

Persistent Homology for Shape Comparison

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Persistent Homology for Shape Comparison

- ◆ *Quick Overview on TDA*
- ◆ *Case Study*

Persistent Homology for Shape Comparison

- ◆ **Quick Overview on TDA**
- ◆ *Case Study*

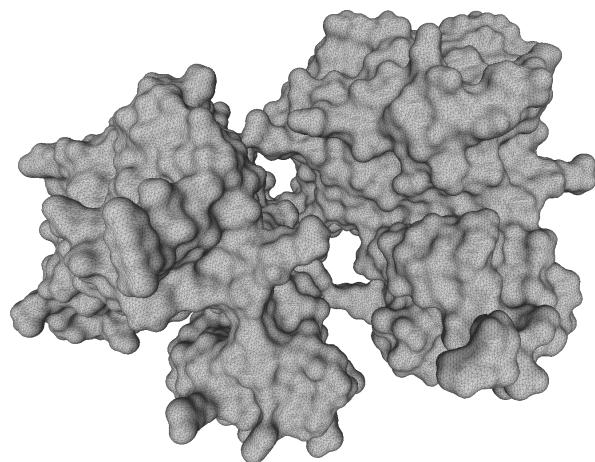
Topological Data Analysis

Topological Data Analysis (TDA) aims at describing, characterizing, and discriminating data on the basis of their shape

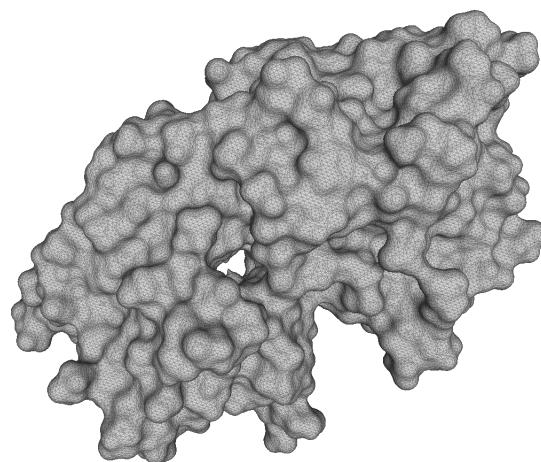
Example:

Consider a dataset consisting of *molecular surfaces* and pick two of them, X and Y

X



Y

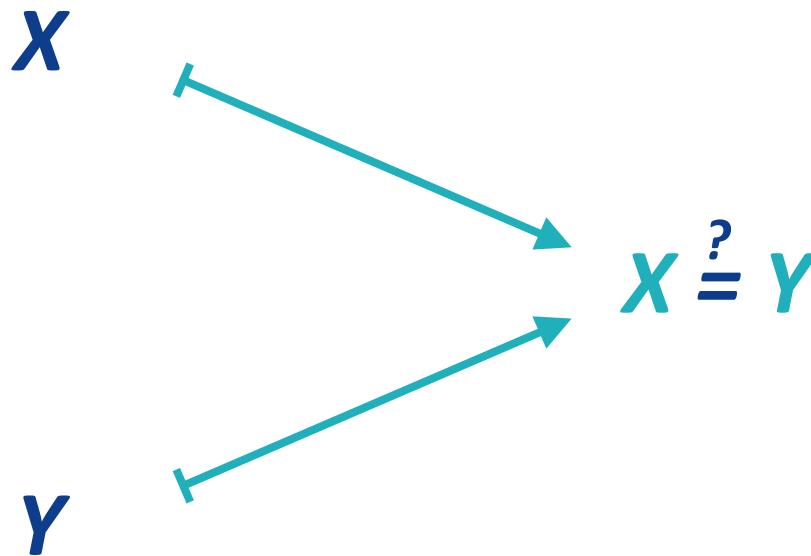


Do X and Y represent the same molecule?

Are X , Y equal?

*Topological
Space*

*Equality
Check*



Do X and Y have the same shape?

