DSC 214
Topological Data Analysis

Topic 7: Persistence in Practice

Instructor: Zhengchao Wan

Persistence-based Framework

- Persistence-based feature representation

Input data:
A collection of point sets, graphs, 2D/3D images, time-series , etc

→

Persistence feature space:
A collection of persistence-based feature representations (e.g, vectors)

→

Further data analysis:
Feed to data analysis pipelines, say SVM, CNN, etc

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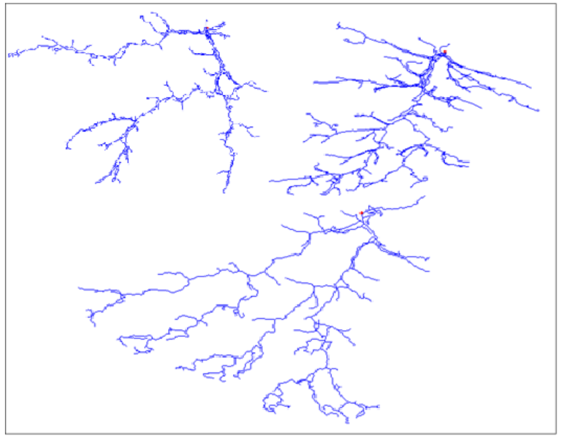

[Li, et al, PLOS One 2017]

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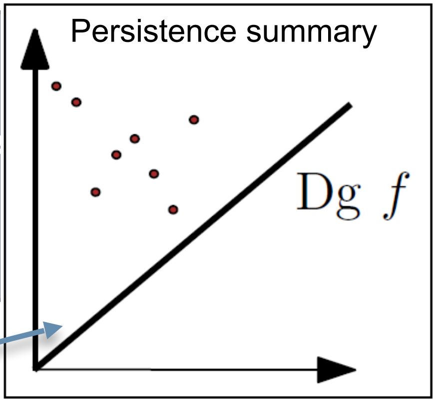

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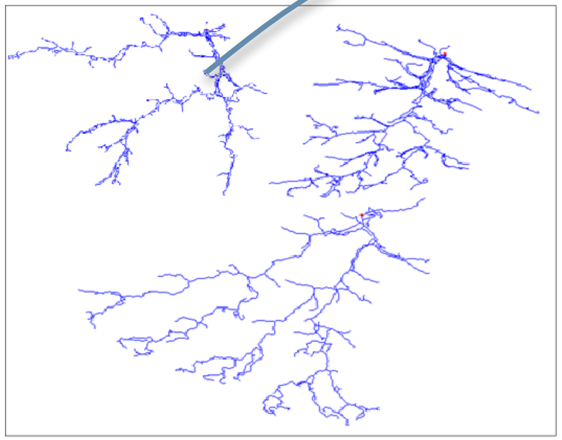

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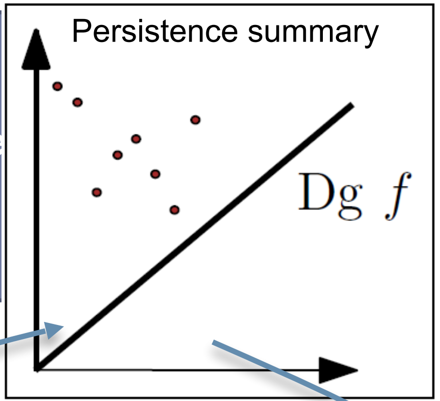

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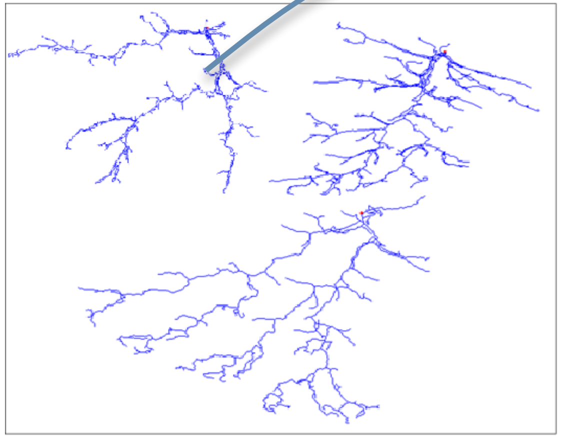

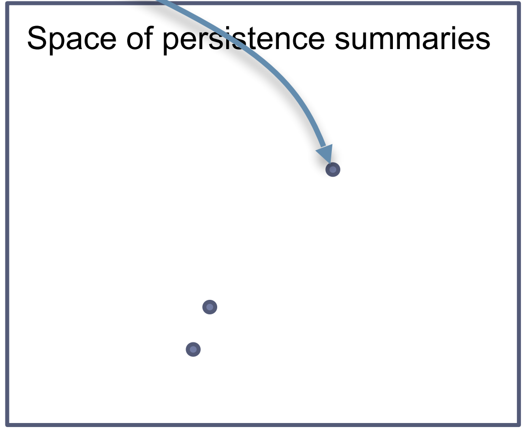

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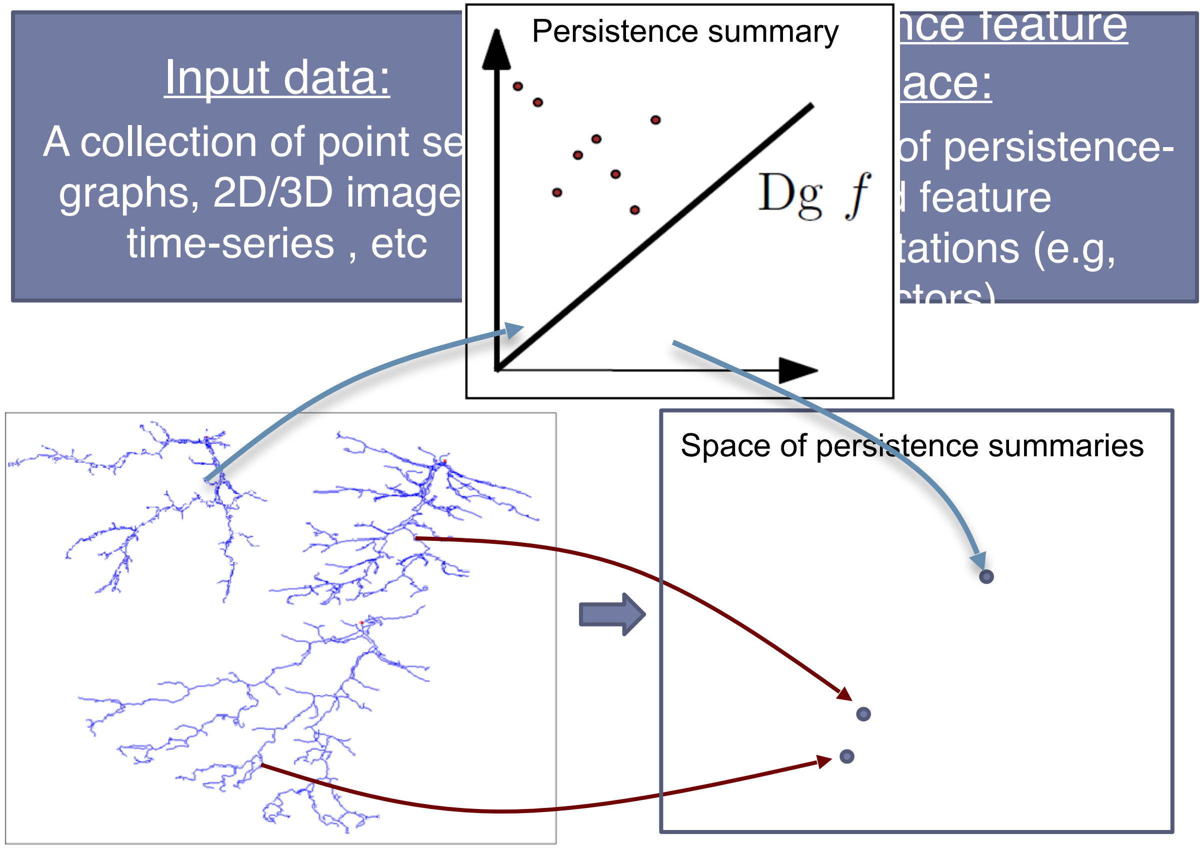

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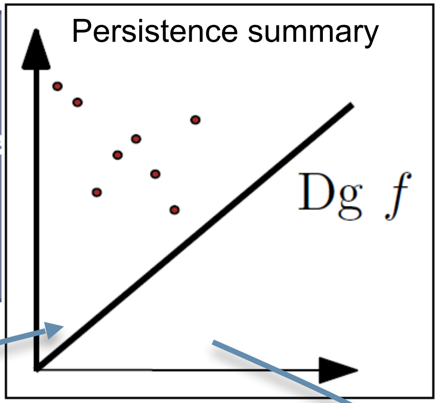

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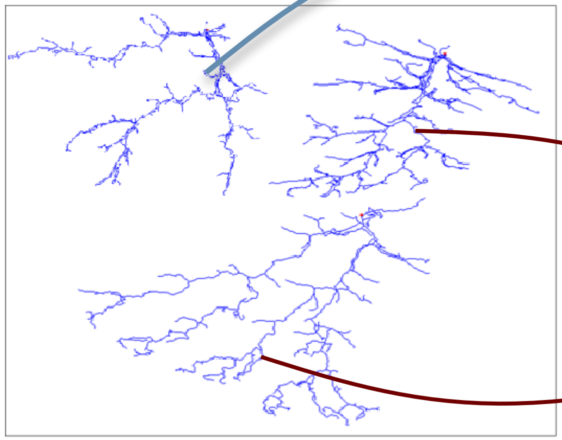

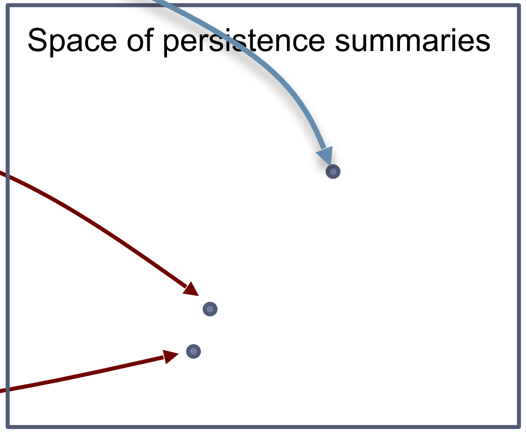

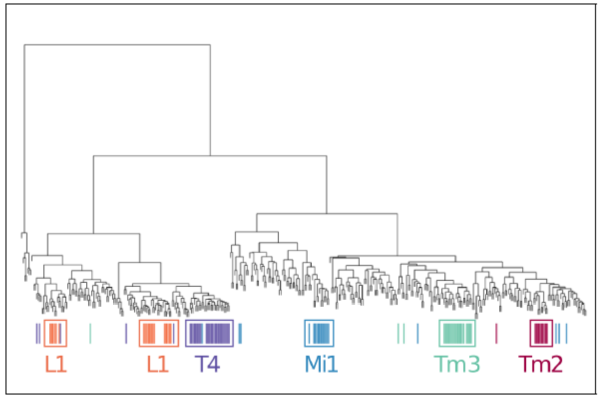

[Li, et al, PLOS One 2017]

- Use PH for different types of data

- Vectorization / kernels for persistence diagrams

Section 1 :
Use PH summaries for different types of data

Point clouds data

- Use Rips or Cech filtrations
  - as approximation of distance field filtration

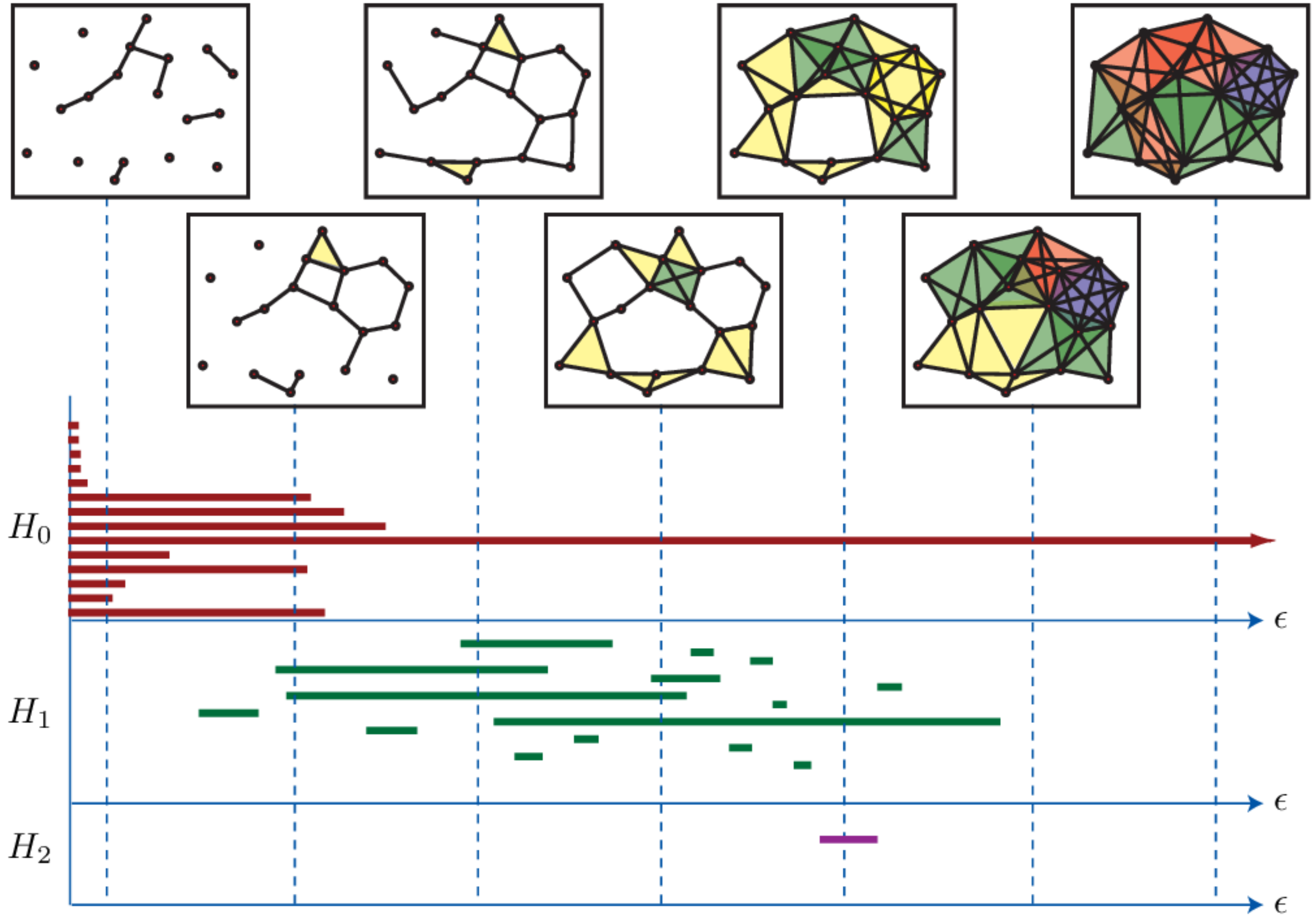

Image courtesy of [Ghrist 05]

General metric spaces

- Input is $P \subseteq (Z,\ d_Z)$, or a special case is that we are given a discrete metric space $(P,\ d_P)$

General metric spaces

$$\mathbb{C}^r_P(P) = \{\sigma = \{p_0, \ldots, p_k\} \mid \cap_{i\in[0,k]} B_P(p; r) \neq \emptyset\}$$

$$\mathbb{VR}^r(P) = \{\sigma = \{p_0, \ldots, p_k\} \mid \mathsf{d}_Z(p_i, p_j) \leq 2r \text{ for any } i, j \in [0, k]\}.$$

General metric spaces

- Input is $P \subseteq (Z,\ d_Z)$, or a special case is that we are given a discrete metric space $(P,\ d_P)$
- Intrinsic Čech complex:

$$\mathbb{C}_P^r(P) = \{\sigma = \{p_0, \ldots, p_k\} \mid \cap_{i\in[0,k]} B_P(p;r) \neq \emptyset\}$$

- Intrinsic Vietoris-Rips complex:

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- We then can use the persistence diagram induced by intrinsic Cech filtration or intrinsic Rips filtration (for increasing r's)

Hausdorff distance, and Gromov-Hausdorff distance

- Hausdorff distance between two sets $A,\ B \subset \left(Z,\ d_Z\right)$
  - $d_H(A,\ B) = \max\{\max_{a\in A}\min_{b\in B} d_Z(a, b), \max_{b\in B}\min_{a\in A} d_Z(a, b)\}$

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Definition 6.3 (Gromov-Hausdorff distance). Given two metric spaces (X, d_X) and (Y, d_Y), a *correspondence* C is a subset $C \subseteq X \times Y$ so that (i) for every $x \in X$, there exists some $(x, y) \in C$; and (ii) for every $y' \in Y$, there exists some $(x', y') \in C$. The *distortion induced by* C is

$$\mathrm{distort}_C(X, Y) := \frac{1}{2} \sup_{(x,y),(x',y')\in C} |\mathsf{d}_X(x, x') - \mathsf{d}_Y(y, y')|.$$

The *Gromov-Hausdorff distance between* (X, d_X) *and* (Y, d_Y) is the smallest distortion possible by any correspondence; that is,

$$\mathsf{d}_{GH}(X, Y) := \inf_{C\subseteq X\times Y} \mathrm{distort}_C(X, Y).$$

Stability

Theorem 6.3. *Čech- and Rips-distances satisfy the following stability statements:*

1. *Given two finite sets* $P, Q \subseteq (Z, \mathsf{d}_Z)$, *we have*

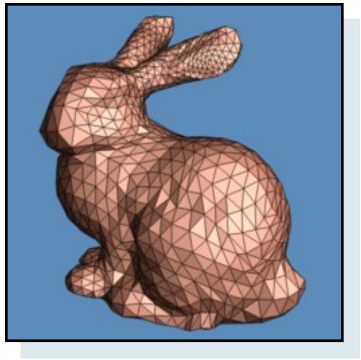
$$\mathsf{d}_{Cech}(P, Q) \leq \mathsf{d}_H(P, Q); \quad \textit{and} \quad \mathsf{d}_{Rips}(P, Q) \leq \mathsf{d}_H(P, Q).$$

2. *Given two finite metric spaces* (P, d_P) *and* (Q, d_Q), *we have*

$$\mathsf{d}_{Cech}(P, Q) \leq 2\mathsf{d}_{GH}((P, \mathsf{d}_P), (Q, \mathsf{d}_Q)), \quad \textit{and} \ \mathsf{d}_{Rips}(P, Q) \leq \mathsf{d}_{GH}((P, \mathsf{d}_P), (Q, \mathsf{d}_Q)).$$

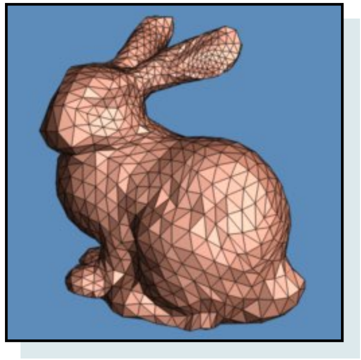
Mesh data

- For example, a triangulation K of surface models



Mesh data

- For example, a triangulation K of surface models
- Idea:
  - Find a meaningful descriptor function $f: K \to R$
  - Compute $dgm_* f$ as its topological summary



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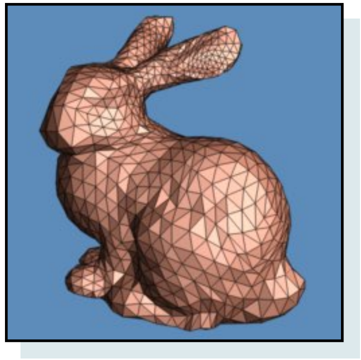
- Examples of choices of descriptor functions:
  - Gaussian curvature
  - Mean curvature
  - Heat-kernel signature function
  - …



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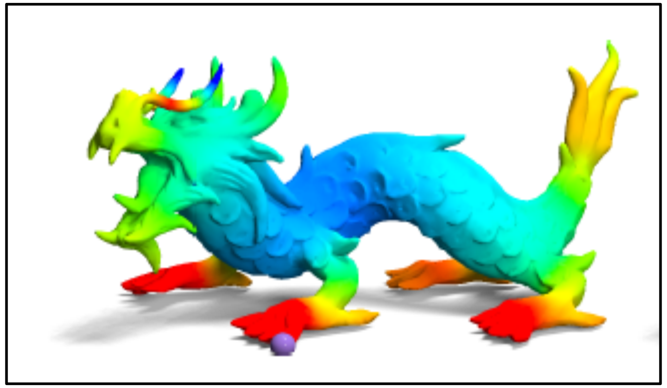
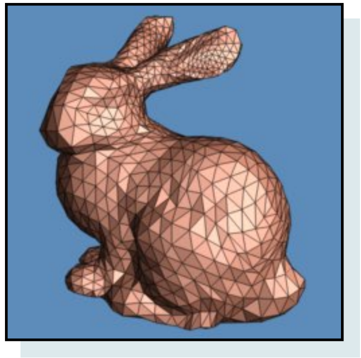
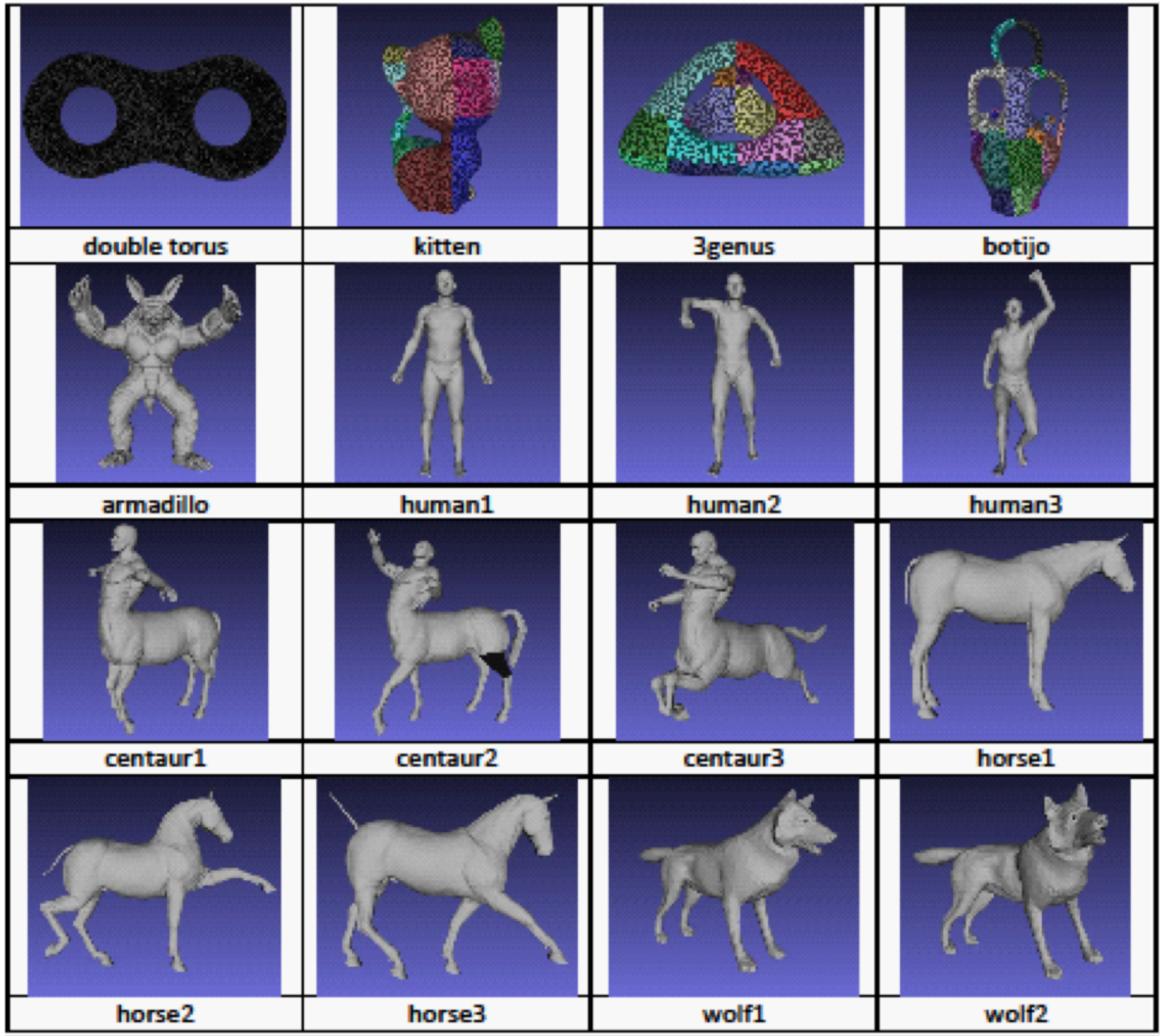




Example


double torus
kitten
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human1
human2
human3
centaur1
centaur2
centaur3
horse1
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horse3
wolf1
wolf2

PD Distance	double torus	kitten	3genus	botijo	armadillo	human1	human2	human3	centaur1	centaur2	centaur3	horse1	horse2	horse3	wolf1	wolf2
double torus	**0.024**	0.235	0.299	0.264	0.307	0.364	0.358	0.340	0.269	0.253	0.245	0.247	0.240	0.250	0.248	0.243
kitten	0.235	**0.037**	0.319	0.268	0.259	0.274	0.268	0.250	0.266	0.249	0.245	0.241	0.242	0.239	0.238	0.238
3genus	0.299	0.319	**0.047**	0.256	0.394	0.388	0.393	0.394	0.394	0.392	0.399	0.401	0.399	0.392	0.386	0.401
botijo	0.264	0.268	0.256	**0.039**	0.276	0.276	0.277	0.278	0.279	0.279	0.277	0.278	0.279	0.278	0.278	0.280
armadillo	0.307	0.259	0.394	0.276	**0.049**	0.159	0.203	0.190	0.127	0.122	0.152	0.114	0.108	0.114	0.125	0.127
human1	0.364	0.274	0.388	0.276	0.159	**0.038**	0.052	0.078	0.207	0.189	0.183	0.195	0.190	0.205	0.176	0.165
human2	0.358	0.268	0.393	0.277	0.203	0.052	**0.038**	0.061	0.213	0.189	0.181	0.200	0.189	0.204	0.176	0.170
human3	0.340	0.250	0.394	0.278	0.190	0.078	0.061	**0.041**	0.210	0.189	0.184	0.199	0.188	0.197	0.176	0.166
centaur1	0.269	0.266	0.394	0.279	0.127	0.207	0.213	0.210	**0.044**	0.057	0.102	0.142	0.161	0.126	0.162	0.180
centaur2	0.253	0.249	0.392	0.279	0.122	0.189	0.189	0.189	0.057	**0.049**	0.085	0.142	0.133	0.117	0.160	0.160
centaur3	0.245	0.245	0.399	0.277	0.152	0.183	0.181	0.184	0.102	0.085	**0.042**	0.127	0.132	0.118	0.139	0.152
horse1	0.247	0.241	0.401	0.278	0.114	0.195	0.200	0.199	0.142	0.142	0.127	**0.042**	0.097	0.079	0.122	0.111
horse2	0.240	0.242	0.399	0.279	0.108	0.190	0.189	0.188	0.161	0.133	0.132	0.097	**0.048**	0.069	0.106	0.105
horse3	0.250	0.239	0.392	0.278	0.114	0.205	0.204	0.197	0.126	0.117	0.118	0.079	0.069	**0.046**	0.117	0.111
wolf1	0.248	0.238	0.386	0.278	0.125	0.176	0.176	0.176	0.162	0.160	0.139	0.122	0.106	0.117	**0.045**	0.066
wolf2	0.243	0.238	0.401	0.280	0.127	0.165	0.170	0.166	0.180	0.160	0.152	0.111	0.105	0.111	0.066	**0.045**

pairwise persistence-based distance between models

- Demo on teeth clustering

Graph Data

- There are different ways to look at graphs
  - Combinatorial graph based
  - Geometric graph based
  - Descriptor function based
  - …

