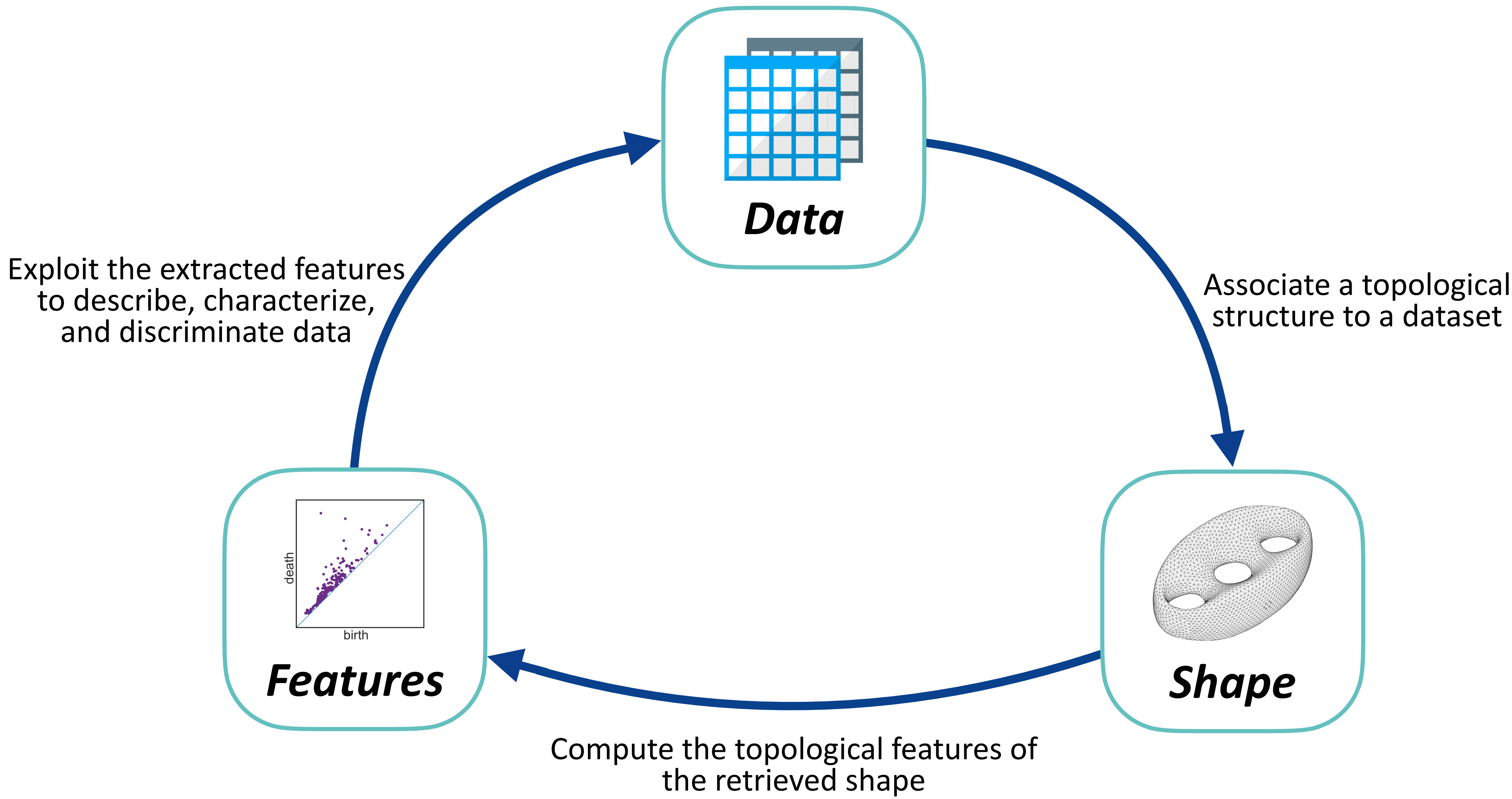
Topological Data Analysis

Persistence & Stability

Ulderico Fugacci

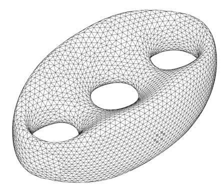
CNR - IMATI

Topological Data Analysis

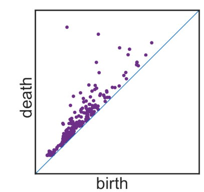


Persistence & Stability

(Persistent) Homology allows for assigning to any (filtered) simplicial complex ***topological information*** ***expressed in terms of*** ***algebraic structures***



Shape



Features

Goal:

Today, we address two main questions:

- ***Can this topological information be characterized in a simpler and "more visualizable" way?***
- ***Is this information stable under small perturbations of the input data?***

Persistence & Stability

- *Persistence Pairs and their Visualizations*
- *Stability Results for Persistent Homology*

Persistence & Stability

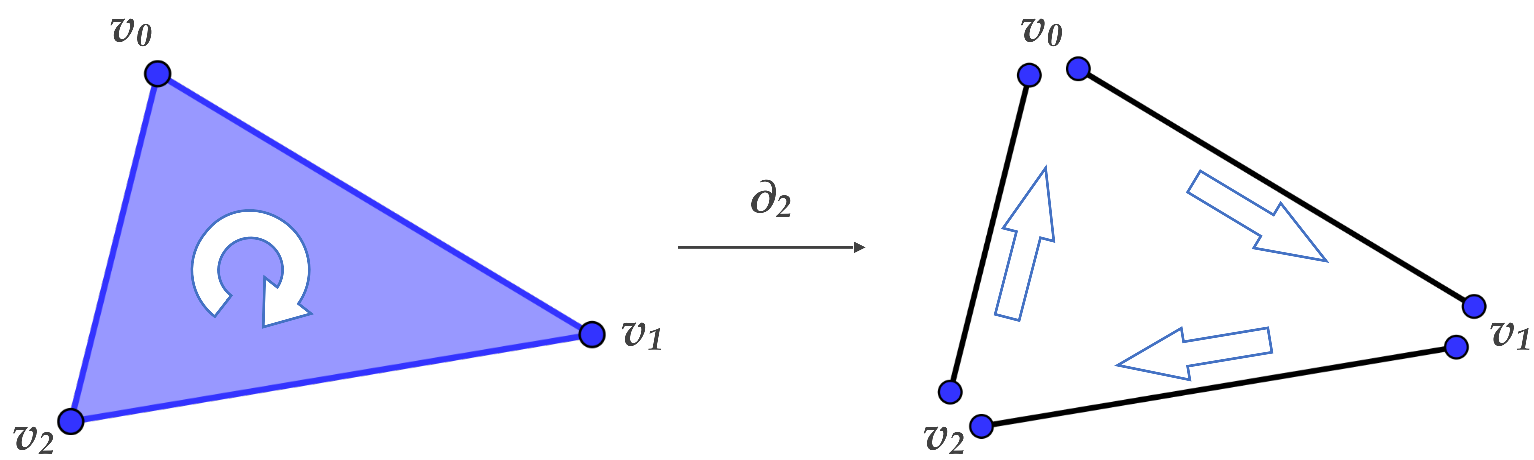
- ***Persistence Pairs* and their Visualizations**
- *Stability Results for Persistent Homology*

Homology

Given a (finite) simplicial complex K,

- a ***k-chain*** is a formal sum (with $\mathbb{Z}$ coefficients) of (oriented) k-simplices of K
- **C_k(K)** is the ***group of the k-chains of K***
- the ***boundary map*** **∂_k : C_k(K) $\longrightarrow$ C_{k-1}(K)** is defined as

$$\partial_k([v_0, \ldots, v_k]) := \sum_{i=0}^{k} (-1)^i [v_0, \ldots, \hat{v}_i, \ldots, v_k]$$



Homology

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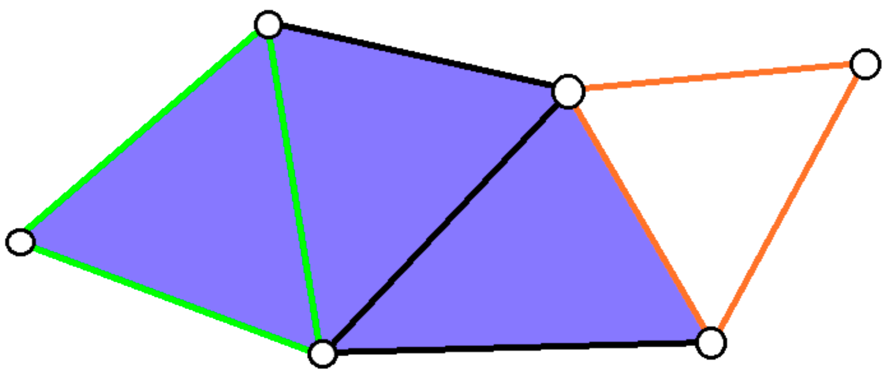


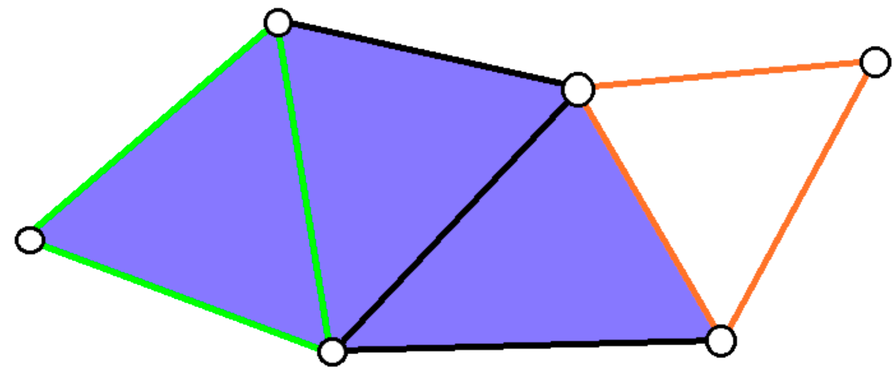
A k-simplex σ is called:

- ***k-cycle*** if $\sigma \in \mathrm{Ker}(\partial_k)$
- ***k-boundary*** if $\sigma \in \mathrm{Im}(\partial_{k+1})$

Homology

Given a (finite) simplicial complex K, the ***k-homology group*** ***$H_k(K)$*** of K is defined as

$$H_k(K) := Z_k(K)/B_k(K)$$



where:

- ***$Z_k(K)$*** is the ***group of k-cycles*** of K
- ***$B_k(K)$*** is the ***group of k-boundaries*** of K

Homology

The ***theorem of structure for finitely generated Abelian groups*** ensures us that

Theorem:

Each homology group can be expressed as

$$H_k(K) \cong \mathbb{Z}^{\beta_k}\langle c_1, \ldots, c_{\beta_k}\rangle \oplus \mathbb{Z}_{\lambda_1}\langle c'_1\rangle \oplus \cdots \oplus \mathbb{Z}_{\lambda_{p_k}}\langle c'_{p_k}\rangle$$

with $\lambda_{i+1} \mid \lambda_i$

We call:

