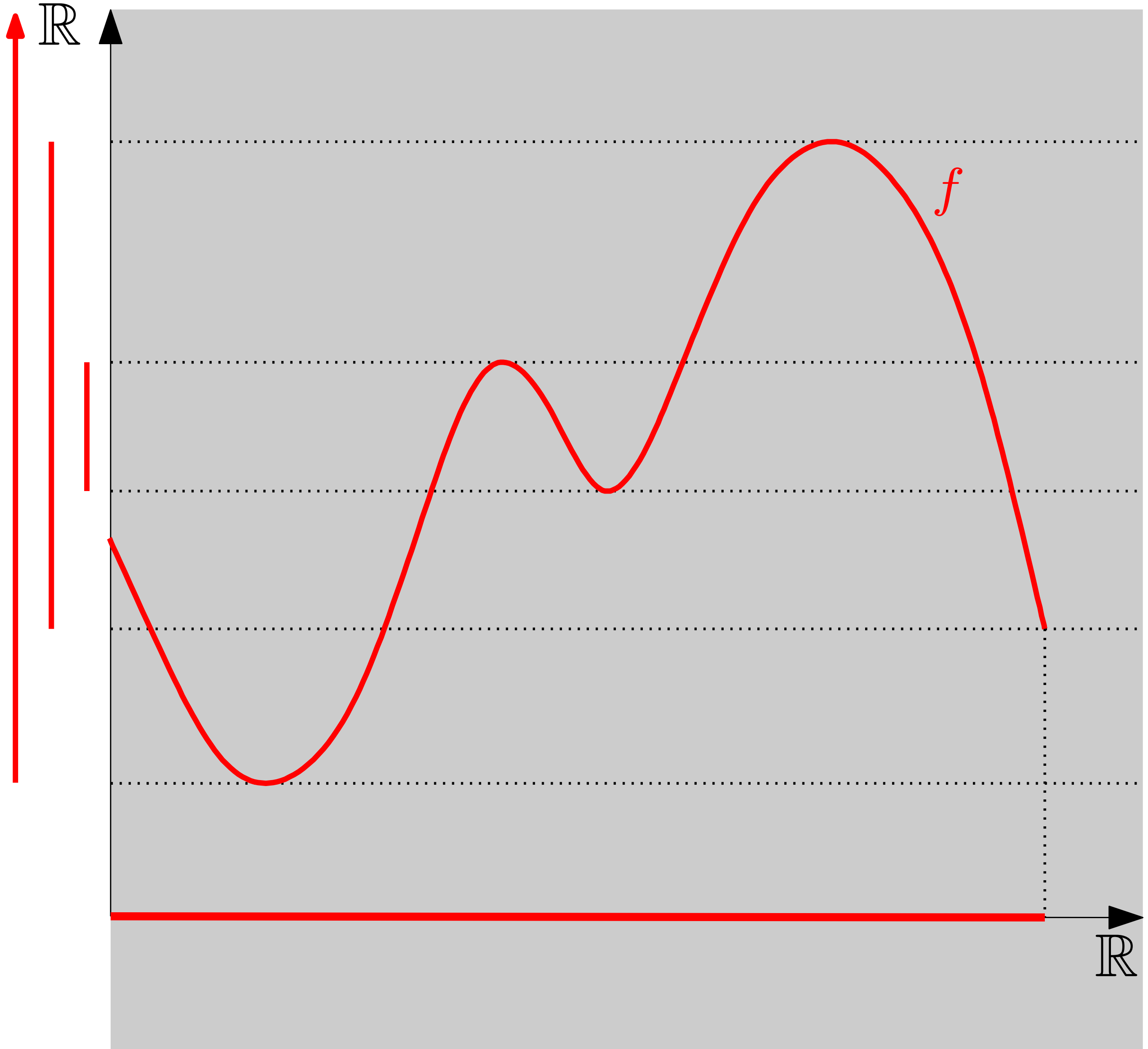

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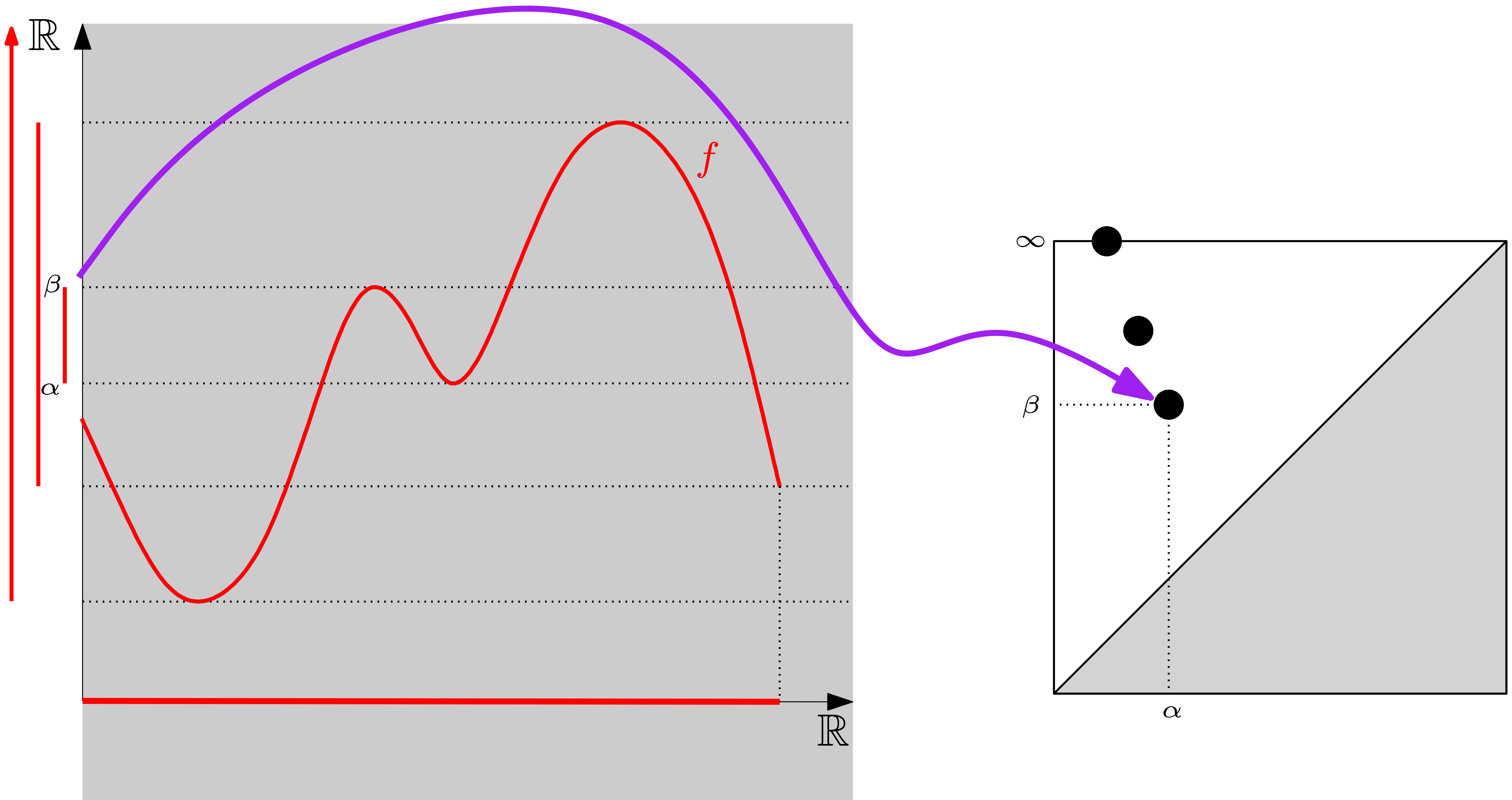
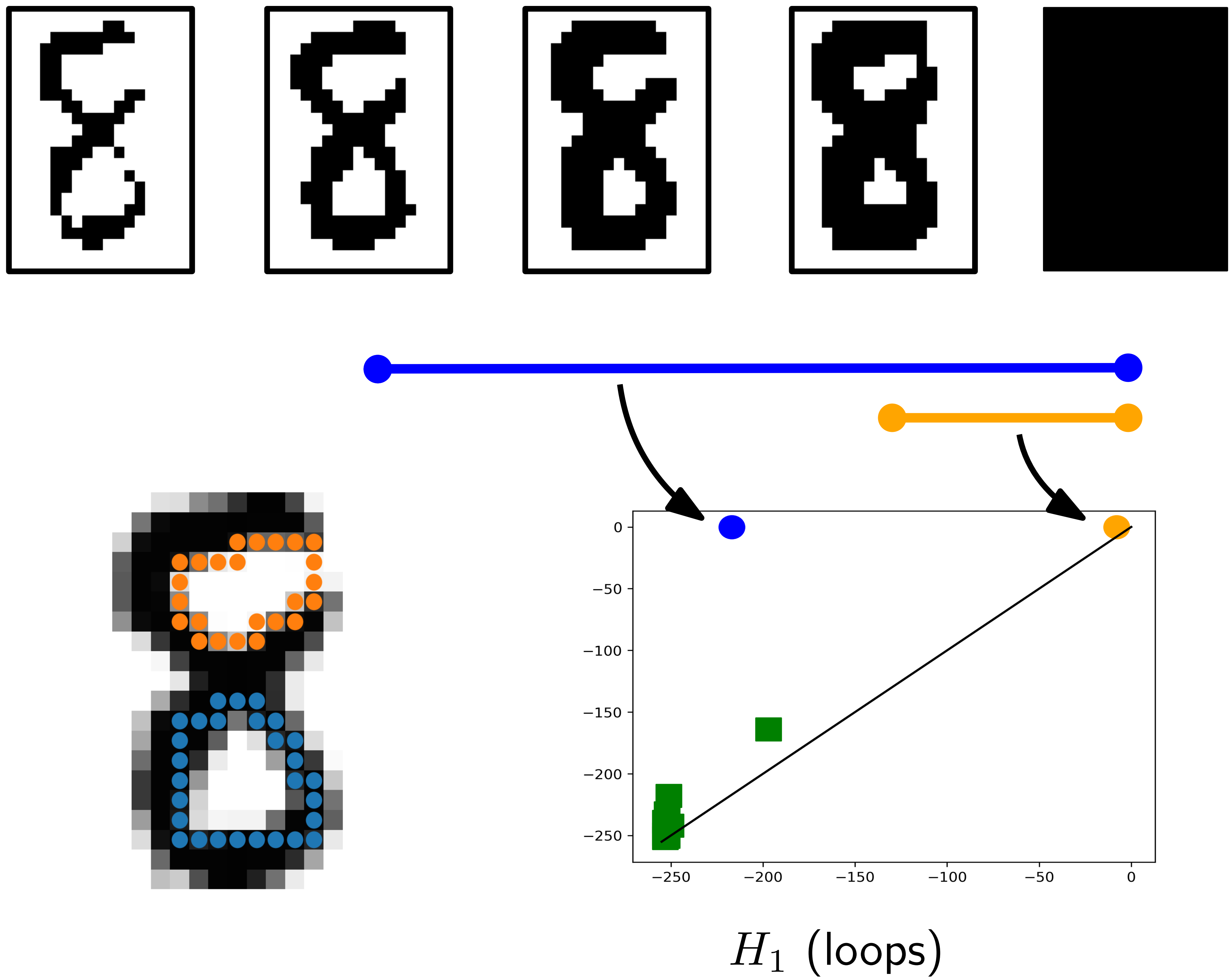
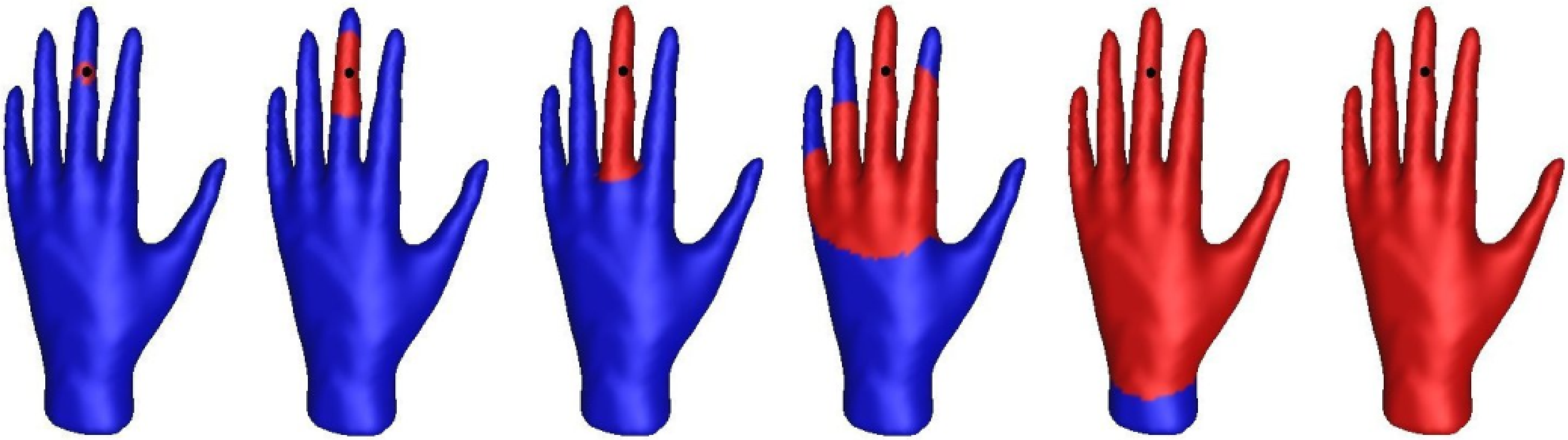