Simplicial homology induced from weighted graphs

- Suppose we are given a weighted graph $G = (V, \; E; w)$
  - This gives us a sequence of graphs $G^a := \left\{ e \in E \mid w(e) \leq a \right\}$
- We can construct simplicial complexes from G
- E.g. 1:
  - clique complex $R^a(G) = \{ \left(v_{i_0}, \ldots, \; v_{i_s} \right) \mid \; v_{i_0}, \ldots, \; v_{i_s}$ forms a clique in $G^a\}$
  - Increasing a then gives us a filtration
    - $R^{a_0}(G) \subseteq R^{a_1}(G) \subseteq \cdots \subseteq R^{a_n}(G)$
  - We can then take the persistence diagram of it as its topological summaries
  - This, for example, has been used in the literature to compare brain networks

Simplicial homology induced from weighted graphs

- Suppose we are given a weighted graph $G = (V,\ E; w)$
  - we can treat this as a metric graph, with shortest path distance d_G induced by w
- E.g 2: intrinsic Čech or Rips complexes induced by d_G

Simplicial homology induced from weighted graphs

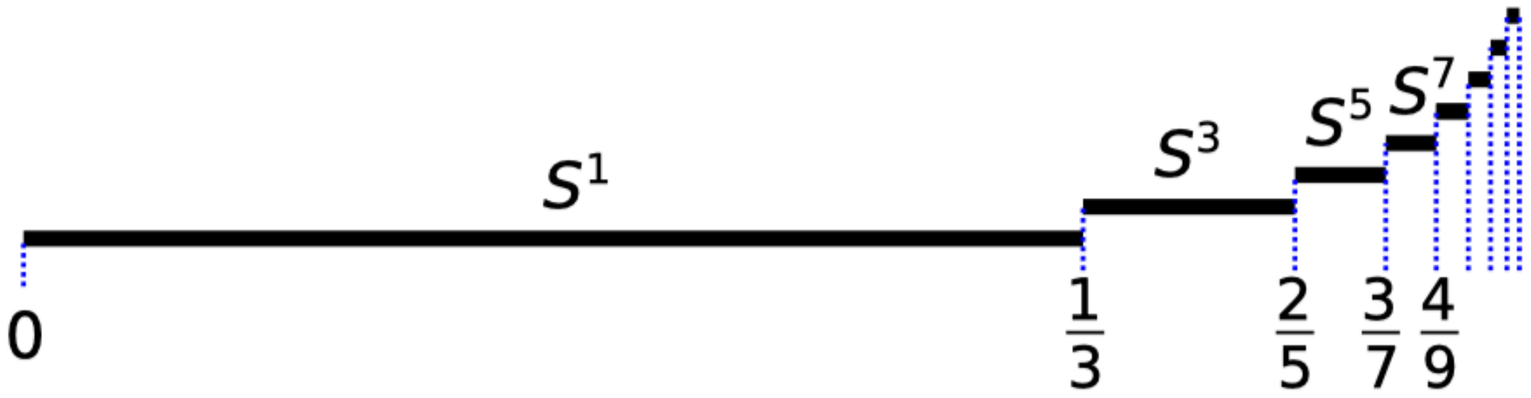
- Suppose we are given a weighted graph $G = (V,\ E; w)$
  - we can treat this as a metric graph, with shortest path distance d_G induced by w
- **Theorem 8.1.** *Let* $0 < r < \frac{1}{2}$. *There are homotopy equivalences: for* $\ell = 0, 1, \ldots,$

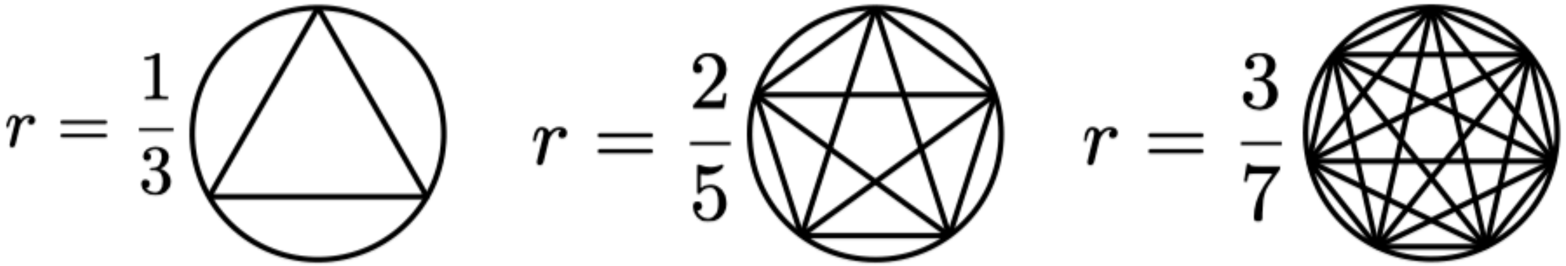
$$\mathbb{C}^r(\mathbb{S}^1) \simeq \mathbb{S}^{2\ell+1} \quad \text{if } \frac{\ell}{2(\ell+1)} < r \leq \frac{\ell+1}{2(\ell+2)}; \quad \text{and}$$

$$\mathbb{VR}^{r/2}(\mathbb{S}^1) \simeq \mathbb{S}^{2\ell+1} \quad \text{if } \frac{\ell}{2\ell+1} < \frac{r}{2} \leq \frac{\ell+1}{2\ell+3}.$$

VR complex of $\mathbb{S}^1$ - circle with unit circumference

- $Rips^r(\mathbb{S}^1) \simeq \mathbb{S}^{2l+1}, \dfrac{l}{2l+1} < r \leq \dfrac{l+1}{2l+3}$





Courtesy of Henry Adams

Simplicial homology induced from weighted graphs

- Suppose we are given a weighted graph $G = (V,\ E; w)$
  - we can treat this as a metric graph, with shortest path distance d_G induced by w

Theorem 8.3. *Let $G = (V, E, \omega)$ be a finite graph with positive weight function $\omega : E \to \mathbb{R}$. Let $\{\gamma_1, \ldots, \gamma_g\}$ be a shortest cycle basis of G where $g = \mathrm{rank}\,(\mathsf{Z}_1(G))$, and for each $i = 1, \ldots, g$, let $\ell_i = length(\gamma_i)$. Then, the 1-st persistence diagram $\mathrm{Dgm}_1\mathcal{C}$ induced by the intrinsic Čech filtration $\mathcal{C} := \{\mathbb{C}^r(|G|)\}_{r\in\mathbb{R}}$ on the metric graph $(|G|, \mathsf{d}_G)$ consists of the following set of points on the y-axis:*

$$\mathrm{Dgm}_1\mathcal{C} = \{(0, \frac{\ell_i}{4}) \mid 1 \le i \le g\}.$$

Descriptor function based

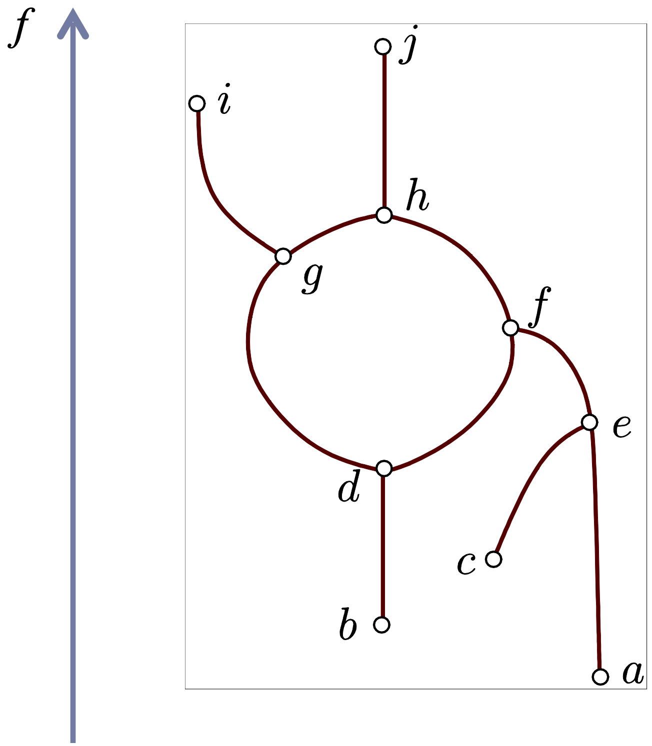
- A graph $G = (V, E)$ can be thought of as a 1-dimensional simplicial complex
- We can thus put a descriptor function on it, and compute its resulting (sub level set) persistence diagram representation

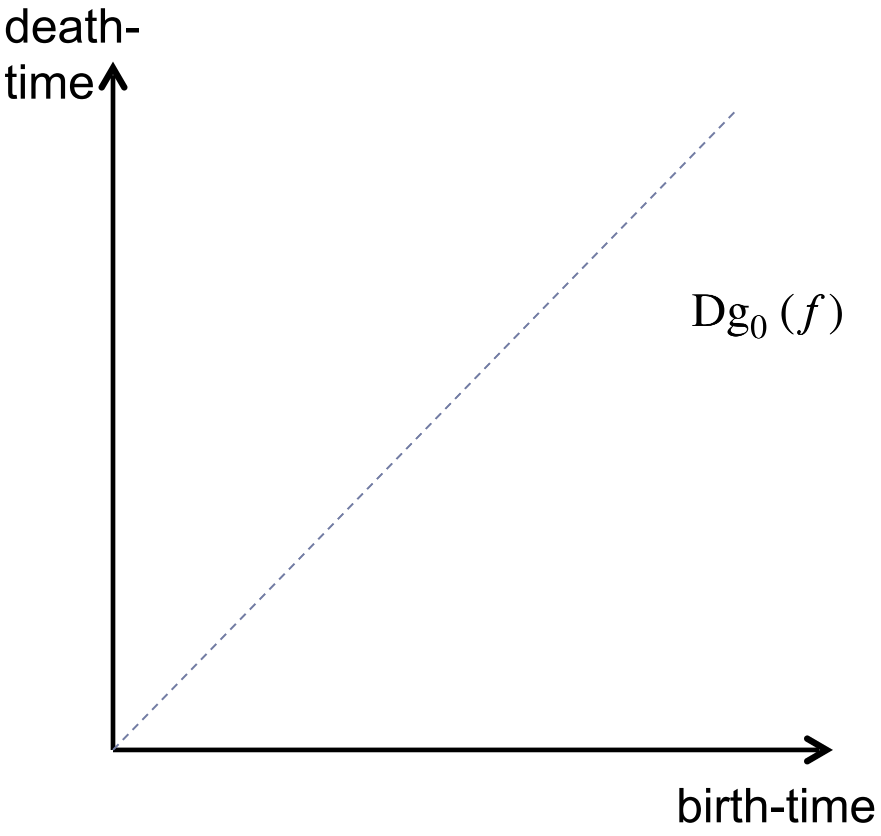
- Some choices of descriptor functions:
  - Discrete Ricci curvature
  - Degree function
  - Heat-kernel signature
  - …

One issue

- There is only 0-th persistent homology for sub-level set filtration
- For 1-dim, cycles created will never die (as there are no triangles)
- Example

A (Very) Simplified Illustration





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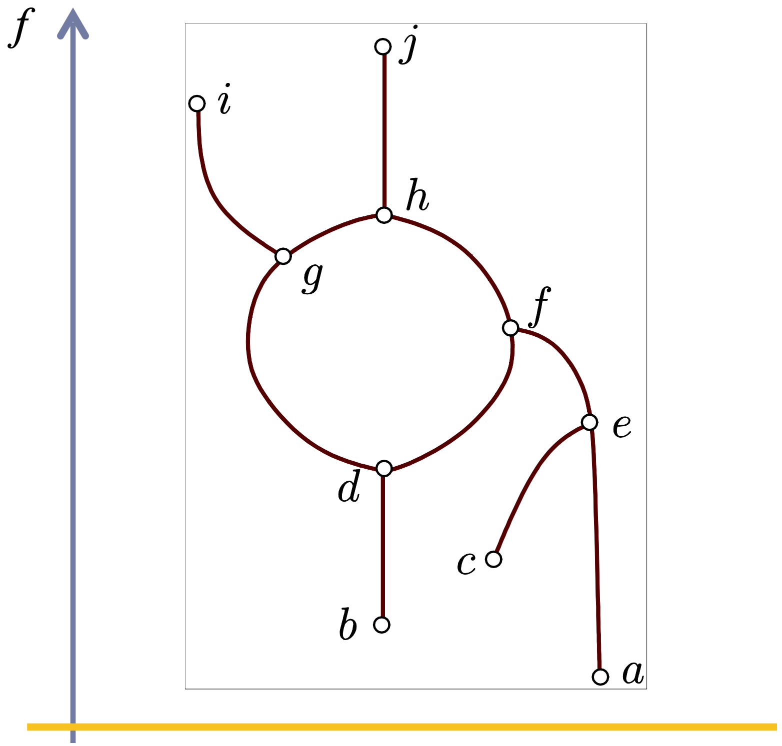

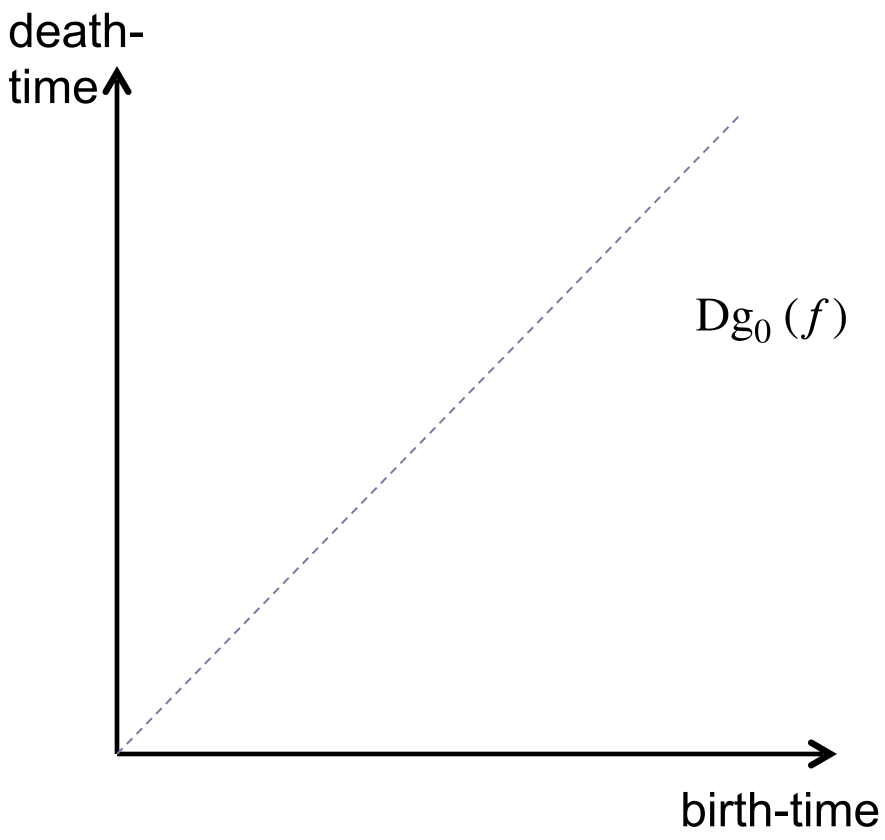

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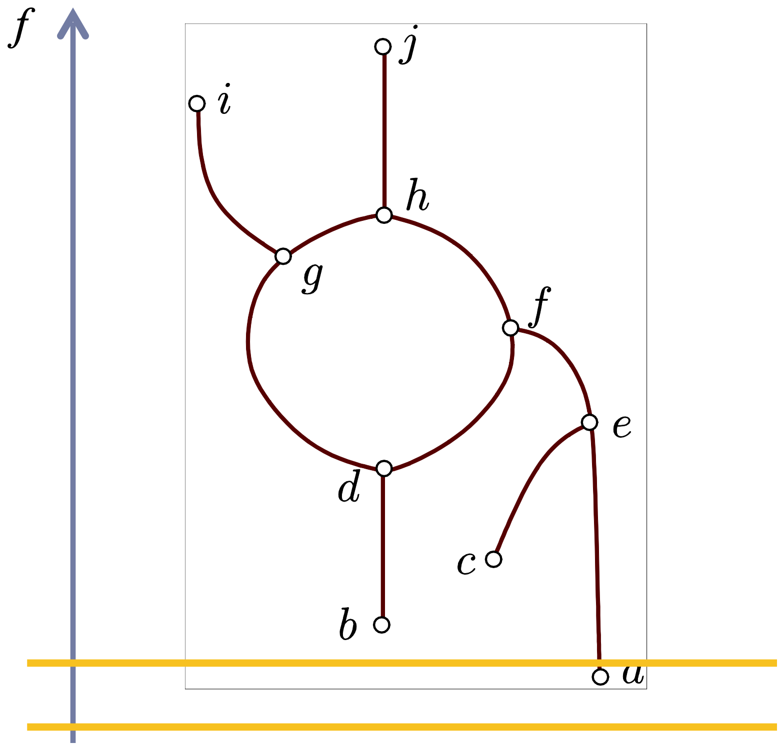

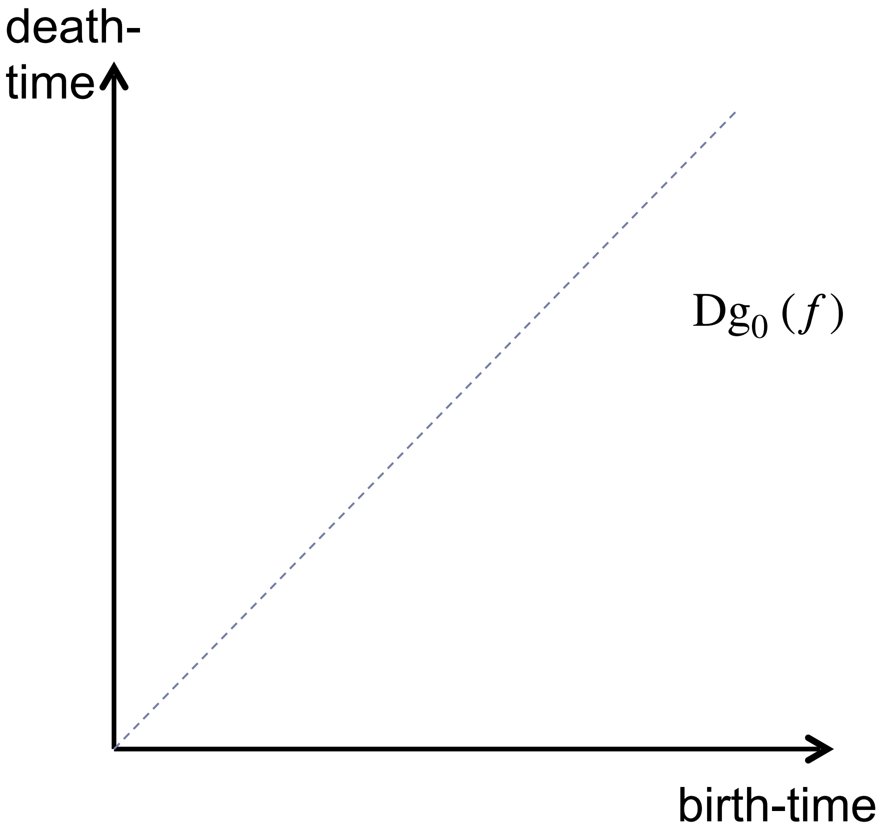

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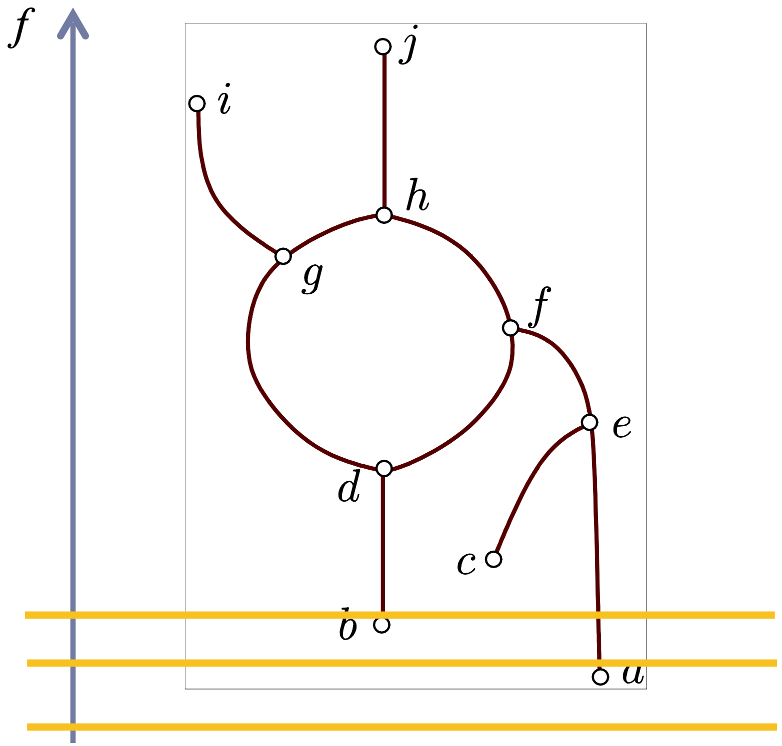

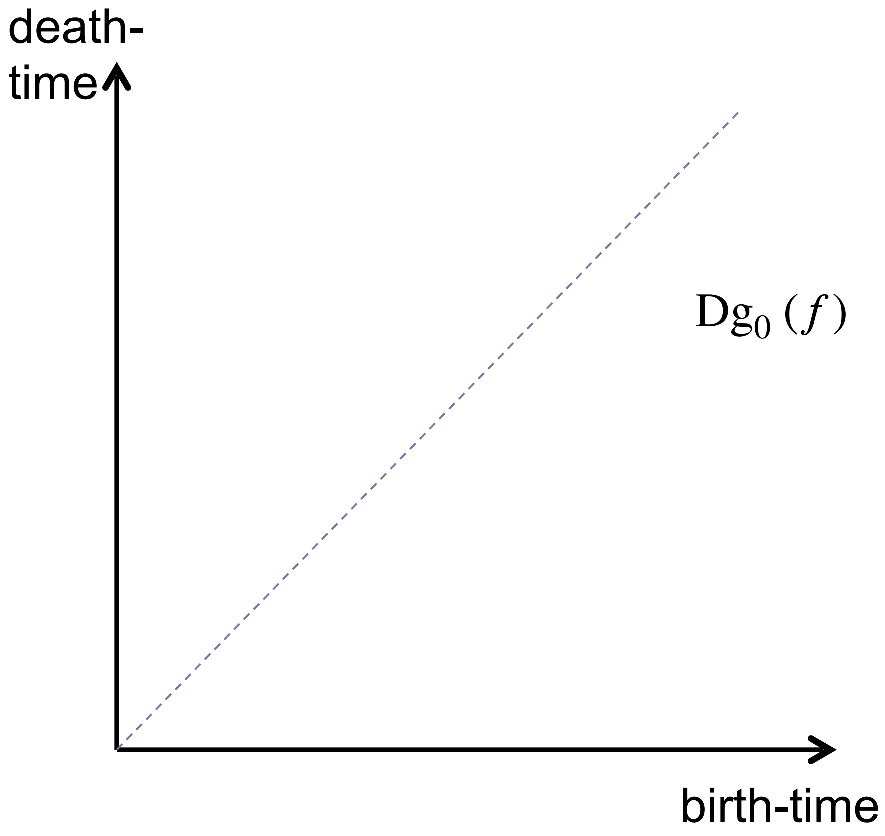

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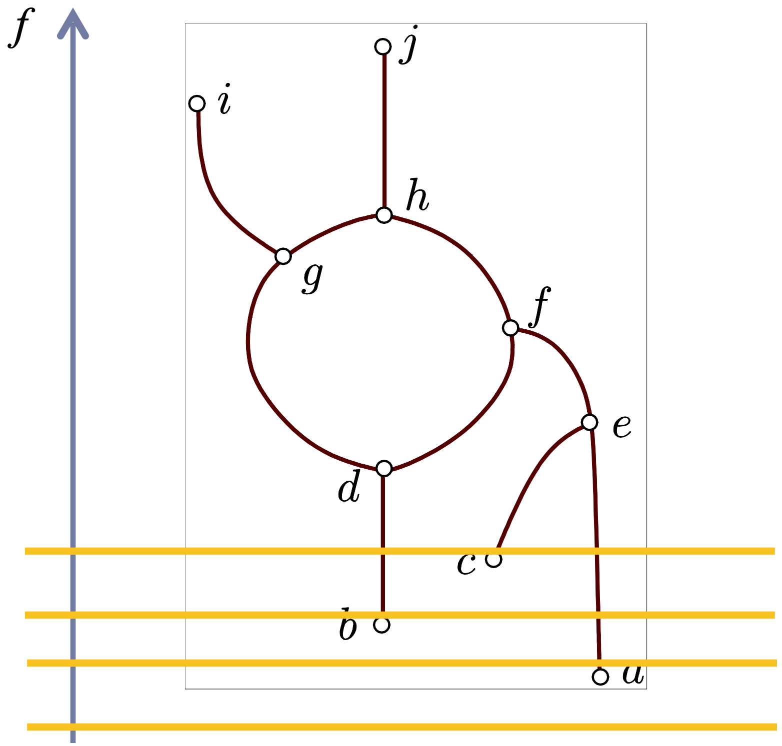