- β_k, the ***k^{th} Betti number*** of K
- $\lambda_1, \ldots, \lambda_{p_k}$, the ***torsion coefficients*** of K
- $c_1, \ldots, c_{\beta_k}, c'_1, \ldots, c'_{p_k}$, the ***homology generators*** of K

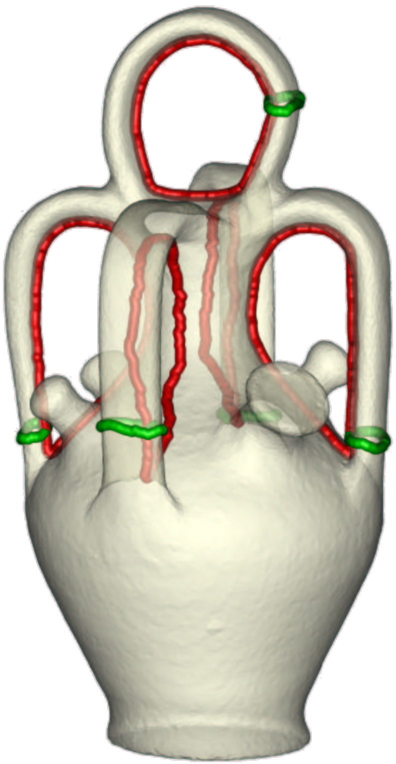


Image from [Dey et al. 2008]

Homology

Hence:

*Up to isomorphism, the **Betti numbers** and the **torsion coefficients** of K **completely characterize** the **homology groups** of K*

Working with coefficients in a field $\mathbb{F}$:

*Up to isomorphism, the **Betti numbers** of K **completely characterize** the **homology groups** of K*

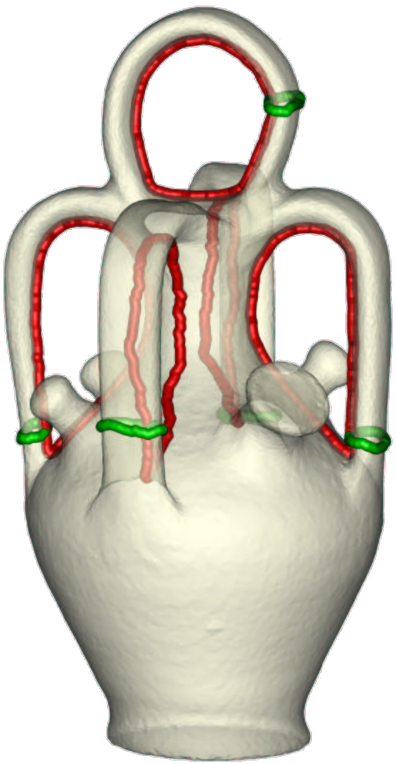
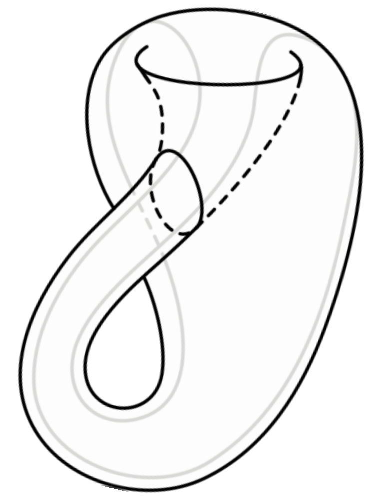


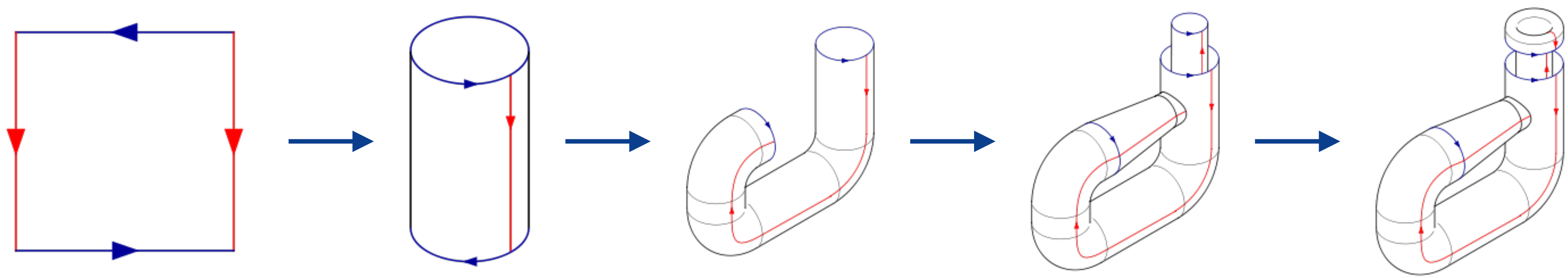
Image from [Dey et al. 2008]

Homology

Example:

*The **Klein bottle** **K** is a non-orientable 2-dimensional manifold embeddable in $\mathbb{R}^4$ which can be built from a unit square by the following construction*



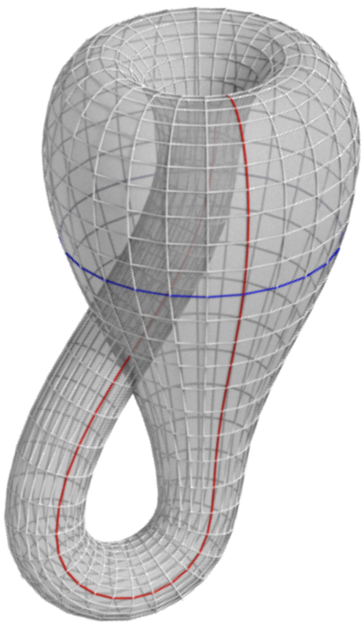


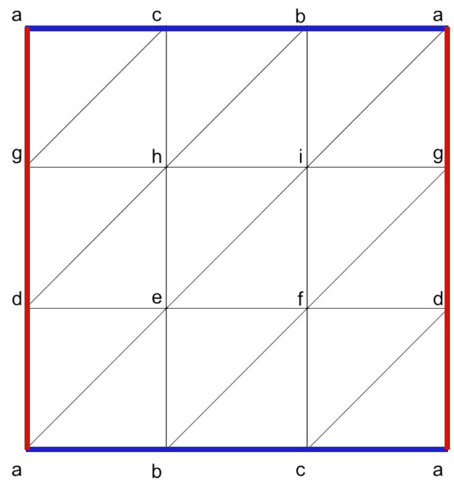
Homology

Example:

K has the following homology groups

$$H_k(K) \cong \begin{cases} \mathbb{Z} & \text{for } k = 0 \\ \mathbb{Z} \oplus \mathbb{Z}_2 & \text{for } k = 1 \\ 0 & \text{for } k \geq 2 \end{cases}$$





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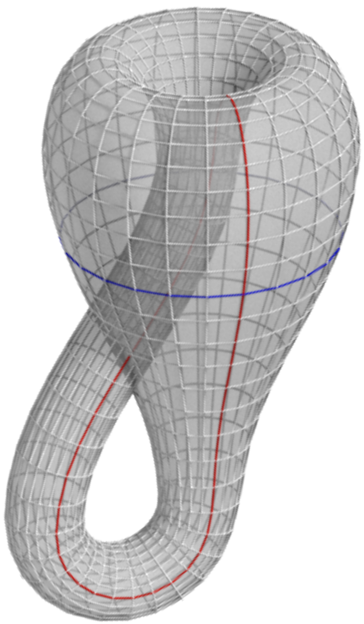
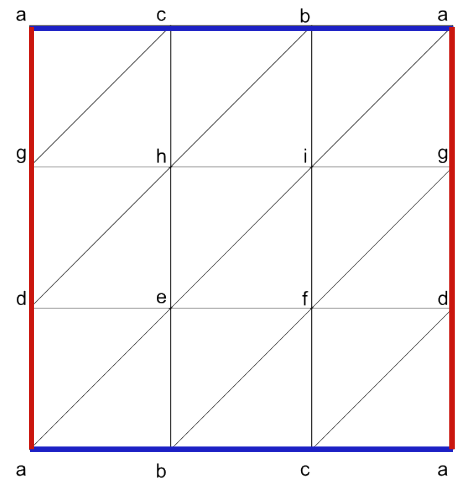
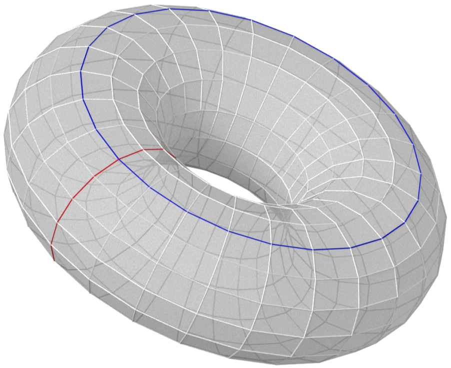




So, it can be distinguished from a torus T

$$H_k(T) \cong \begin{cases} \mathbb{Z} & \text{for } k = 0 \\ \mathbb{Z}^2 & \text{for } k = 1 \\ \mathbb{Z} & \text{for } k = 2 \\ 0 & \text{for } k > 2 \end{cases}$$

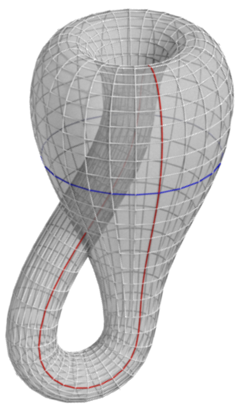


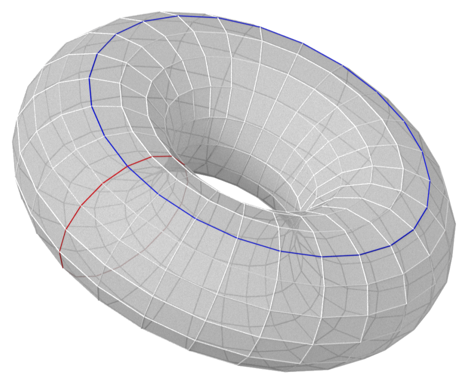
Homology

Example:

By considering $\mathbb{Z}_2$ as coefficient group,

the Klein bottle K and the torus T have isomorphic homology groups





$$H_k(K;\mathbb{Z}_2) \cong \left\{ \begin{array}{ll} \mathbb{Z}_2 & \text{for } k=0 \\ \mathbb{Z}_2 \oplus \mathbb{Z}_2 & \text{for } k=1 \\ \mathbb{Z}_2 & \text{for } k=2 \\ 0 & \text{for } k>2 \end{array} \right\} \cong H_k(T;\mathbb{Z}_2)$$

Persistent Homology

In a Nutshell:

Persistent homology allows for
describing the changes in the shape of an evolving object