Persistence of images



Persistence of meshes



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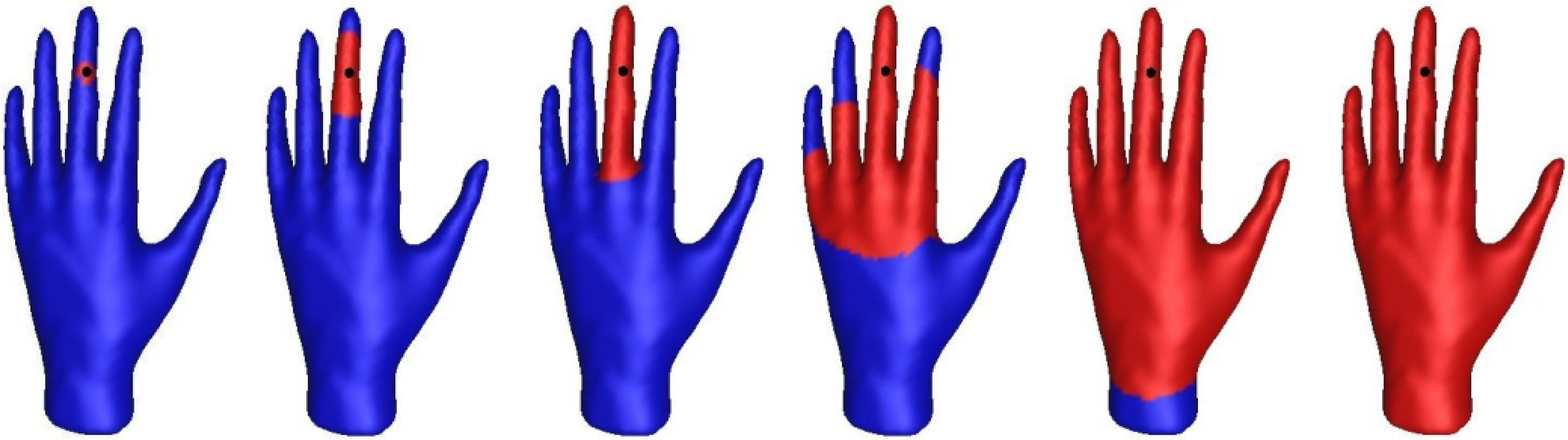
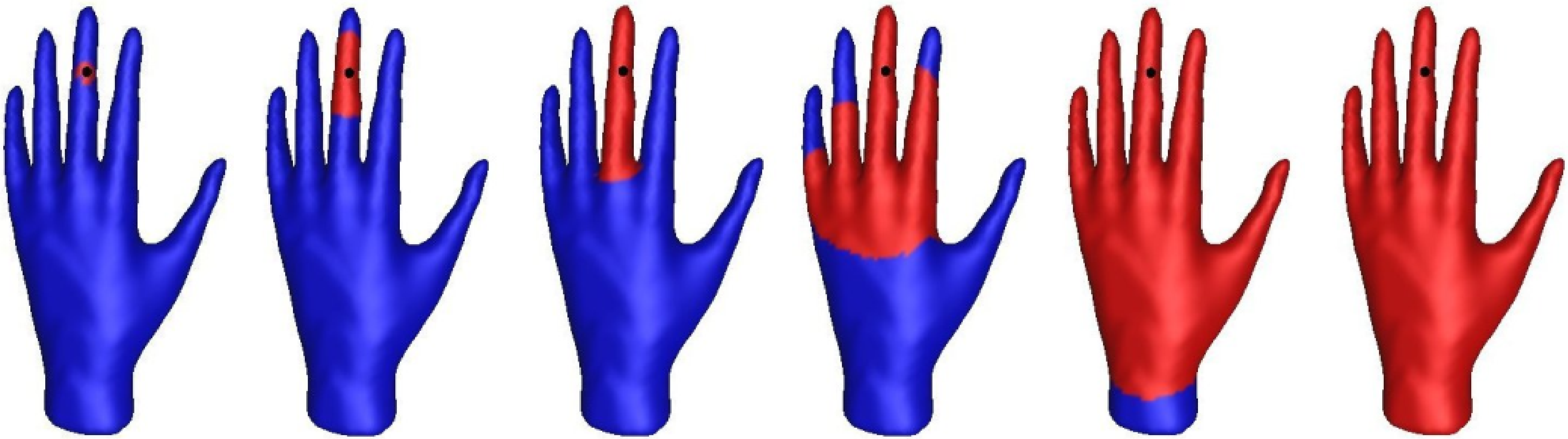


```
In [ ]: st = get_simplex_tree_from_faces(faces)
        filtration = geodesic_distances(base_vertex)
        for v in range(len(vertices)):
            st.assign_filtration([v], filtration[v])
        st.make_filtration_non_decreasing()
        st.persistence()
        dgm = st.persistence_intervals_in_dimension(1)
```