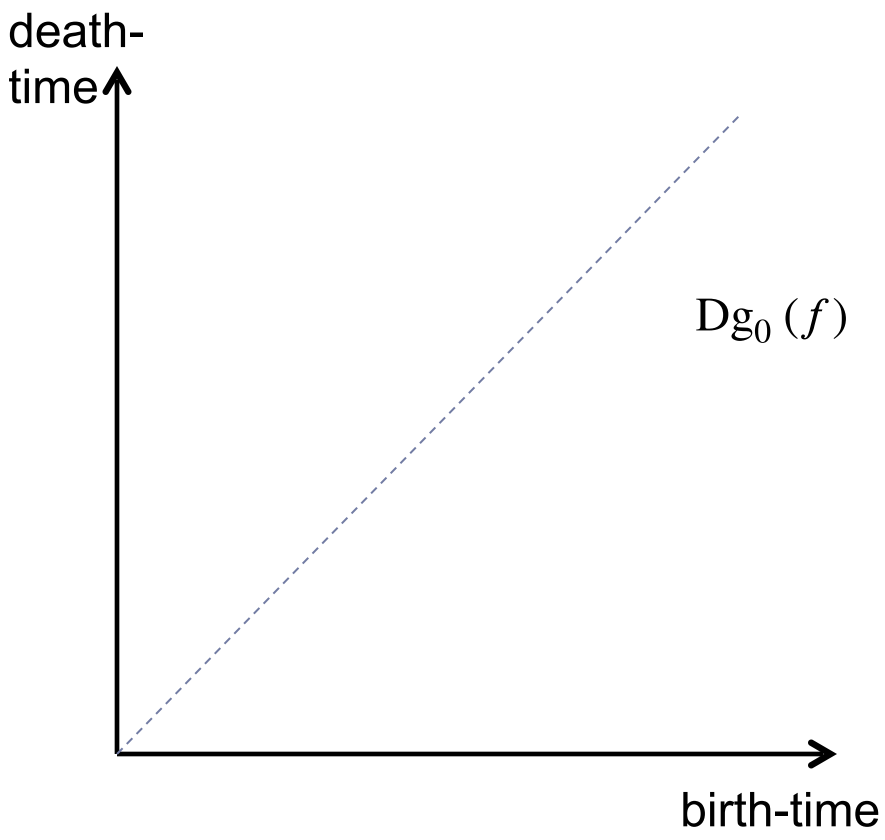

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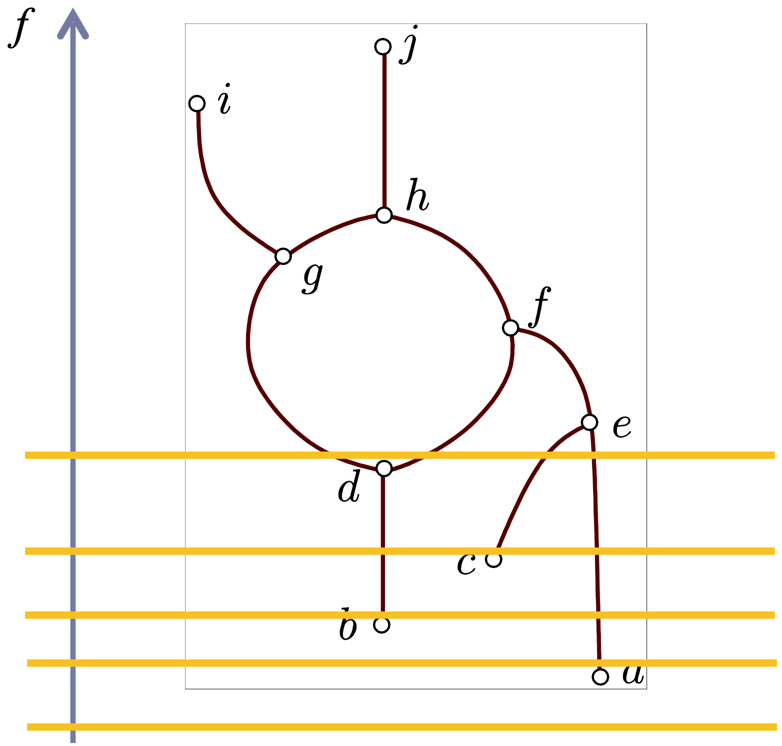

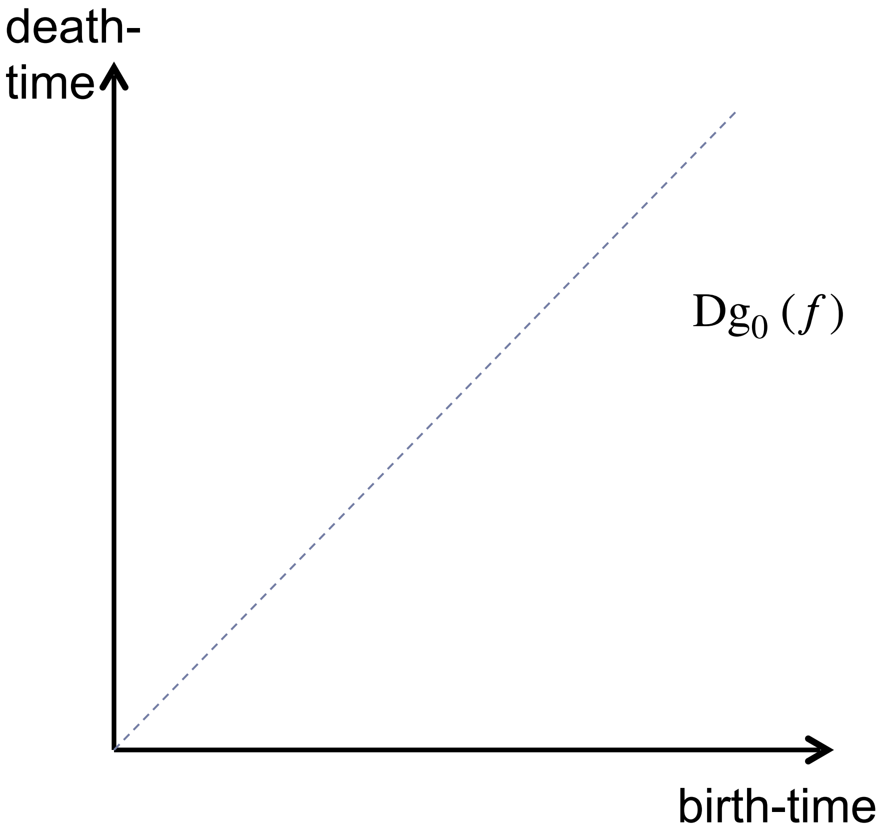

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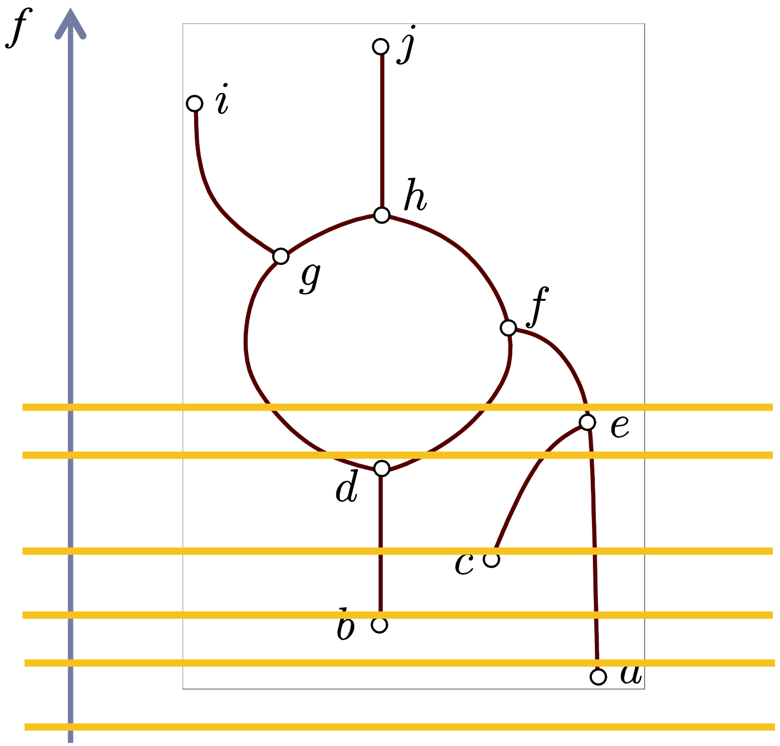

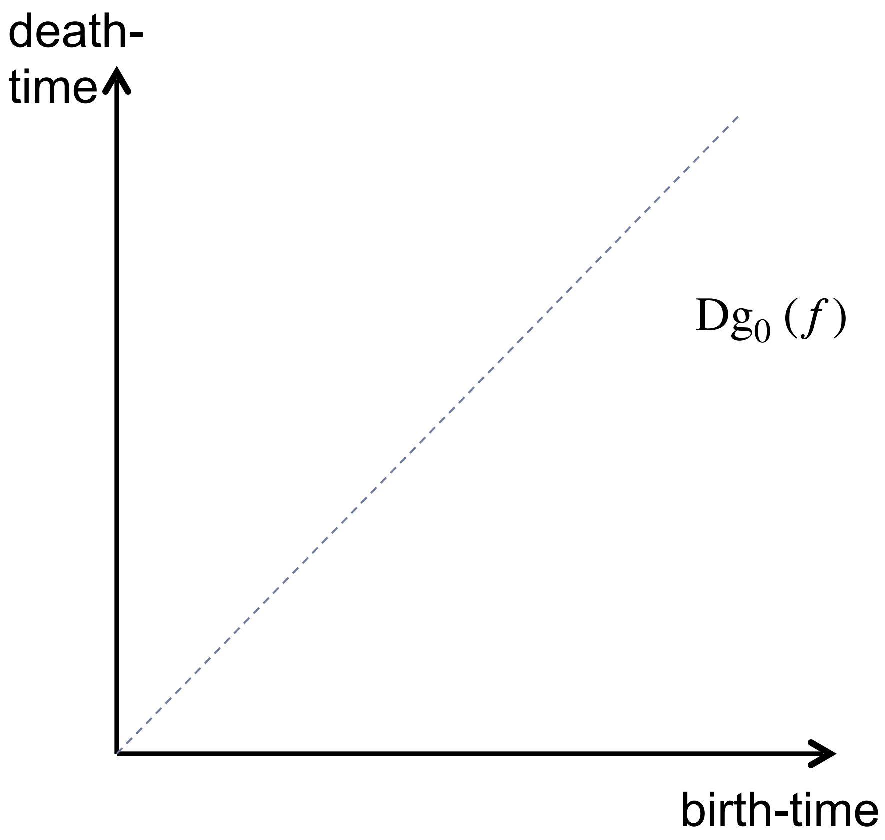

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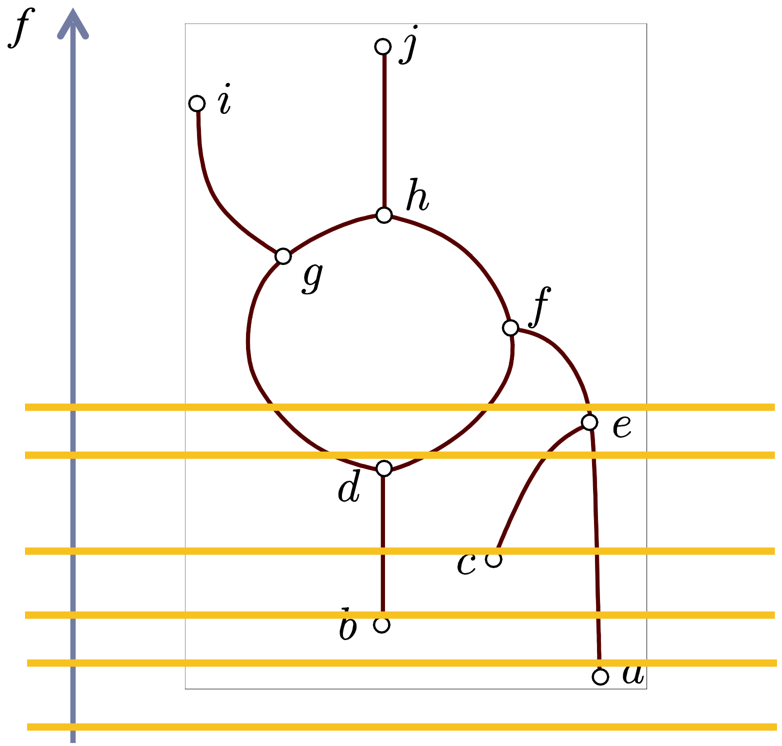

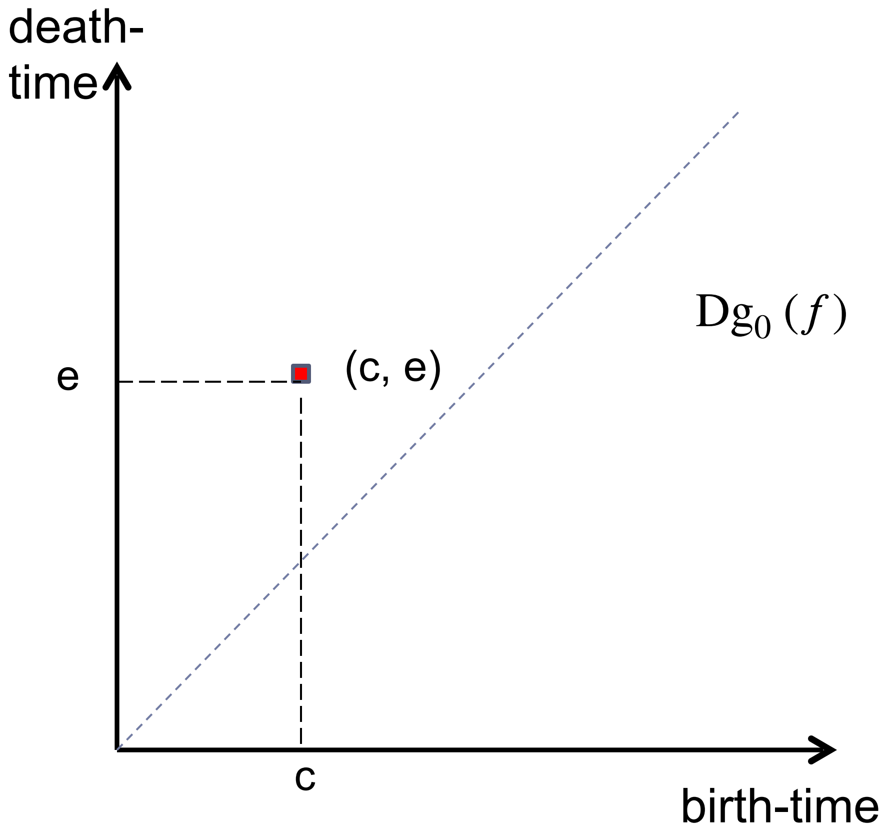

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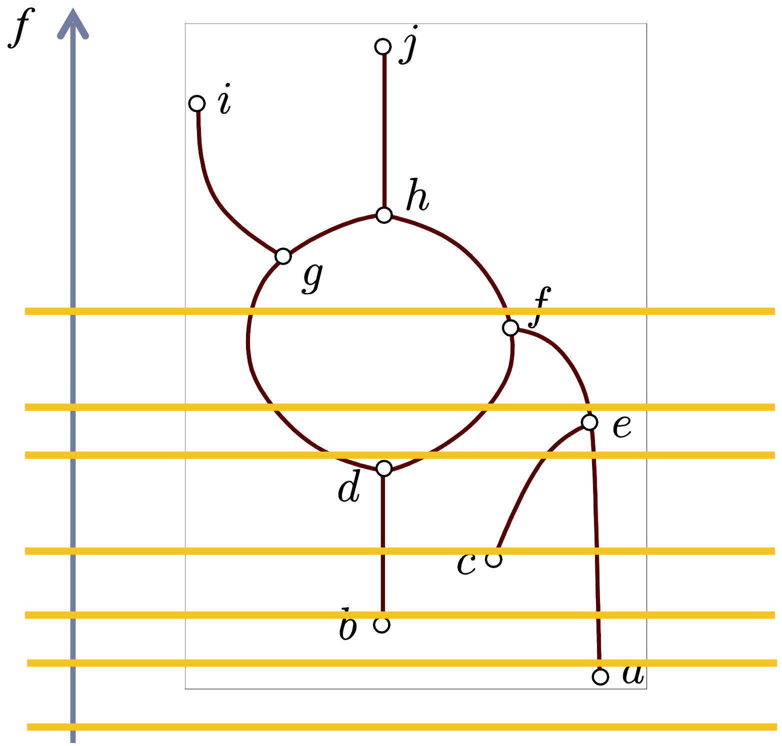

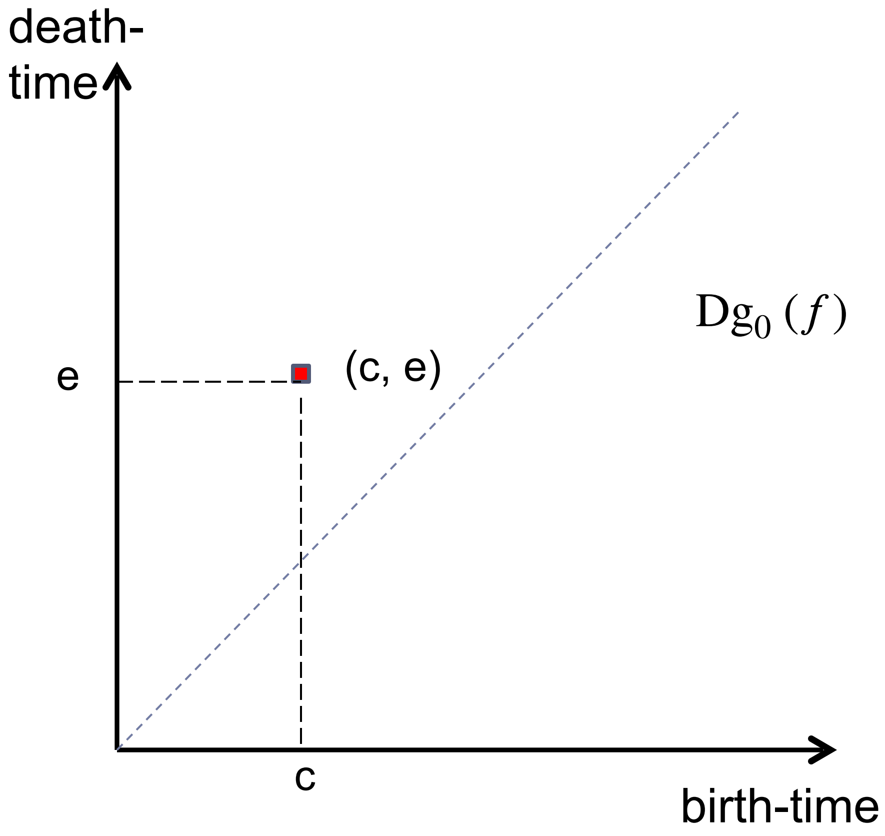

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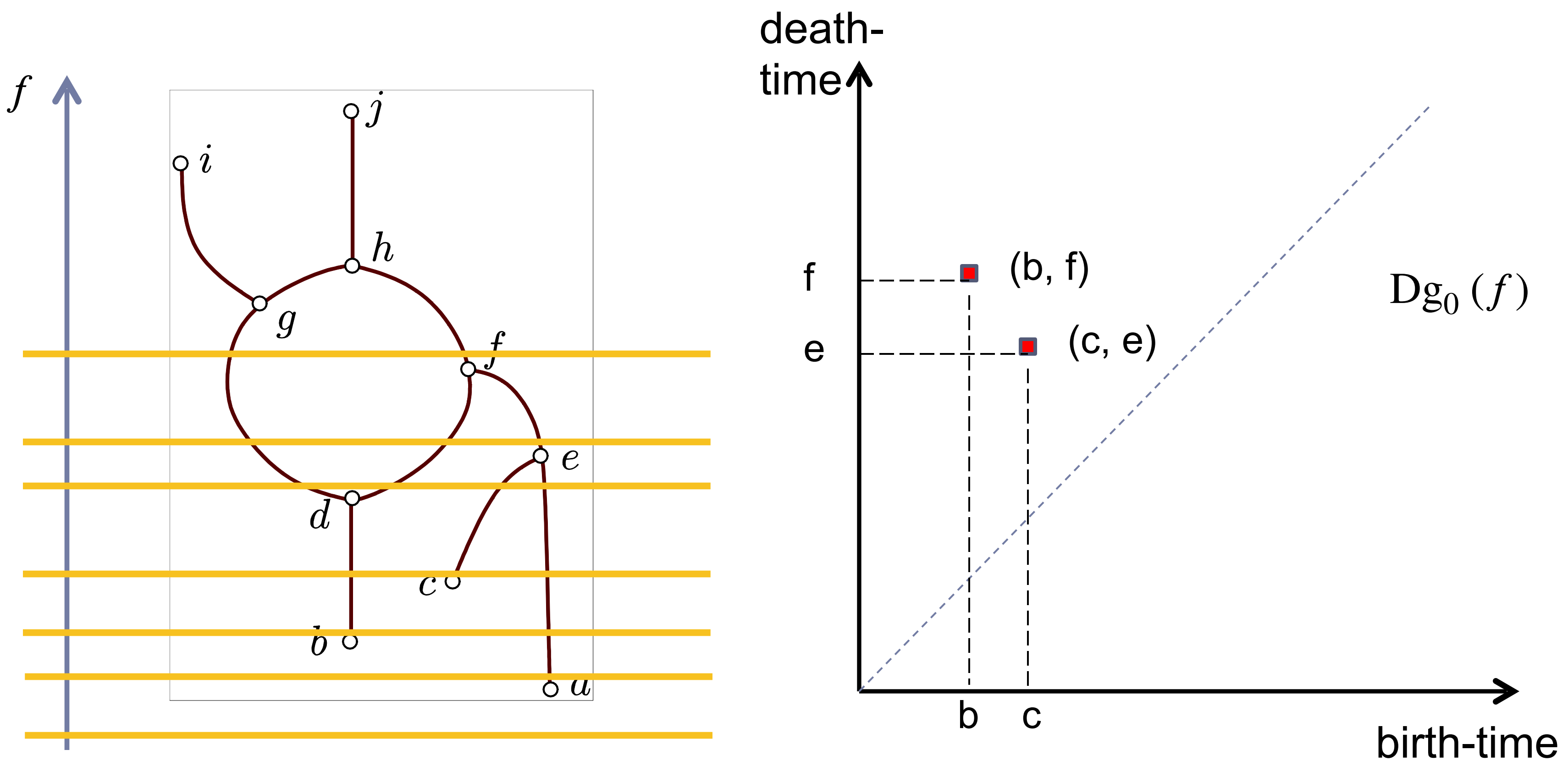

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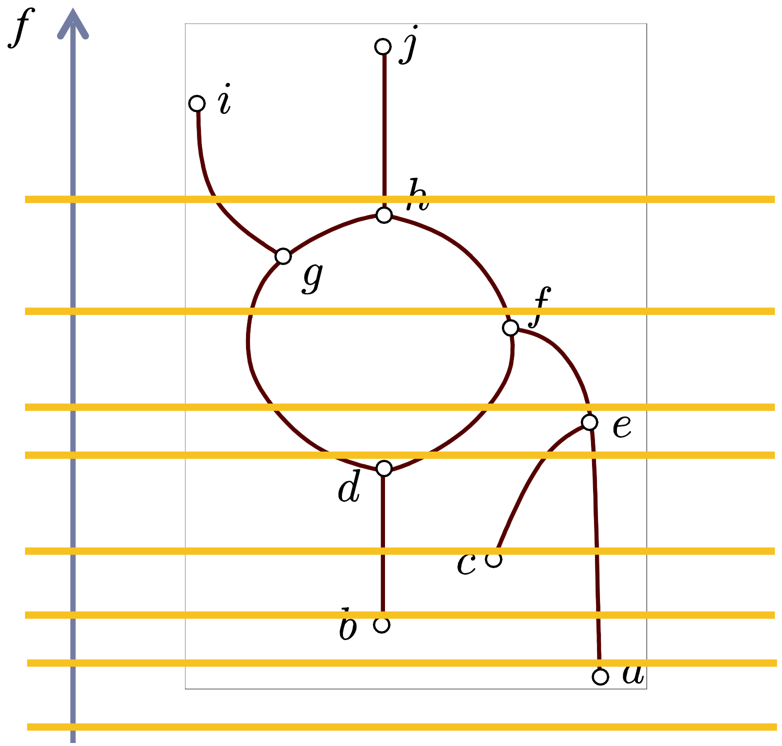