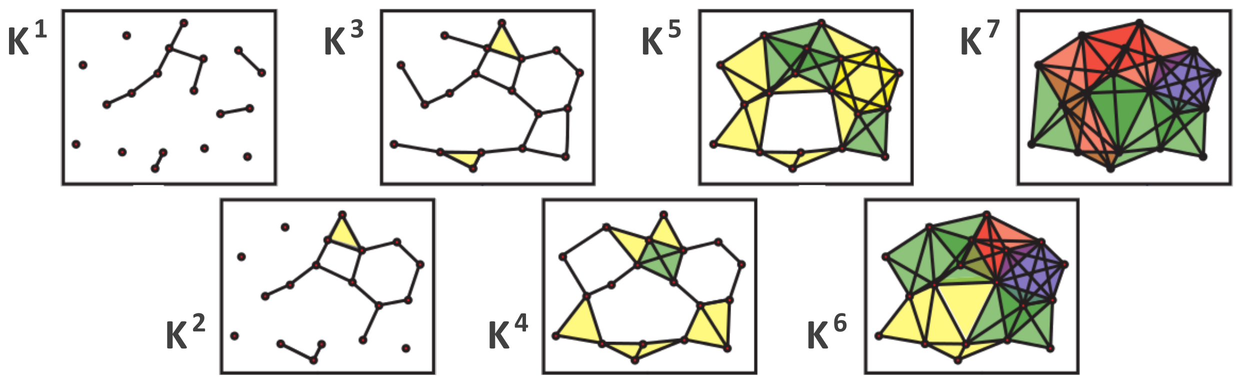


Image from [Ghrist 2008]

Persistent Homology

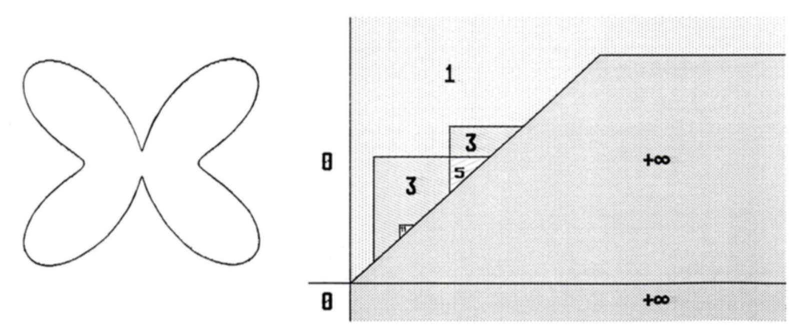
An Evolving Notion:

1990

Frosini

Size Functions:

- ***Estimation of natural pseudo-distance*** between shapes endowed with a function *f*
- Tracking of the ***connected components*** of a shape along its evolution induced by *f*



Actually, this coincides with ***persistent homology in degree 0***

Image from [Frosini 1992]

Persistent Homology

An Evolving Notion:

1990 — Frosini

1994 — Delfinado, Edelsbrunner

Incremental Algorithm for Betti Numbers:

- Introduction of the notion of ***filtration***
- De facto computation of ***persistence pairs***

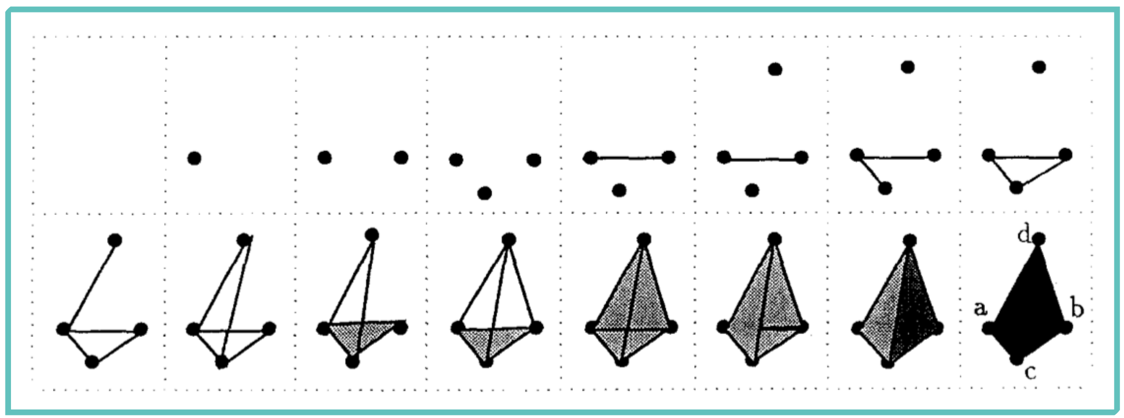


Image from [Delfinado, Edelsbrunner 1995]

Persistent Homology

An Evolving Notion:

1990 — Frosini

1994 — Delfinado, Edelsbrunner

1999 — Robins

Homology from Finite Approximations:

- ***Extrapolation of the homology*** of a metric space from a ***finite point-set approximation***
- Introduction of ***persistent Betti numbers***

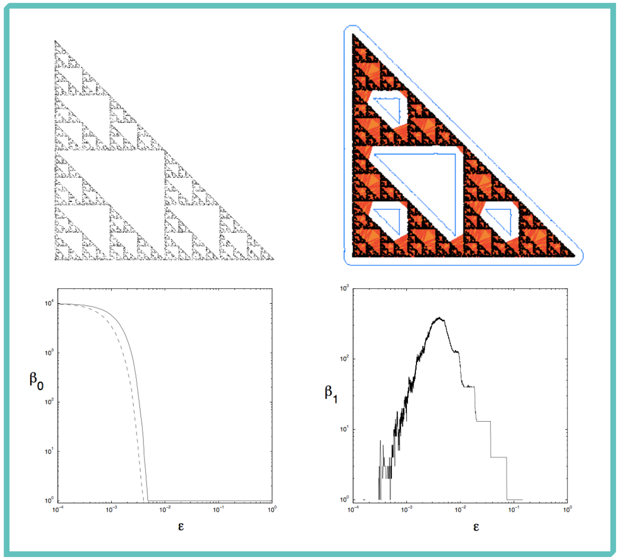


Image from [Robins 1999]

Persistent Homology

An Evolving Notion:

1990	1994	1999	2002
Frosini	Delfinado, Edelsbrunner	Robins	Edelsbrunner, Letscher, Zomorodian

Topological Persistence:

- Introduction and algebraic formulation of the notion of ***persistent homology***
- ***Description of an algorithm*** for computing persistent homology

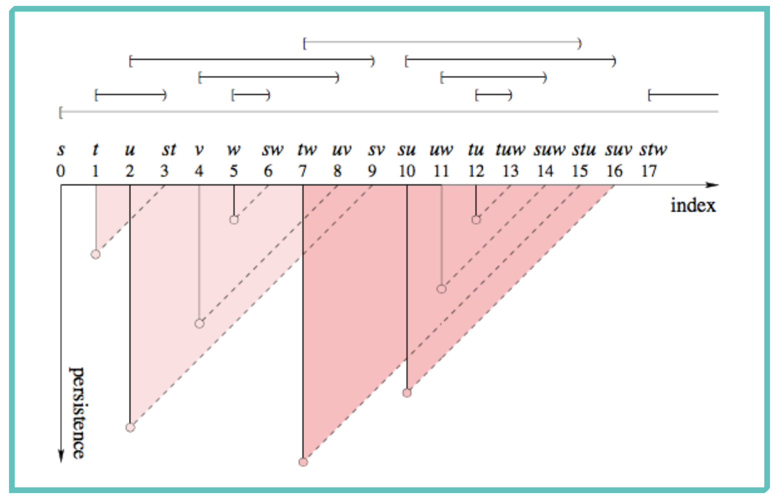


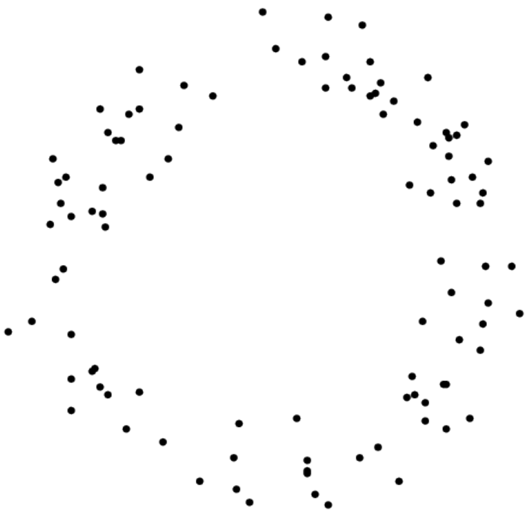
Image from [Edelsbrunner et al. 2002]

Persistent Homology

A Twofold Purpose:

Shape Description

- *Which is the shape of a given data?*



Persistent Homology

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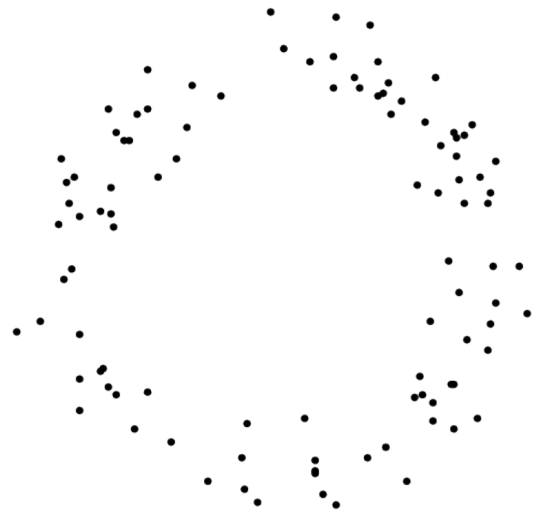
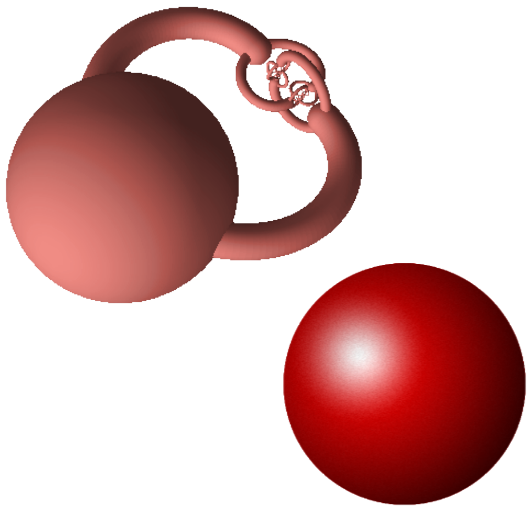




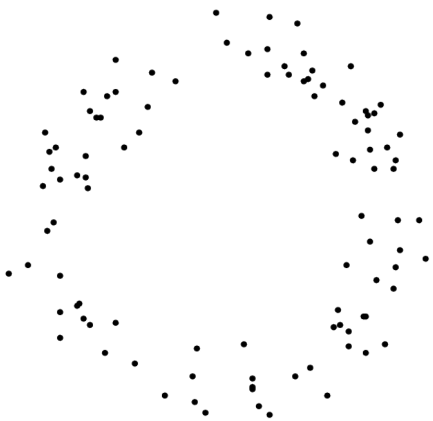
Shape Comparison

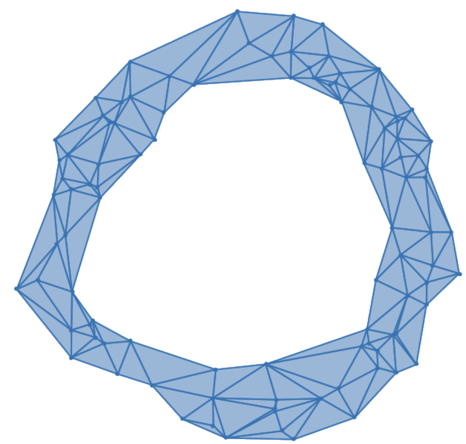
- *Given two data, do they have the same shape?*

Persistent Homology

✦ ***Which is the shape of a given data?***

Persistent homology allows for the retrieval of the ***"actual"*** homological information of a data





Point Cloud Dataset → ***Topological Nature of the "Underlying" Shape***

Image from [Bauer 2015]

Persistent Homology

Which is the shape of a given data?