Topological
Space

Algebraic
Structure

Equality
Check

X \longmapsto

$Shape(X)$



$Shape(X) \stackrel{?}{=} Shape(Y)$

Y \longmapsto

$Shape(Y)$



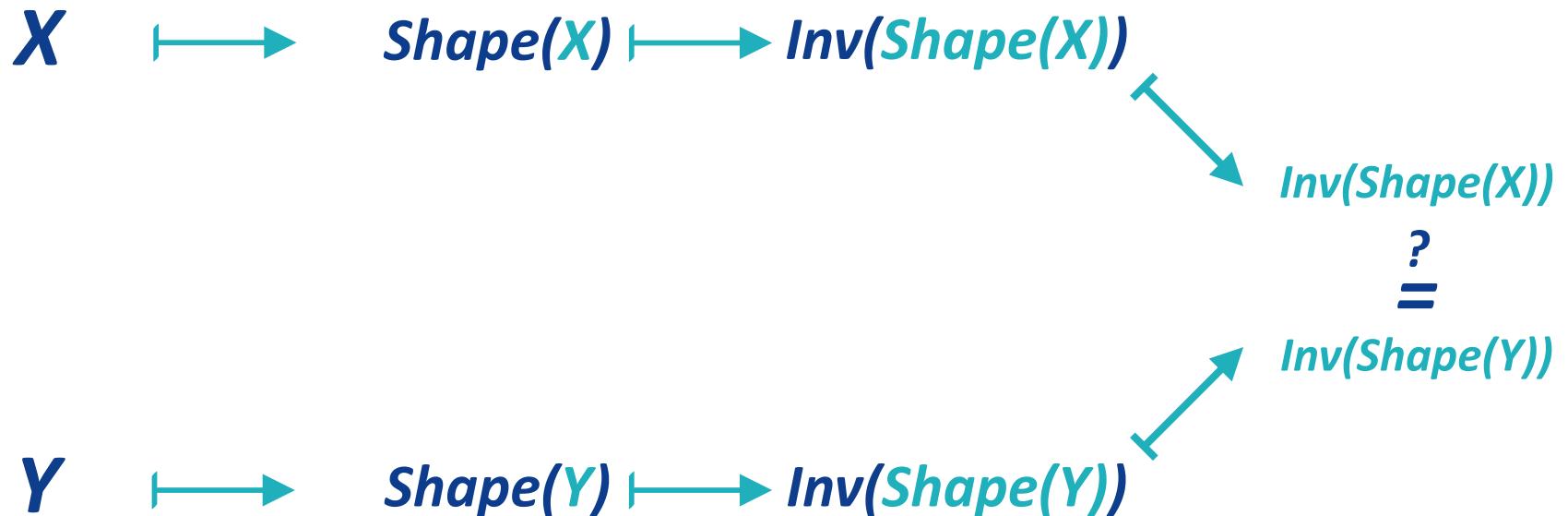
Do X and Y have the same shape?

Topological
Space

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Invariant

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Homology

Given a topological space X and a field \mathbb{F} , the *homology of X* is a *topological invariant*

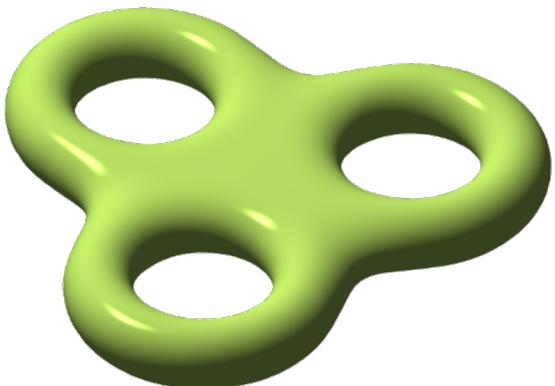
↑
intuition

detecting the “holes” of X

↓
formalism

capturing the independent non-bounding cycles of X

measuring how far the chain complex associated with X is from being exact



$$H_i(X; \mathbb{F}) \cong \begin{cases} \mathbb{F} & \text{for } i = 0 \\ \mathbb{F}^6 & \text{for } i = 1 \\ \mathbb{F} & \text{for } i = 2 \\ 0 & \text{otherwise} \end{cases}$$

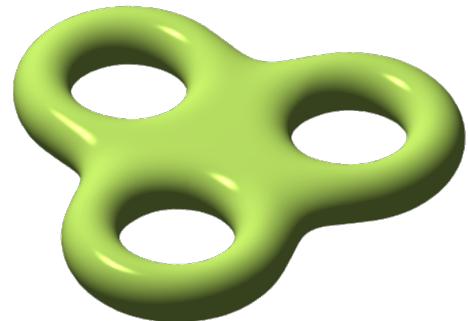
Homology

Theorem:

Any homology group of X with coefficients in \mathbb{F} can be expressed as

$$H_i(X; \mathbb{F}) \cong \mathbb{F}^{\beta_i}$$

where β_i is called the **i^{th} Betti number** of X



$$\beta_i = \begin{cases} 1 & \text{for } i = 0 \\ 6 & \text{for } i = 1 \\ 1 & \text{for } i = 2 \\ 0 & \text{otherwise} \end{cases}$$

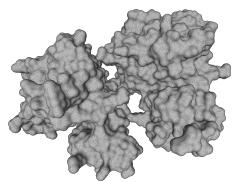
Do X and Y have the same shape?