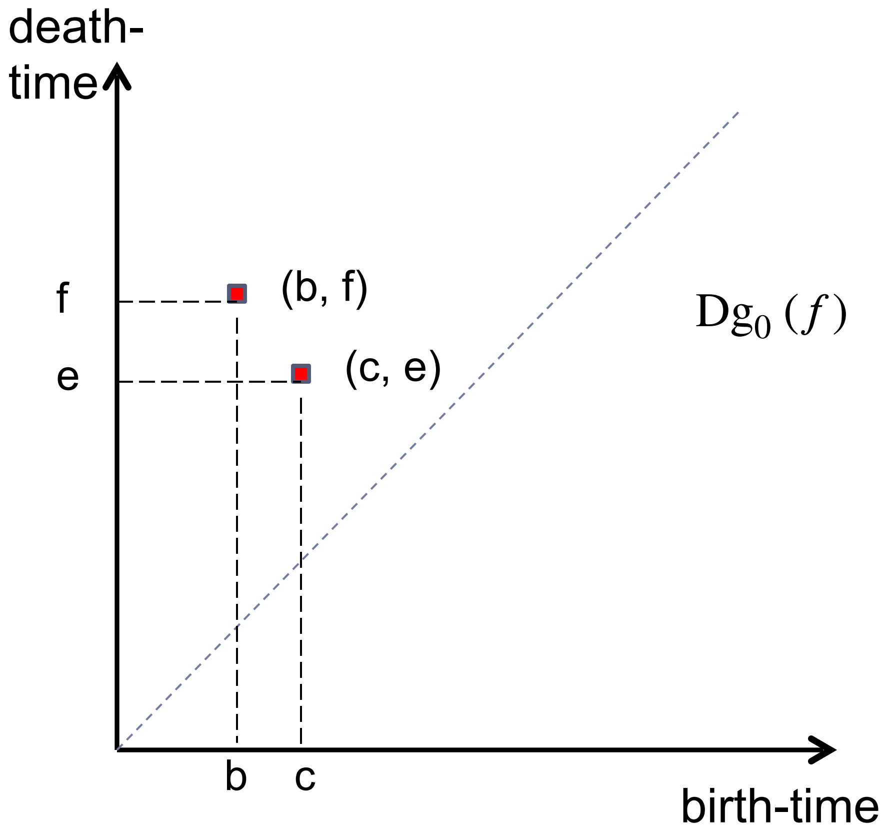

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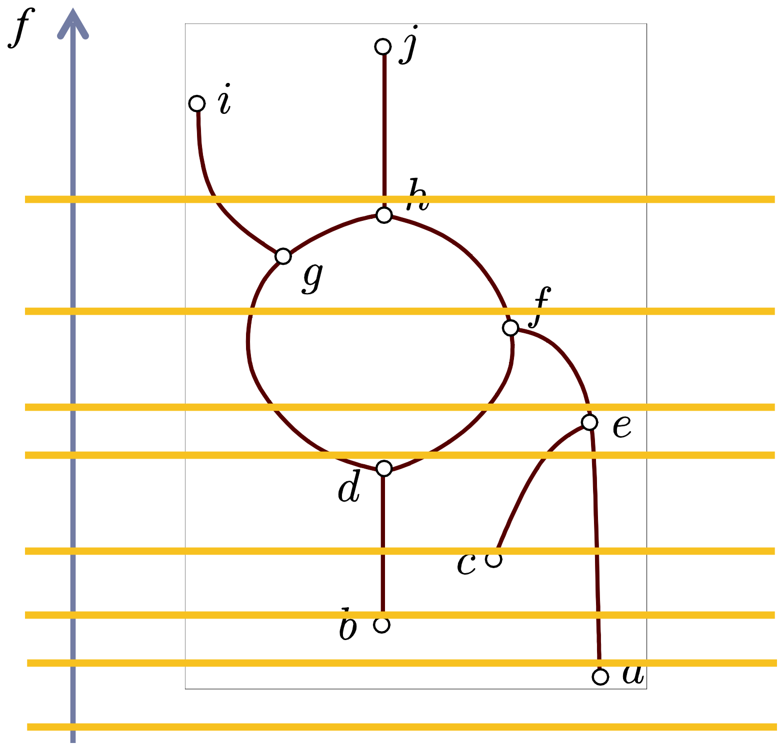

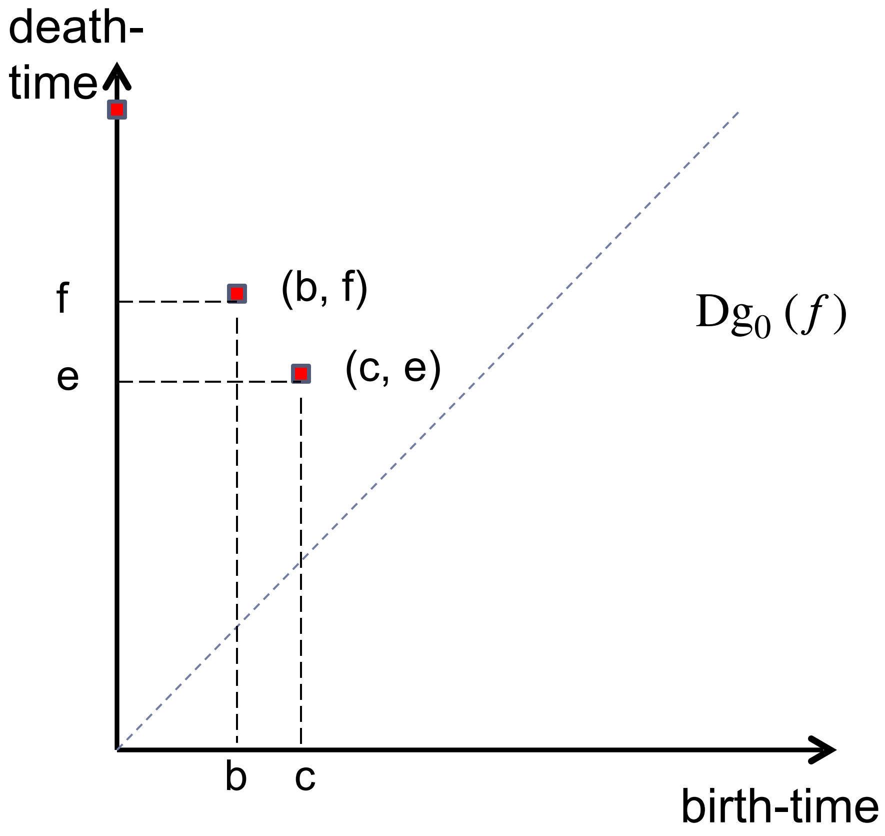

Loop Features

- Captured by Extended persistence:
  - *[Cohen-Steiner, Edelsbrunner and Harer, FoCM 2009]*

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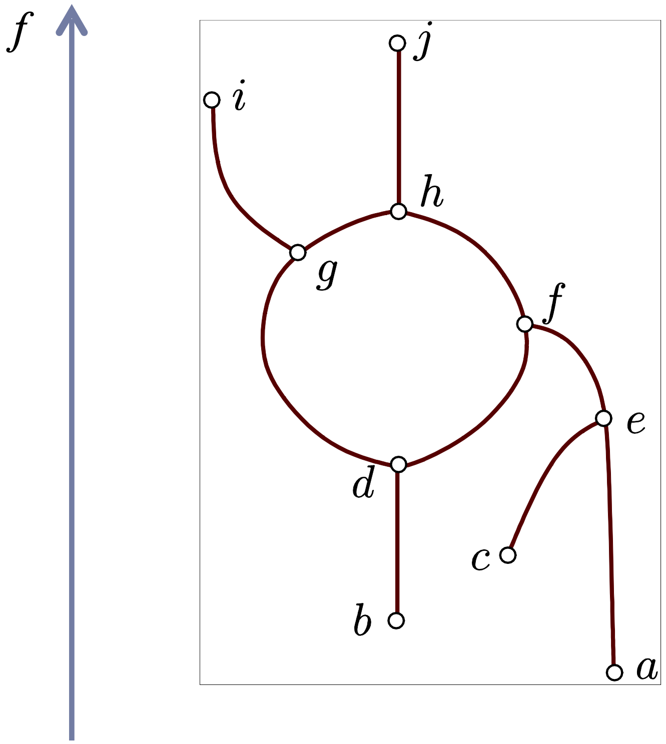

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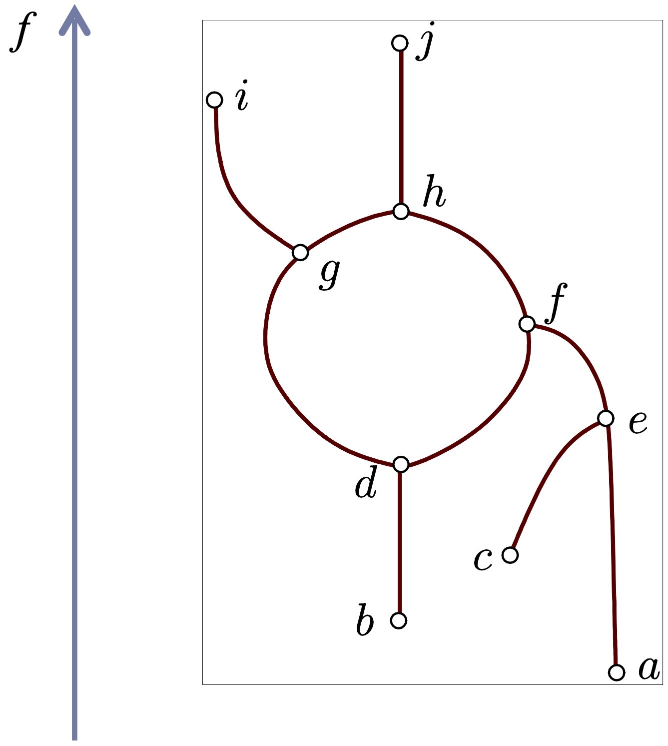

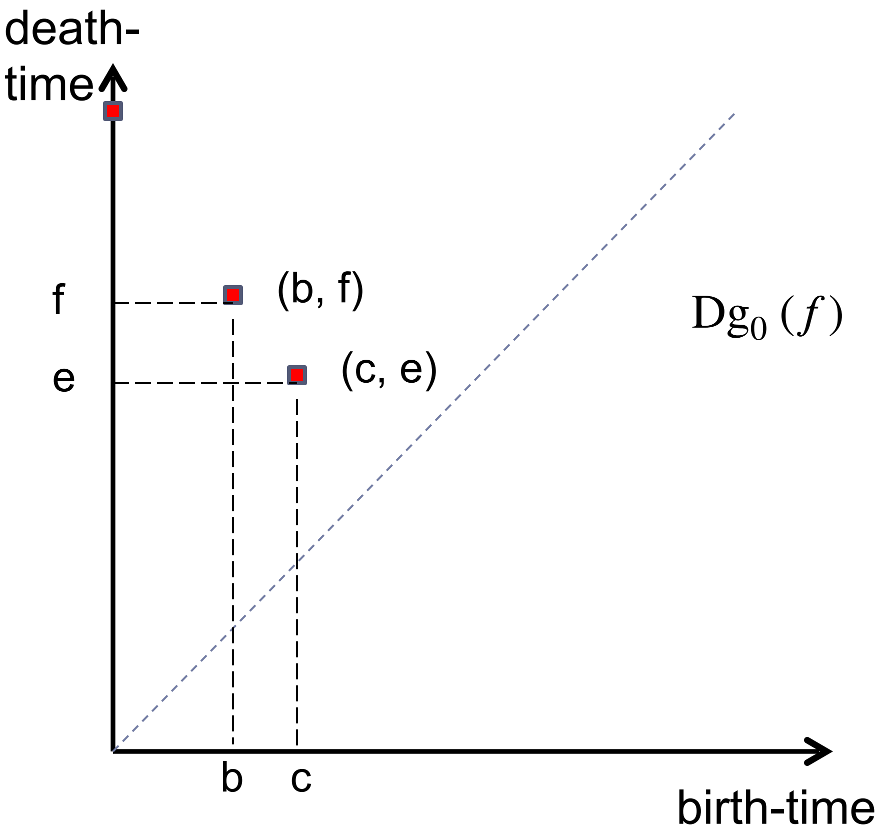

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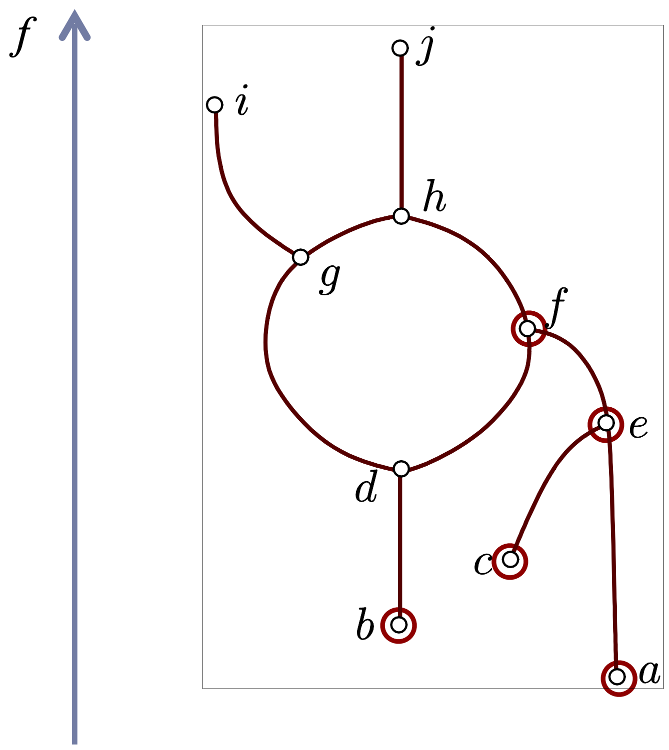

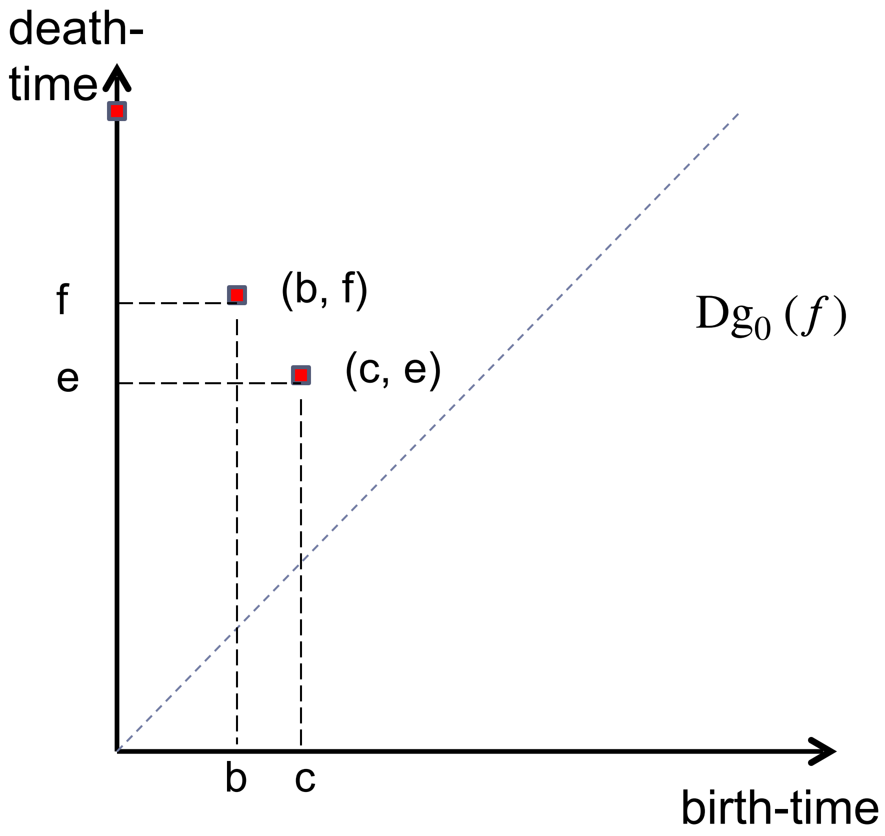

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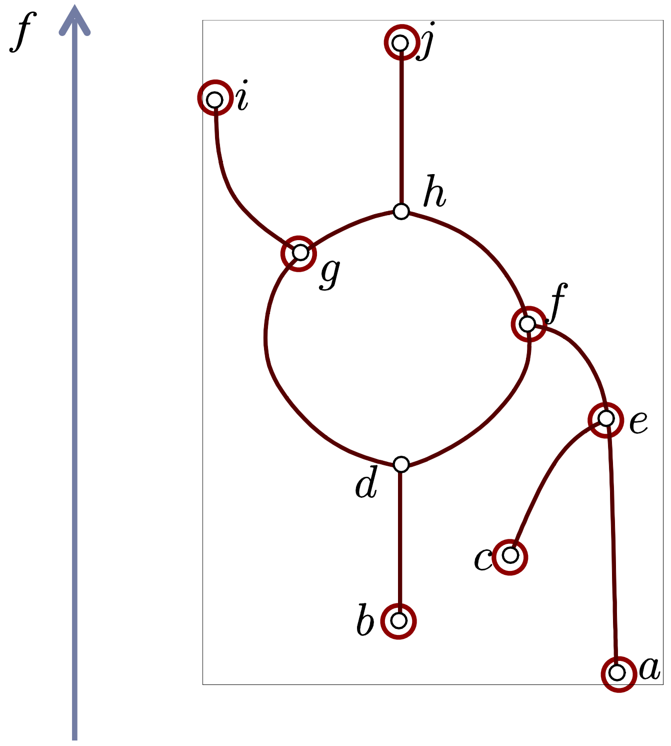

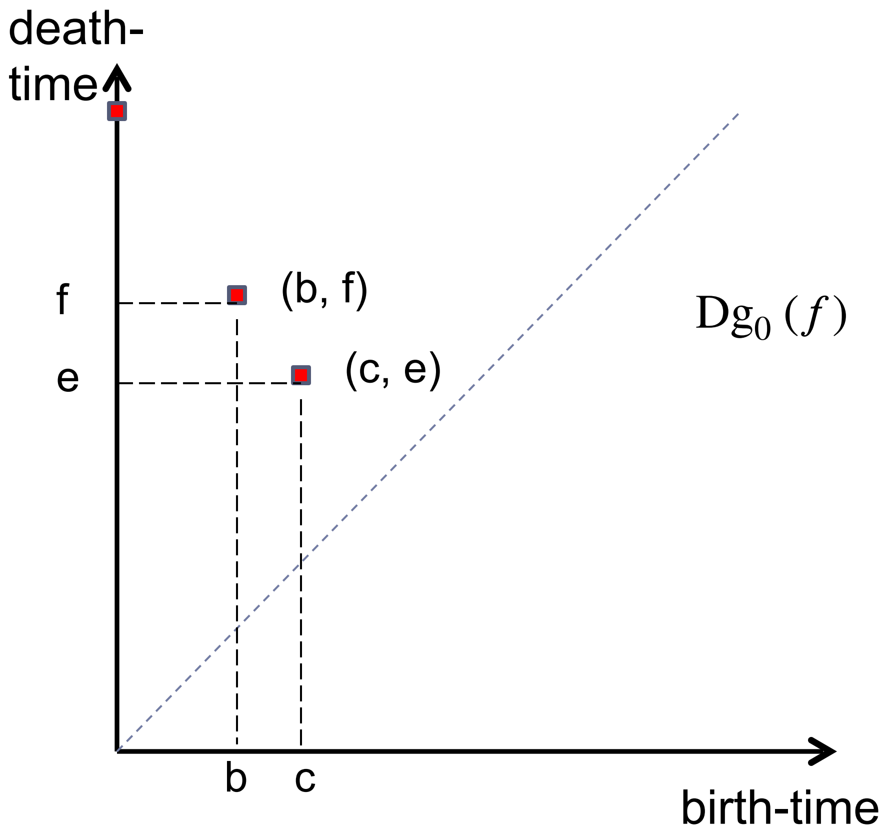

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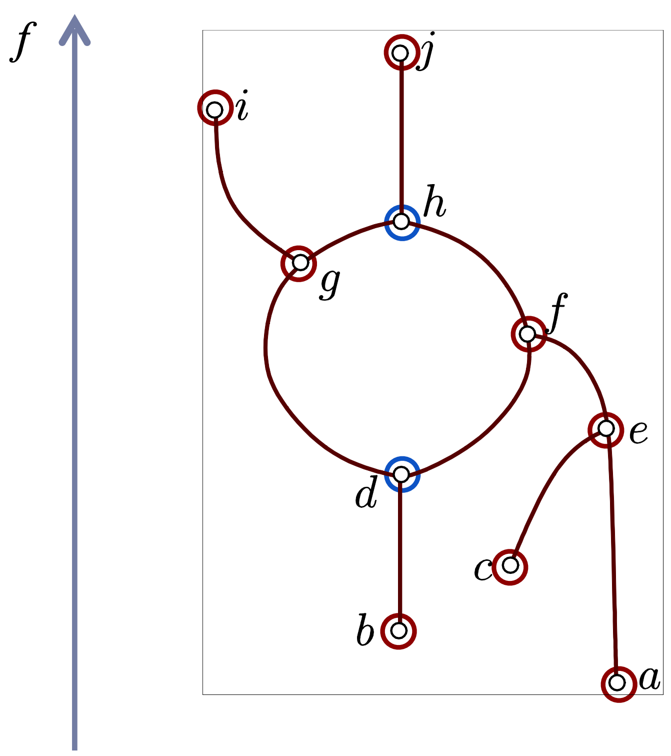

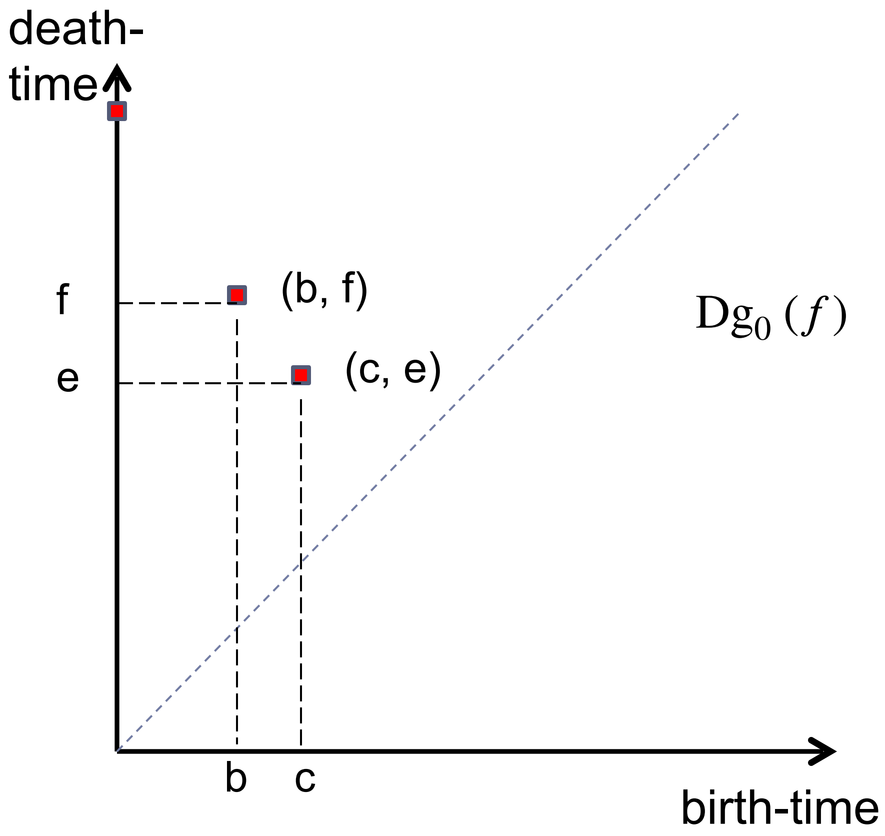

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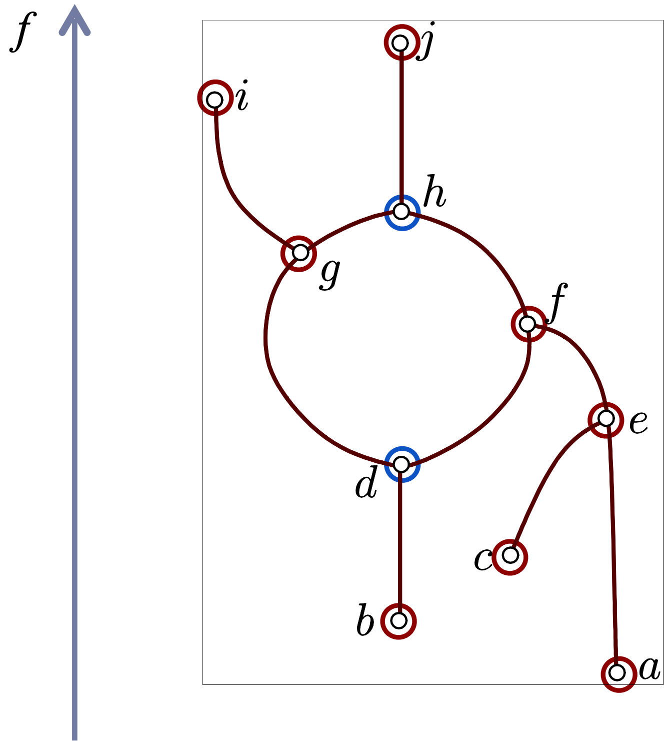
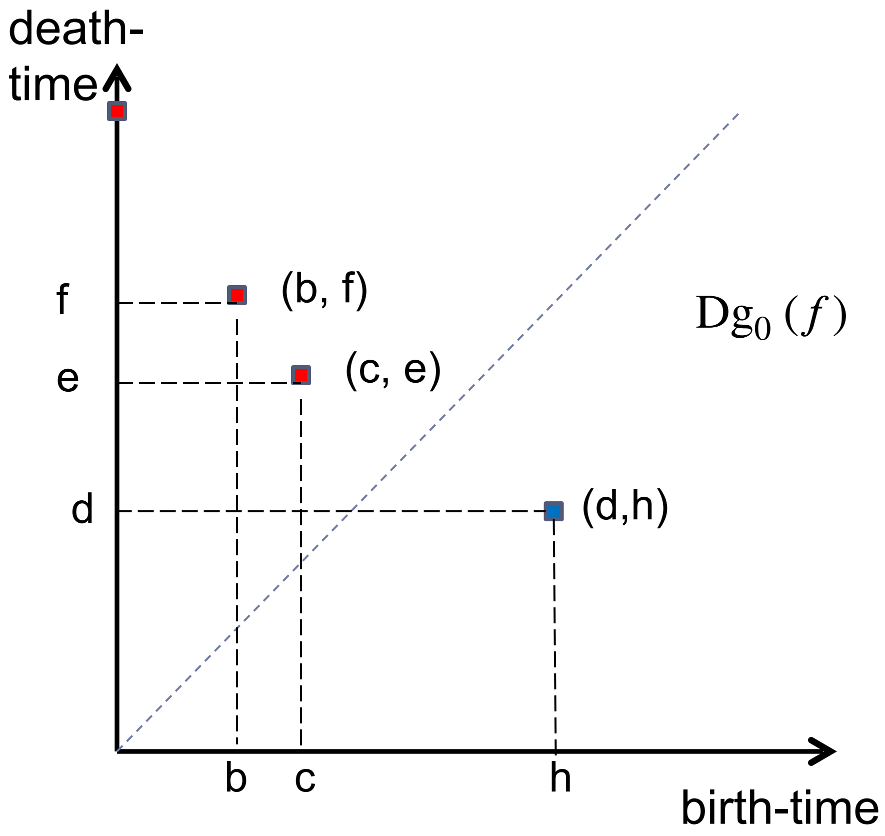
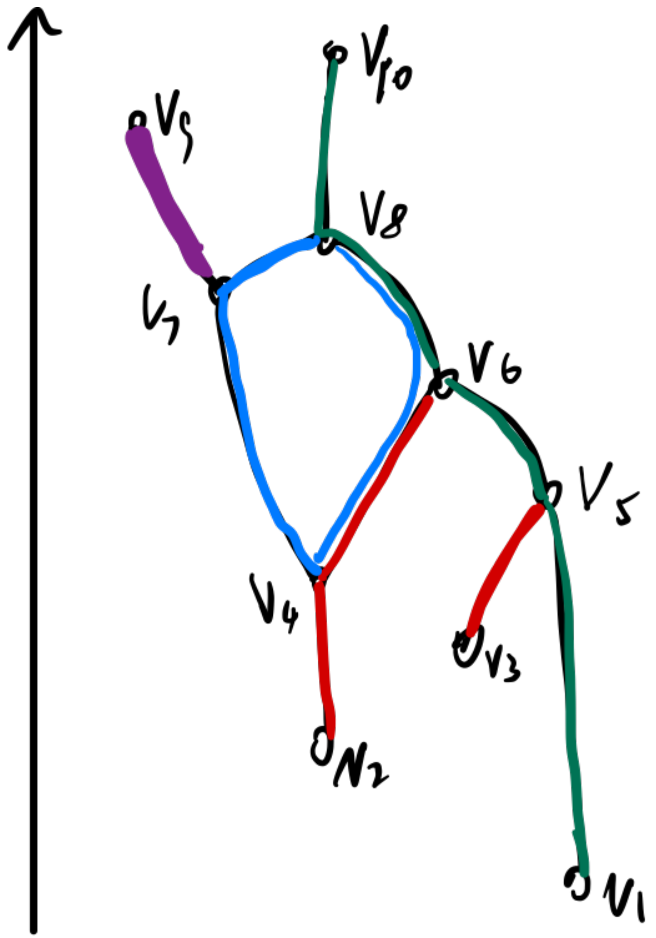
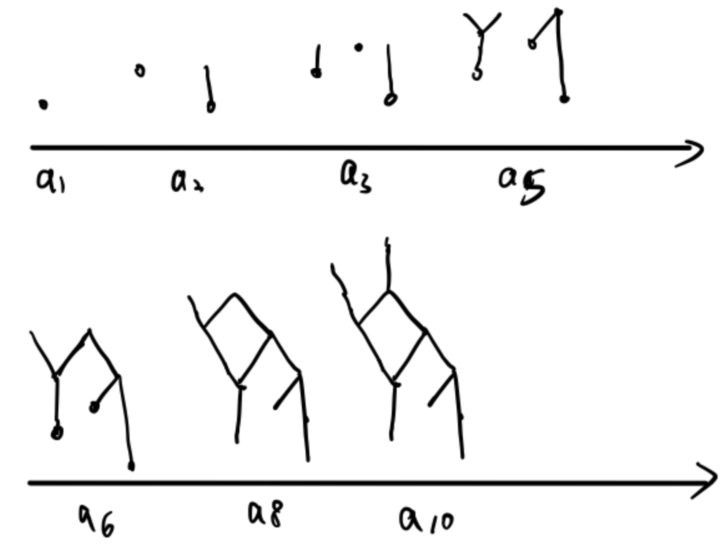