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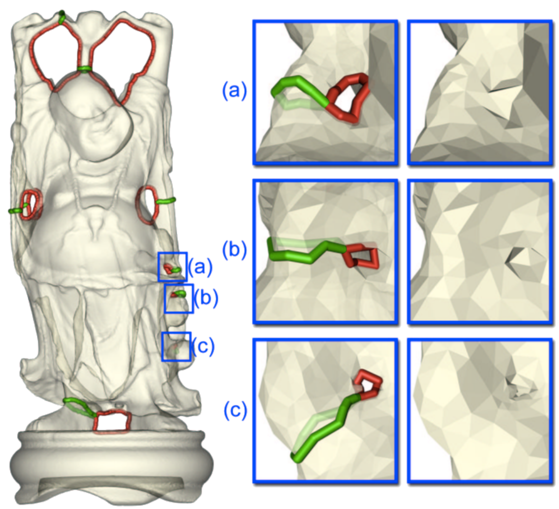


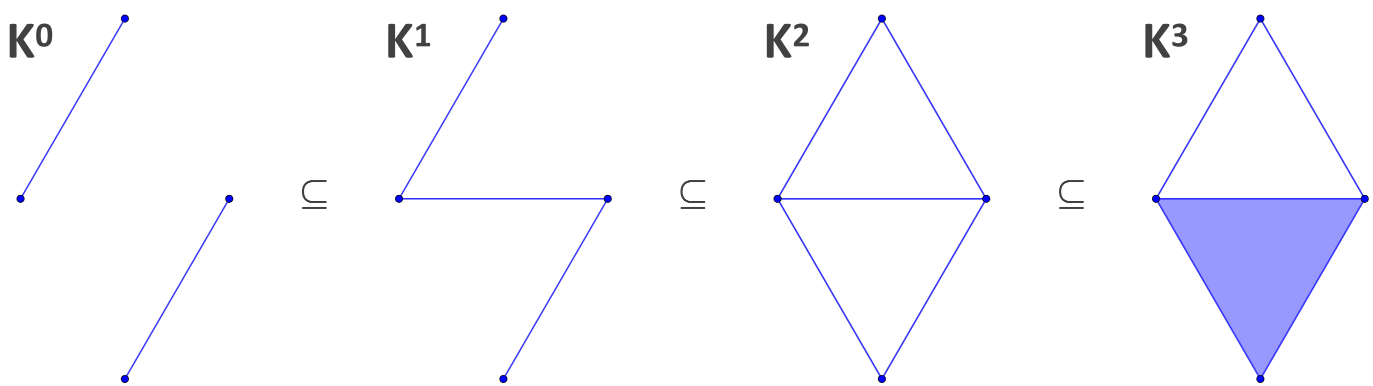
Noisy Dataset → ***Relevant Homological Information***

Image from [Dey et al. 2008]

Persistence Pairs

The *core information* of persistent homology is given by the ***persistence pairs***

Given a filtration $K^0 \subseteq K^1 \subseteq \ldots \subseteq K^m$,



A **persistence pair *(p, q)*** is an element in $\{0, \ldots, m\} \times (\{0, \ldots, m\} \cup \{\infty\})$ such that $p < q$ representing a **homological class** that is **born at step *p*** and **dies at step *q***

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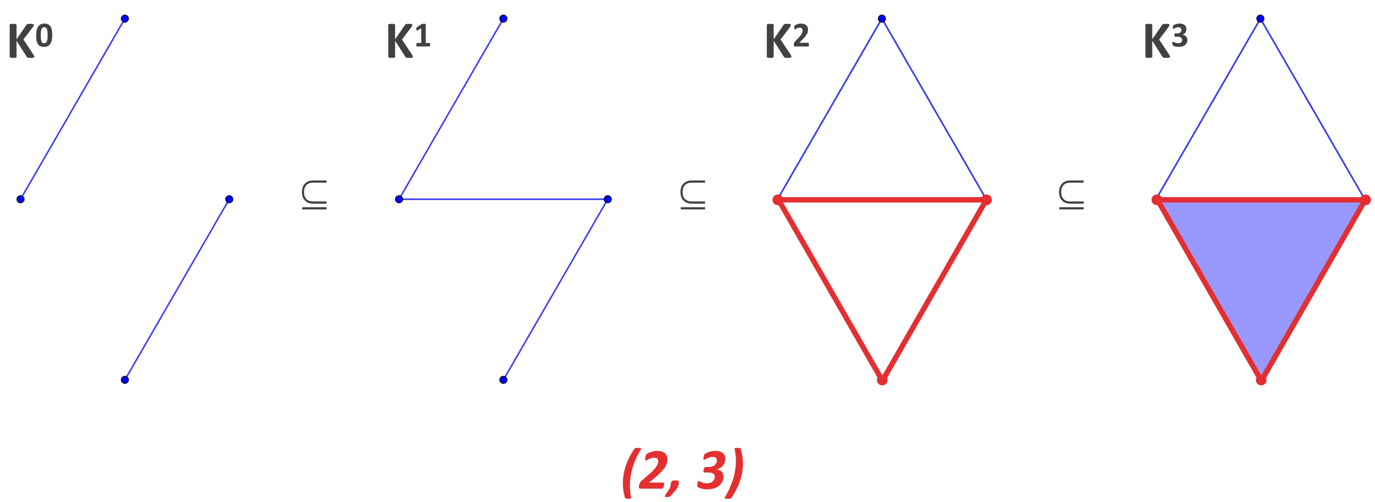

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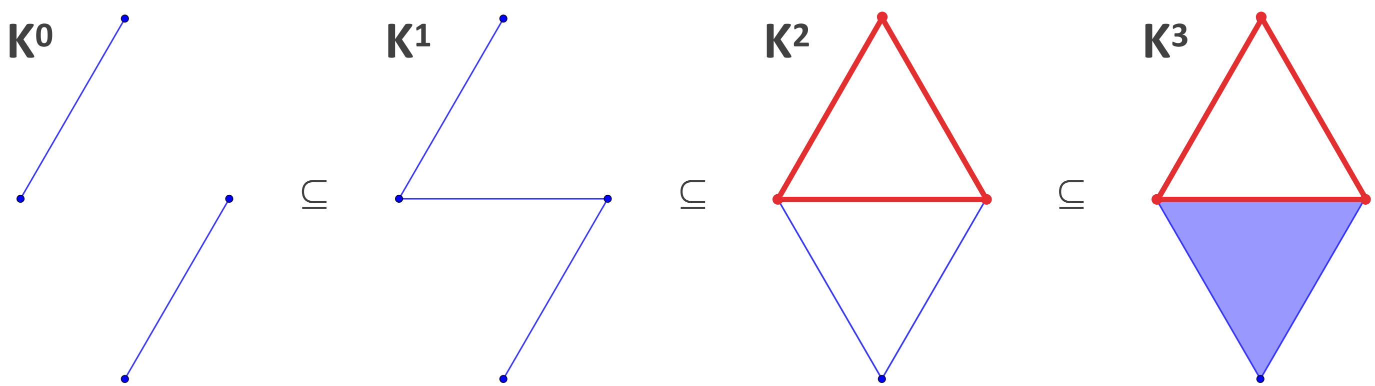

(2, ∞) essential pair

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Persistence Pairs

Given a filtered simplicial complex K, a field $\mathbb{F}$, and k ∈ $\mathbb{N}$,

its ***persistence module*** $M := \bigoplus_{t \in \mathbb{N}} H_k(K^t; \mathbb{F})$ is a ***finitely generated*** $\mathbb{F}$***[x]-module***

The corresponding structure theorem ensures us that

Theorem:

The persistence module M can be expressed as

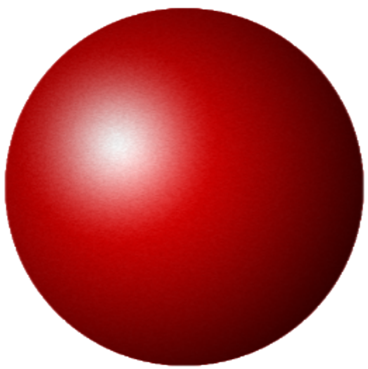
$$M \cong \bigoplus_{j=1}^{n} \mathbb{F}[x](-a_j) \bigoplus_{i=1}^{m} \mathbb{F}[x](-c_i)/x^{d_i}$$

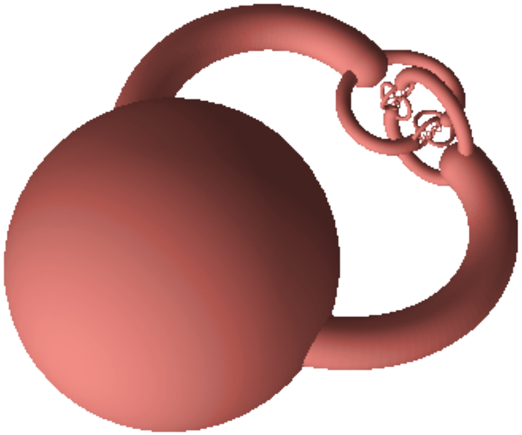
So, the persistence module M is completely determined by its persistence pairs

I.e., the collection of the pairs (c_i, d_i), (a_j, ∞)

Persistence Pairs

- *Do they have the same shape?*





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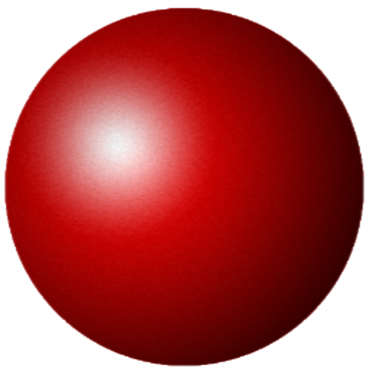
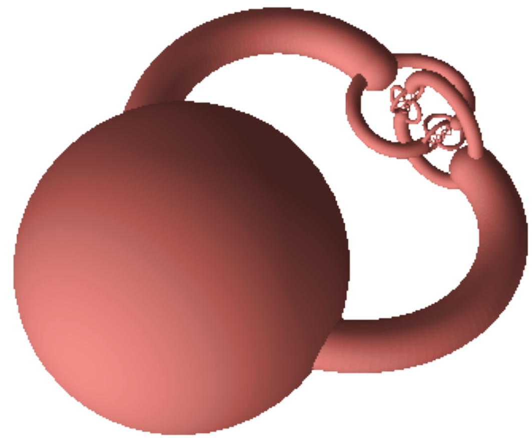
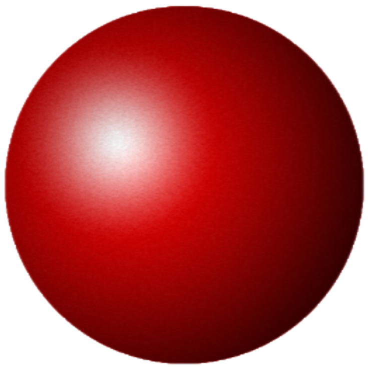


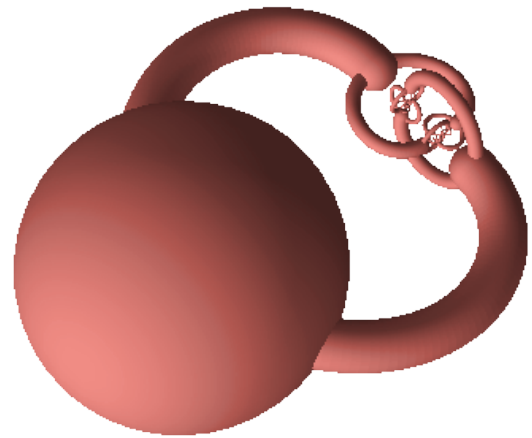


In Practice?	In Theory?