Persistence of meshes



In [ ]:
```
st = get_simplex_tree_from_faces(faces)
filtration = geodesic_distances(base_vertex)
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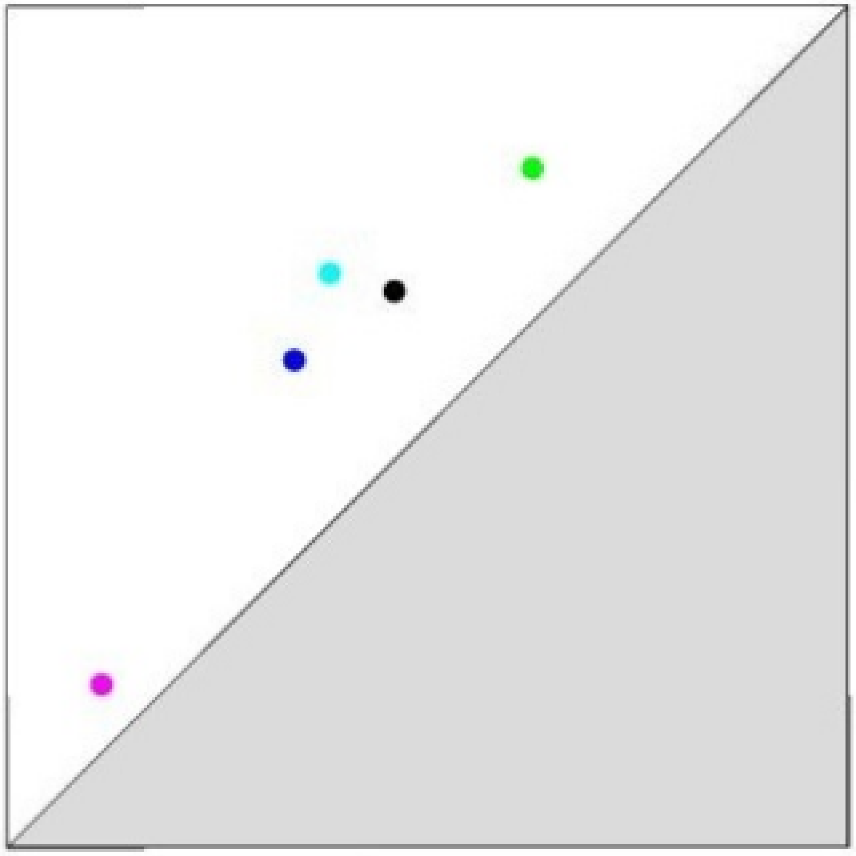

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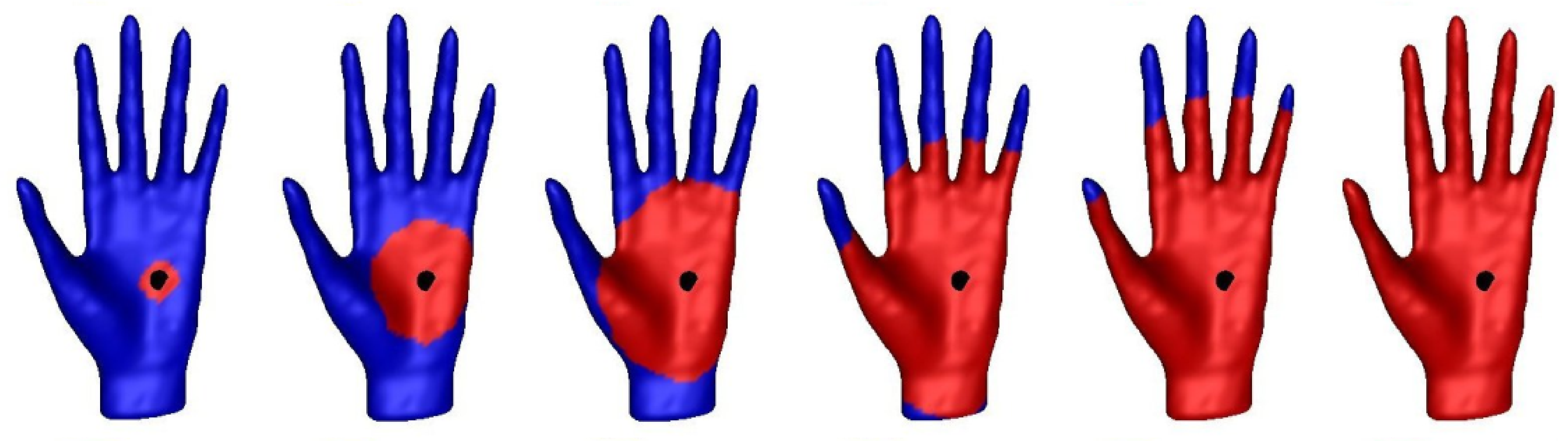

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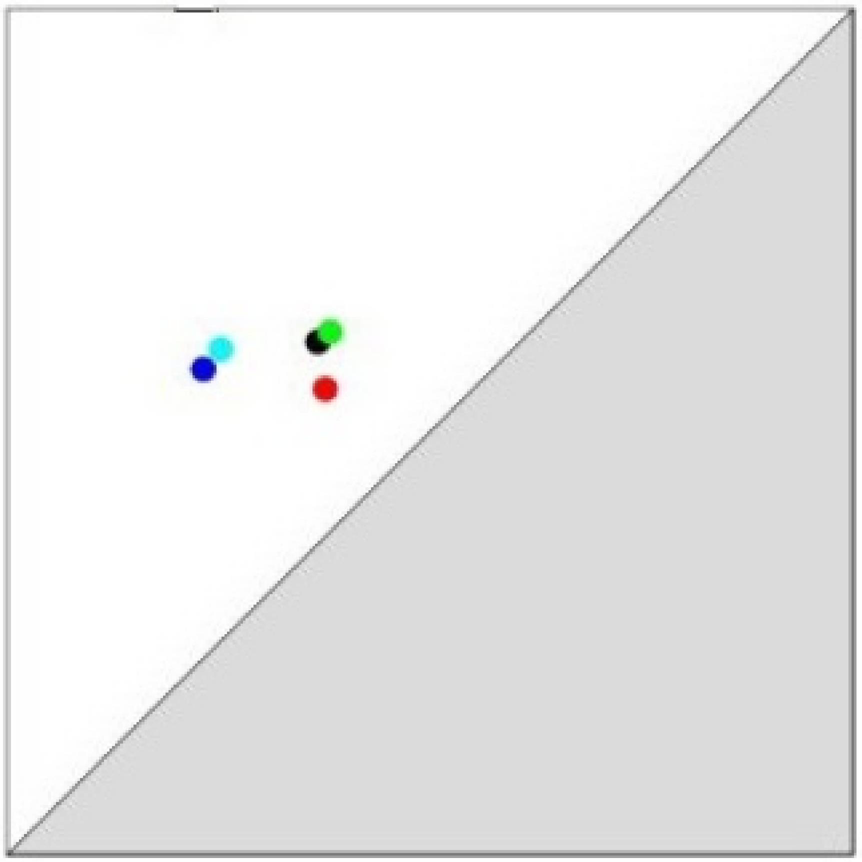
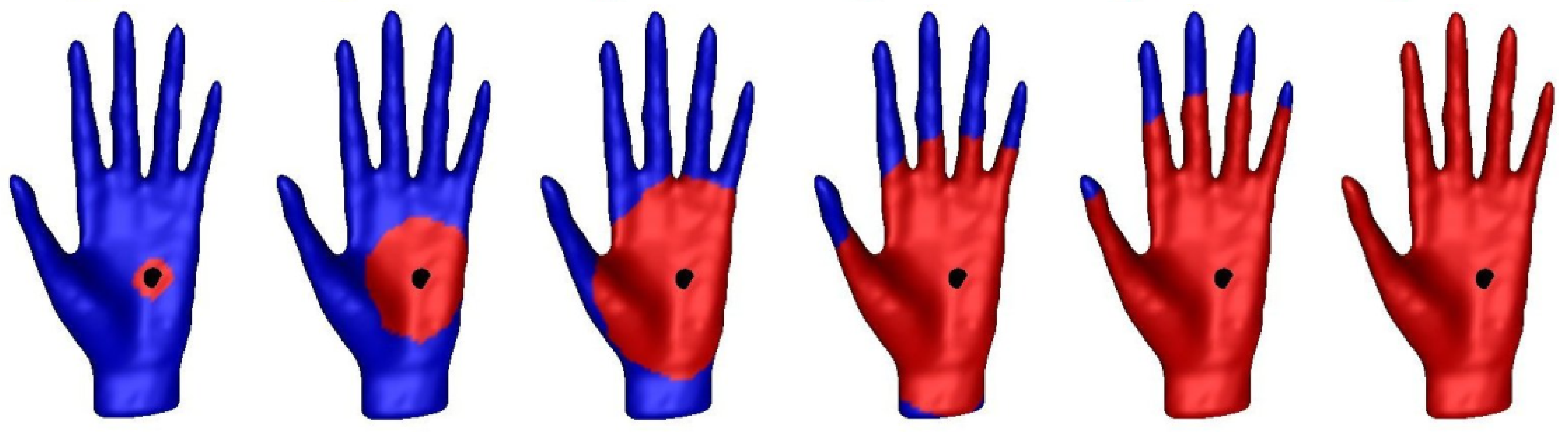


Persistence of meshes



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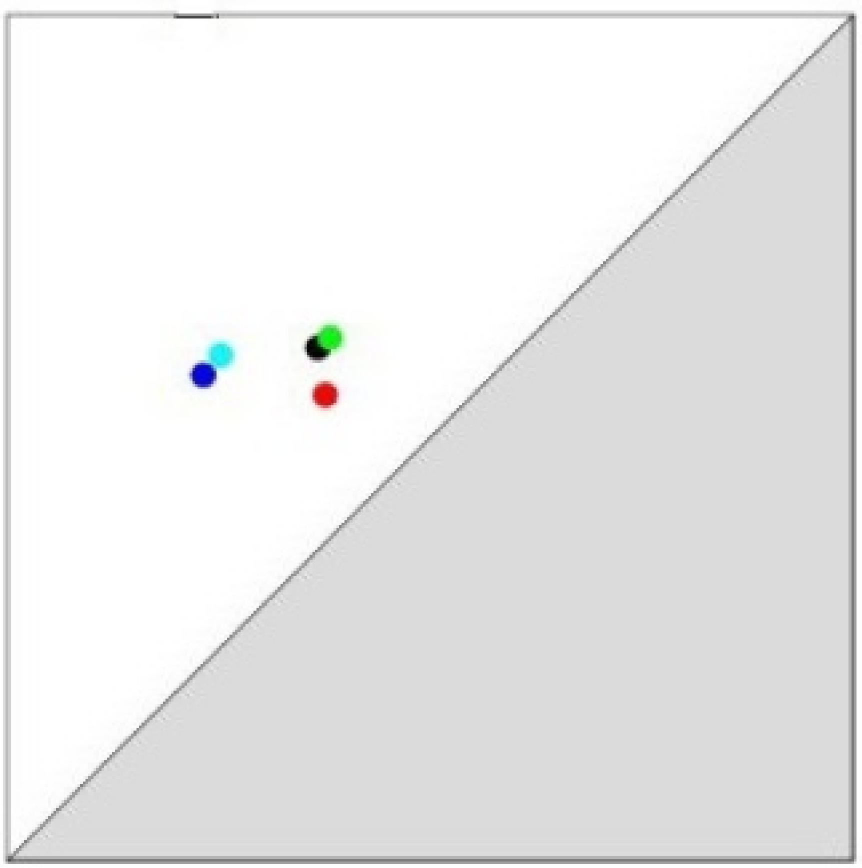
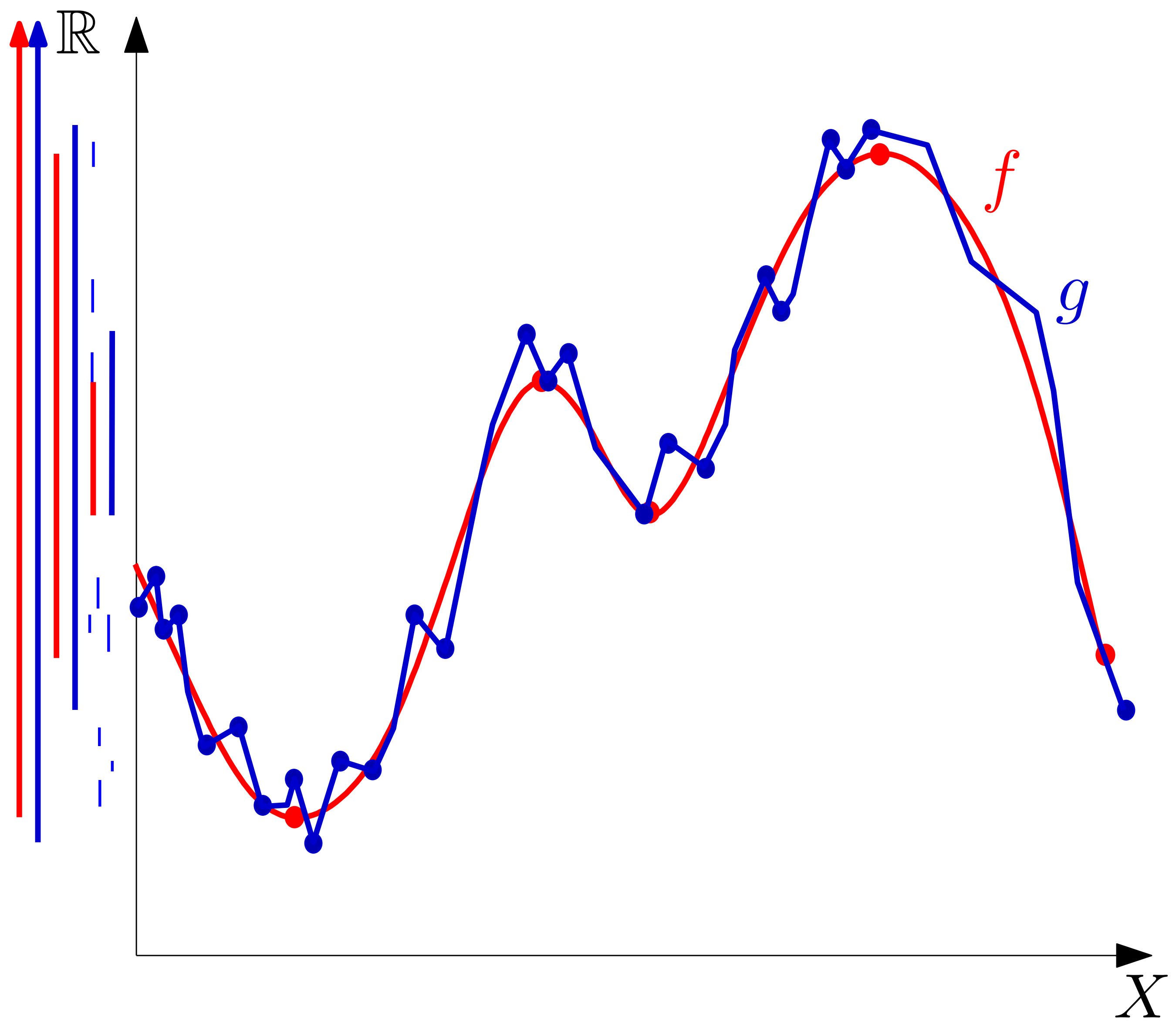
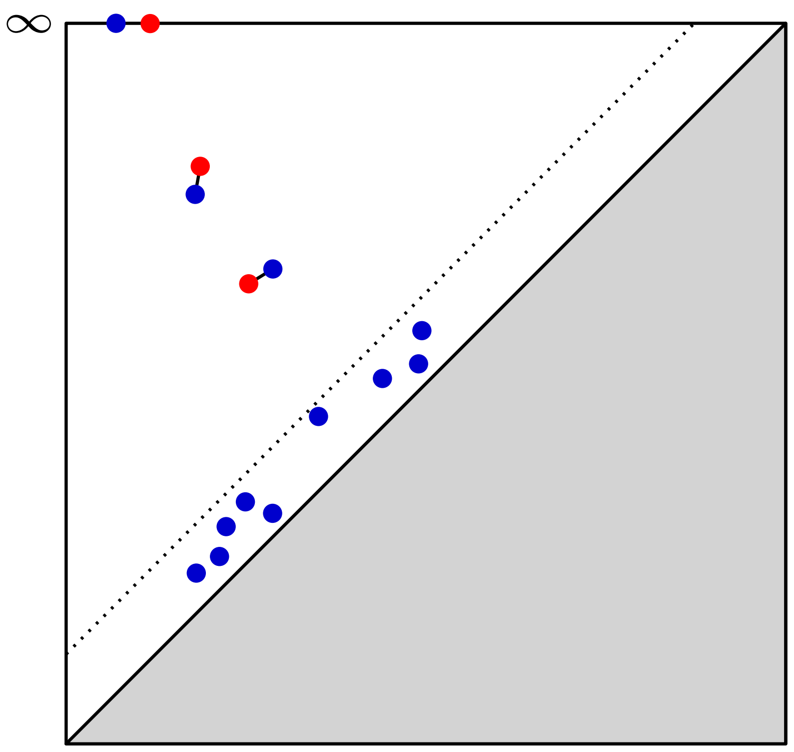


Thm: $d_b(D(f), D(g)) \leq \|f - g\|_\infty$

Stability and distance between PDs





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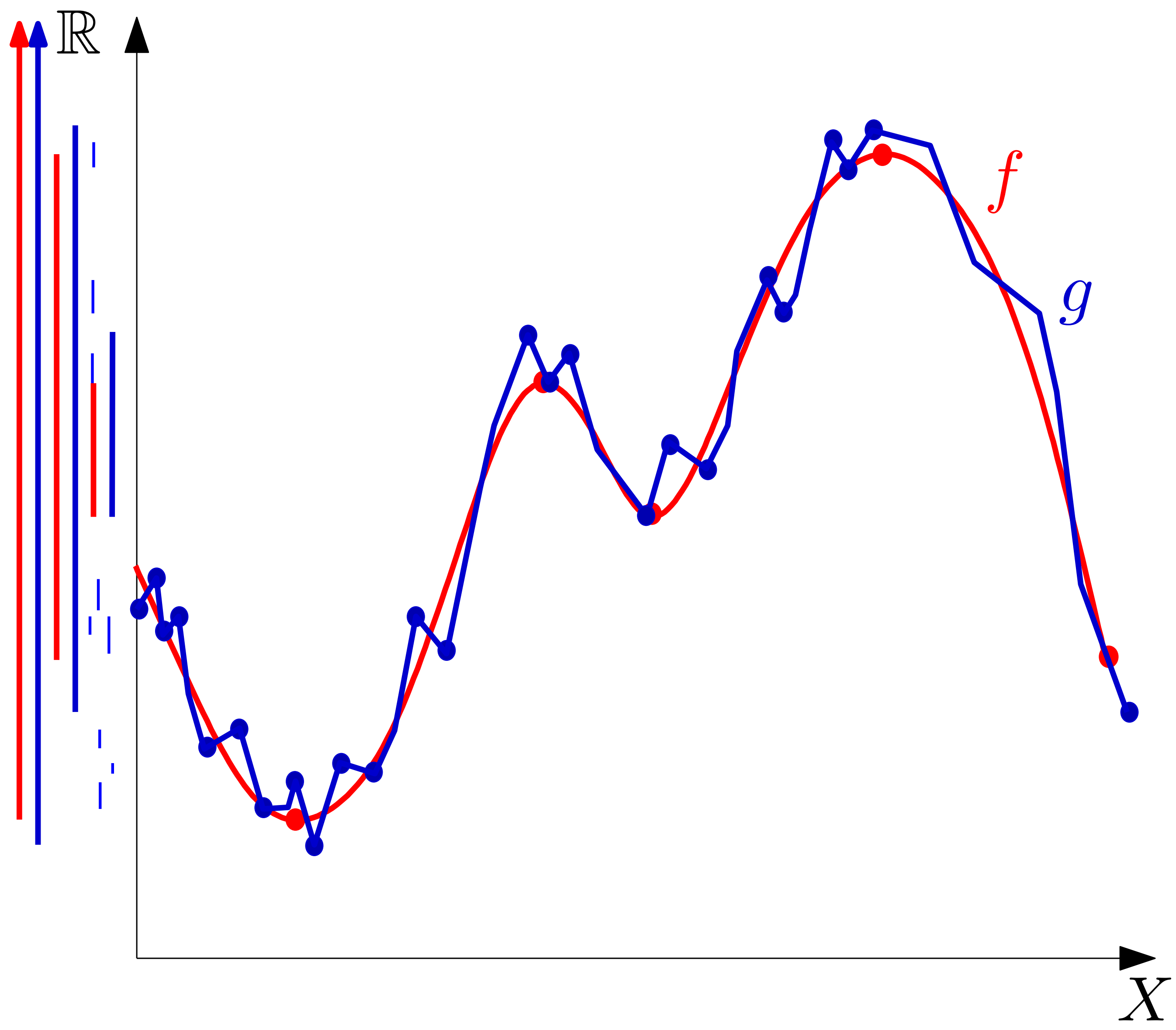
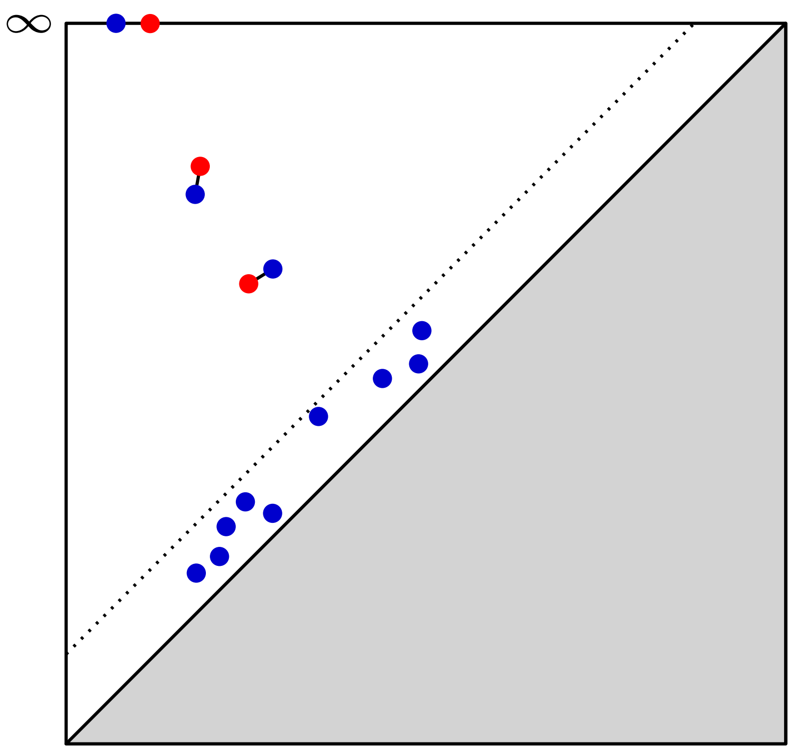




Thm: $d_b(D(f), D(g)) \leq \|f - g\|_\infty$

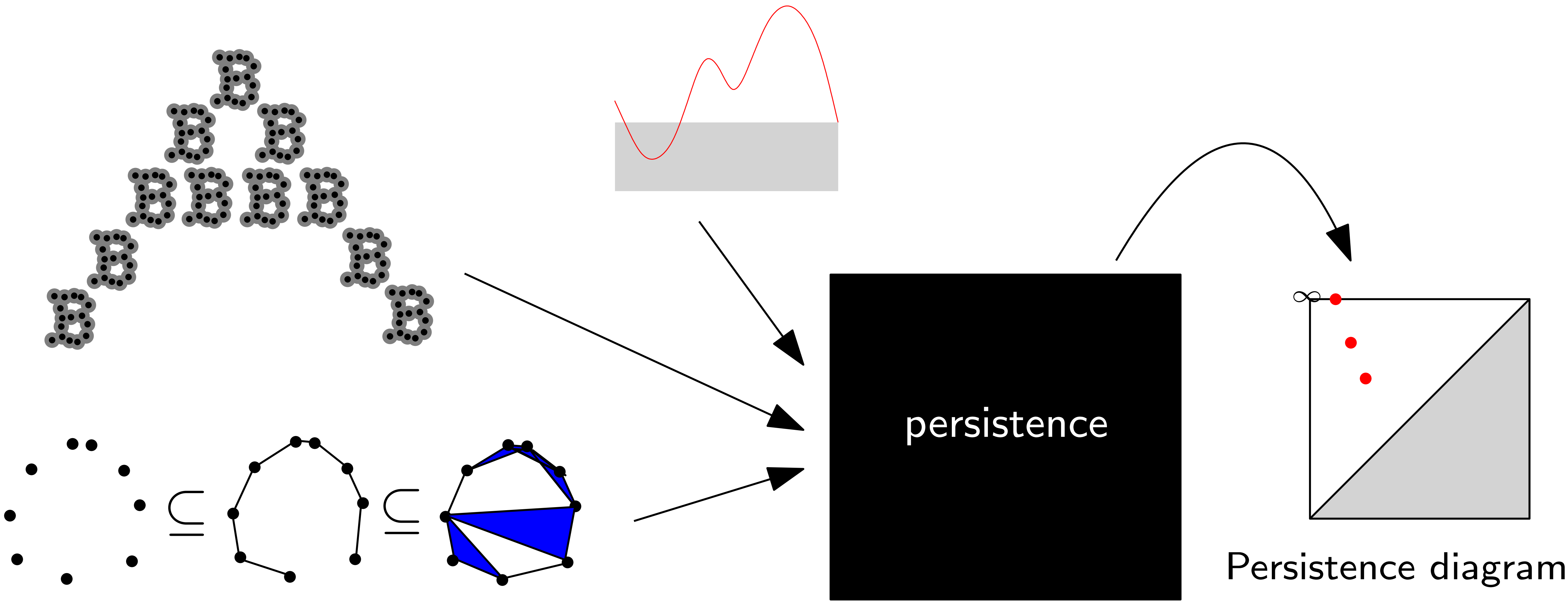
In [ ]:
```
BD = gudhi.representations.BottleneckDistance(epsilon=.001)
BD.fit([st1.persistence_intervals_in_dimension(1)])
bd = BD.transform([st2.persistence_intervals_in_dimension(1)])