0-dim

(a_0, a_{10})

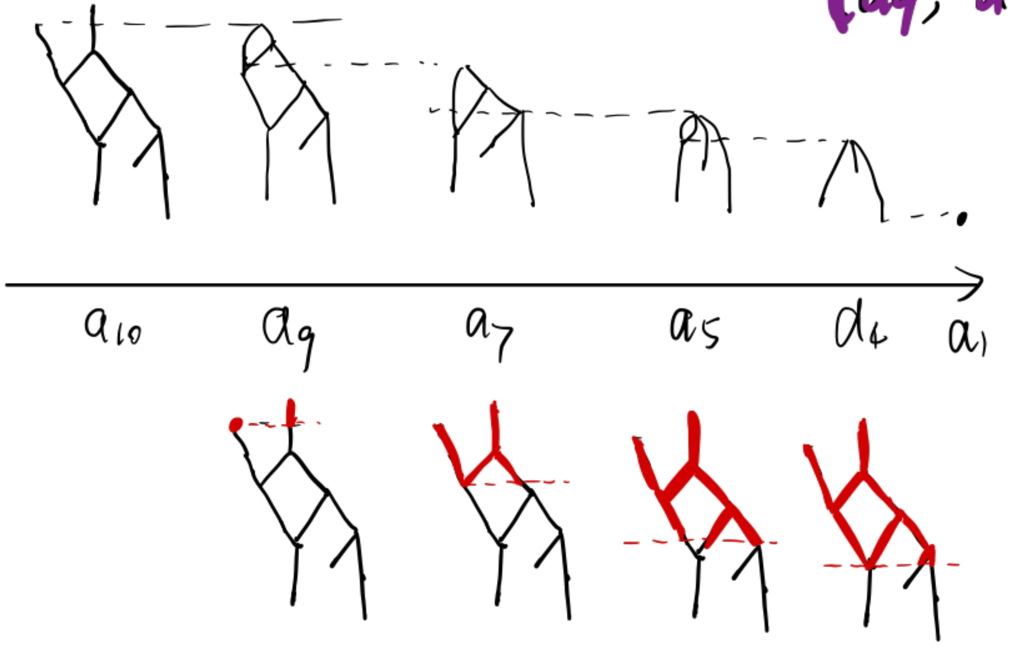
(a_2, a_6)

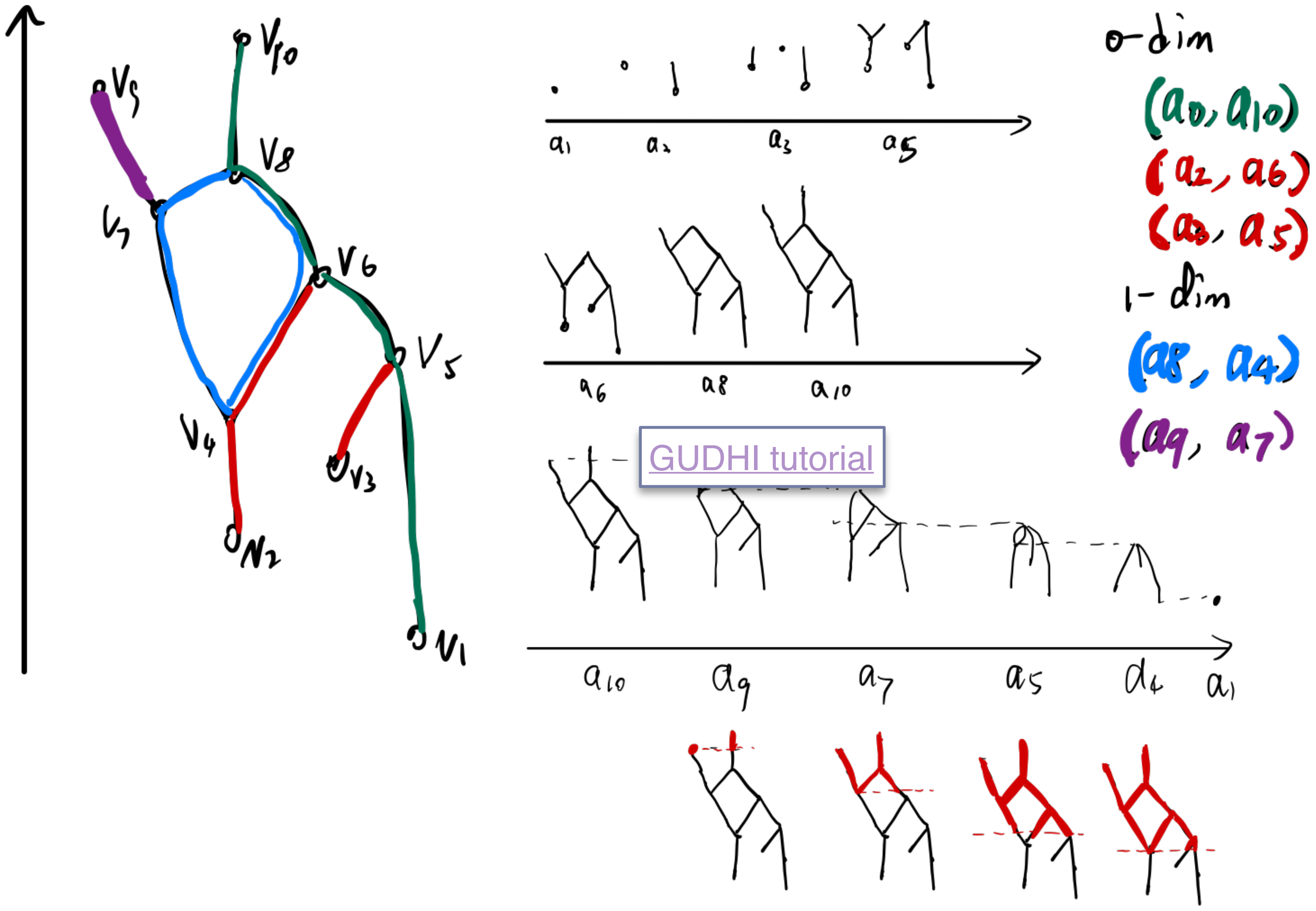
(a_3, a_5)

1-dim

(a_8, a_4)

(a_9, a_7)





V_{10}
V_9
V_8
V_7
V_6
V_5
V_4
V_3
V_2
V_1
a_1 a_2 a_3 a_5
a_6 a_8 a_{10}
GUDHI tutorial
a_{10} a_9 a_7 a_5 a_4 a_1
0-dim
(a_0, a_{10})
(a_2, a_6)
(a_3, a_5)
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A simple application: neuron classification

- For each neuron cell:
  - its morphology is represented by a rooted tree T

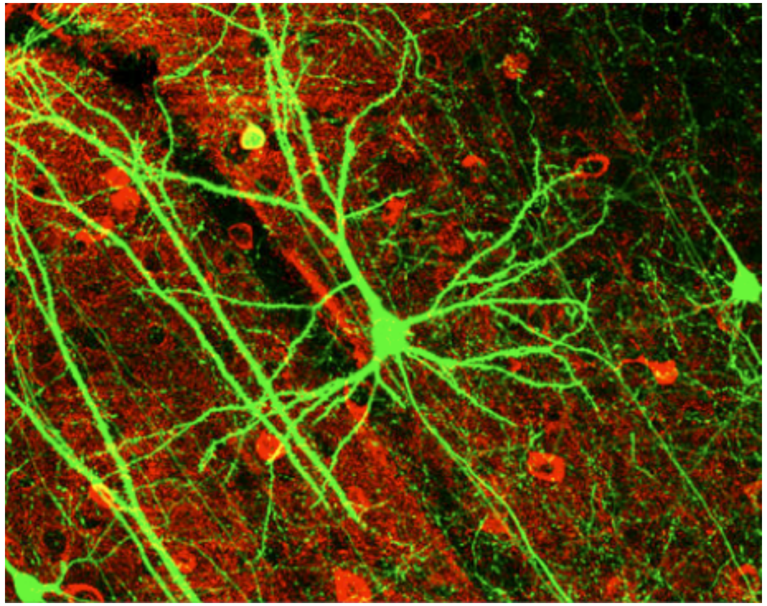


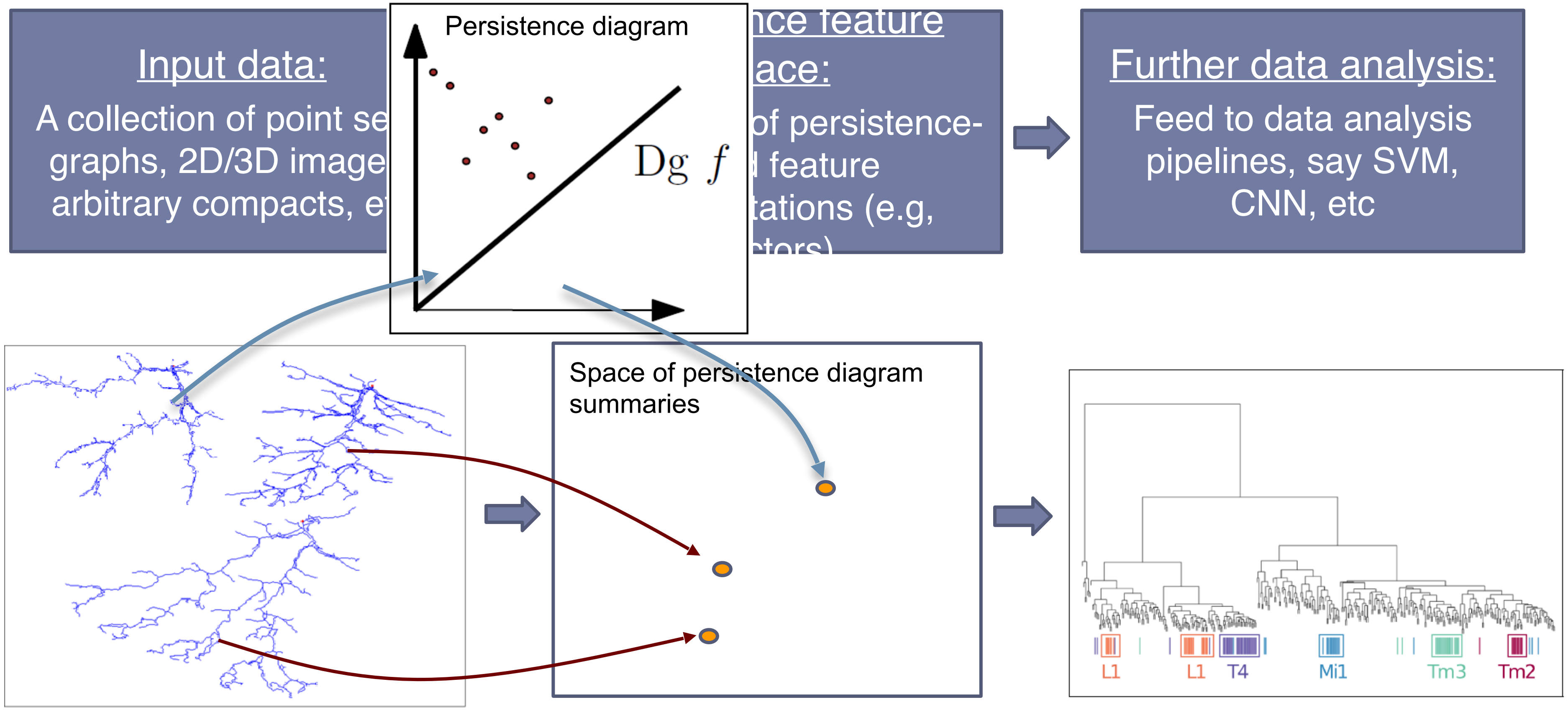
Image taken from Wikipedia

Neuron classification

- For each neuron cell:
  - its morphology is represented by a rooted tree T
- For a neuron tree T, choices of descriptor function $f: T \to R$:
  - Euclidean distance function to root; i.e, $f(x) = \left|\left|x - r\right|\right|_2$
  - Geodesic distance function to root

Persistence-based Framework

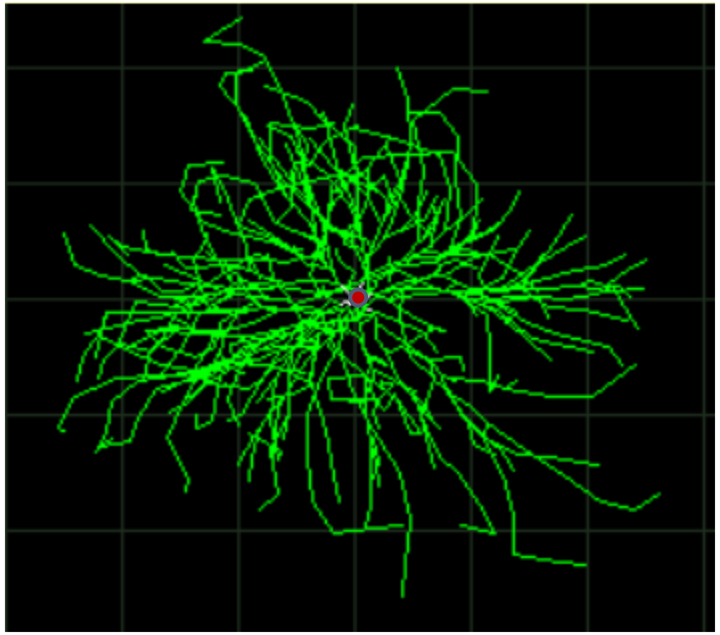
- Persistence-based feature vectorization



[Li, et al, PLOS One 2017]

Connection to Sholl-like Analysis

- Sholl function $N: R^+ \to R^+$
  - $N(\lambda) :=$ number of intersection of T with a circle (sphere) centered at the root r with radius λ



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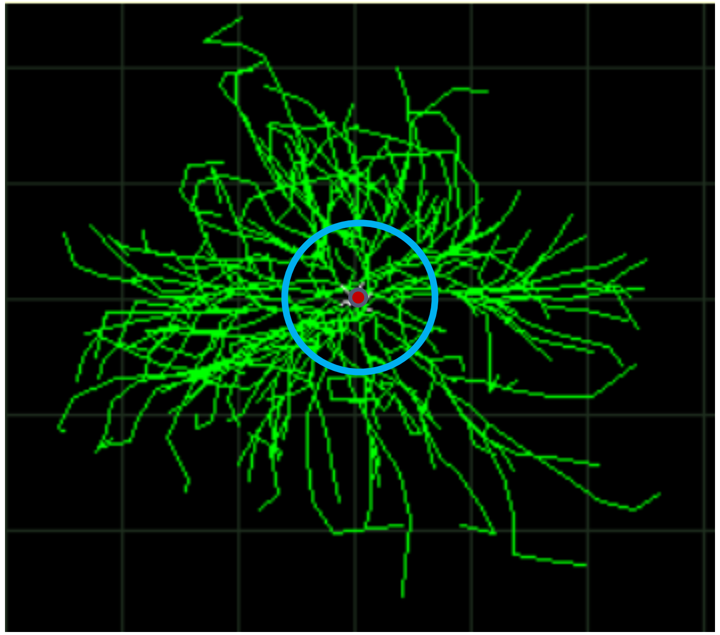

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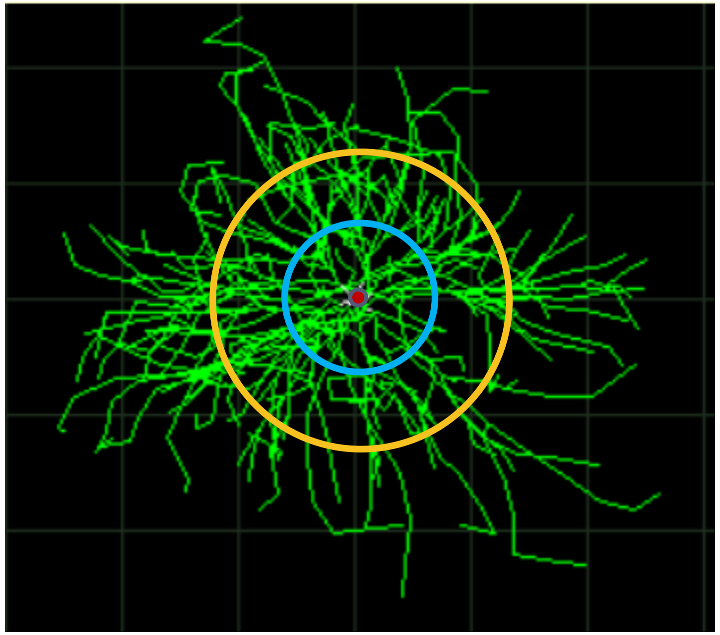

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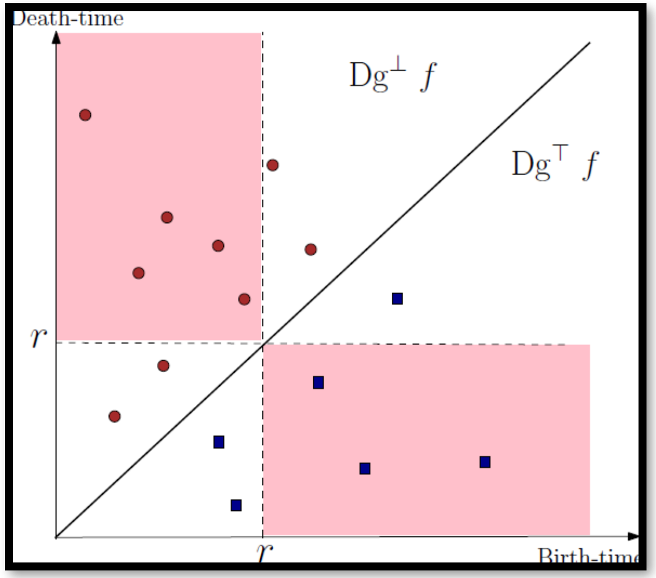

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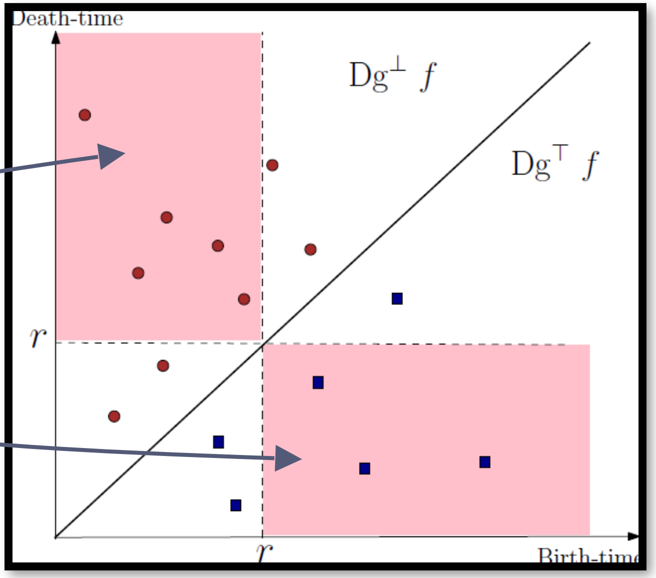
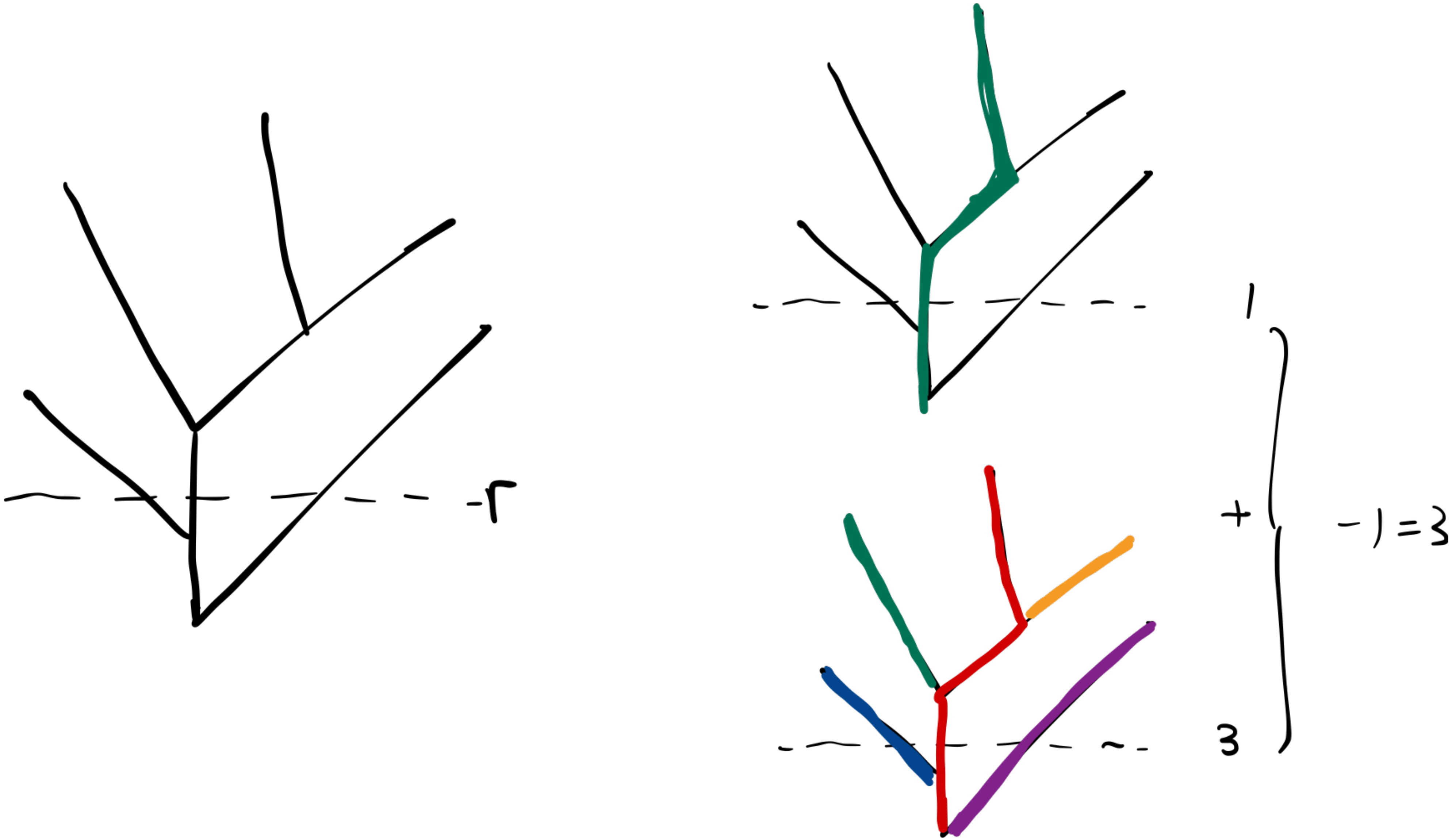
$N(r) =$ total number of points in these two regions - 1