Persistence Pairs

- ***Do they have the same shape?***





In Practice?

In Theory?

*They are **homeomorphic***

Persistence Pairs

- *Do they have the same shape?*

Persistence Pairs

- *Do they have the same shape?*

In Practice?

In Theory?

Persistence Pairs

- ***Do they have the same shape?***

In Practice?

In Theory?

*They are **not homeomorphic***

Persistence Pairs

Differently from homology, persistent homology provides
a notion of "shape" closer to our everyday perception

It is possible to ***compare two shapes*** by comparing their ***homology groups***

Persistence Pairs

Differently from homology, persistent homology provides
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It is possible to ***compare two shapes*** by comparing their ***hom*** … ***ups***

PERSISTENCE PAIRS

Persistence Pairs

Differently from homology, persistent homology provides
a notion of "shape" closer to our everyday perception

It is possible to ***compare two shapes*** by comparing their ***hom*** … ***ups***

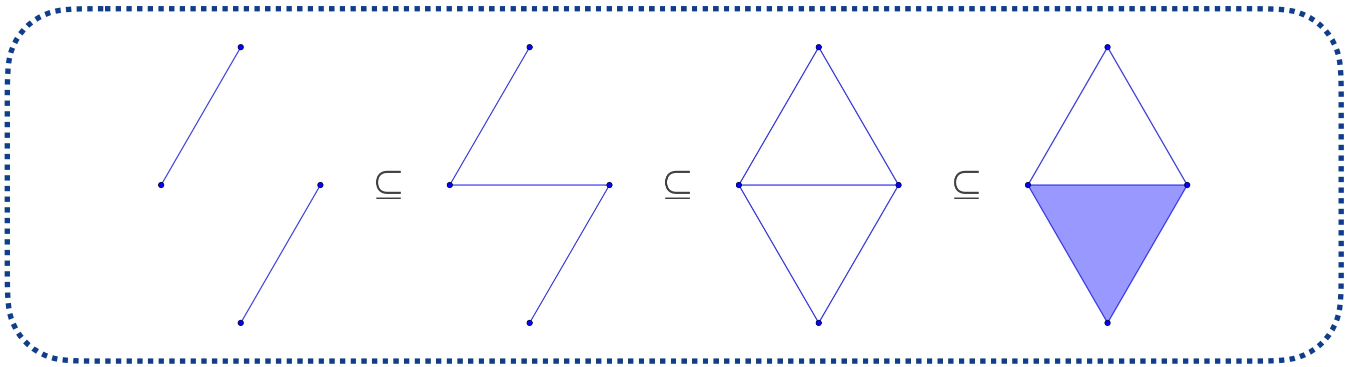
PERSISTENCE PAIRS

In order to better perform the above task, we need:

- ***Visual*** and ***descriptive representations*** for persistence pairs
- Notions of ***distance*** between sets of persistence pairs and ***stability results***

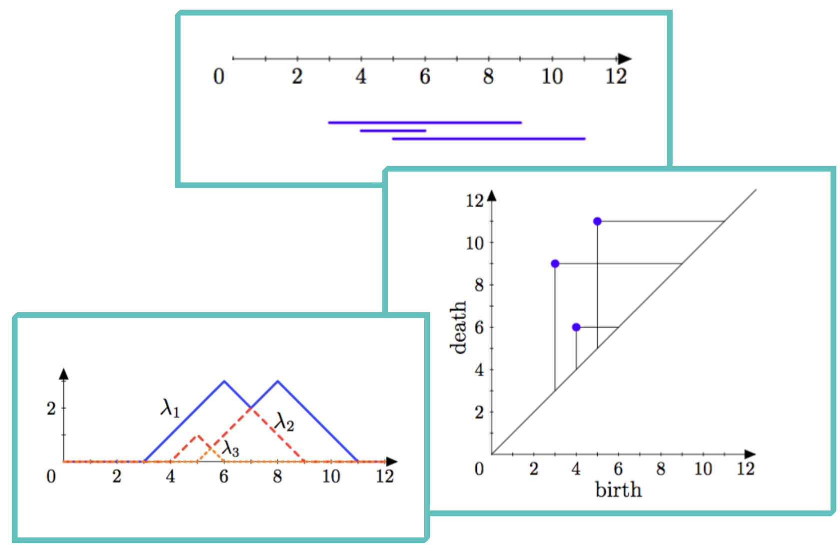
Visualizing Persistence Pairs

Given a filtered simplicial complex K,



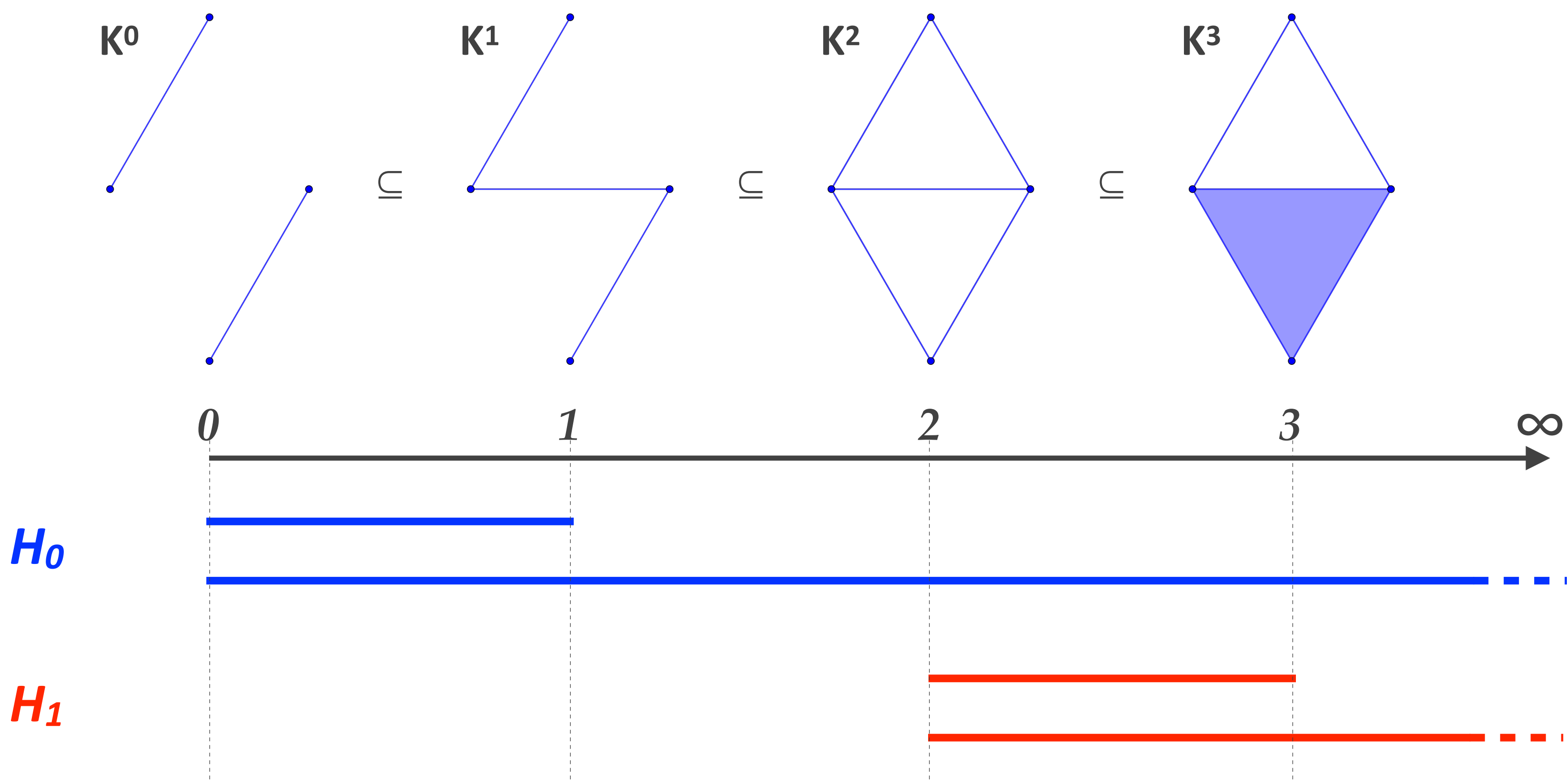
Persistent pairs of K can be visualized through:

- **Barcodes** [Carlsson et al. 2005; Ghrist 2008]
- **Persistence diagrams** [Edelsbrunner, Harer 2008]
- **Persistence landscapes** [Bubenik 2015]
- *Corner points and lines* [Frosini, Landi 2001]
- *Half-open intervals* [Edelsbrunner et al. 2002]
- *k-triangles* [Edelsbrunner et al. 2002]