WD = gudhi.representations.WassersteinDistance(internal_p=2, order=2)
WD.fit([st1.persistence_intervals_in_dimension(1)])
wd = WD.transform([st2.persistence_intervals_in_dimension(1)])
```

I. Turn datasets into simplicial complexes

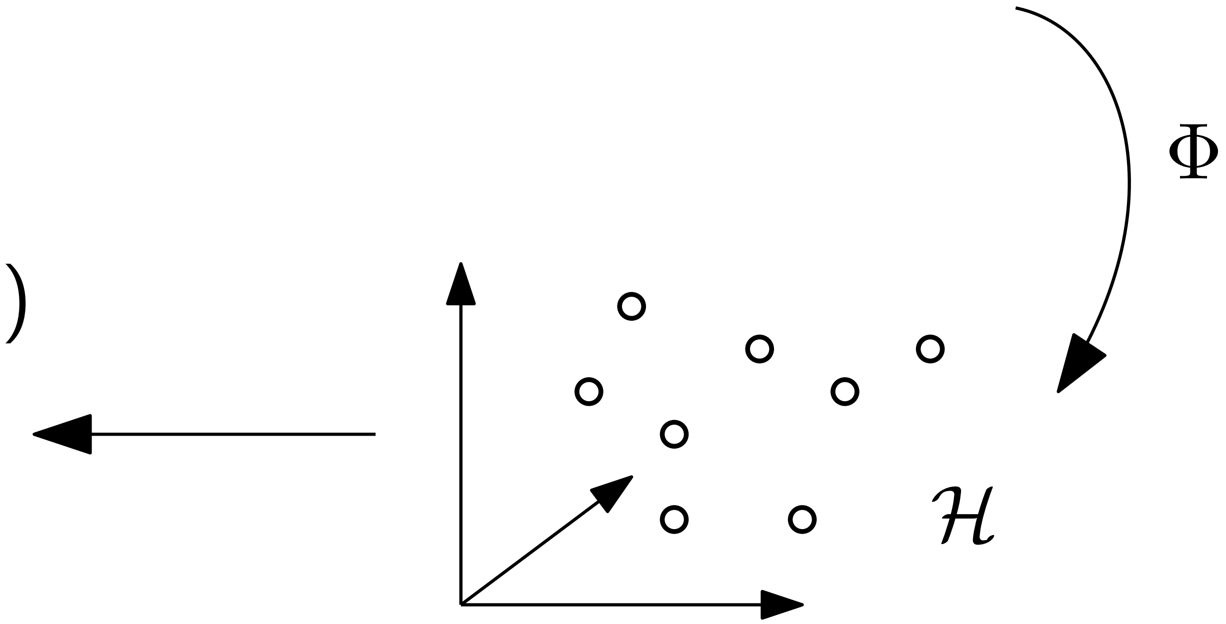
II. Compute and compare persistence diagrams

III. Feed / regularize ML models w/ topology

Persistence diagrams and ML



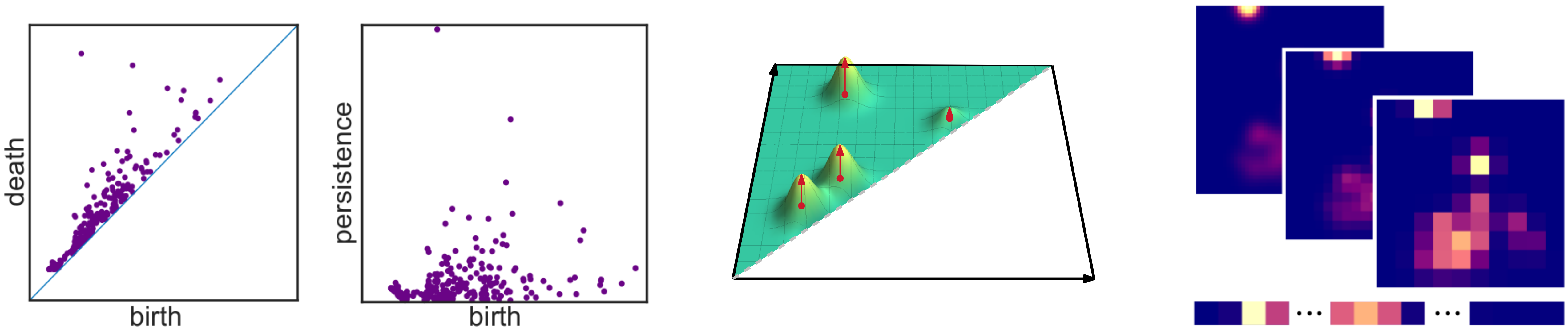
- Classifier (RF, SVM, NN etc.)
- Dim. red. (PCA, MDS, UMAP, t-SNE)
- Clustering (DBSCAN, K-means, etc.)



Etc.

Persistence representations

[*Persistence Images: A Stable Vector Representation of Persistent Homology*, Adams et al., JMLR, 2017]



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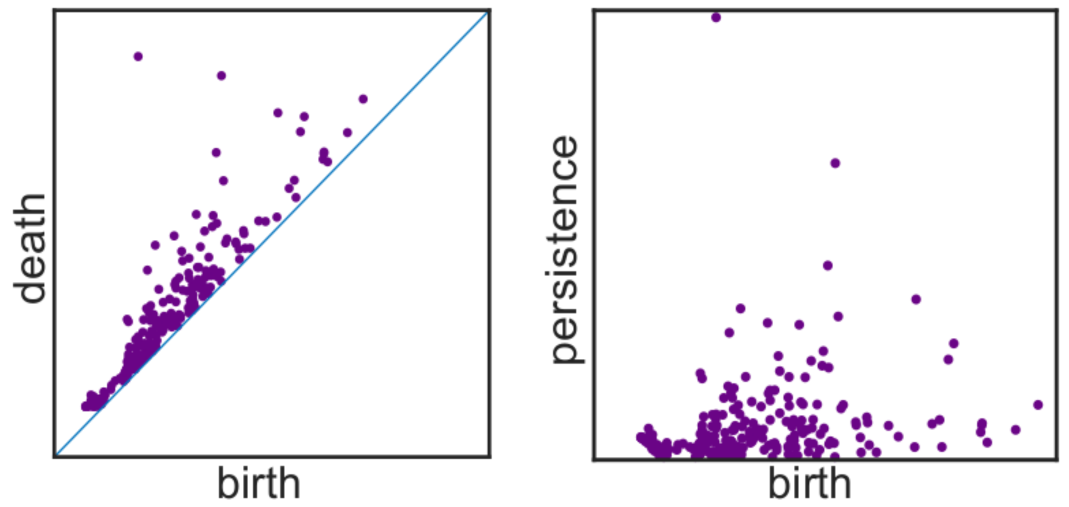
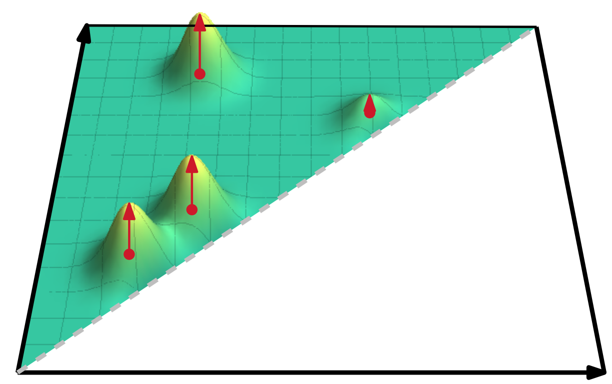
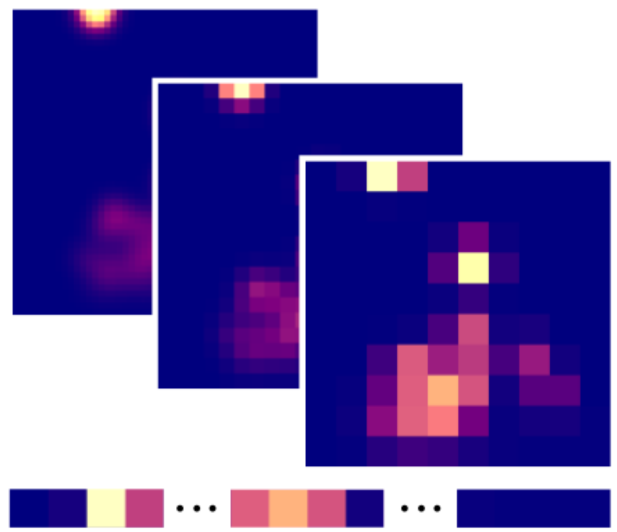
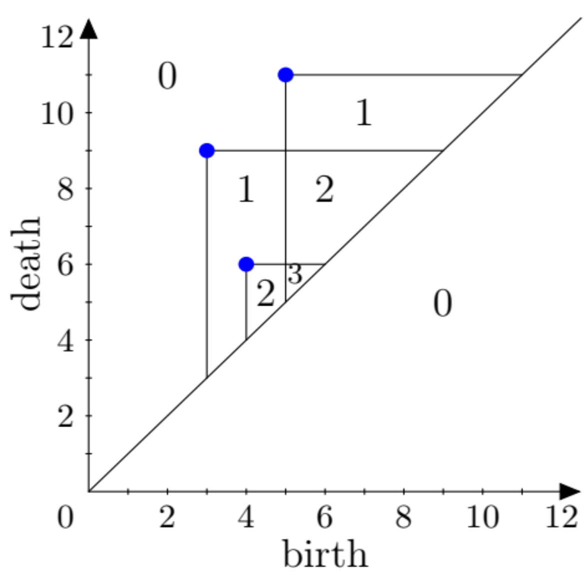
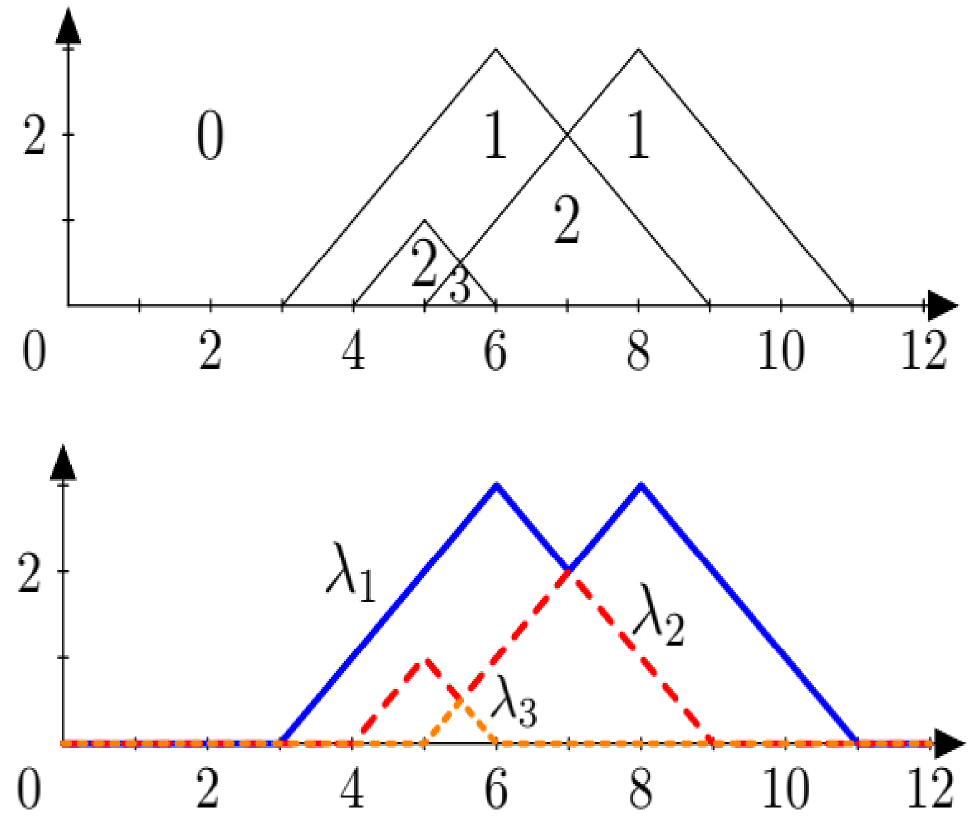
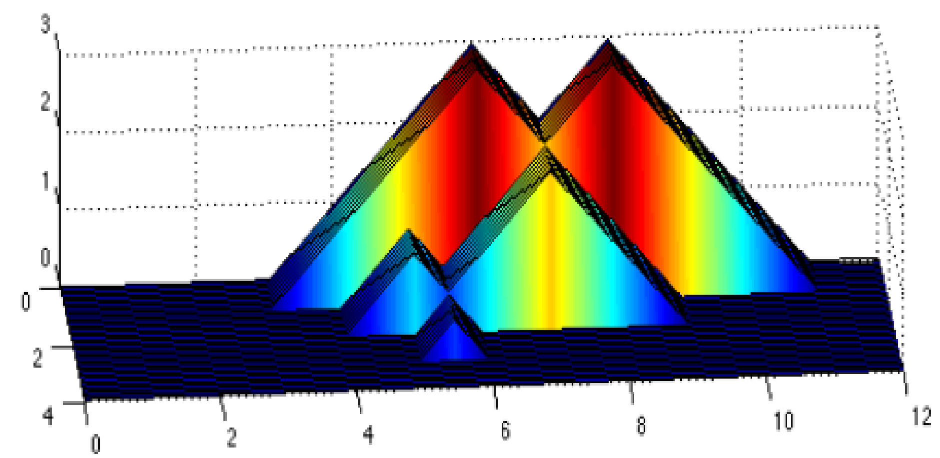








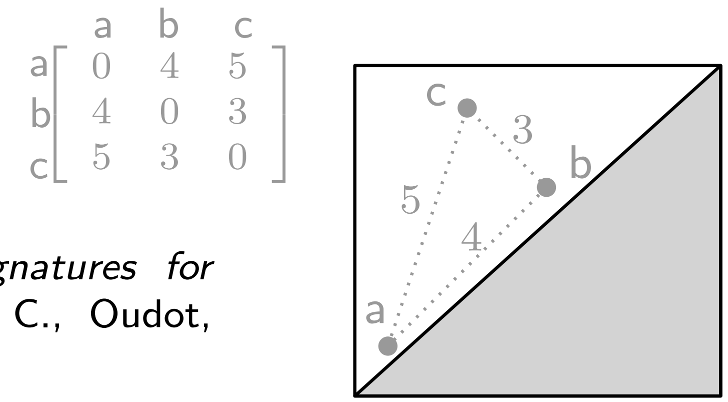


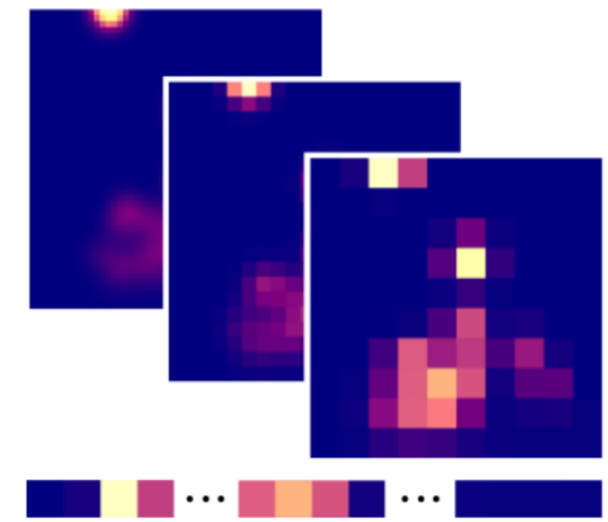


[*Statistical Topological Data Analysis using Persistence Landscapes*, Bubenik, JMLR, 2015]

Persistence representations

- images [*Persistence Images: A Stable Vector Representation of Persistent Homology*, Adams et al., JMLR, 2017]



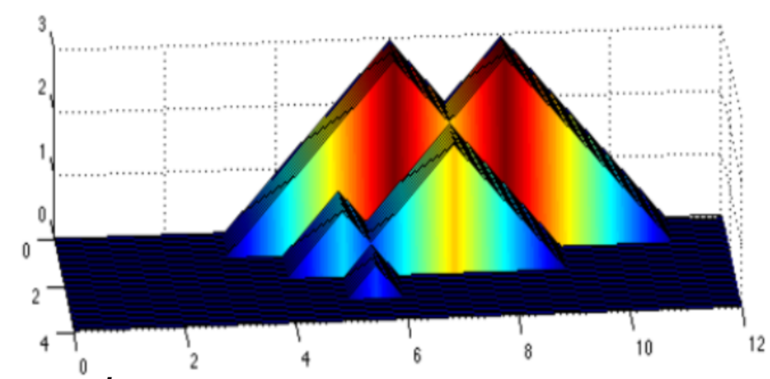


- finite metric spaces [*Stable topological signatures for points on 3D shapes*, C., Oudot, Ovsjanikov, SGP, 2015]

- polynomial roots or evaluations [*Tropical coordinates on the space of persistence barcodes*, Kalisnik, FoCM, 2018]

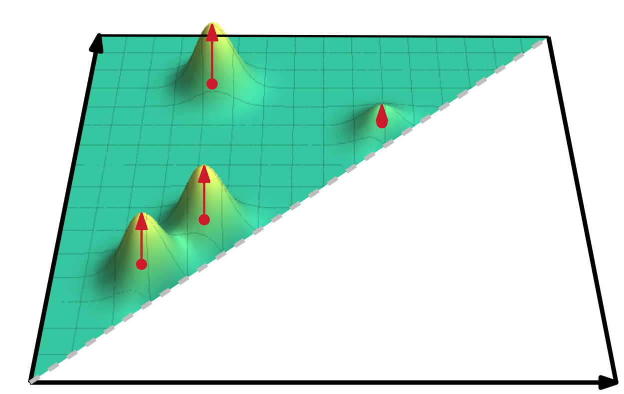
$$\{p_1, \ldots, p_n\} \mapsto (P_1(p_1, \ldots, p_n), \ldots, P_r(p_1, \ldots, p_n), \ldots)$$

- landscapes [*Statistical Topological Data Analysis using Persistence Landscapes*, Bubenik, JMLR, 2015]



- discrete measures:

→ Fisher information [*Persistence Fisher kernel: a Riemannian manifold kernel for persistence diagrams*, Le, Yamada, NeurIPS, 2018]



→ convolution with weighted kernel [*Persistence weighted Gaussian kernel for topological data analysis*, Kusano, Hiraoka, Fukumizu, ICML, 2016]

→ heat diffusion [*A stable multi-scale kernel for topological machine learning*, Reininghaus et al., CVPR, 2015]

→ optimal transport [*Sliced Wasserstein distance between PDs*, C., Cuturi, Oudot, ICML, 2017]

Persistence representations

In [20]:

```
from sklearn.preprocessing   import MinMaxScaler
from sklearn.pipeline        import Pipeline
from sklearn.svm             import SVC
from sklearn.ensemble        import RandomForestClassifier
from sklearn.neighbors       import KNeighborsClassifier

# Definition of pipeline
pipe = Pipeline([("Separator", gd.representations.DiagramSelector(limit=np.inf, point_type="finite")),
                 ("Scaler",    gd.representations.DiagramScaler(scalers=[([0,1], MinMaxScaler())])),
                 ("TDA",       gd.representations.PersistenceImage()),
                 ("Estimator", SVC())])

# Parameters of pipeline. This is the place where you specify the methods you want to use to handle diagrams
param =    [{"Scaler__use":         [False],
             "TDA":                 [gd.representations.SlicedWassersteinKernel()],
             "TDA__bandwidth":      [0.1, 1.0],
             "TDA__num_directions": [20],
             "Estimator":           [SVC(kernel="precomputed", gamma="auto")]},

            {"Scaler__use":         [False],
             "TDA":                 [gd.representations.PersistenceWeightedGaussianKernel()],
             "TDA__bandwidth":      [0.1, 0.01],
             "TDA__weight":         [lambda x: np.arctan(x[1]-x[0])],
             "Estimator":           [SVC(kernel="precomputed", gamma="auto")]},

            {"Scaler__use":         [True],
             "TDA":                 [gd.representations.PersistenceImage()],
             "TDA__resolution":     [ [5,5], [6,6] ],
             "TDA__bandwidth":      [0.01, 0.1, 1.0, 10.0],
             "Estimator":           [SVC()]},

            {"Scaler__use":         [True],
             "TDA":                 [gd.representations.Landscape()],
             "TDA__resolution":     [100],
             "Estimator":           [RandomForestClassifier()]},

            {"Scaler__use":         [False],
             "TDA":                 [gd.representations.BottleneckDistance()],
             "TDA__epsilon":        [0.1],
             "Estimator":           [KNeighborsClassifier(metric="precomputed")]}
           ]
```

Learn persistence representations

Learn persistence representations

[*PersLay: A Neural Network Layer for Persistence Diagrams and New Graph Topological Signatures*, C., Chazal, Ike, Lacombe, Royer, Umeda, AISTATS, 2019]

$$\mathrm{PersLay}(D) = \rho\left(\mathsf{op}\{w(p) \cdot \phi(p)\}_{p \in D}\right)$$

Permutation-invariant operation

Weight function

Point transformation

Learn persistence representations

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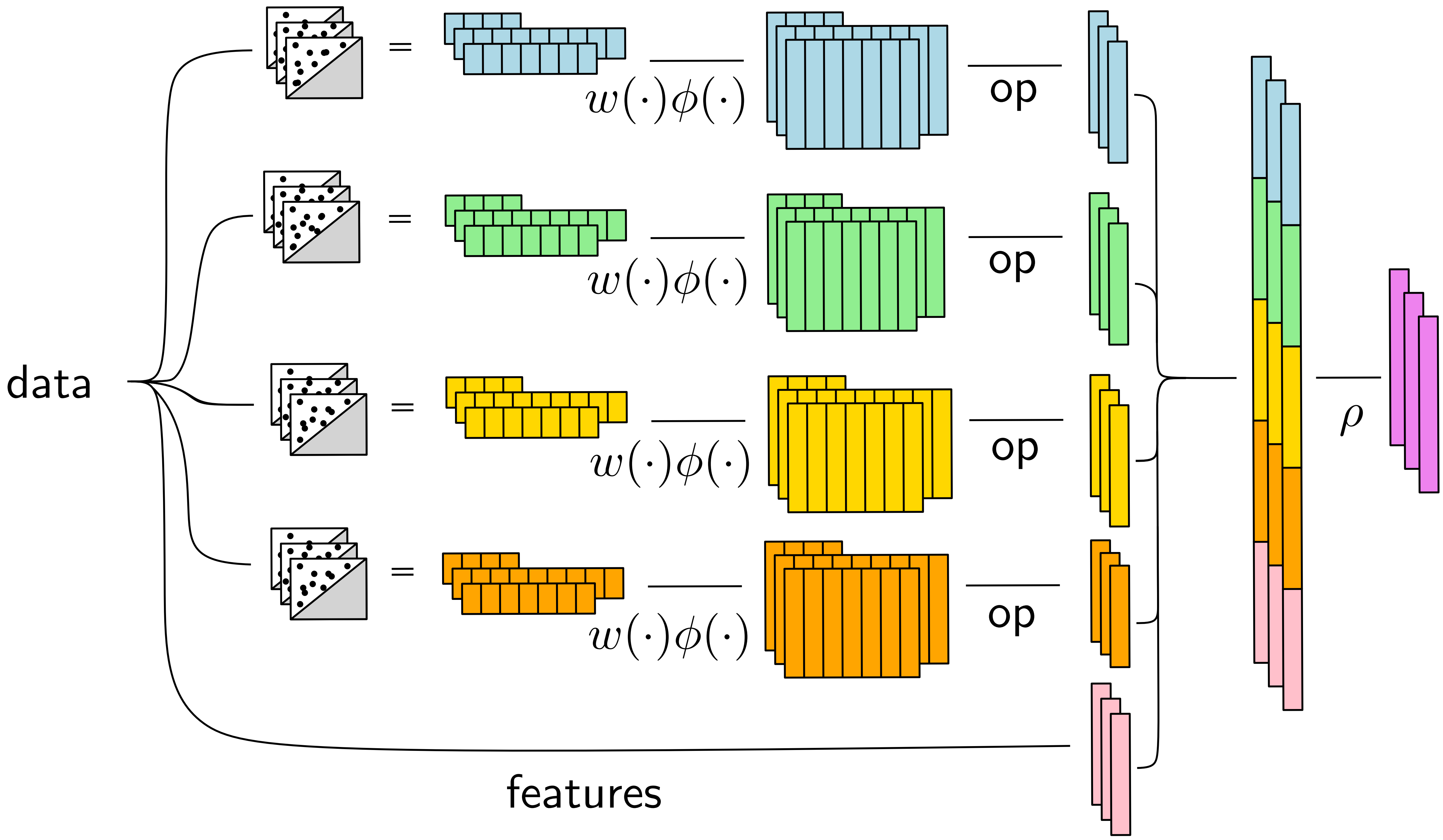

Learn persistence representations

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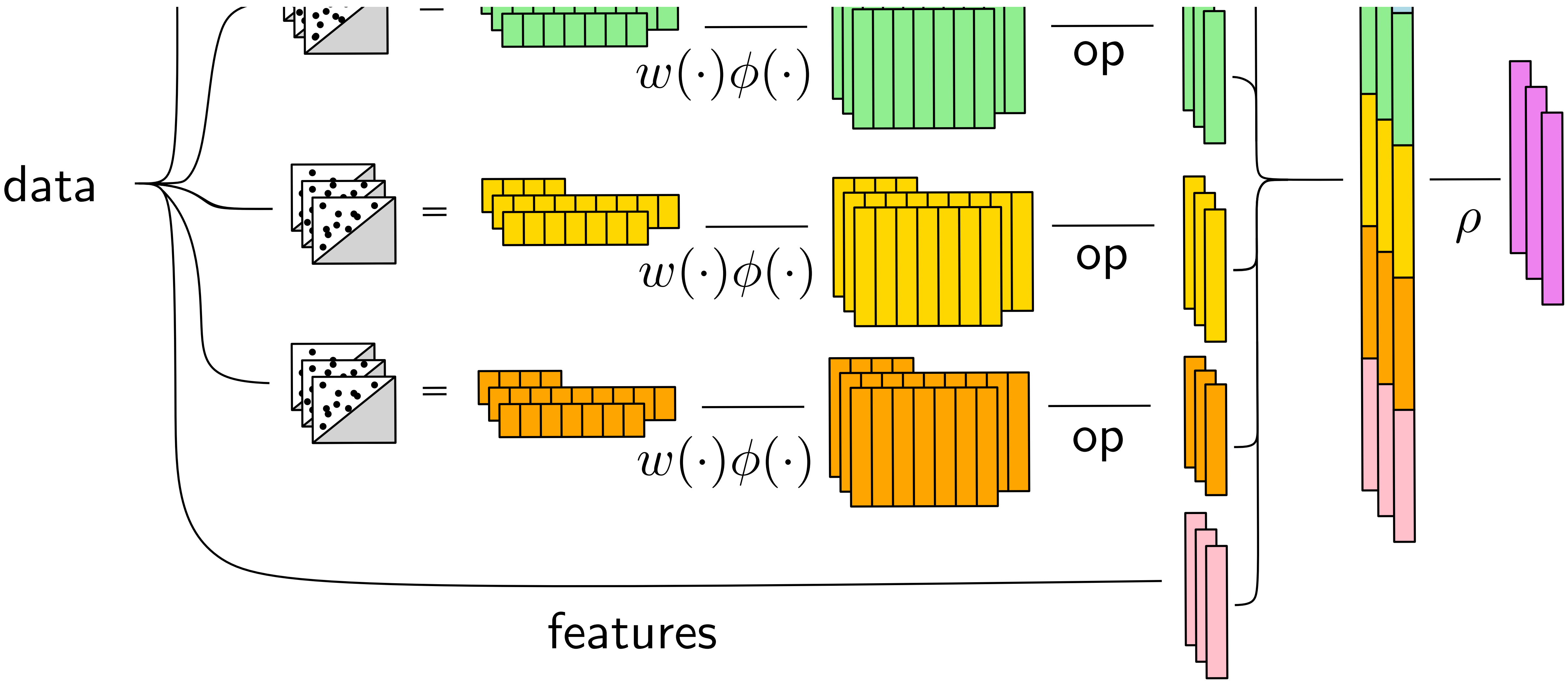
```
In [ ]: rho = tensorflow.identity
        phi = gudhi.tensorflow.perslay.GaussianPerslayPhi((100, 100), ((-.5, 1.5), (-.5, 1.5)), .1)
        weight = gudhi.tensorflow.perslay.GridPerslayWeight(np.array(
                    numpy.random.uniform(size=[100,100]),dtype=np.float32),((-0.01, 1.01),(-0.01, 1.01)))
        perm_op = tensorflow.math.reduce_sum