r
1
+
3
-1 = 3

Directed graphs / asymmetric networks

- Directed clique complex
- Path homology

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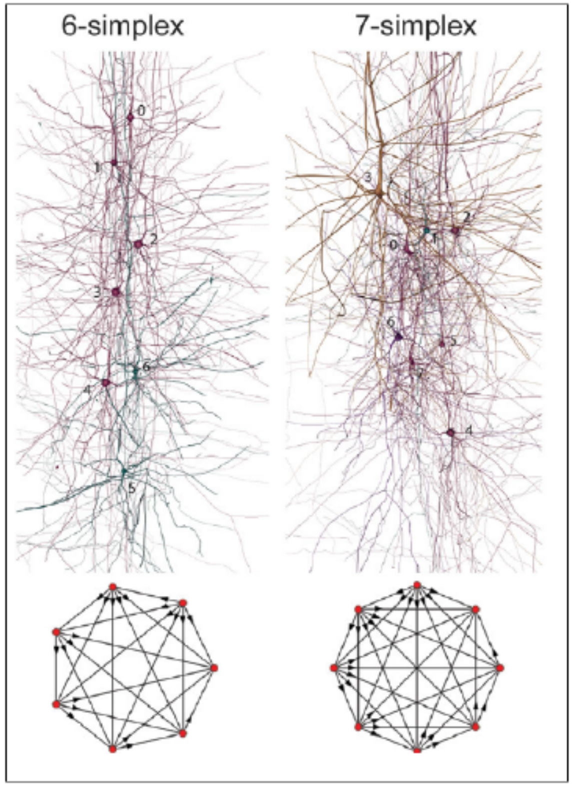
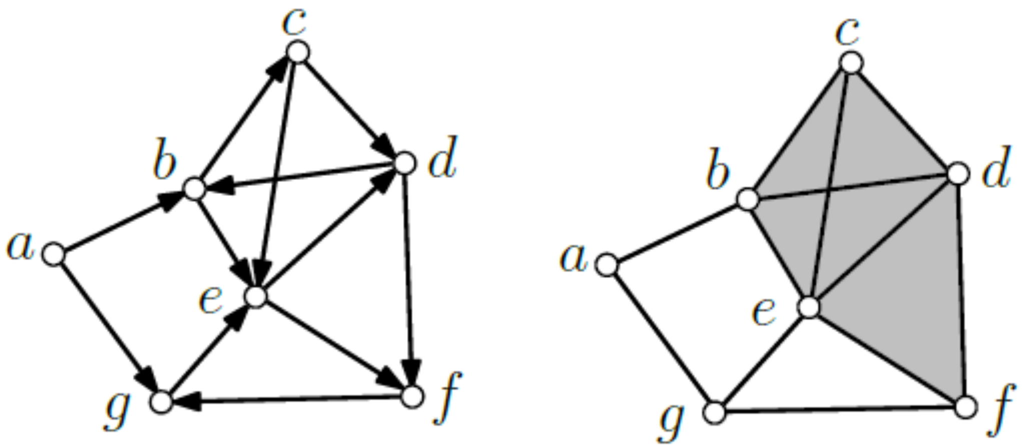
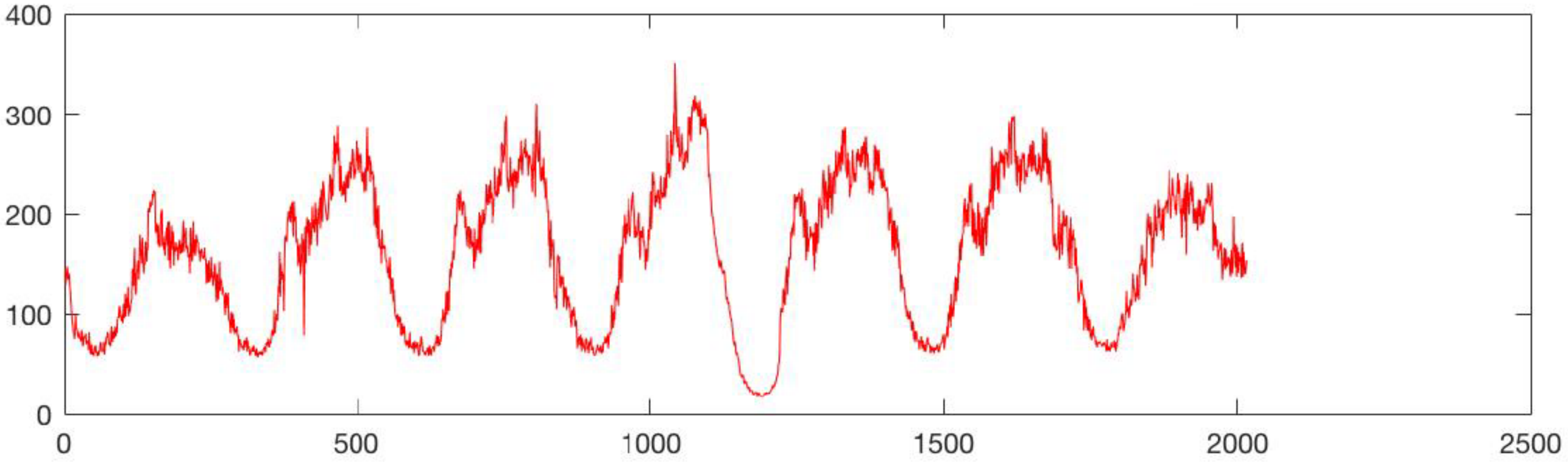


[Reimann et al., 2017]



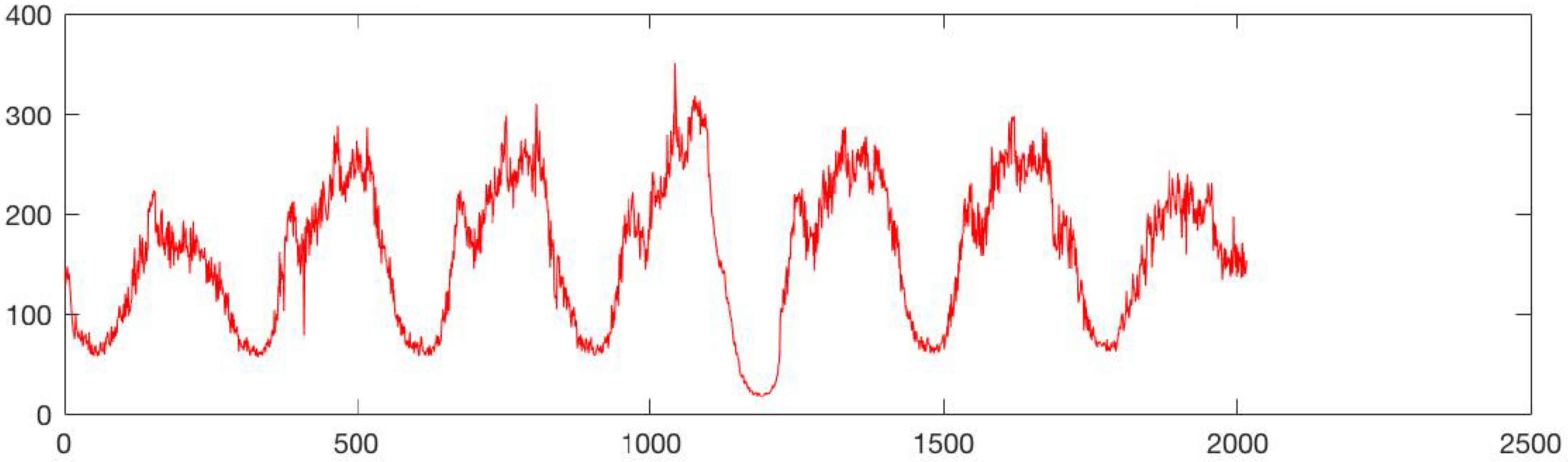
Time series data

- How do we create a filtration on top of a time series data?



Time series data

- How do we create a filtration on top of a time series data?
- Use some sort of "sliding window" embedding
  - Often one aims to capture quasi-periodic features



Time-delay embedding

- Map a time-series data $f: R \to R$ to a point cloud data

Given a time-series $f: R \to R$ and a parameter τ, a time-delay embedding is a lift to a time-series $\phi: R \to R^{M+1}$ defined by

$$\phi(t) = (f(t),\ f(t+\tau),\ \ldots,\ f(t+M\tau))$$

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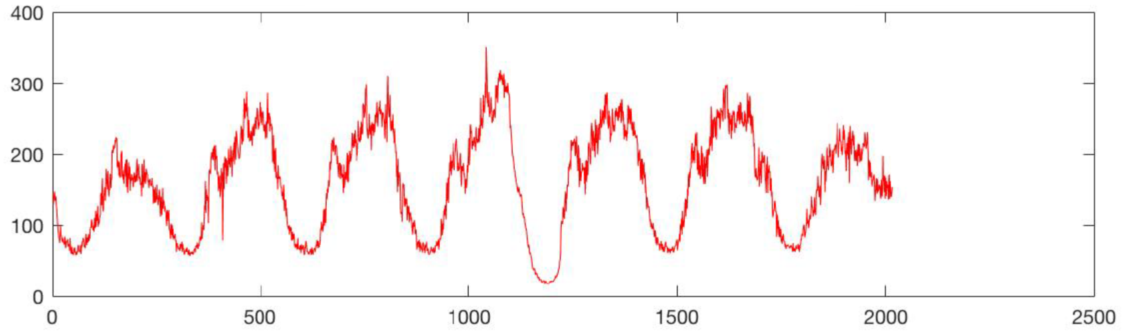
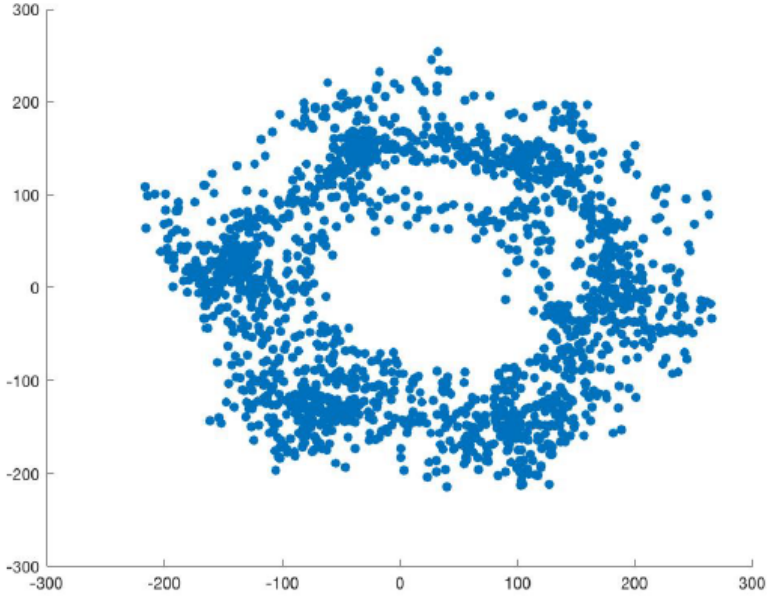
If the time-series is discrete time, then this will give a point cloud data.

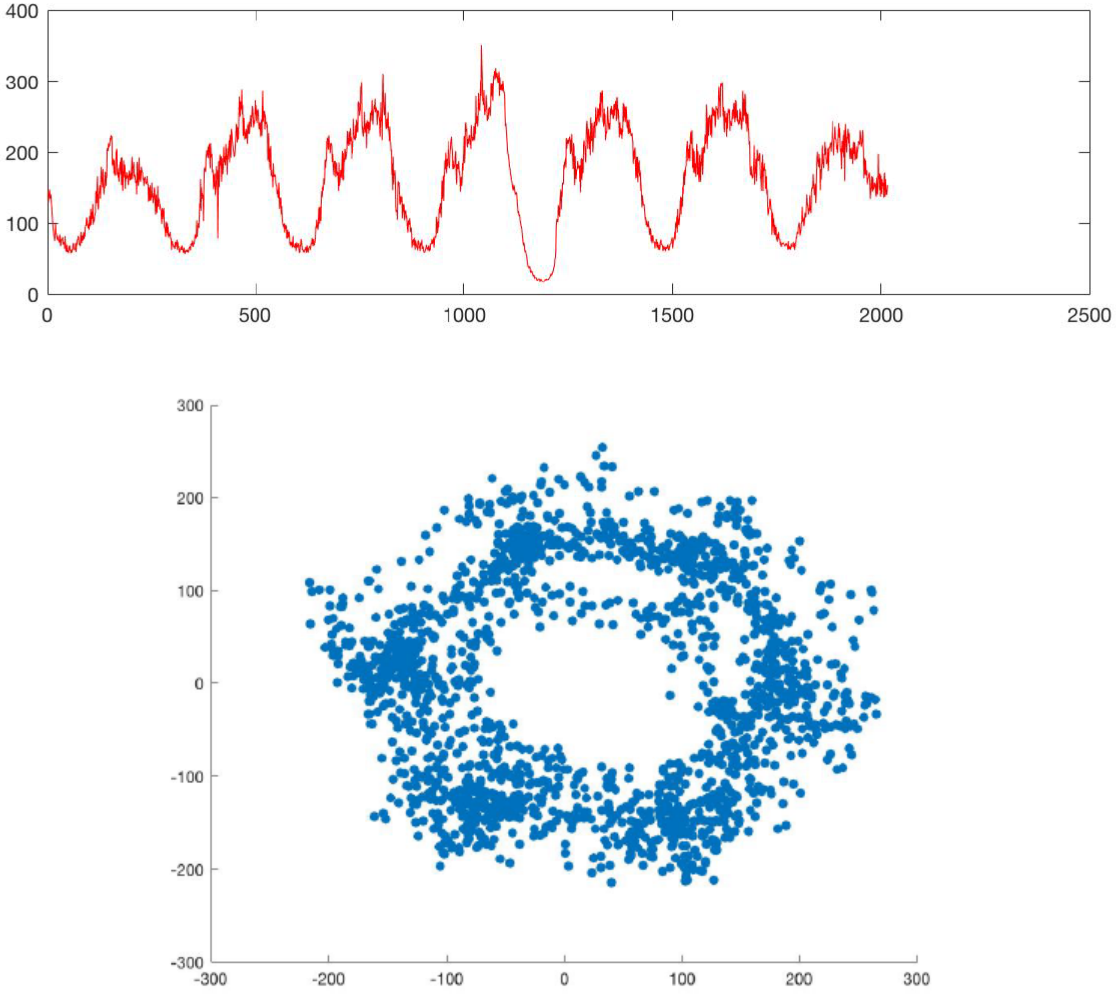
Examples



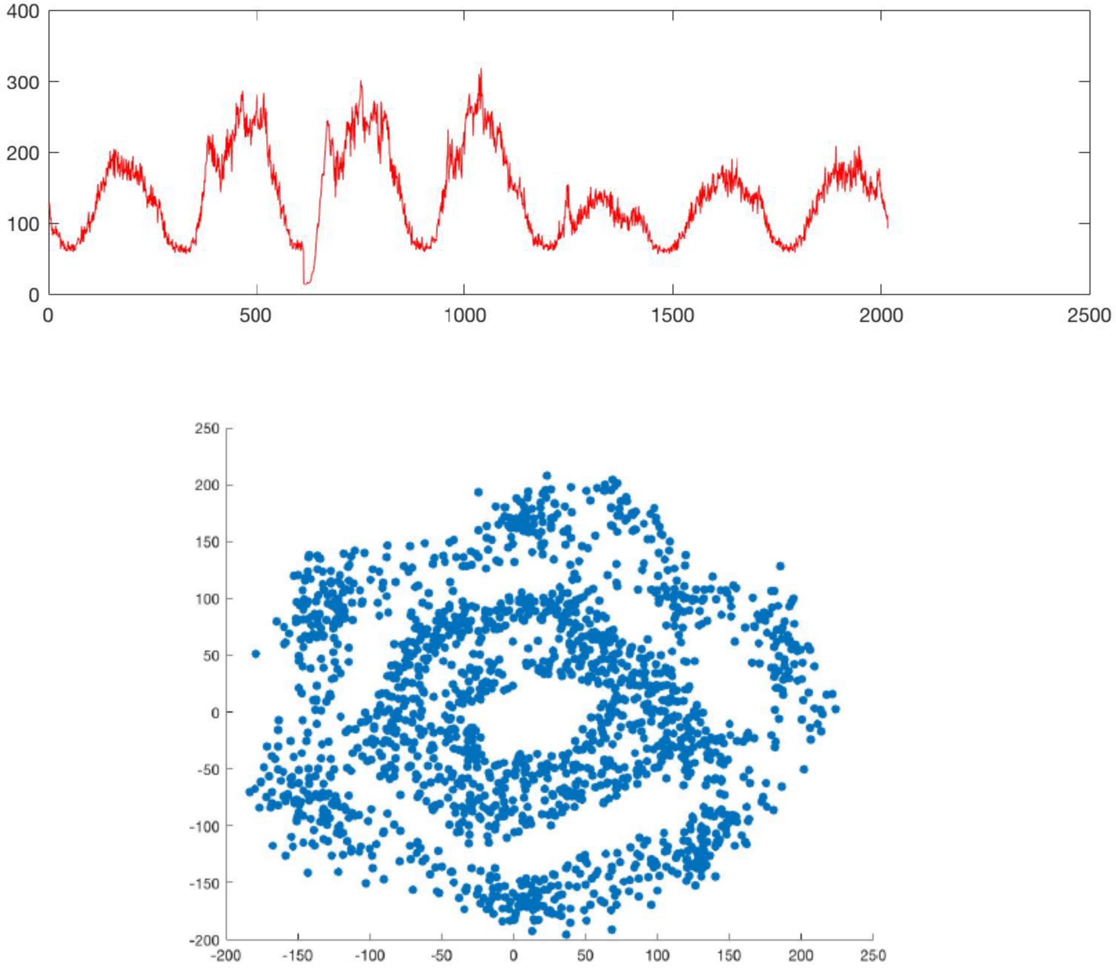


(a) Week 1

Examples

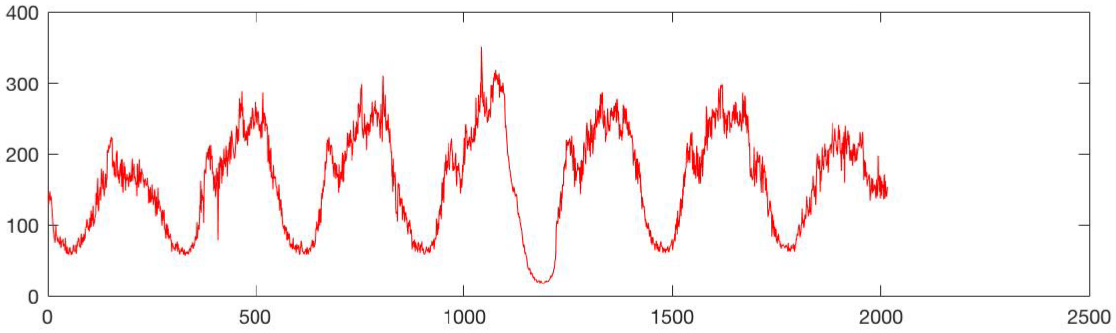


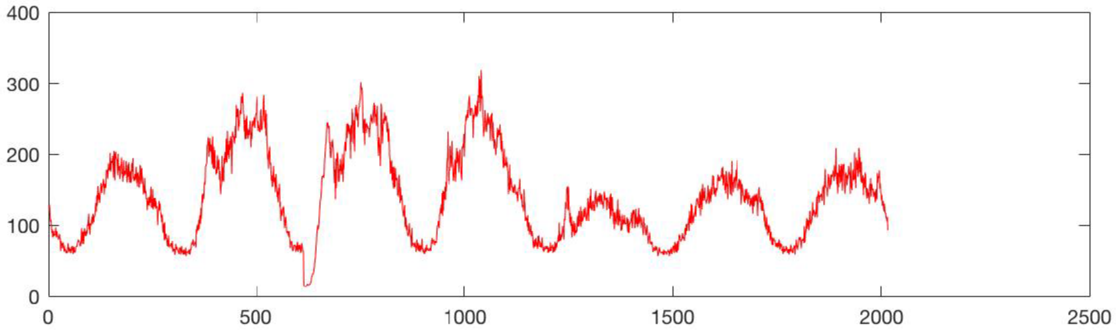
(a) Week 1

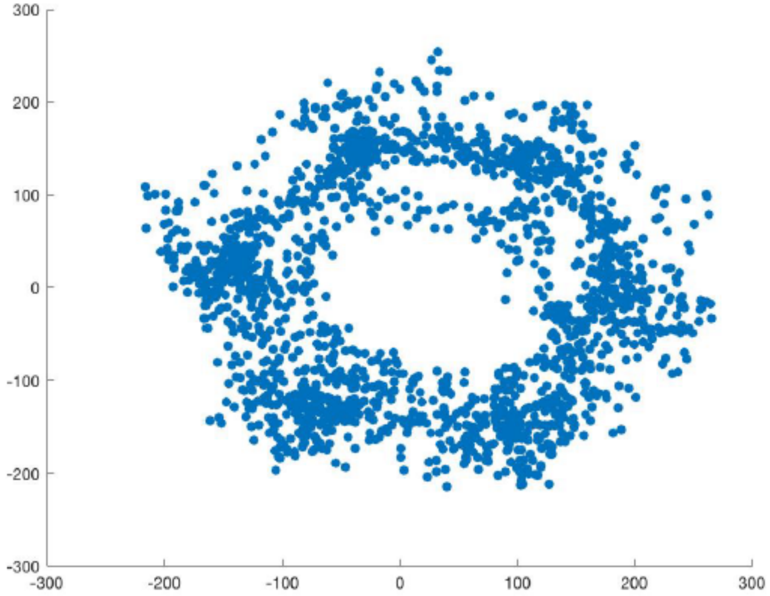


(b) Week 8

Examples

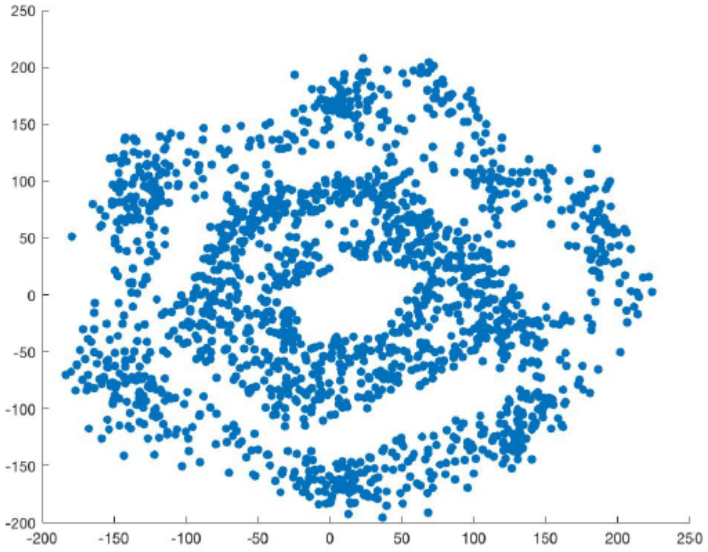






(a) Week 1

See a demo



(b) Week 8

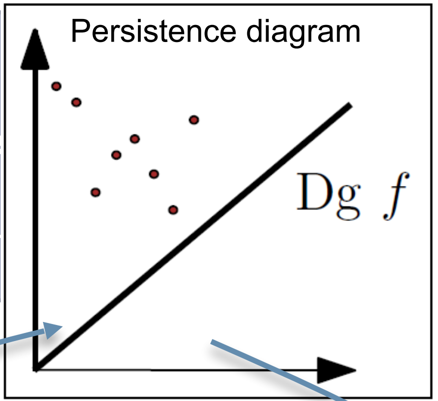
Section 2 :
Vectorization of persistence diagram summaries

Persistence-based Framework

- Persistence-based feature vectorization

Input data:

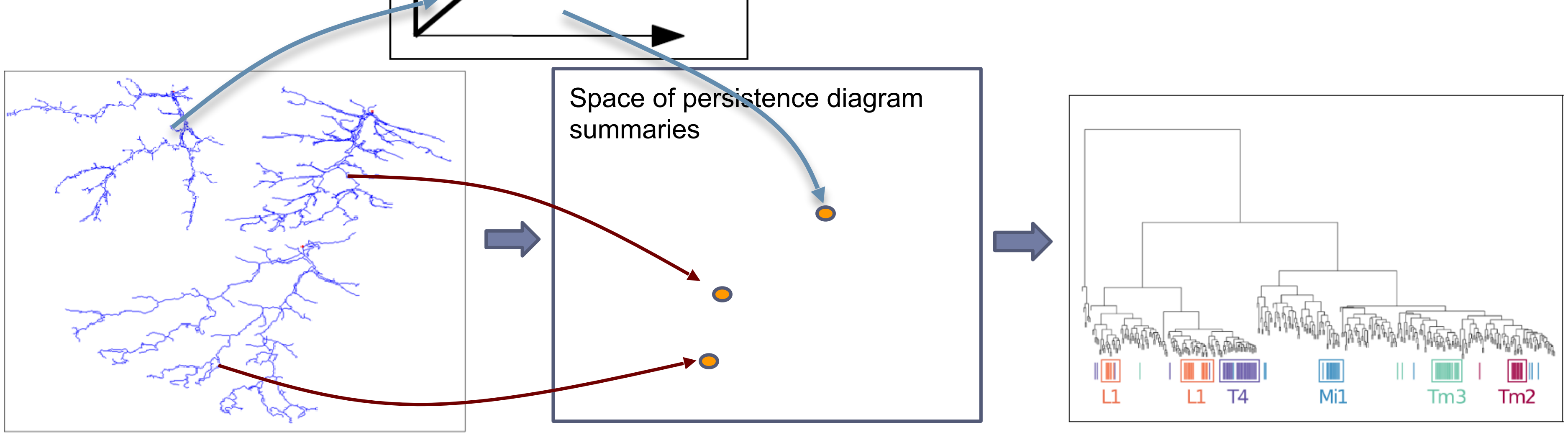
A collection of point se
graphs, 2D/3D image
arbitrary compacts, e



nce feature
ace:
of persistence-
l feature
tations (e.g,
ctors)

Further data analysis:

Feed to data analysis pipelines, say SVM, CNN, etc



[Li, et al., PLOS One 2017]

- Classical distance measure for persistence
  - e.g, bottleneck distance and Wasserstein distance, has stability properties,
  - but does not have nice (e.g, inner product) structure

- Map the space of persistence diagrams to yet another (finite or infinite dimensional) vector space

Persistence feature representation

- Persistence landscapes
  - [Bubenik 2012]
- Persistence scale space kernel
  - [Reininghause et al., 2014]
- Persistence images
  - [Adams et al., 2015, 2017]
- Persistence weighted Gaussian kernel
  - [Kusano et al., 2017]
- Sliced Wasserstein kernel
  - [Carriere et al., 2017]
- Persistence Fisher kernel
  - [Le and Yamada 2018]
- ....

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Gudhi package contains most of these

- Wonderful slides

Persistence landscapes

- Map persistence diagrams to a function space [Bubenik 2012]

Definition 13.1 (Persistence landscape). Given a finite persistence diagram $D = \{(b_i, d_i)\}_{i\in[1,n]}$ from $\mathbb{D}$, the *persistence landscape w.r.t. D* is a function $\lambda_D : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$ where

$$\lambda_D(k, t) := k\text{-th largest value of } [\min\{t - b_i, d_i - t\}]_+ \text{ for } i \in [1, n].$$

Here, $[c]_+ = max(c, 0)$.