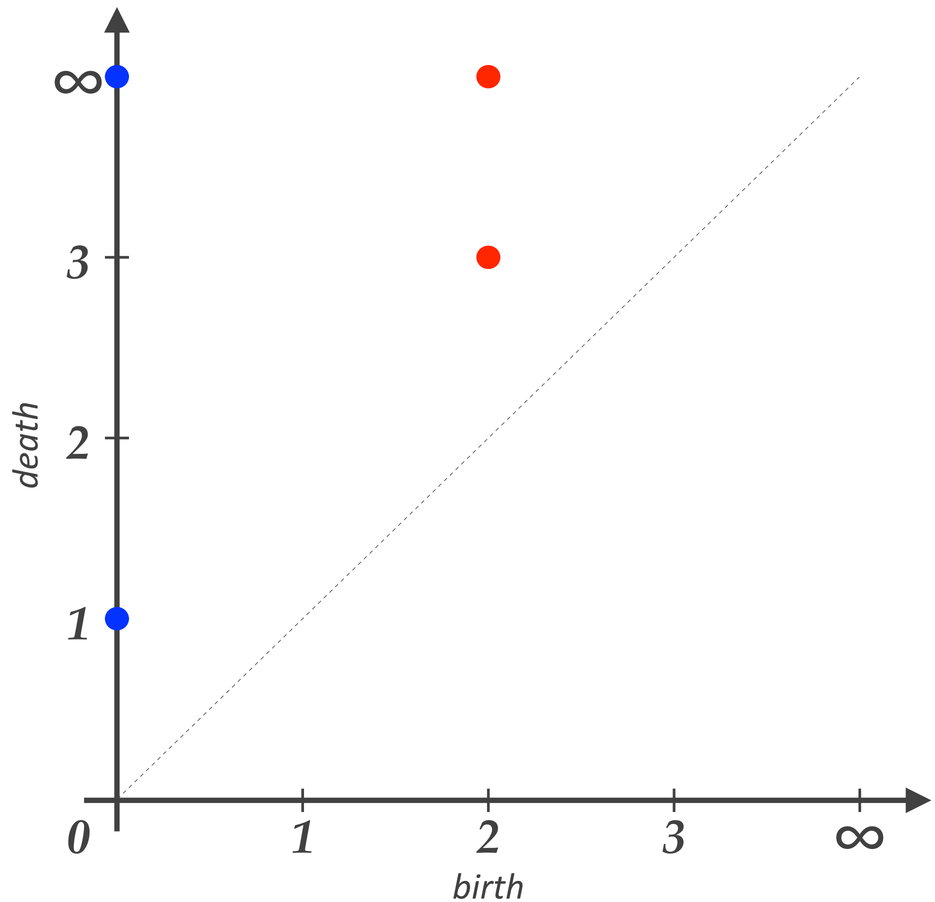
Visualizing Persistence Pairs

Barcodes: *Persistence pairs are represented as* ***intervals in*** $\mathbb{R}$



Visualizing Persistence Pairs

Persistence Diagrams: *Persistence pairs are represented as **points in** $\mathbb{R}^2$*

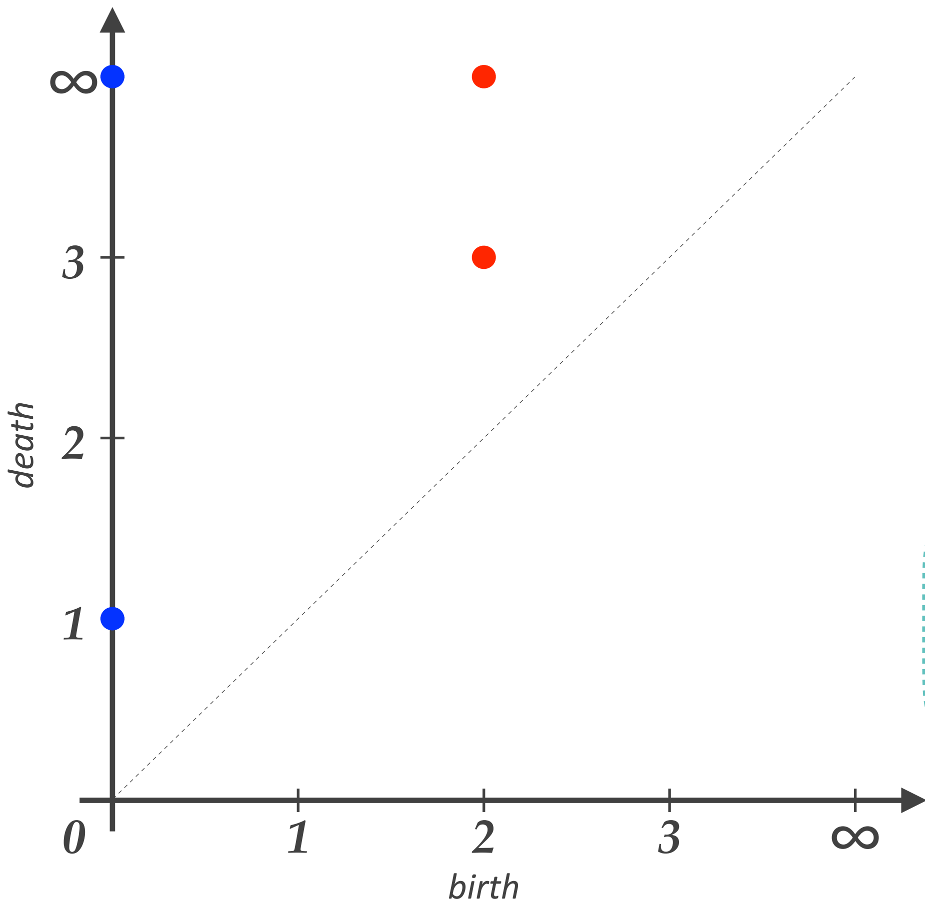


H_0 (0, 1) (0, ∞)

H_1 (2, 3) (2, ∞)

Visualizing Persistence Pairs

Persistence Diagrams: *Persistence pairs are represented as* ***points in*** $\mathbb{R} \times (\mathbb{R} \cup \{\infty\})$



H_0 $(0, 1)$ $(0, \infty)$

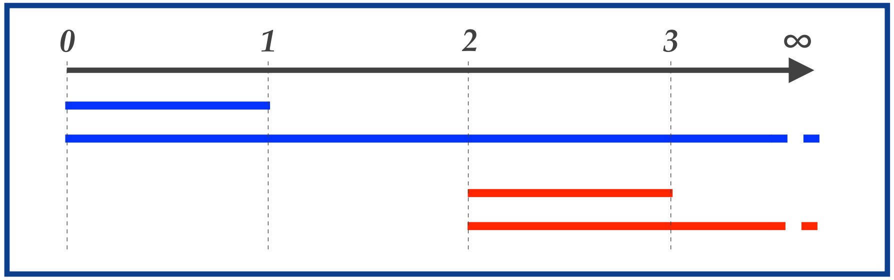
H_1 $(2, 3)$ $(2, \infty)$

Formally, a persistence diagram is a ***multiset***

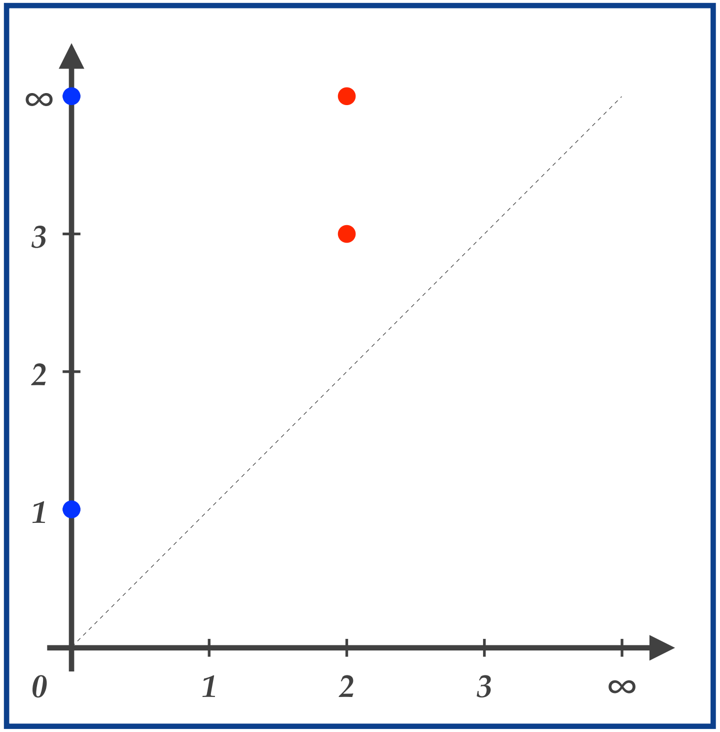
- Points are endowed with **multiplicity**

Visualizing Persistence Pairs

*Both tools **visually represent** the **lifespan** of the homology classes:*



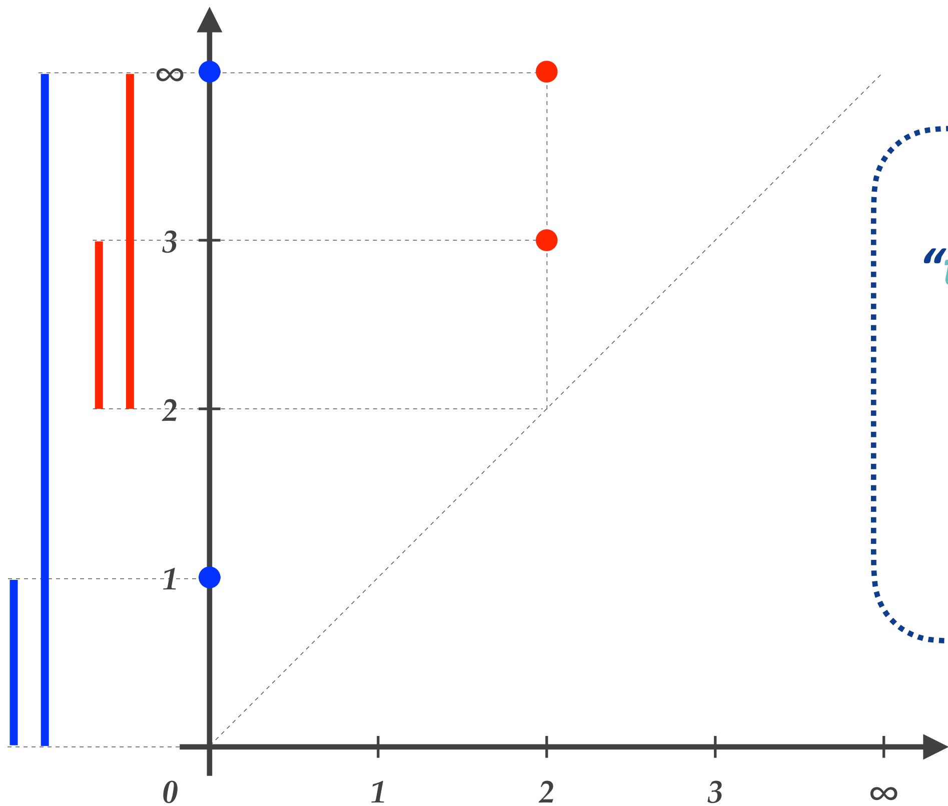
- **Barcode:** ***length of the intervals***
- **Persistence Diagram:** ***distance from the diagonal***



Barcodes and Persistence Diagrams ***encode equivalent information***

Visualizing Persistence Pairs

Barcodes and Persistence Diagrams ***encode equivalent information***



A visualization can be easily ***"translated"*** into the other one:

[p, q]	⟷	***(p, q)***
[p, ∞)		***(p, ∞)***

Visualizing Persistence Pairs

Example: ***Brain functional networks from fMRI*** (functional magnetic resonance imaging)