        perslay = gudhi.tensorflow.perslay.Perslay(phi=phi, weight=weight, perm_op=perm_op, rho=rho)
        vectors = perslay(diagrams)
```



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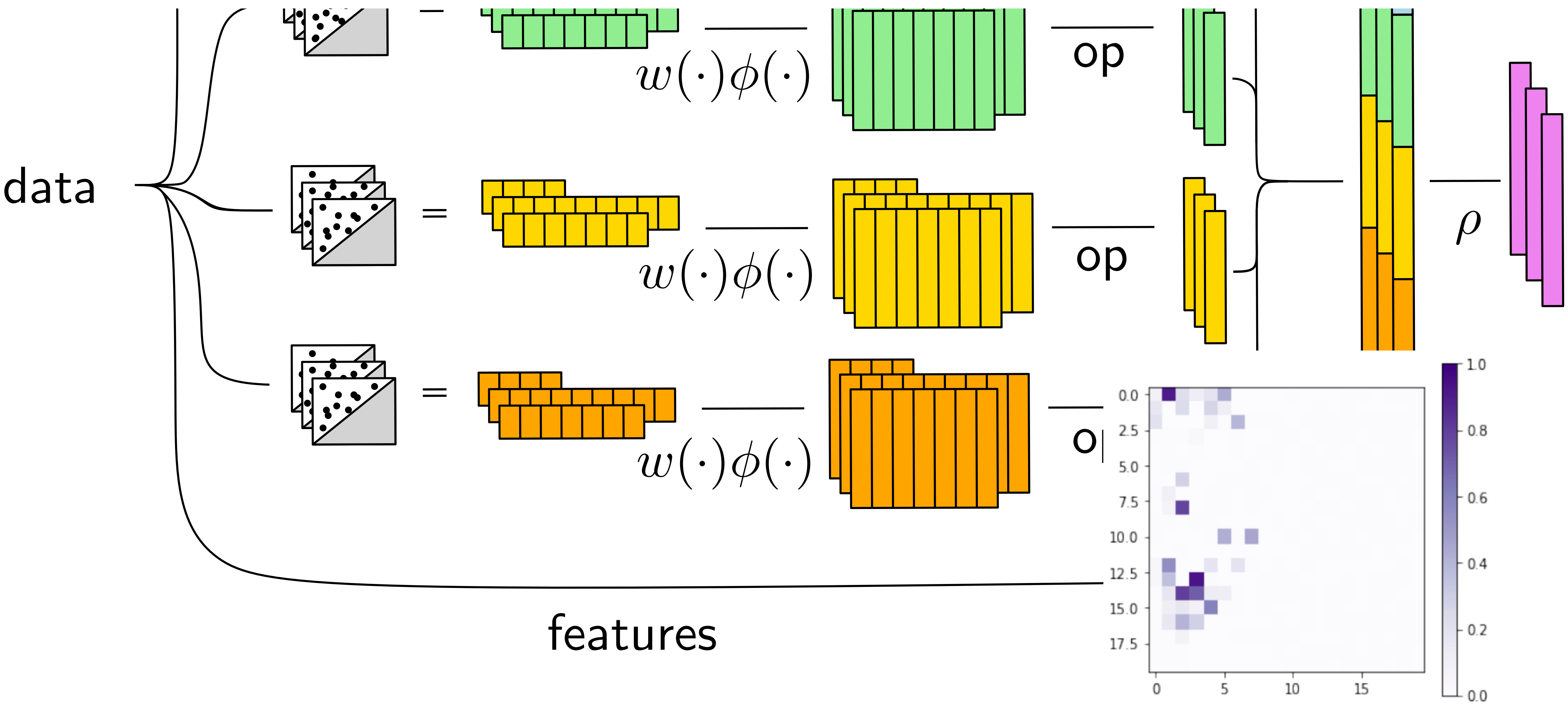

Weight function learnt

Learn filtrations

Learn filtrations

A persistence diagram D is made of all $(\mathcal{F}(\sigma_+), \mathcal{F}(\sigma_-)) \in \mathbb{R}^2$ where σ_+ (resp. σ_-) is positive (resp. negative), and $\mathcal{F}$ is the filtration function.

Thus we can define the gradient of a point $p = (\mathcal{F}(\sigma_+), \mathcal{F}(\sigma_-)) \in D$ as

$$\nabla p = [\nabla \mathcal{F}(\sigma_+), \nabla \mathcal{F}(\sigma_-)]$$

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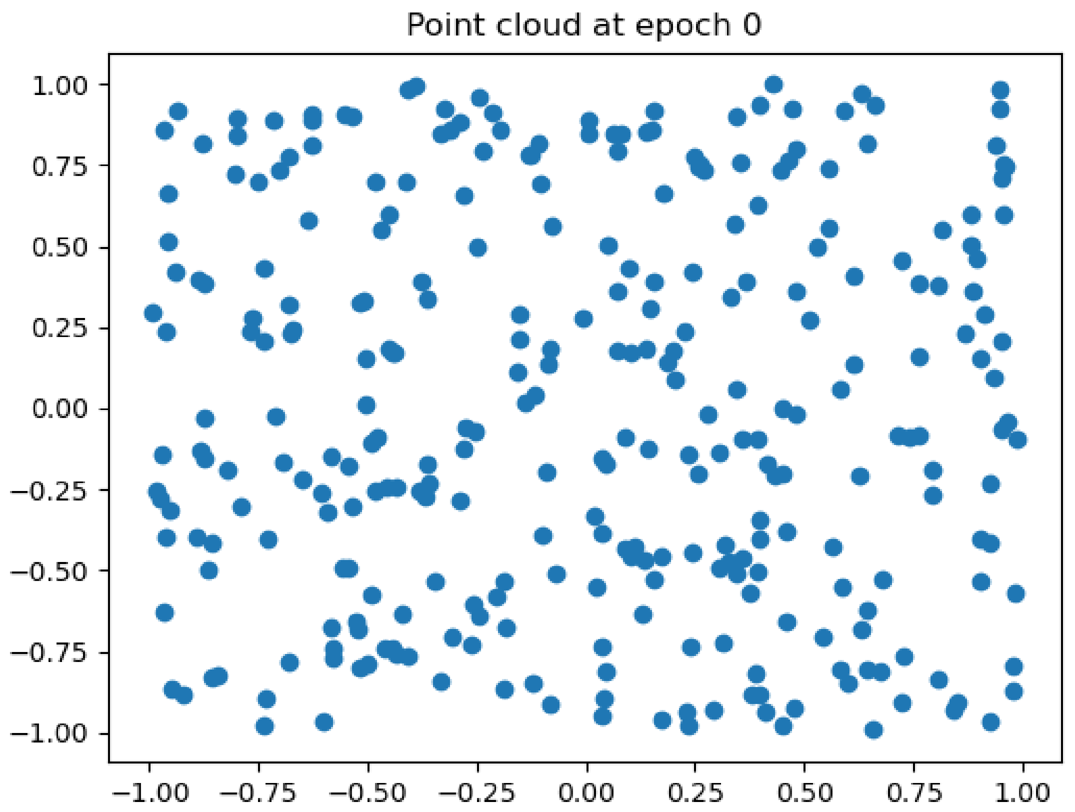

Ex: VR filtration parametrized by a point cloud

Learn filtrations

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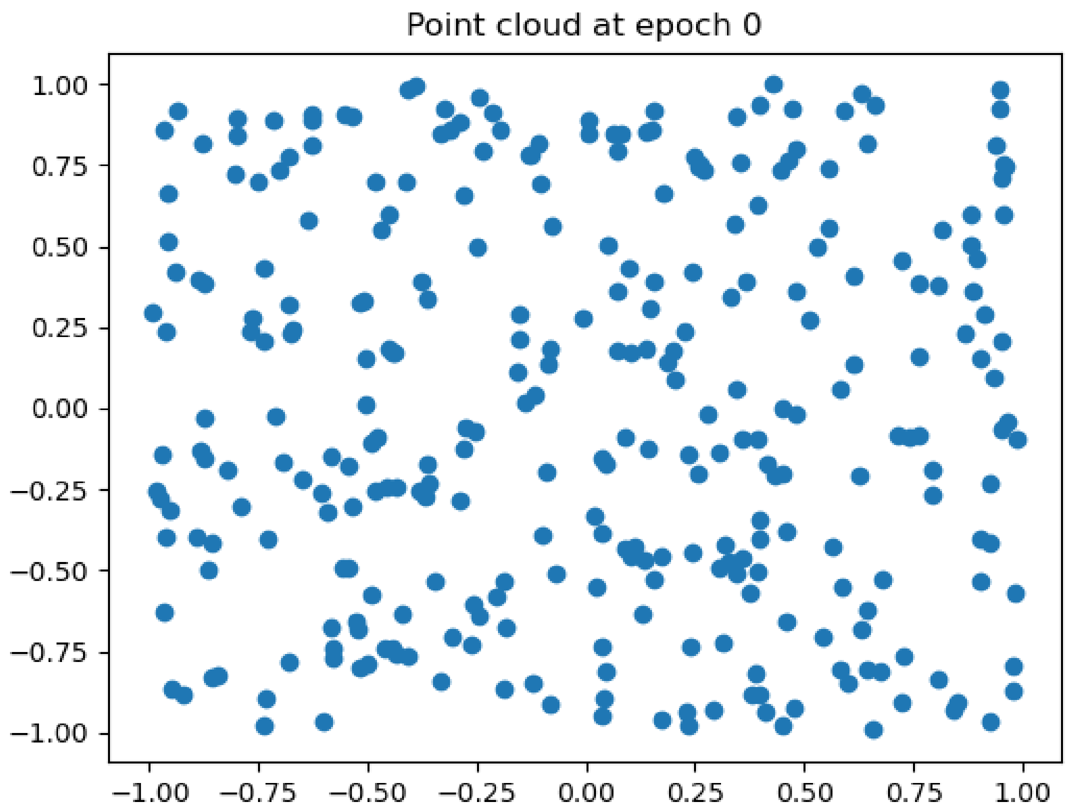

In [ ]:
```
optimizer = tensorflow.keras.optimizers.SGD(learning_rate=0.1)
for epoch in tqdm(range(200+1)):

    with tensorflow.GradientTape() as tape:
        dgm = gudhi.tensorflow.RipsLayer(maximum_edge_length=1., homology_dimensions=[1]).call(X)[0][0]
        # Opposite of the squared distances to the diagonal
        persistence_loss = -tensorflow.math.reduce_sum(tf.square(.5*(dgm[:,1]-dgm[:,0])))
        # Unit square regularization
        regularization = tensorflow.reduce_sum(tf.maximum(tf.abs(X)-1, 0))
        loss = persistence_loss + regularization
    gradients = tape.gradient(loss, [X])

    # We also apply a small random noise to the gradient to ensure convergence
    np.random.seed(epoch)
    gradients[0] = gradients[0] + numpy.random.normal(loc=0., scale=.001, size=gradients[0].shape)