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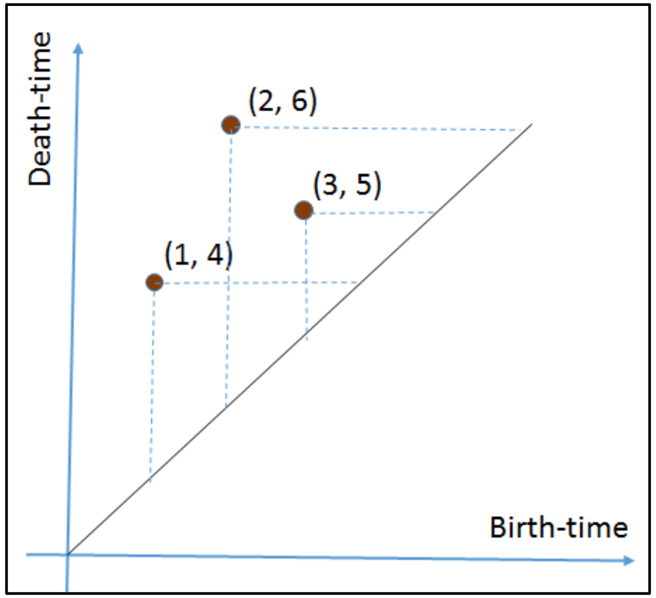

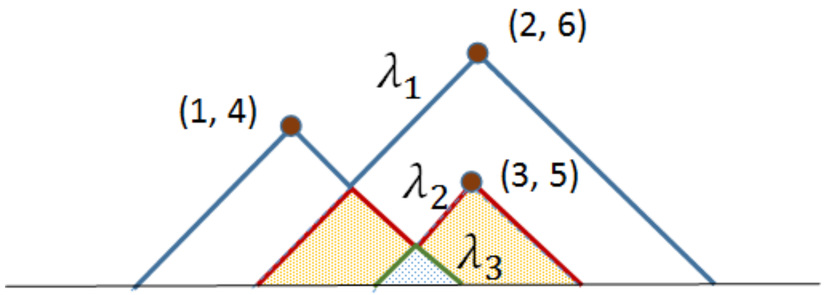

Metric for persistence landscapes

- p-norm: $$\|\lambda_D\|_p^p = \sum_{k=1}^{\infty} \|\lambda_D(k,\cdot)\|_p^p.$$

- p-landscape distance:

Metric for persistence landscapes

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- p-landscape distance:

$$\Lambda_p(D_1, D_2) = \|\lambda_{D_1} - \lambda_{D_2}\|_p$$

Some results

Claim *Given a persistence diagram D, let λ_D be its persistence landscape. Then from λ_D one can uniquely recover the persistence diagram D.*

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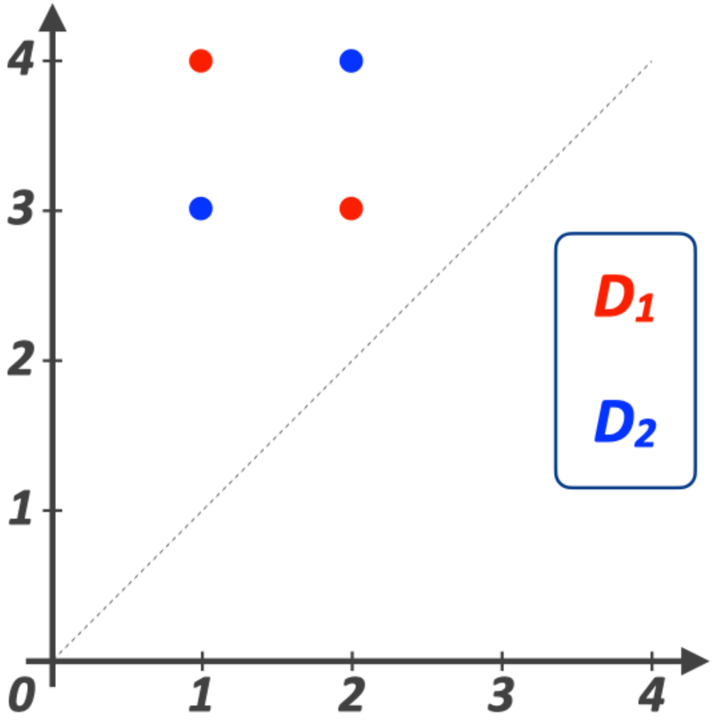
Theorem *For persistence diagrams D and D', $\Lambda_\infty(D, D') \leq d_B(D, D')$.*

Statistics for TDA

- There is no well-defined notion of mean for persistence diagrams



Courtesy of Fugacci

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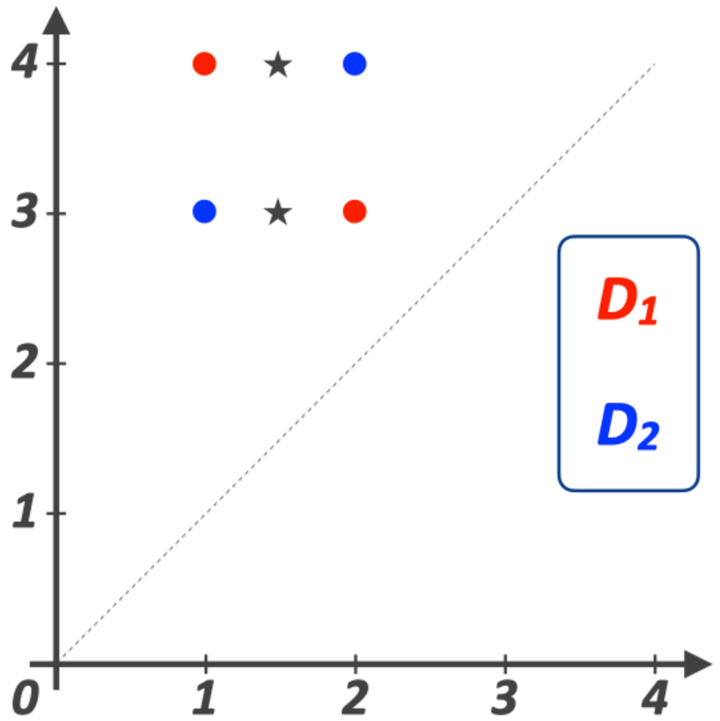

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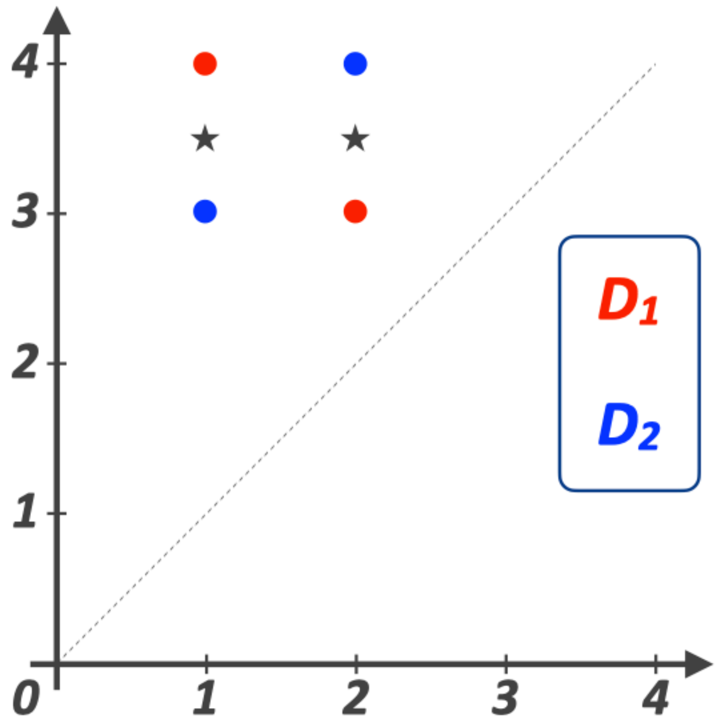

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Statistics for TDA

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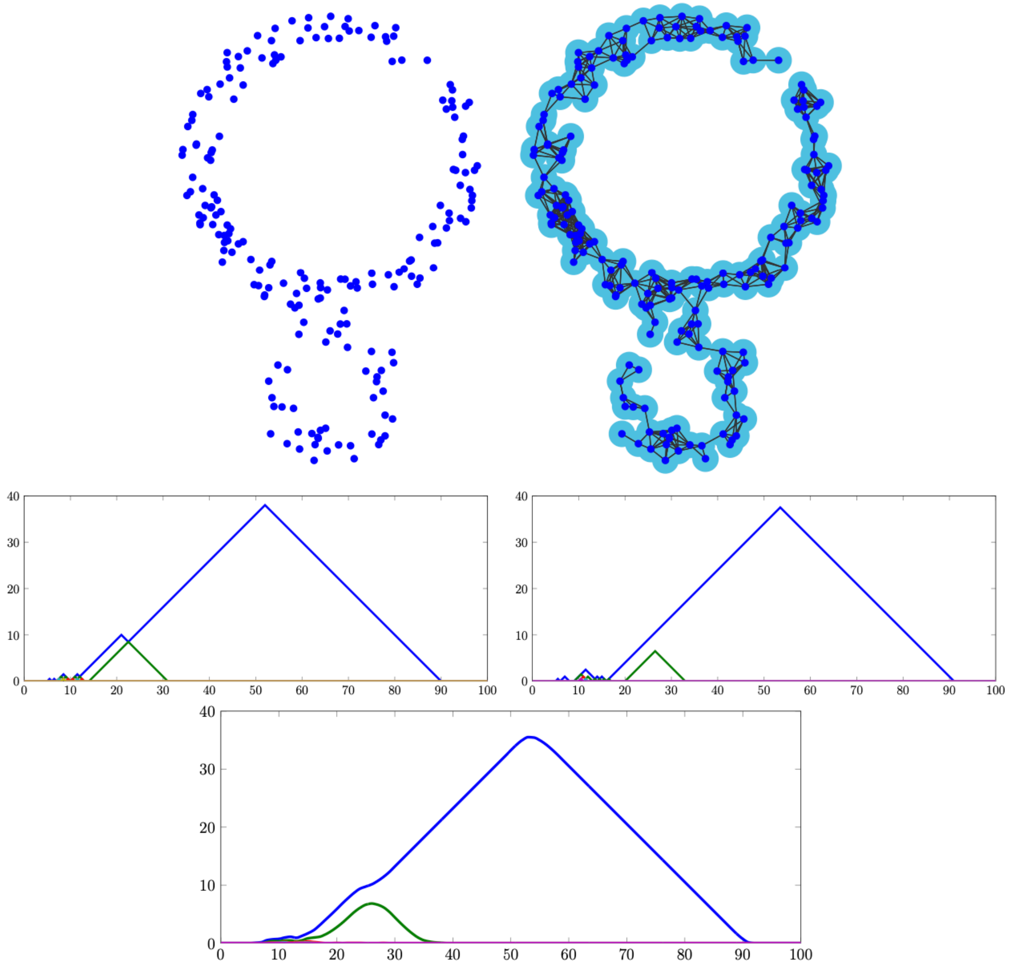
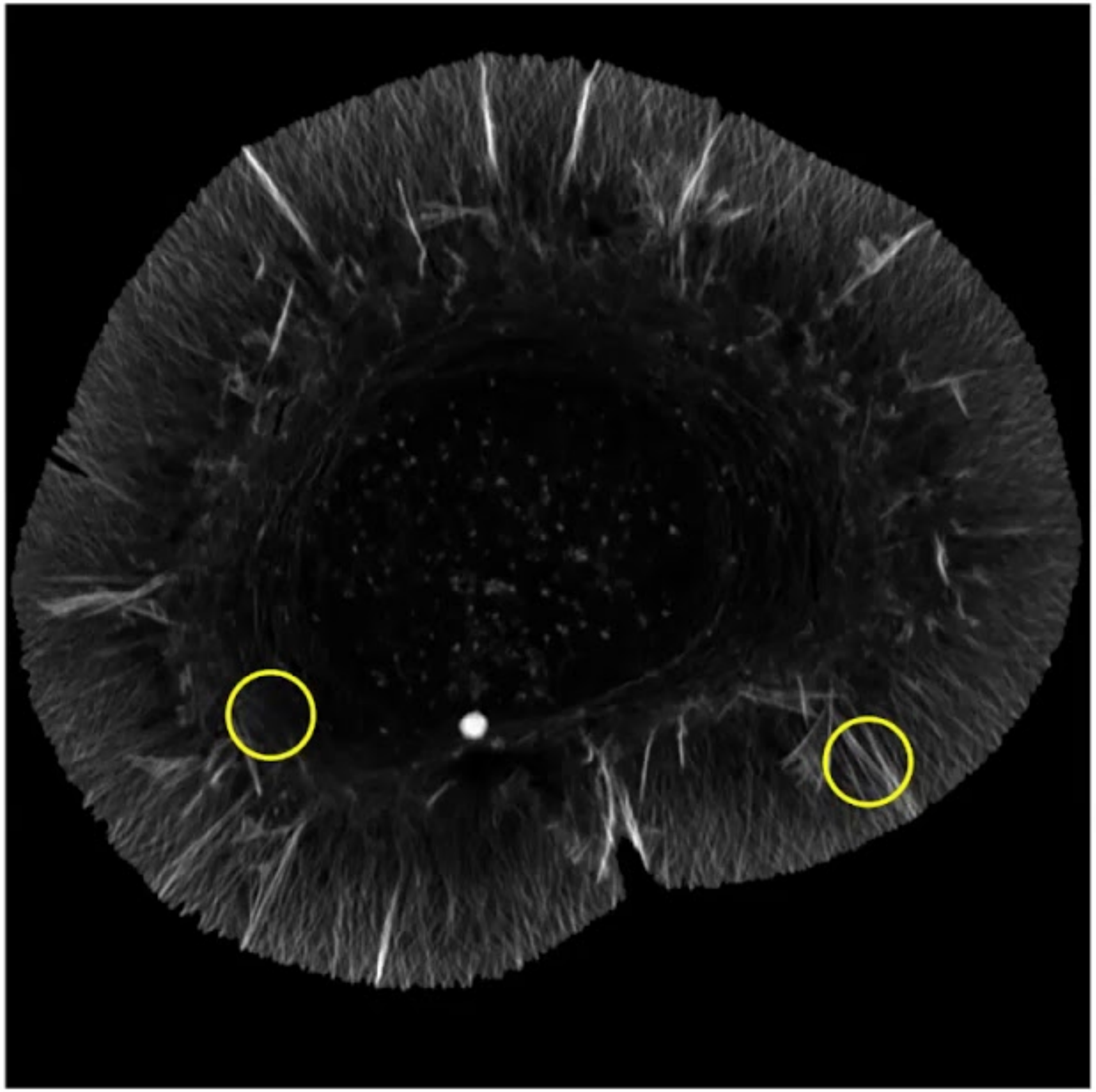
- mean landscape of $\lambda_{D_1}, \lambda_{D_2}, \ldots, \lambda_{D_\ell}$

$$\overline{\lambda}(k, t) = \frac{1}{n} \sum_{i=1}^{\ell} \lambda_{D_i}(k, t).$$

Average of persistence landscapes



e biological images



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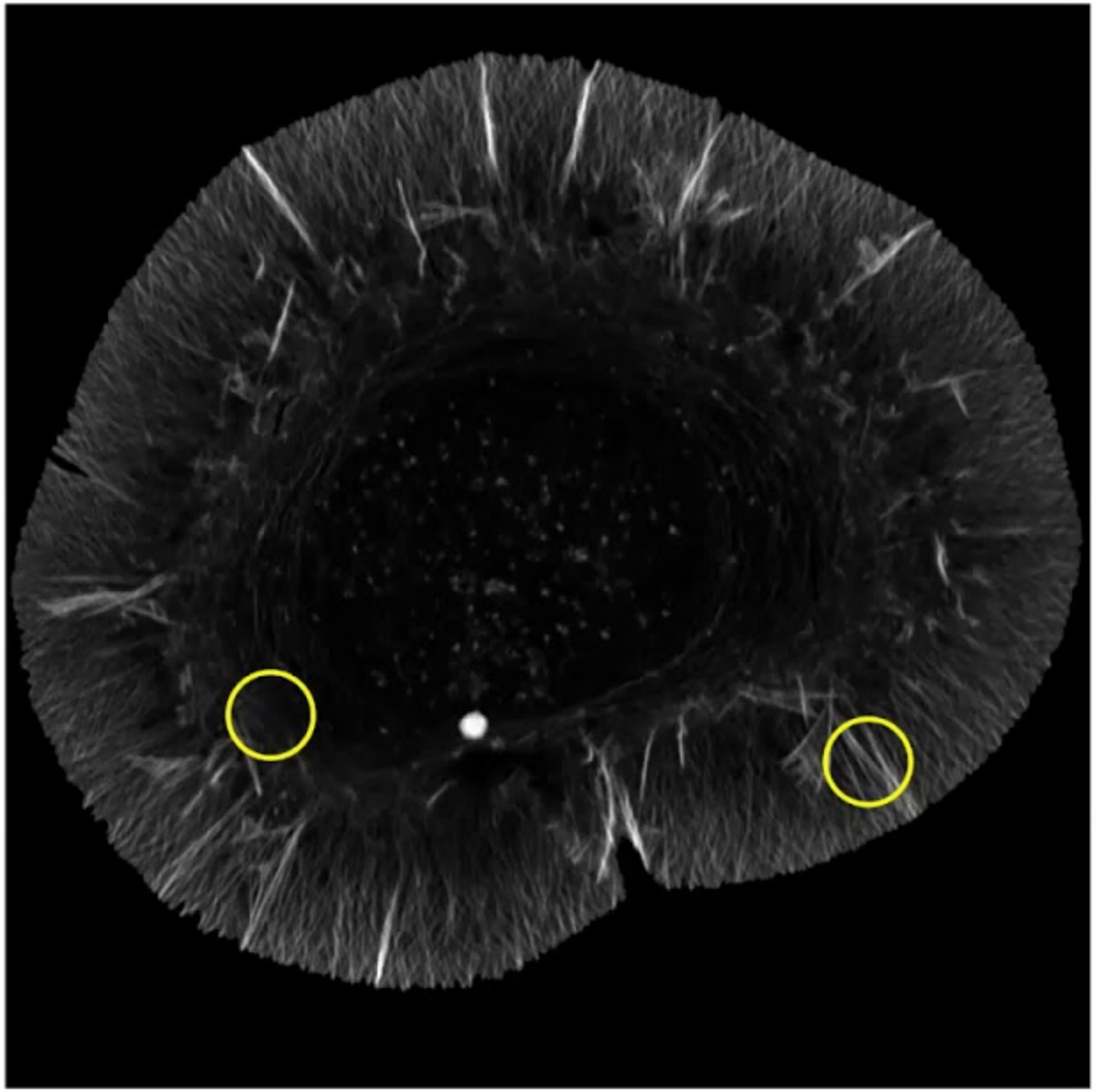

Next

- Kernel-based approach
- SVM for classification
- PCA for dimension reduction, visualization

Kernels

- Given a topological space X, a kernel is simply a function $k: X \times X \rightarrow R$
  - i.e., given any $x, \ y \in X$, it sends them to a real value $k\left(x, y\right)$
- In practice, we often use positive (semi-)definite kernels:
- A Hilbert space is intuitively a vector space (over real or complex number) equipped with an inner product, and it is a complete metric space w.r.t. the distance induced by the inner product.

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  - i.e., given any $x,\ y \in X$, it sends them to a real value $k(x, y)$
- In practice, we often use positive (semi-)definite kernels:

Definition 13.2 (Positive, negative semi-definite kernel)**.** Given a topological space X, a function $\mathsf{k} : X \times X \to \mathbb{R}$ is a *positive semi-definite kernel* if it is symmetric and for any integer $n > 0$, any $x_1, \ldots, x_n \in X$, and any $a_1, \ldots, a_n \in \mathbb{R}$ with $\sum_i a_i = 0$, it holds that $\sum_{i,j} a_i a_j \mathsf{k}(x_i, x_j) \geq 0$. Analogously, k is a *negative semi-definite kernel* if it is symmetric and any integer $n > 0$, any $x_1, \ldots, x_n \in X$ and any $a_1, \ldots, a_n \in \mathbb{R}$ with $\sum_i a_i = 0$, it holds that $\sum_{i,j} a_i a_j \mathsf{k}(x_i, x_j) \leq 0$.

- A Hilbert space is intuitively a vector space (over real or complex number) equipped with an inner product, and it is a complete metric space w.r.t. the distance induced by the inner product.

- A positive semi-definite kernel can be thought of the inner product $k\left(x, y\right) = \langle\Phi(x),\ \Phi(y)\rangle_{\mathscr{H}}$ after mapping X to some Hilbert space $\mathscr{H}$ via a feature map $\Phi: X \to\ \mathscr{H}$
- Hence given a positive semi-definite kernel, we can induce a (pseudo-)metric:
  - $d_k^2(x,\ y) = \left\langle x - y, x - y \right\rangle = k(x,\ x) + k\left(y,\ y\right)\ - 2k\left(x, y\right)$
- In what follows, we will define kernel (distance) for persistence diagrams by either explicitly specifying the kernel; or specifying the feature map.

PSSK (Persistence scale space kernel)

- [Reininghaus et al. 2015]

Definition 13.3 (Persistence scale space kernel (PSSK)). Define the feature map $\Phi_\sigma : \mathbb{D} \to \mathcal{L}^2(\Omega)$ at scale $\sigma > 0$ as follows: for a persistence diagram $D \in \mathbb{D}$ and $x \in \Omega$, set:

$$\Phi_\sigma(D)(x) = \frac{1}{4\pi\sigma} \sum_{y \in D} [e^{-\frac{\|x-y\|^2}{4\sigma}} - e^{-\frac{\|x-\bar{y}\|^2}{4\sigma}}],$$

where $\bar{y} = (y_2, y_1)$ if $y = (y_1, y_2)$ (i.e, $\bar{y}$ is the reflection of y across the diagonal). This feature map induces the following *persistence scale space kernel (PSSK)* $k_\sigma : \mathbb{D} \times \mathbb{D} \to \mathbb{R}$ using the inner product structure on $\mathcal{L}^2(\Omega)$: given two diagrams $D, E \in \mathbb{D}$,

$$k_\sigma(D, E) = \langle \Phi_\sigma(D), \Phi_\sigma(E) \rangle_{\mathcal{L}^2(\Omega)} = \frac{1}{8\pi\sigma} \sum_{y \in D;\, z \in E} [e^{-\frac{\|y-z\|^2}{8\sigma}} - e^{-\frac{\|y-\bar{z}\|^2}{8\sigma}}].$$

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$$\|\Phi_\sigma(D) - \Phi_\sigma(E)\|_{\mathcal{L}^2(\Omega)} = \sqrt{k_\sigma(D, D) + k_\sigma(E, E) - 2k_\sigma(D, E)}.$$

- Hence a persistence diagram D is mapped to a function $\Phi_\sigma(D)$ under the feature map Φ_σ
- Induced metric:

$$\|\Phi_\sigma(D) - \Phi_\sigma(E)\|_{\mathcal{L}^2(\Omega)} = \sqrt{k_\sigma(D, D) + k_\sigma(E, E) - 2k_\sigma(D, E)}.$$

- Stability:

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- Stability:

Theorem 13.2. *Given two persistence diagrams $D, E \in \mathbb{D}$, we have*

$$\|\Phi_\sigma(D) - \Phi_\sigma(E)\|_{\mathcal{L}^2(\Omega)} \le \frac{1}{2\pi\sigma} \mathrm{d}_{W,1}(D,E).$$

PWGK (Persistence weighted Gaussian kernel)

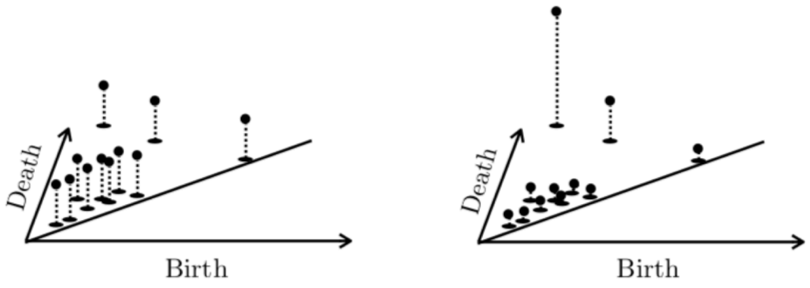
- [Kusano et al. 2017]

Definition 13.5 (Persistence weighted kernel)**.** Let $k : \Omega \to \mathbb{R}$ be a C_0-universal kernel on Ω (e.g, a Gaussian), and $\omega : \Omega \to \mathbb{R}^+$ a strictly positive (weight) function on Ω. The following feature map $\Psi_{k,\omega} : \mathbb{D} \to \mathcal{H}_k$ maps each persistence diagram $D \in \mathbb{D}$ to the RKHS $\mathcal{H}_k$ associated to k:

$$\Psi_{k,\omega}(D) = \sum_{x \in D} \omega(x) k(\cdot, x).$$

This feature map induces the following *persistence weighted kernel (PWK)* $K_{k,\omega} : \mathbb{D} \times \mathbb{D} \to \mathbb{R}$:

$$K_{k,\omega}(D, E) = \langle \Psi_{k,\omega}(D), \Psi_{k,\omega}(E) \rangle_{\mathcal{H}_k} = \sum_{x \in D;\ y \in E} \omega(x)\omega(y)k(x, y). \tag{13.4}$$



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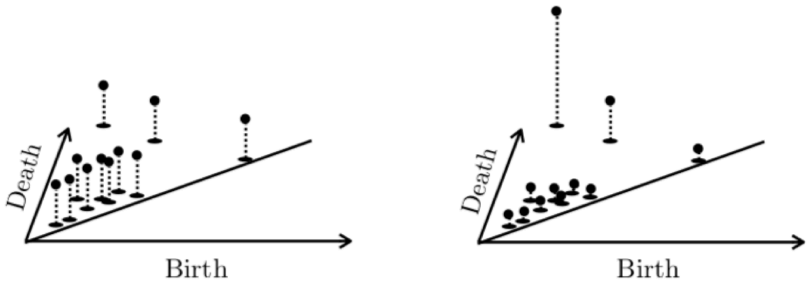

PWGK (Persistence weighted Gaussian kernel)

- Specific choice of the weight function ω:
  - given a persistence point $x = (b, d)$, let $pers(x) = \left| d - b \right|$
  - then, we define $\omega_{arc}(x) = \arctan\left(C \cdot pers(x)^p\right)$, where C is some constant and p a positive integer.