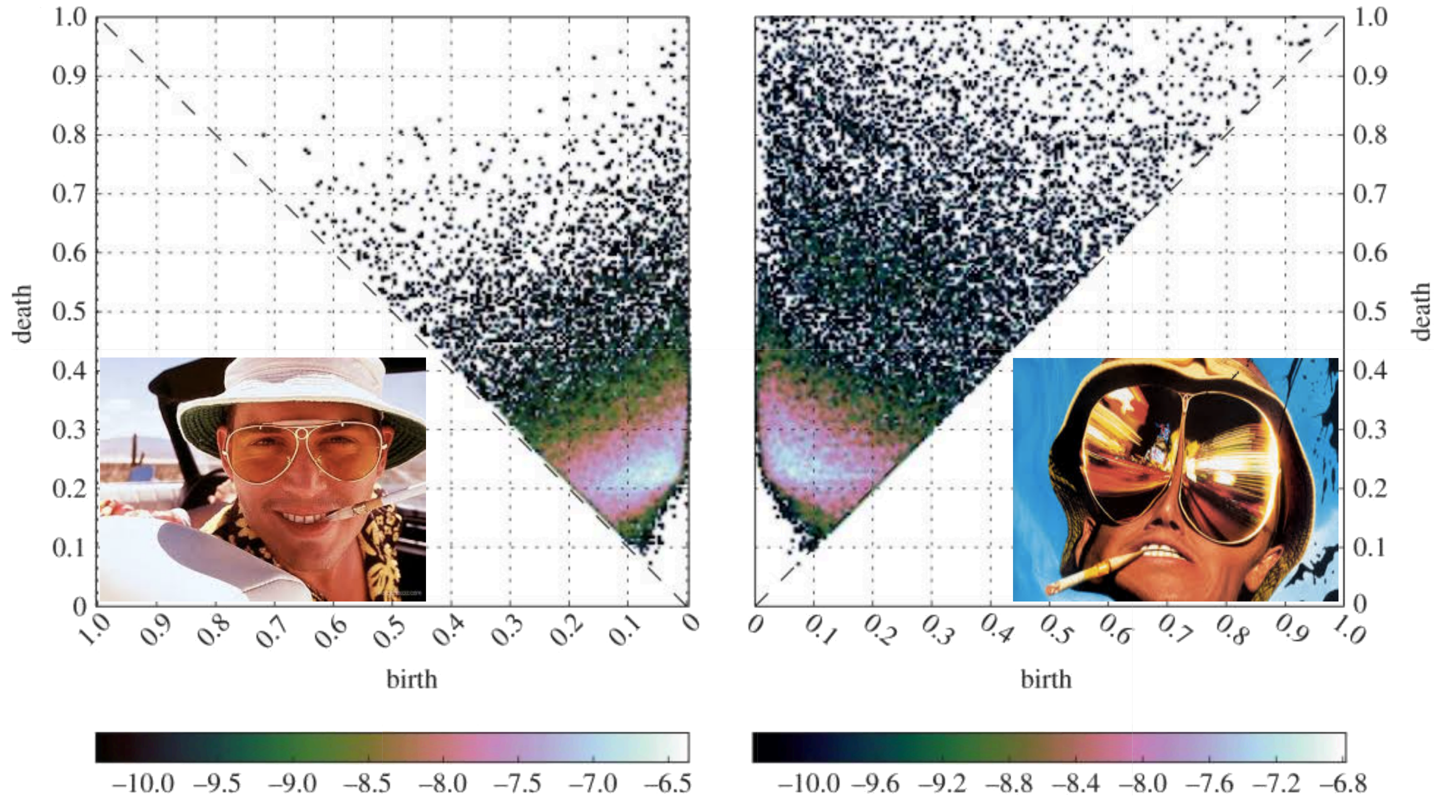


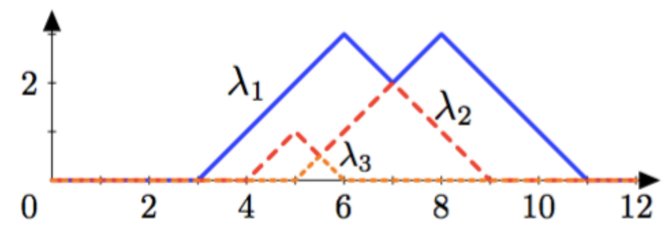
Image from [Petri et al. 2014]

(log-)Probability densities of H_1 for the placebo (left) and the psilocybin (right) groups

Visualizing Persistence Pairs

Persistence Landscapes:

Persistence landscapes *are statistics-friendly representations of persistence pairs*



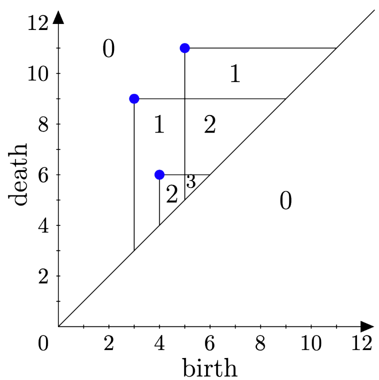
Given a persistence module M, persistence landscapes

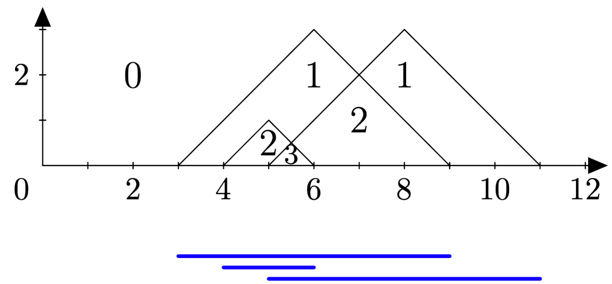
- Consist of a collection of ***1-Lipschitz functions***
- Lie in a ***vector space***
- Are ***stable*** (under small perturbations of the input filtration)

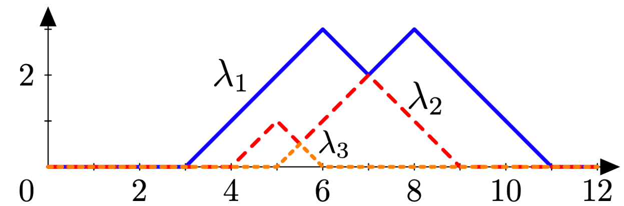
Image from [Bubenik 2015]

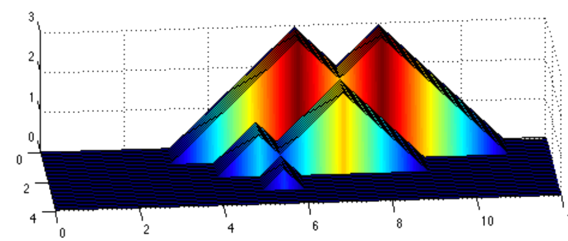
Visualizing Persistence Pairs

Persistence Landscapes: Given a persistence module M,









Images from [Bubenik 2015]

Formally,

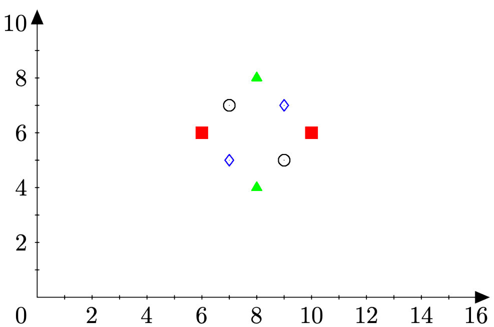
$$\lambda_i(x) := \sup\{m \geq 0 \mid \beta^{x-m,x+m} \geq i\}$$

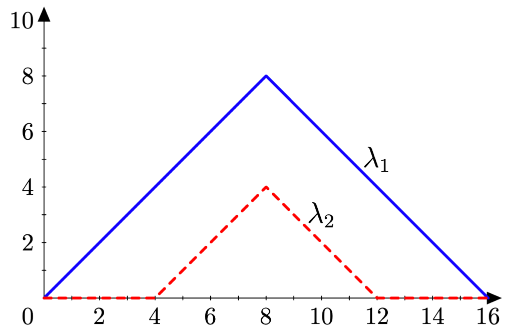
where $\beta^{a,b} := \dim\Big(\mathrm{im}(\iota_{a,b} : M_a \to M_b)\Big)$

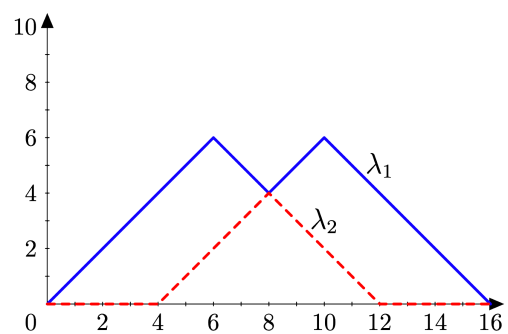
Visualizing Persistence Pairs

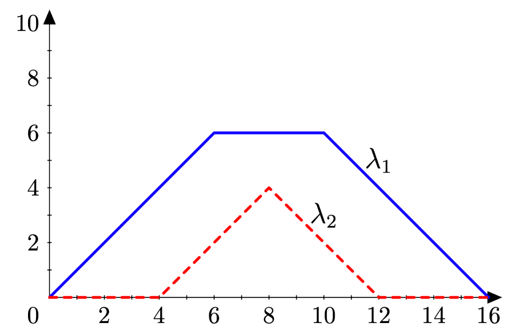
Persistence Landscapes: *Mean of persistence diagrams is **not unique**, but …*

Mean** of persistence landscapes is **well-defined









Images from [Bubenik 2015]

Persistence & Stability

- *Persistence Pairs and their Visualizations*
- ***Stability Results for Persistent Homology***

Stability of Persistence Pairs

In order to be adopted in real applicative domains, it is crucial that

persistent homology is not affected by noisy data and small perturbations

Stability Result:

*By defining **distances*** for both domains,*

Similar Data → ***Similar Persistent Homology***

**The term "distance" is intended in a broad sense, including pseudo-metrics and dissimilarity measures*

Stability of Persistence Pairs

Distances:

- ***For the Data in Input*:**
  - ***Natural pseudo-distance*** *of shapes*
  - ***L_∞-distance*** *of filtering functions*
  - ***Gromov-Hausdorff distance*** *of metric spaces/point clouds*
- ***For the retrieved Persistent Homology Information*:**
  - ***Interleaving distance*** *of persistence modules*
  - ***Bottleneck distance*** *of persistence diagrams*
  - ***Hausdorff distance*** *of persistence diagrams*
  - *Matching distance of persistence diagrams*
  - *Wasserstein distances of persistence diagrams*

Stability of Persistence Pairs

Distances for Input Data:

Let (X, f) be a *pair* such that:

- X is a ***(triangulable) topological space***
- f: X $\longrightarrow \mathbb{R}$ is a ***continuous function***

A pair (X, f) induces a *filtration*:

- $X^t := f^{-1}((-\infty, t])$

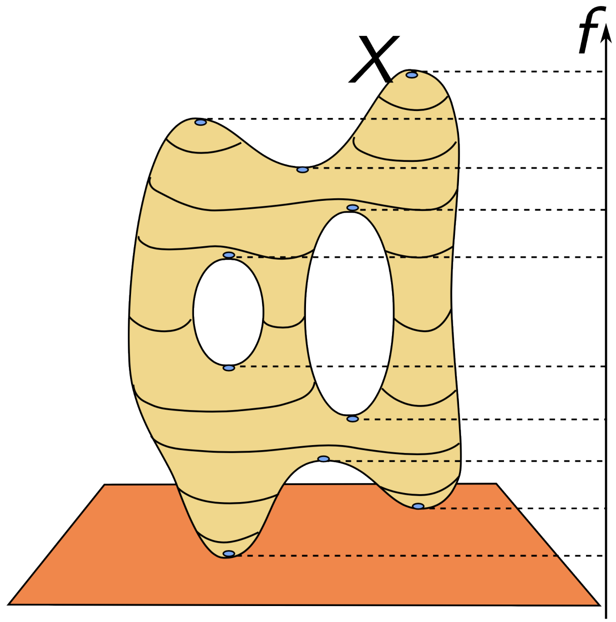


Image from [Ferri et al. 2015]

Definition:

*The function f is called **tame** if:*

- *f has a **finite number of homological critical values** (i.e. the "time" steps in which homology changes)*
- *For any $k \in \mathbb{N}$ and $t \in \mathbb{R}$, the **homology group $H_k(X^t, \mathbb{F})$ has finite dimension***

Stability of Persistence Pairs

Distances for Input Data:

Definition:

*Given two pairs (X, f) and (Y, g), their **natural pseudo-distance** d_N is defined as:*

$$d_N\Big((X,f),(Y,g)\Big) := \begin{cases} \inf_{h\in H(X,Y)}\{\max_{x\in X}\{|f(x)-g\circ h(x)|\}\} \\ +\infty & \text{if } H(X,Y)=\emptyset \end{cases}$$

*where **H(X, Y)** is the set of all the **homeomorphisms between X and Y***

Stability of Persistence Pairs

Distances for Input Data:

Working with two functions f, g: $X \longrightarrow \mathbb{R}$ defined on the same topological space X, one can simply consider the ***L_∞-distance*** between f and g

$$\|f-g\|_\infty := \sup_{x\in X}\{|f(x)-g(x)|\}$$

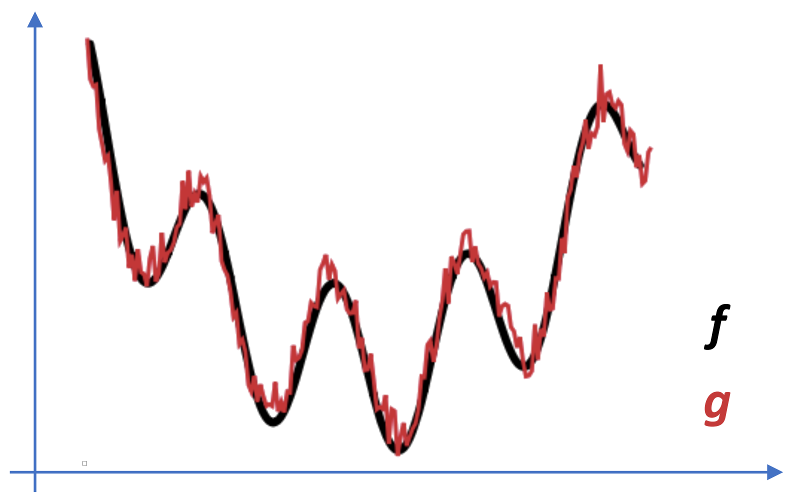


Image from [Rieck 2016]

Stability of Persistence Pairs

Distances for Input Data:

Given two ***finite metric spaces*** (X, d_X), (Y, d_Y) (e.g. two finite point clouds in $\mathbb{R}^n$),

Definitions:

*A **correspondence** $C: X \rightrightarrows Y$ from X to Y is a subset of $X \times Y$ such that*

*the **canonical projections** $\pi_X: C \longrightarrow X$ and $\pi_Y: C \longrightarrow Y$ are both **surjective***

*The **distortion dis(C)** of a correspondence $C: X \rightrightarrows Y$ is defined as:*

$$dis(C) := \sup\left\{|d_X(x,x') - d_Y(y,y')| : (x,y),(x',y') \in C\right\}$$

*The **Gromov-Hausdorff distance d_{GH}** between (X, d_X) and (Y, d_Y) is defined as:*

$$d_{GH}(X,Y) := \frac{1}{2}\inf\{dis(C) \,|\, C : X \rightrightarrows Y \text{ is a correspondence}\}$$

Stability of Persistence Pairs

Distances for Persistent Homology Information:

Two persistence modules M and N are called ***ε-interleaved*** with $\varepsilon \geq 0$ if there exist f and g such that, for any p, q $\in \mathbb{R}$ with p $\leq$ q, the following **diagrams commute**

$$
\begin{tikzcd}
 & M_p \arrow[dr, "f_p"] & \\
N_{p-\varepsilon} \arrow[ur, "g_{p-\varepsilon}"] \arrow[rr] & & N_{p+\varepsilon}
\end{tikzcd}
\qquad
\begin{tikzcd}
M_p \arrow[rr] \arrow[dr, "f_p"'] & & M_q \arrow[dr, "f_q"] & \\
 & N_{p+\varepsilon} \arrow[rr] & & N_{q+\varepsilon}
\end{tikzcd}
$$

$$
\begin{tikzcd}
M_{p-\varepsilon} \arrow[rr] \arrow[dr, "f_{p-\varepsilon}"'] & & M_{p+\varepsilon} \\
 & N_p \arrow[ur, "g_p"'] &
\end{tikzcd}
\qquad
\begin{tikzcd}
 & M_{p+\varepsilon} \arrow[rr] & & M_{q+\varepsilon} \\
N_p \arrow[ur, "g_p"] \arrow[rr] & & N_q \arrow[ur, "g_q"'] &
\end{tikzcd}
$$

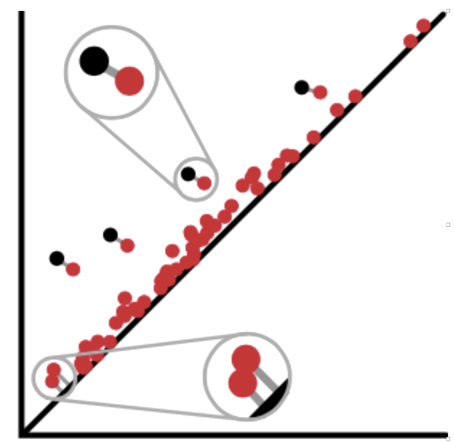
Definition:

Given two persistence modules M and N, their ***interleaving distance d_I*** *is defined as:*

$$d_I(M, N) := \inf\{\varepsilon \geq 0 \,|\, \text{M and N are } \varepsilon\text{-interleaved}\}$$

Stability of Persistence Pairs

Distances for Persistent Homology Information:



Definitions:

Given two persistence diagrams D_1 and D_2,

*their **bottleneck distance** d_B and **Hausdorff distance** d_H are defined as:*

$$d_B(D_1, D_2) := \inf_{\gamma} \left\{ \sup_{x \in D_1} \{\|x - \gamma(x)\|_\infty\} \right\}$$

$$d_H(D_1, D_2) := \max \left\{ \sup_{x \in D_1} \left\{ \inf_{y \in D_2} \{\|x - y\|_\infty\} \right\}, \sup_{y \in D_2} \left\{ \inf_{x \in D_1} \{\|y - x\|_\infty\} \right\} \right\}$$

where γ ranges over all bijections from D_1 to D_2

Stability of Persistence Pairs

Distances for Persistent Homology Information:

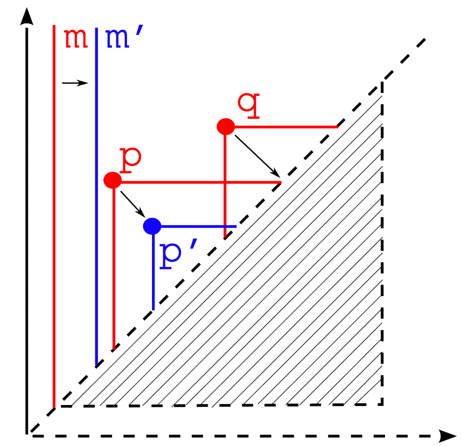


Image from [Ferri et al. 2015]

Definitions:

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their ***bottleneck distance*** $\boldsymbol{d_B}$ *and* ***Hausdorff distance*** $\boldsymbol{d_H}$ *are defined as:*

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where γ ranges over all bijections from D_1 to D_2

Stability of Persistence Pairs

Stability Results:

Given two pairs (X, f), (Y, g) of topological spaces and ***tame*** functions and $k \in \mathbb{N}$, let M, N be the induced k^{th} persistence modules and let D_1, D_2 be the corresponding persistence diagrams

- $d_H(D_1, D_2) \leq d_B(D_1, D_2)$
- $d_I(M, N) = d_B(D_1, D_2)$

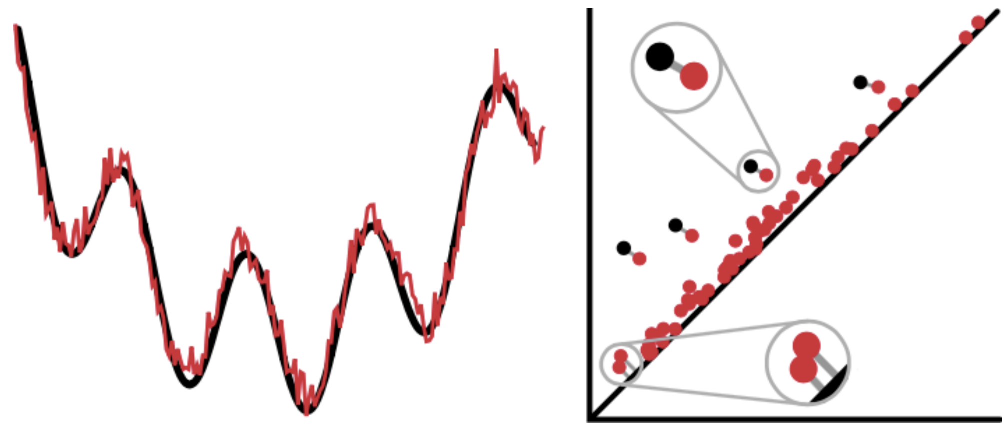
Theorem:

*Under the above hypothesis, the following **optimal lower bound** holds*

$$d_I(M, N) \leq d_N\Big((X, f), (Y, g)\Big)$$

Stability of Persistence Pairs

Stability Results:



Theorem:

*Given two **tame** continuous functions f, g: $X \longrightarrow \mathbb{R}$*

on a topological space X, $k \in \mathbb{N}$, and D_f, D_g the induced k^{th} persistence diagrams,

$$d_B(D_f, D_g) \leq \|f - g\|_\infty$$

Images from [Rieck 2016]

Stability of Persistence Pairs

Stability Results:

Theorem:

*Given two finite metric spaces (X, d_X), (Y, d_Y), $k \in \mathbb{N}$, and D_X, D_Y the k^{th} persistence diagrams of the **filtrations of the Vietoris-Rips complexes generated by X and Y**,*

$$d_B(D_X, D_Y) \leq d_{GH}(X, Y)$$

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