    optimizer.apply_gradients(zip(gradients, [X]))
```

Learn filtrations

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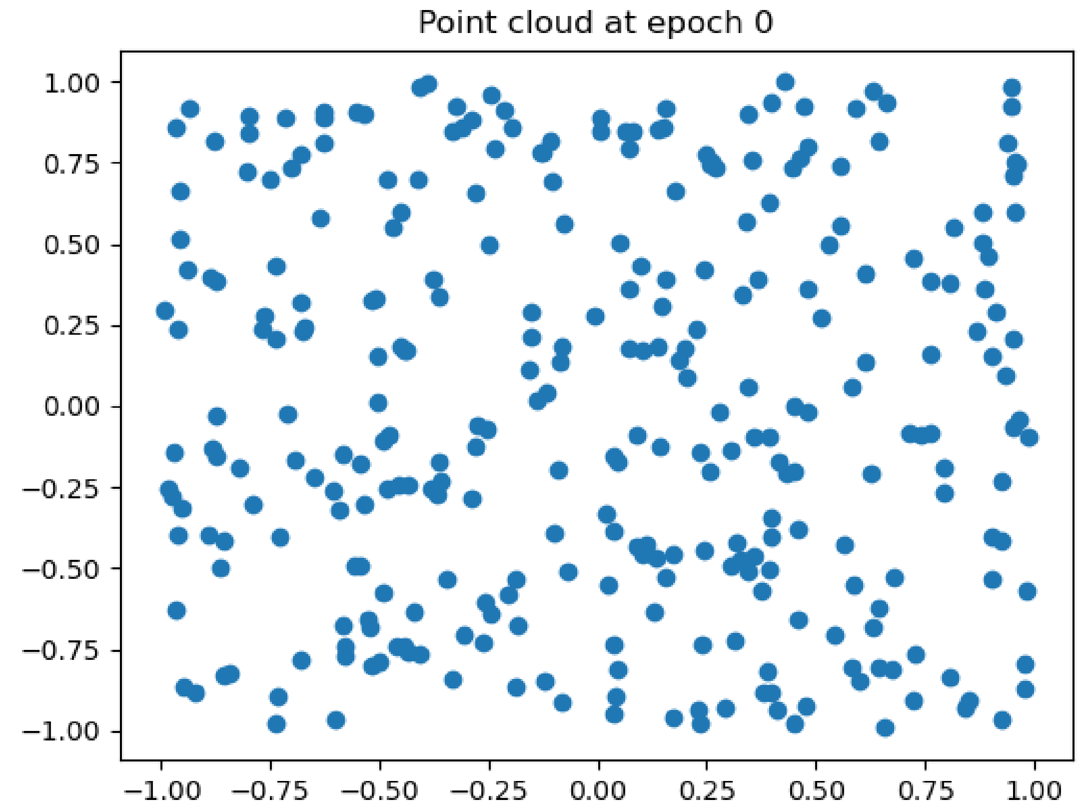
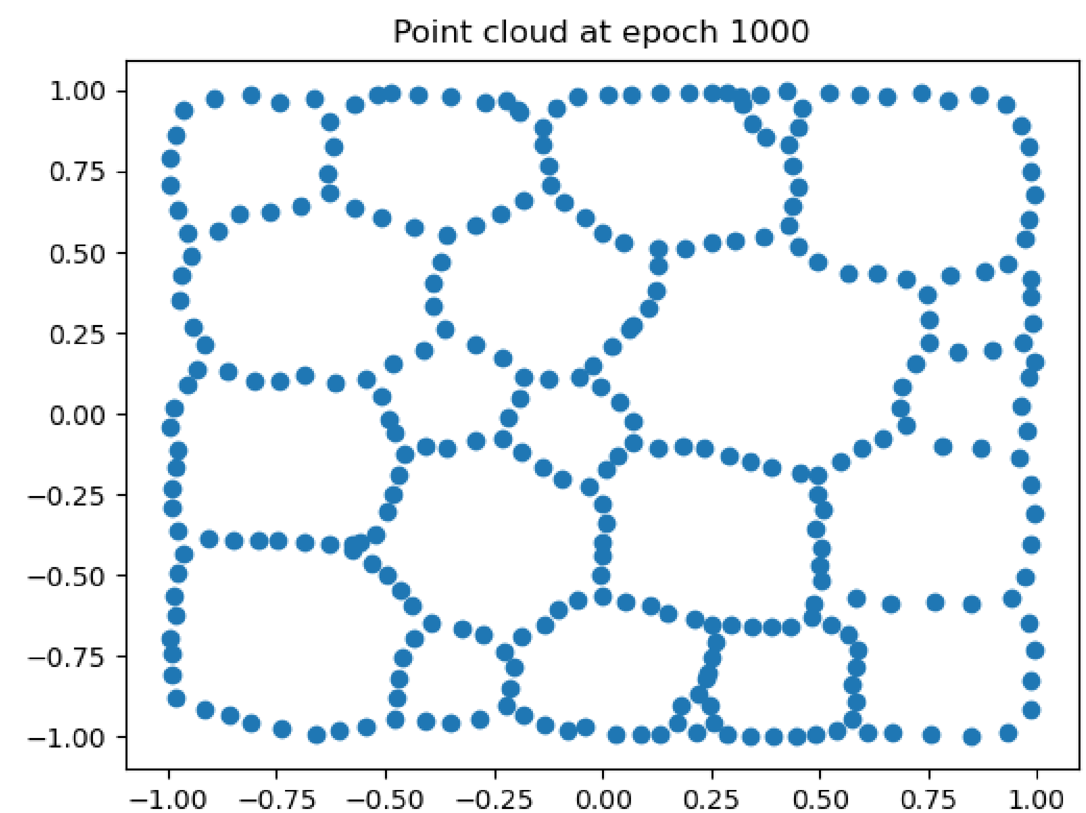
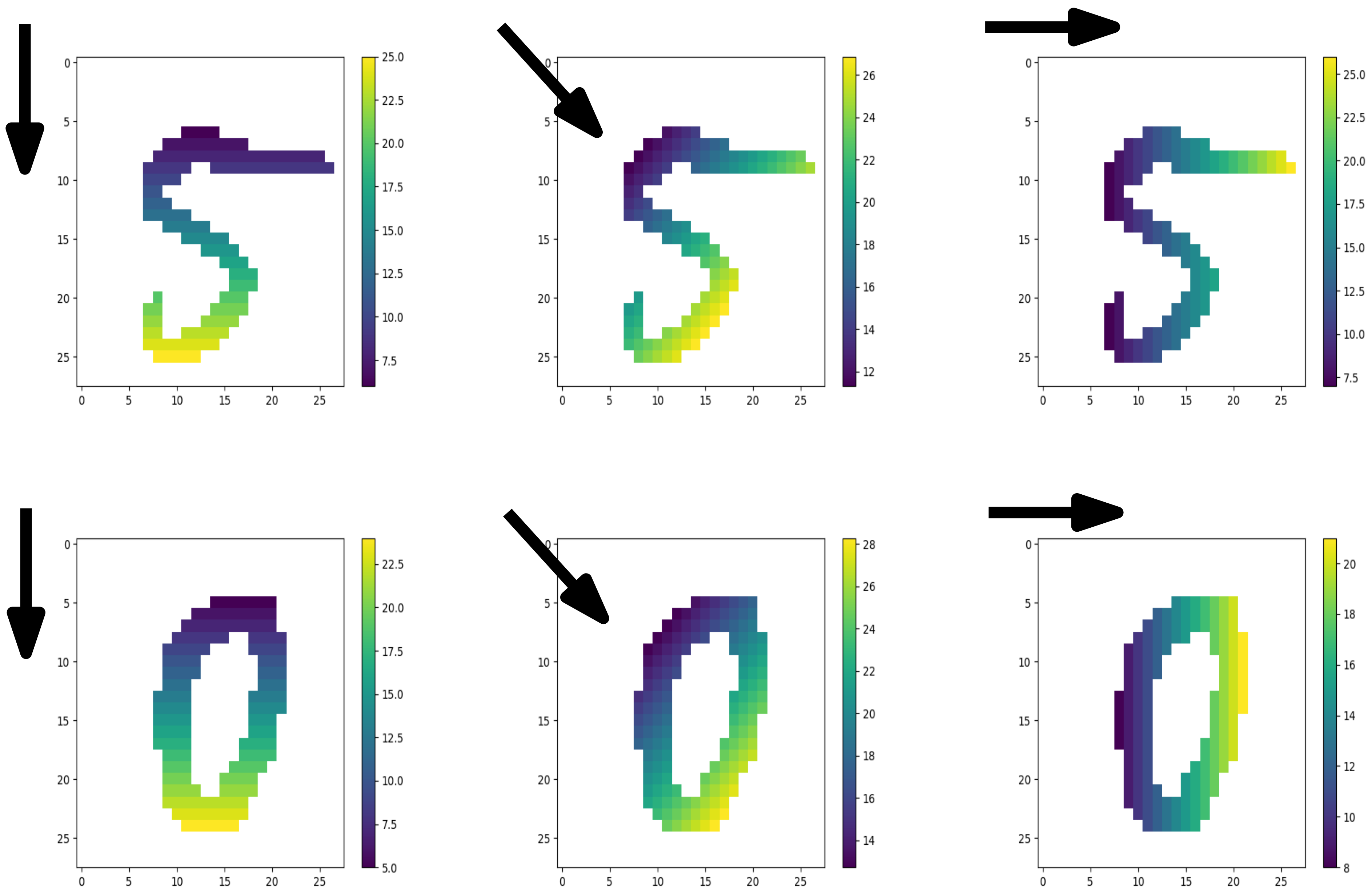




Learn filtrations

Ex: images filtered by a direction parameterized by angle



Learn filtrations

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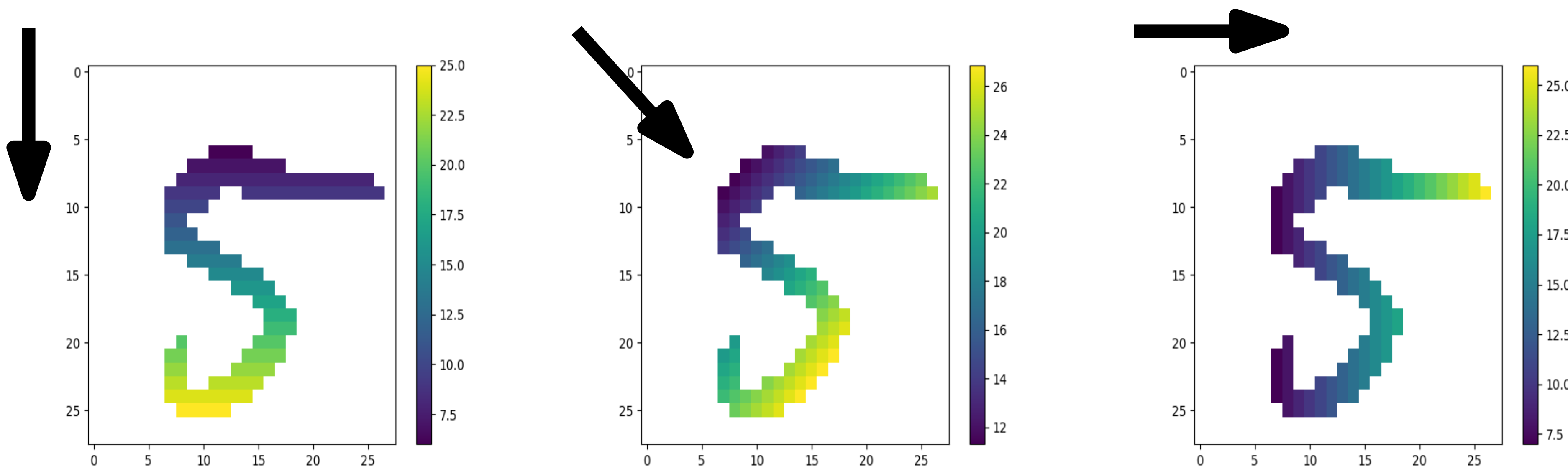
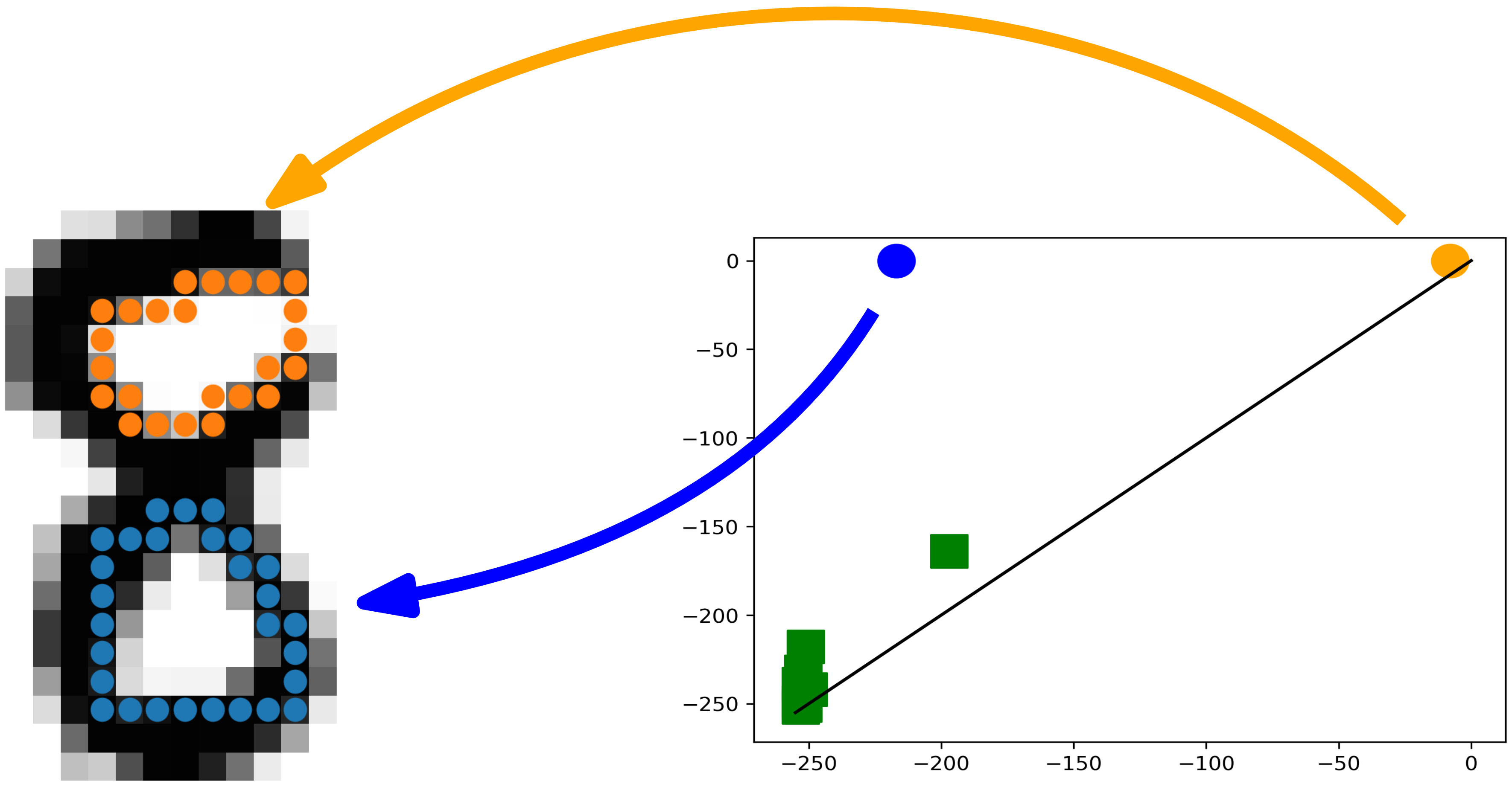


Dataset	Baseline	Before	After	Difference	Dataset	Baseline	Before	After	Difference
vs01	100.0	61.3	99.0	**+37.6**	vs26	99.7	98.8	98.2	-0.6
vs02	99.4	98.8	97.2	-1.6	vs28	99.1	96.8	96.8	0.0
vs06	99.4	87.3	98.2	**+10.9**	vs29	99.1	91.6	98.6	**+7.0**
vs09	99.4	86.8	98.3	**+11.5**	vs34	99.8	99.4	99.1	-0.3