- Using the 2D Gaussian kernel $k_G\left(x, y\right) = e^{-\frac{||x-y||^2}{2\tau^2}}$, and weight function ω_{arc}, the resulting kernel for persistence diagrams is called PWGK
  - i.e, $k_G^{\omega_{arc}}\left(x, y\right) = \omega_{arc}(x)\omega_{arc}\left(y\right)k_G(x, y)$

Other kernels

- Sliced Wasserstein kernel = OT + TDA
- Persistence Fisher kernel = Information Geometry + TDA

Sliced Wasserstein kernel (SW)

- [Carriere et al., 2017] define a kernel like $k(x, y) = \exp(-\frac{f(x, y)}{2\sigma^2})$
- Here it constructs a positive kernel via exponentiating a negative kernel!

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Theorem 13.4. *Given X and $\phi : X \times X \to \mathbb{R}$, the kernel ϕ is negative semi-definite if and only if $e^{-t\phi}$ is positive semi-definite for all $t > 0$.*

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Theorem 13.4. *Given X and $\phi : X \times X \to \mathbb{R}$, the kernel ϕ is negative semi-definite if and only if $e^{-t\phi}$ is positive semi-definite for all $t > 0$.*

- First construct the so-called Sliced Wasserstein distance d_{SW}, which turns out to be negative (semi-)definite.
- Then use d_{SW} to construct SW kernel via the above theorem.

Wasserstein Distance

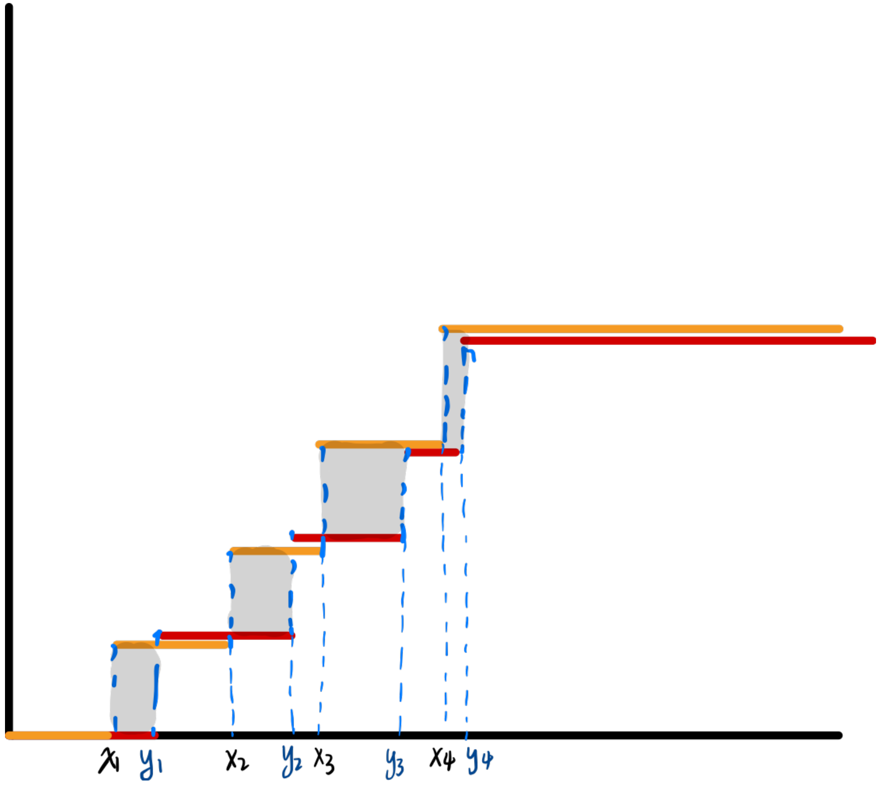
- A *transport plan* between two probability measures $\mu, \ \nu$ on $\mathbb{R}^d$ is a probability measure π on $\mathbb{R}^d \times \mathbb{R}^d$ such that for every $A, B \subseteq \mathbb{R}^d$, $\pi(A \times \mathbb{R}^d) = \mu(A)$ and $\pi(\mathbb{R}^d \times B) = \mu(B)$.
- The p-cost of a transport plan π is:

$$C_p(\pi) = \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p \pi(dx \times dy) \right)^{1/p}$$

- The *Wasserstein distance* of order p between $\mu, \ \nu$ on $\mathbb{R}^d$ with finite p -moment
  - $W_p(\mu, \ \nu) =$ the minimum p-cost $C_p(\pi)$ of any transport plan π between μ and ν .

Wasserstein distance on real line

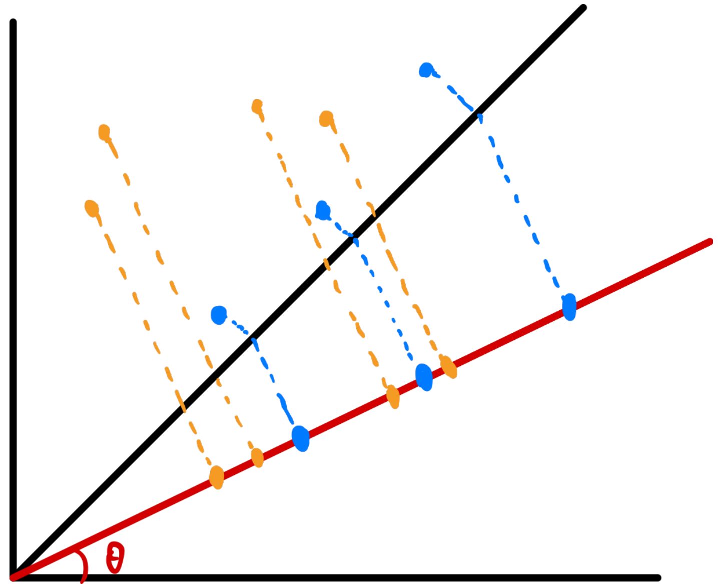
Remark 2.2. *For two unnormalized uniform empirical measures* $\mu = \sum_{i=1}^{n} \delta_{x_i}$ *and* $\nu = \sum_{i=1}^{n} \delta_{y_i}$ *of the same size, with ordered* $x_1 \leq \cdots \leq x_n$ *and* $y_1 \leq \cdots \leq y_n$*, one has:* $\mathcal{W}(\mu, \nu) = \sum_{i=1}^{n} |x_i - y_i| = \|X - Y\|_1$*, where* $X = (x_1, \cdots, x_n) \in \mathbb{R}^n$ *and* $Y = (y_1, \cdots, y_n) \in \mathbb{R}^n$*.*



Sliced-Wasserstein distance

Definition 13.6 (Sliced-Wasserstein distance)**.** Given a unit vector $\theta \in \mathbb{S}^1 \subseteq \mathbb{R}^2$, let $L(\theta)$ denote the line $\{\lambda\theta \mid \lambda \in \mathbb{R}\}$. Let $\pi_\theta : \mathbb{R}^2 \to L(\theta)$ be the orthogonal projection of the plane onto $L(\theta)$. Given two persistence diagrams D and E, set $\mu_D^\theta := \sum_{p \in D} \delta_{\pi_\theta(p)}$ and $\overline{\mu}_D^\theta := \sum_{p \in D} \delta_{\pi_\theta \circ \pi_\Delta(p)}$, where $\pi_\Delta : \mathbb{R}^2 \to \Delta$ is the orthogonal projection onto the diagonal $\Delta = \{(x, x) \mid x \in \mathbb{R}\}$. Set μ_E^θ and $\overline{\mu}_E^\theta$ in a symmetric manner. Then the *Sliced Wasserstein distance* between D and E is defined as:

$$\mathsf{d}_{SW}(D, E) := \frac{1}{2\pi} \int_{\mathbb{S}^1} \mathcal{W}(\mu_D^\theta + \overline{\mu}_E^\theta,\ \mu_E^\theta + \overline{\mu}_D^\theta) d\theta.$$



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- The positive semi-definite *Sliced Wasserstein kernel* k_{SW} is defined as:
  - $k_{SW}(D,\ E) := e^{-\frac{d_{SW}(D,\ E)}{2\tau^2}}$ for some $\tau > 0$

Persistence Images

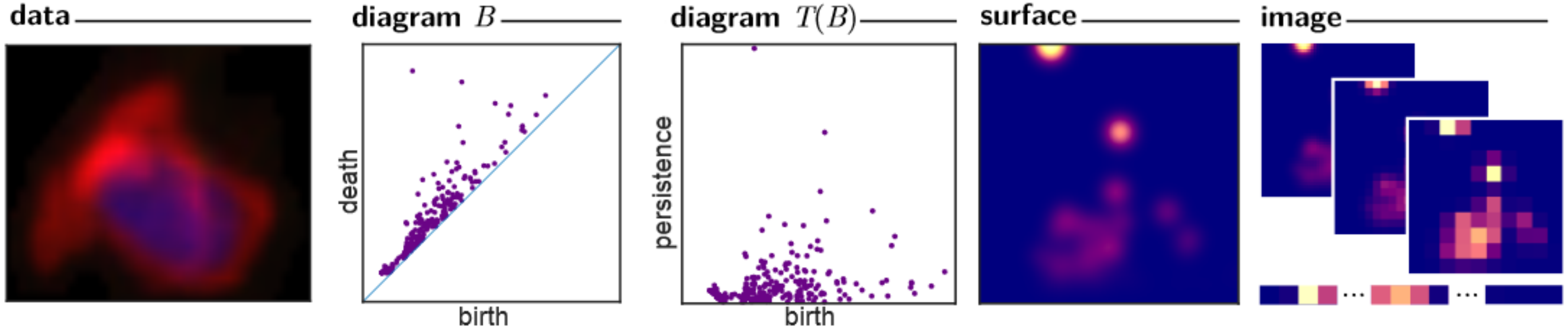
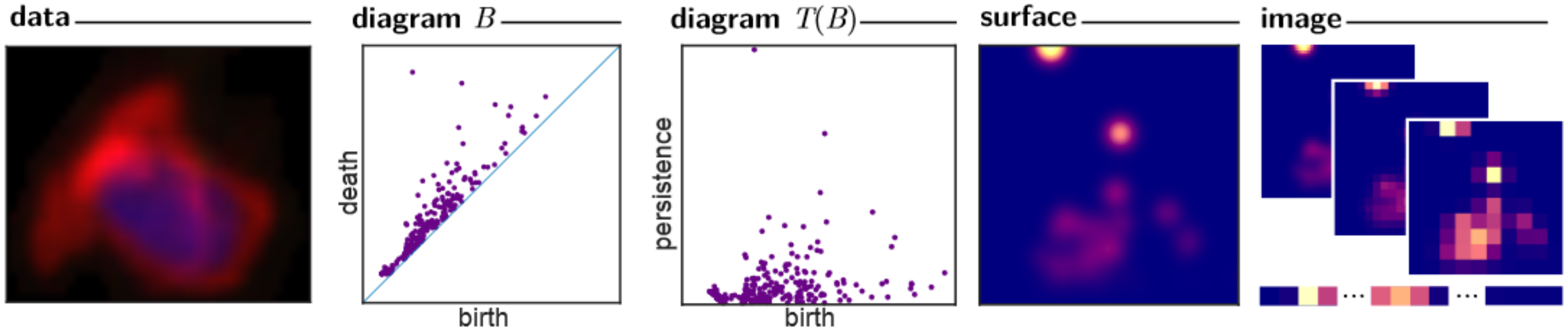


Figure 1: Algorithm pipeline to transform data into a persistence image.

Image taken from [Adams et al., 2017]

- Given a persistence diagram B
  - $T : \mathbb{R}^2 \to \mathbb{R}^2$ such that $T(x, y) = (x, y - x)$
  - Persistence surface ρ_B: $R^2 \to R$ where
    - $$\rho_B(z) = \sum_{u \in T(B)} f(u) \cdot \phi_u(z)$$

Persistence Images



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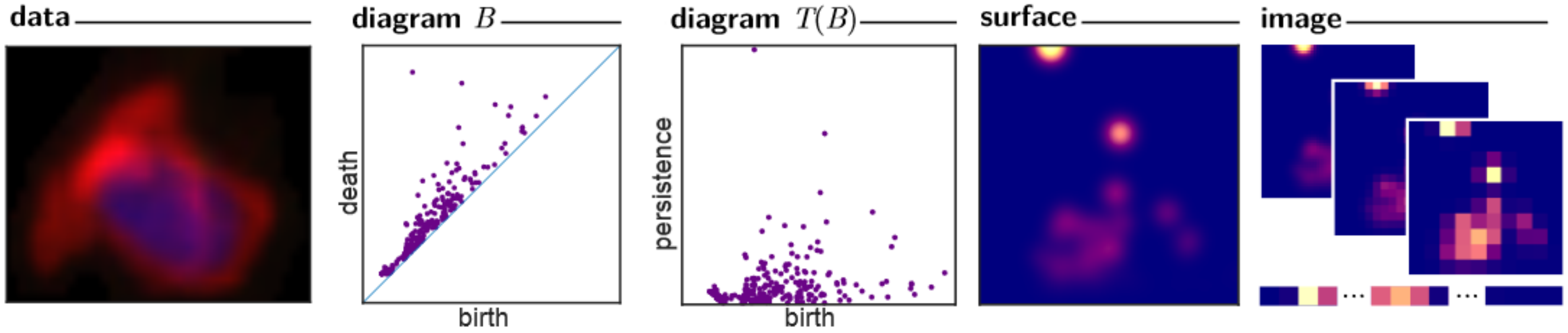

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weight function

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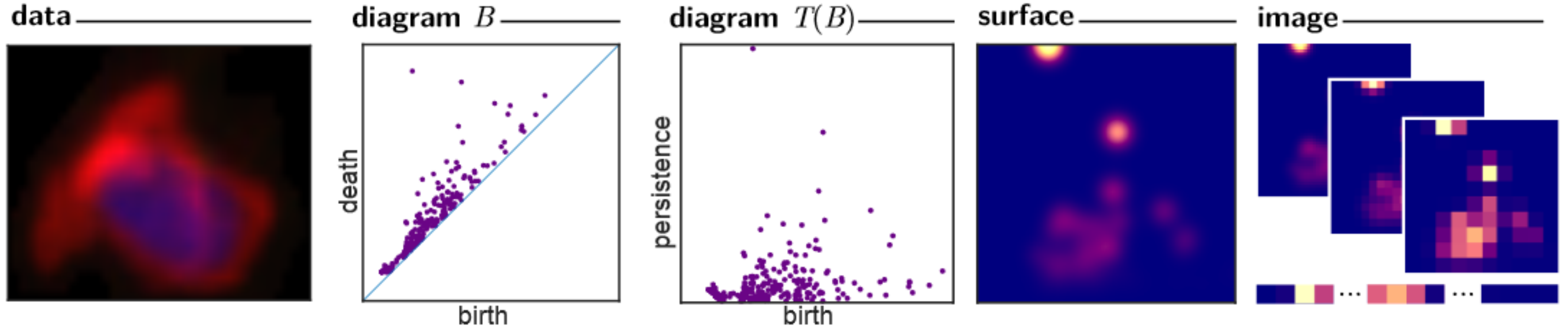

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    - $\rho_B(z) = \sum_{u \in T(B)} f(u) \cdot \phi_u(z)$
  - Persistence image:
    - I_B: a discretization of ρ_B: $I_B[p] = \int_p \rho_B dxdy$

- Metric:
  - We can simply use p-norms of vector difference $||I_D - I_E||_p$

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  - We can simply use p-norms of vector difference $||I_D - I_E||_p$

Theorem 13.3. *Suppose persistence images are computed with the normalized Gaussian distribution with variance σ^2 and weight function $\omega : \mathbb{R}^2 \to \mathbb{R}$. Then the persistence images are stable w.r.t. the* 1*-Wasserstein distance between persistence diagrams. More precisely, given two finite and bounded persistence diagrams D and E, we have:*

$$|| \mathrm{I}_D - \mathrm{I}_E||_1 \leq \left(\sqrt{5}|\nabla\omega| + \sqrt{\frac{10}{\pi}} \frac{||\omega||_\infty}{\sigma} \right) \cdot \mathrm{d}_{W,1}(D, E).$$

Here, $\nabla\omega$ stands for the gradient of ω, and $|\nabla\omega| = \sup_{z\in\mathbb{R}^2} ||\nabla\omega||_2$ is the maximum norm of the gradient vector of ω at any point in $\mathbb{R}^2$. The same upper bound holds for $|| \mathrm{I}_D - \mathrm{I}_E||_2$ and $|| \mathrm{I}_D - \mathrm{I}_E||_\infty$ as well.

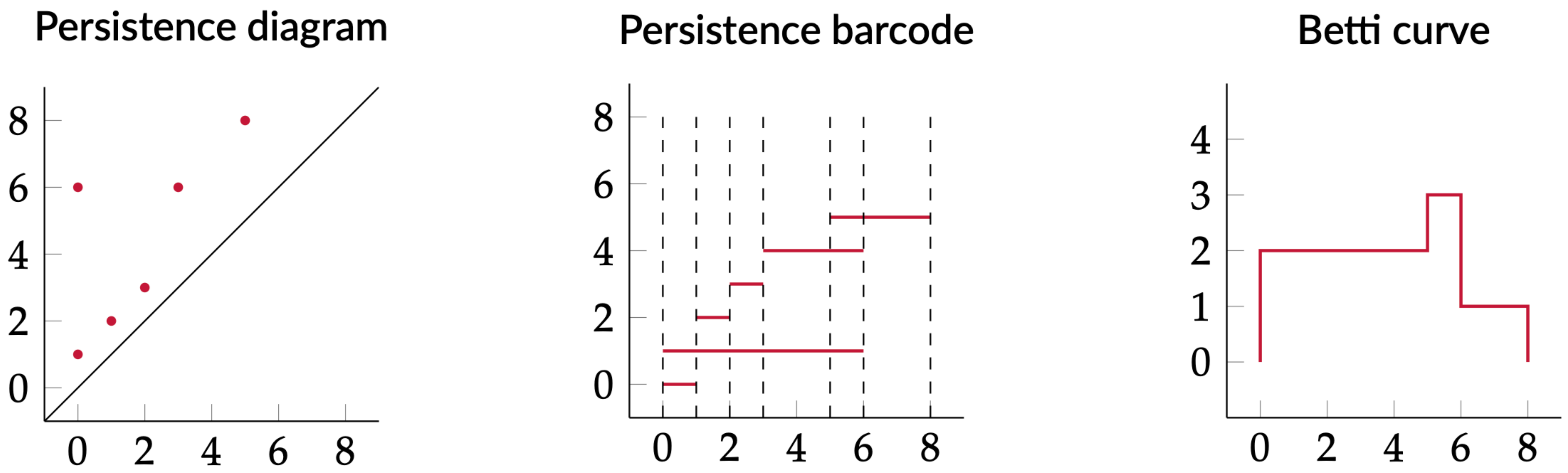
Packages

- scikit-tda persistence image
- Tutorial based on giotto-tda

Other methods

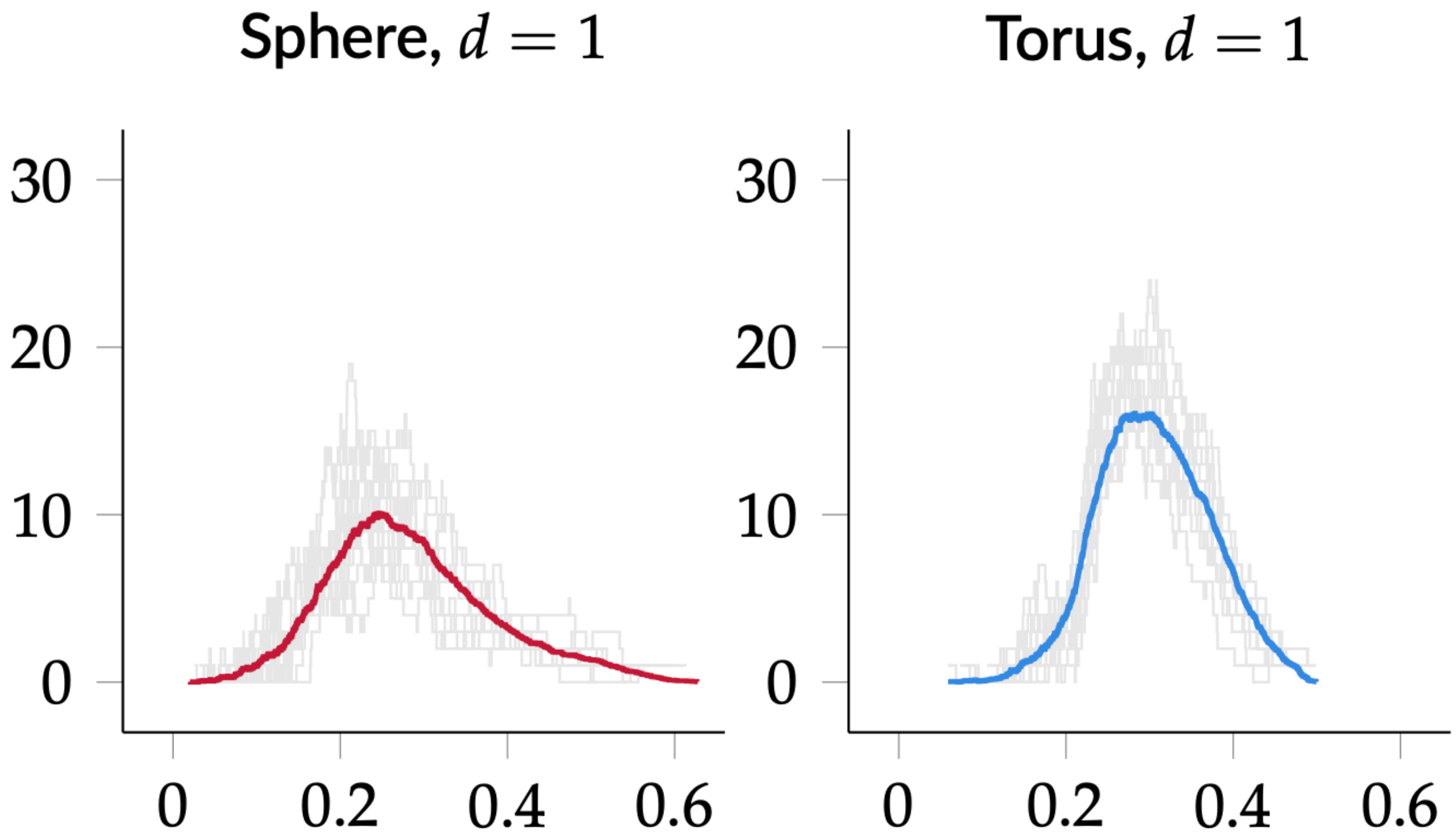
Betti curve

- [Rieck et al. 2019]



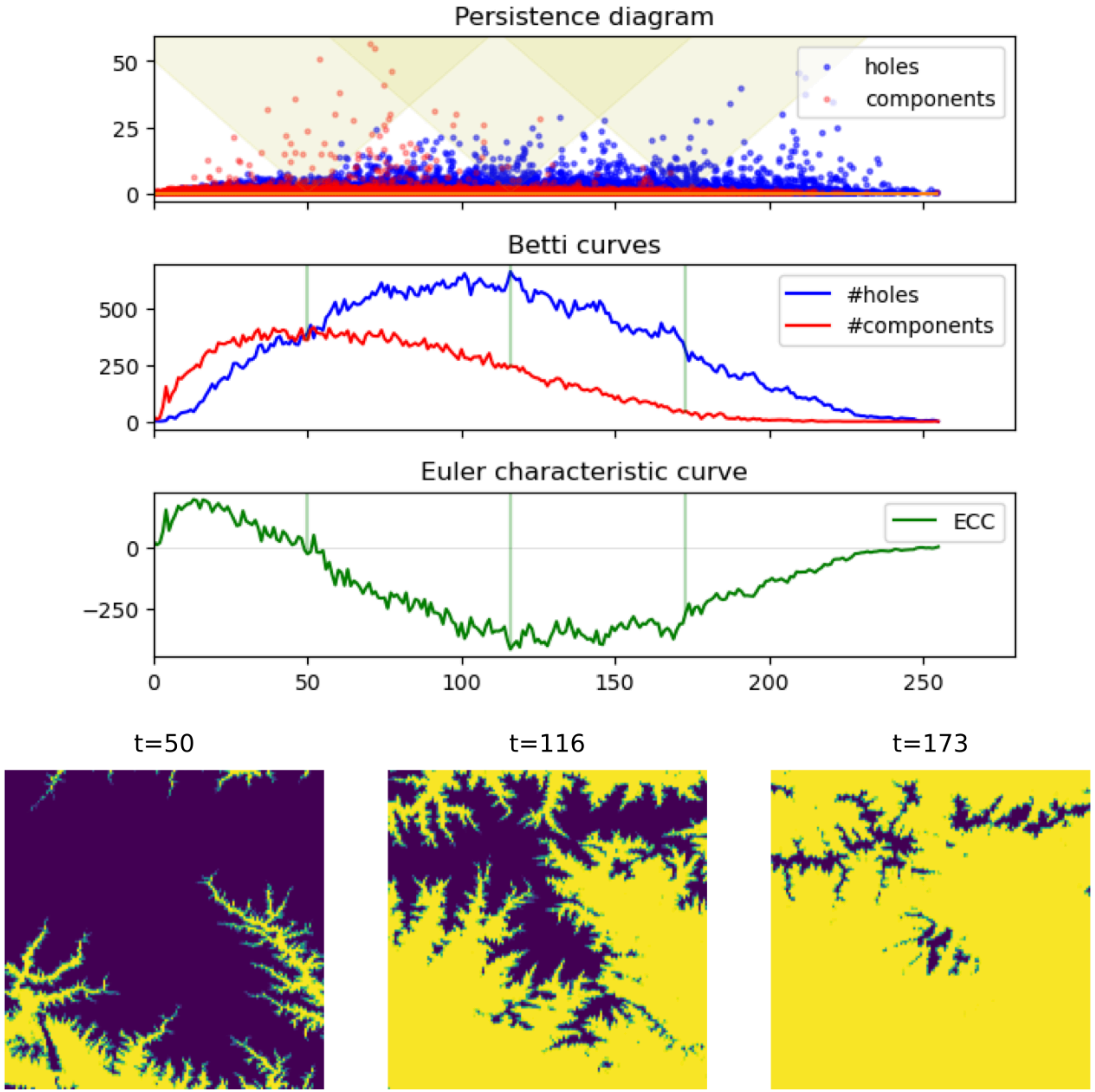
Courtesy of Bastian Rieck

Betti curve - bootstrap



Euler characteristic curve

- [Wang et al. 2023]
- $\chi(X) = \sum (-1)^i \beta_i(X)$
- GPU implementation
- Kernel available



Concluding remarks

- These kernels / vector representations make it easier to use ML methods on persistence-based features.
- Later we will talk about neural network architectures for handling PDs.

FIN