vs16	99.7	89.0	97.3	**+8.3**	vs36	99.7	99.3	99.3	-0.1
vs19	99.6	84.8	98.0	**+13.2**	vs37	98.9	94.9	97.5	**+2.6**
vs24	99.4	98.7	98.7	0.0	vs57	99.7	90.5	97.2	**+6.7**
vs25	99.4	80.6	97.2	**+16.6**	vs79	99.1	85.3	96.9	**+11.5**

What's next?

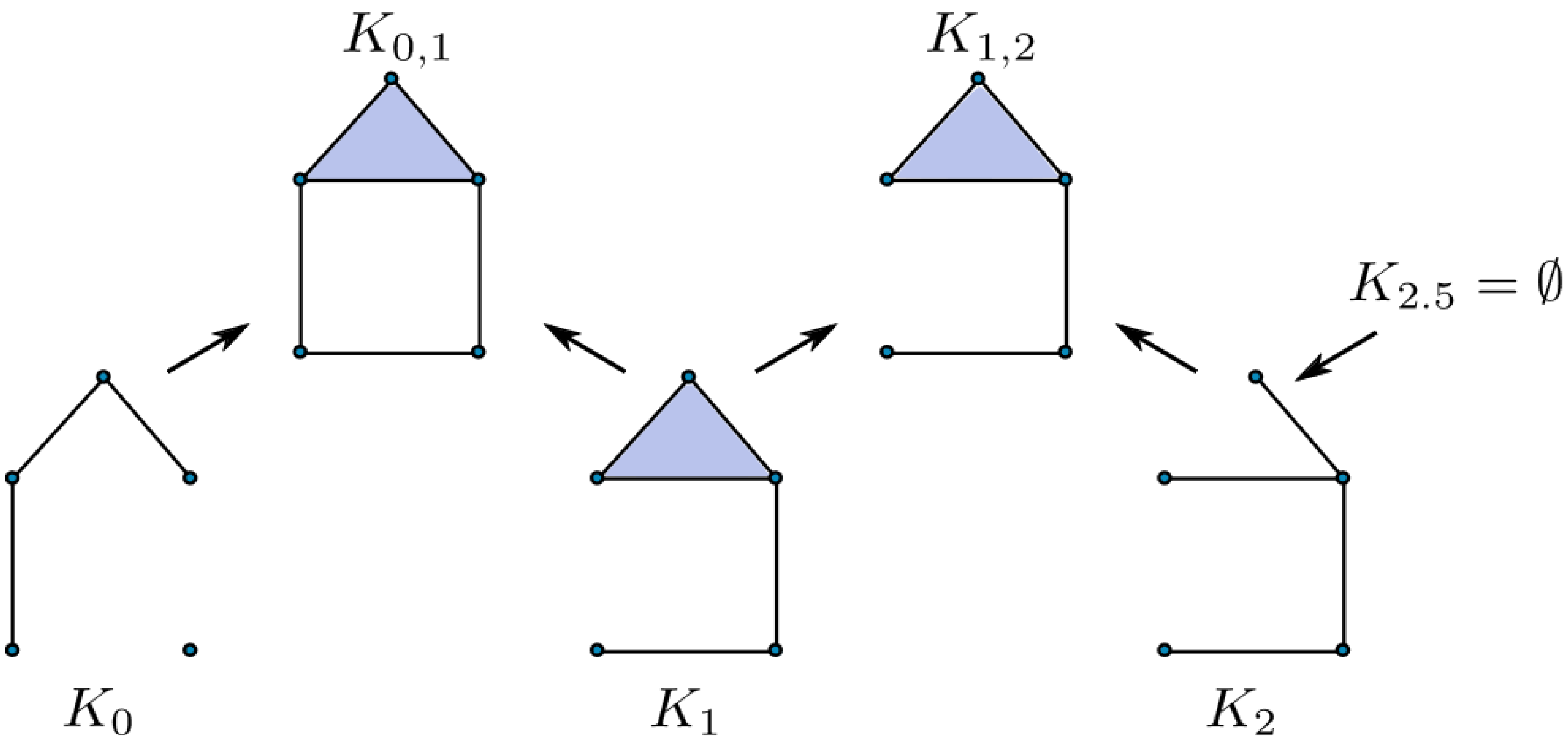
What's next?

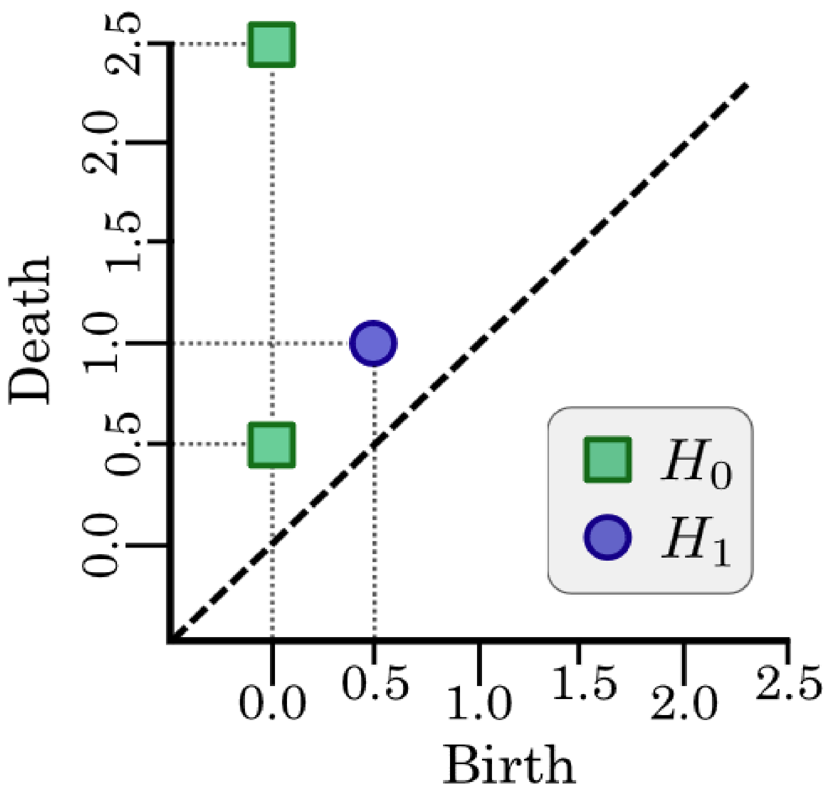
- Representative cycles



What's next?

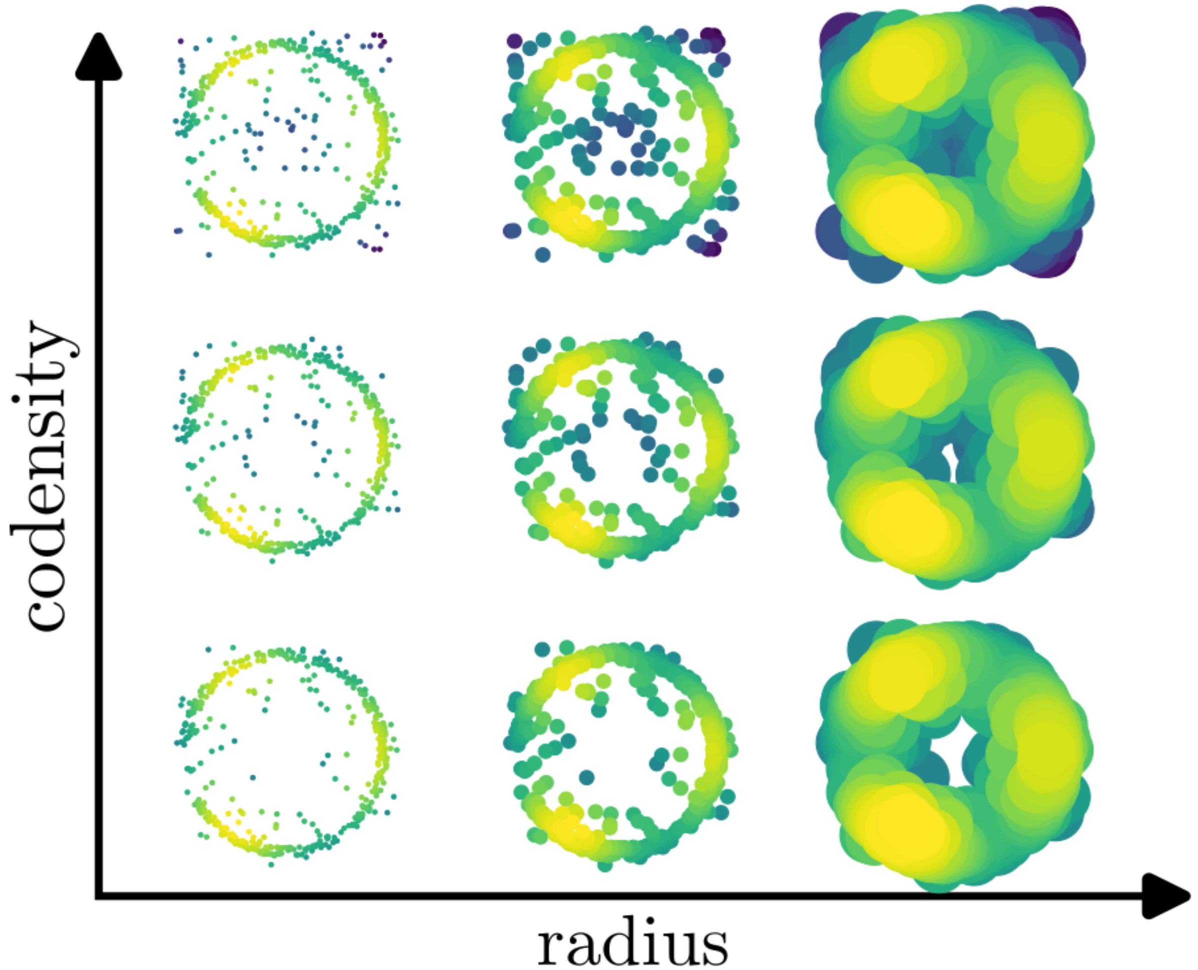
- Representative cycles
- Zigzag persistence





What's next?

- Representative cycles
- Zigzag persistence
- Multi-parameter persistence



What's next?

- Representative cycles
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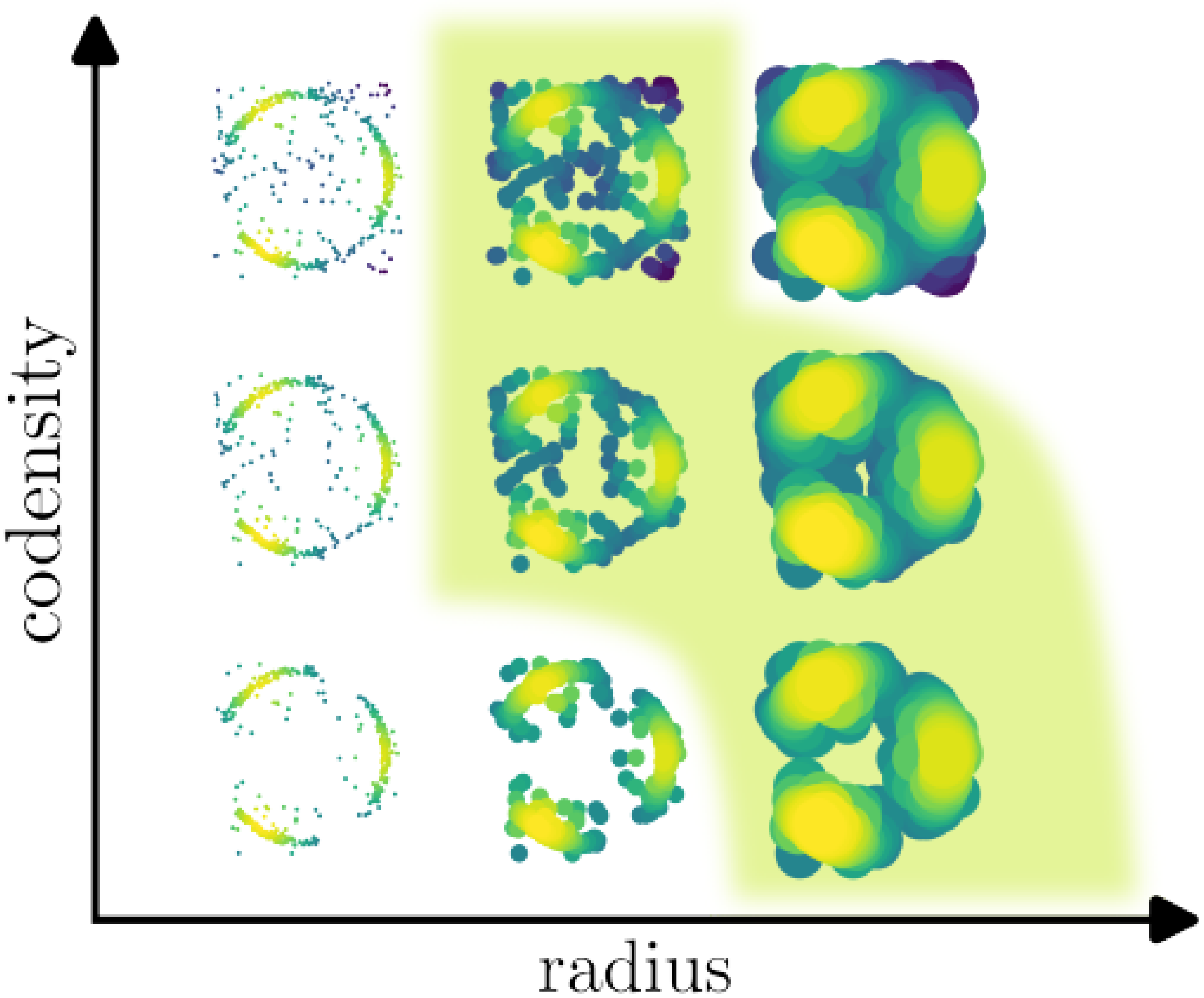

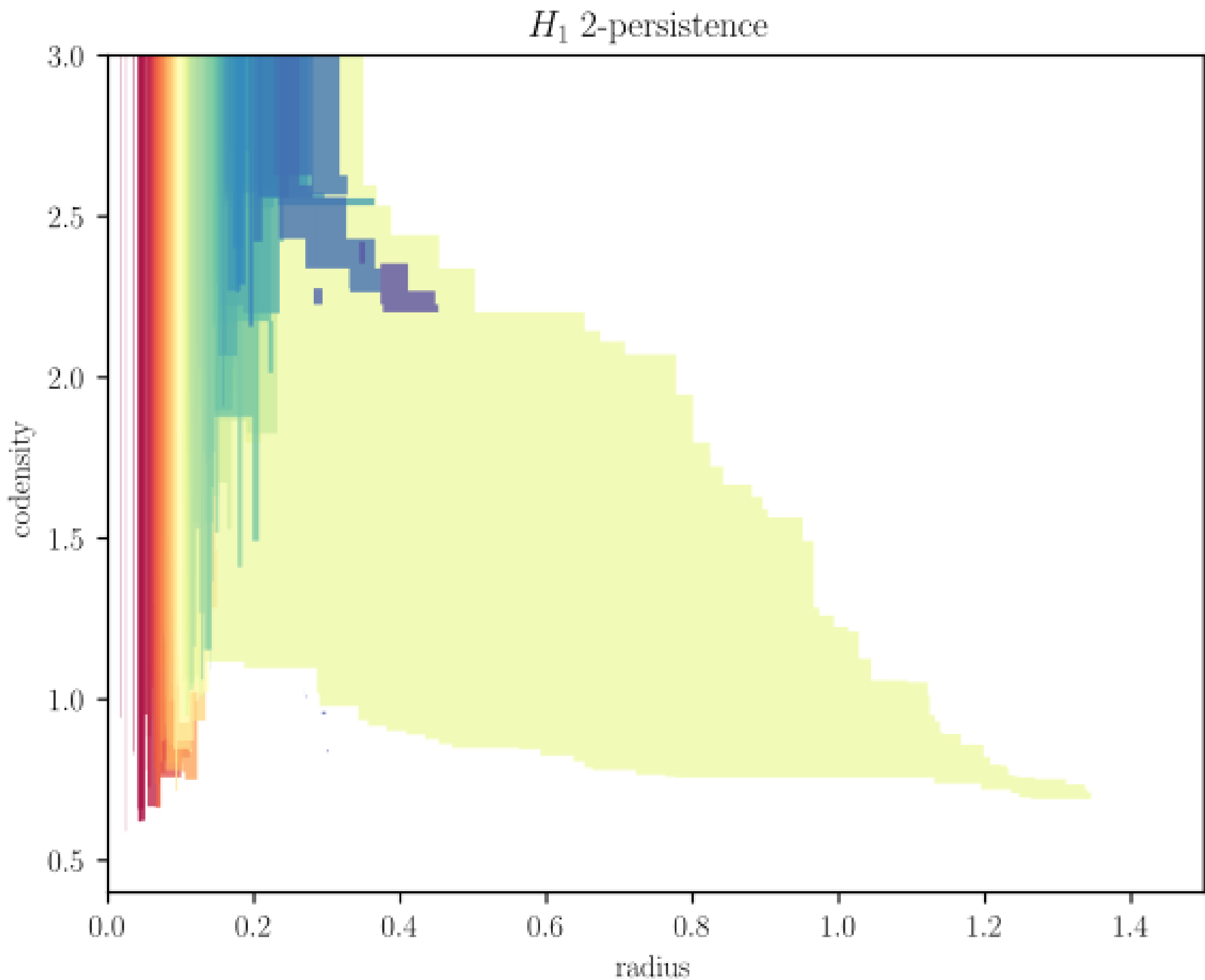

Thanks!!