Topological Space

Algebraic Structure

Algebraic Invariant

Equality Check

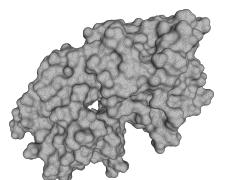


$$H_i(X; \mathbb{Z}_2) \cong \begin{cases} \mathbb{Z}_2 & \text{for } i = 0 \\ (\mathbb{Z}_2)^4 & \text{for } i = 1 \\ \mathbb{Z}_2 & \text{for } i = 2 \end{cases}$$

$$(1, 4, 1)$$



$X \neq Y$



$$H_i(Y; \mathbb{Z}_2) \cong \begin{cases} \mathbb{Z}_2 & \text{for } i = 0 \\ (\mathbb{Z}_2)^2 & \text{for } i = 1 \\ \mathbb{Z}_2 & \text{for } i = 2 \end{cases}$$

$$(1, 2, 1)$$



Homology Fails

Do they have the same shape?



In Practice?

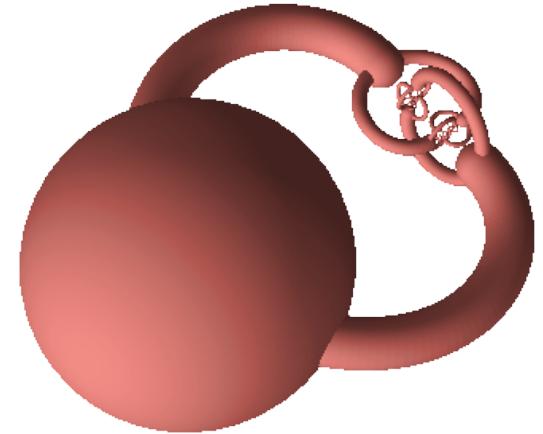
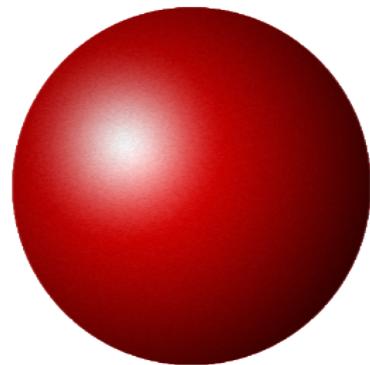


In Theory?



Homology Fails

Do they have the same shape?



In Practice?



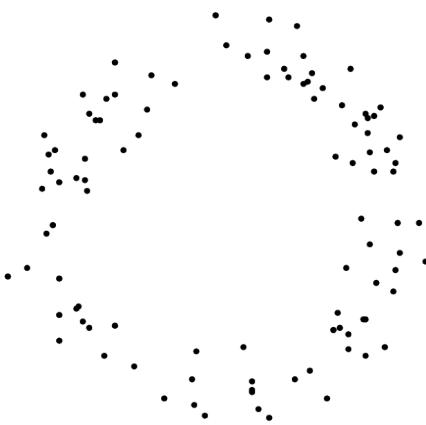
In Theory?



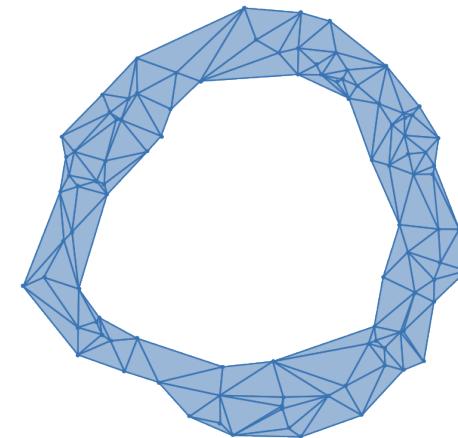
Homology Fails

Which is the shape of a given data?

We would like to retrieve the “*actual*” homological information of a data



Point Cloud Dataset



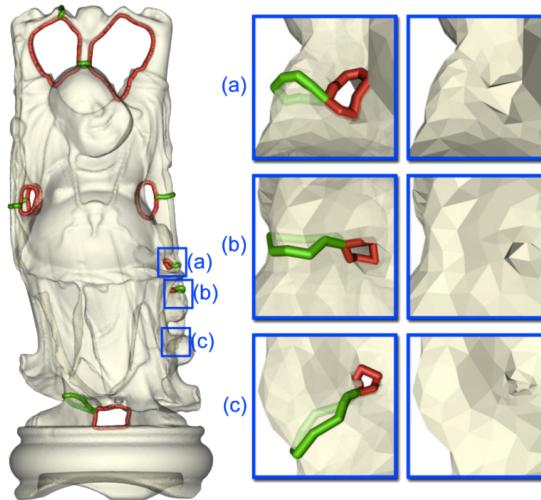
*Topological Nature of
the “Underlying” Shape*

Image from [Bauer 2015]

Homology Fails

Which is the shape of a given data?

We would like to retrieve the “*actual*” homological information of a data



Noisy Dataset

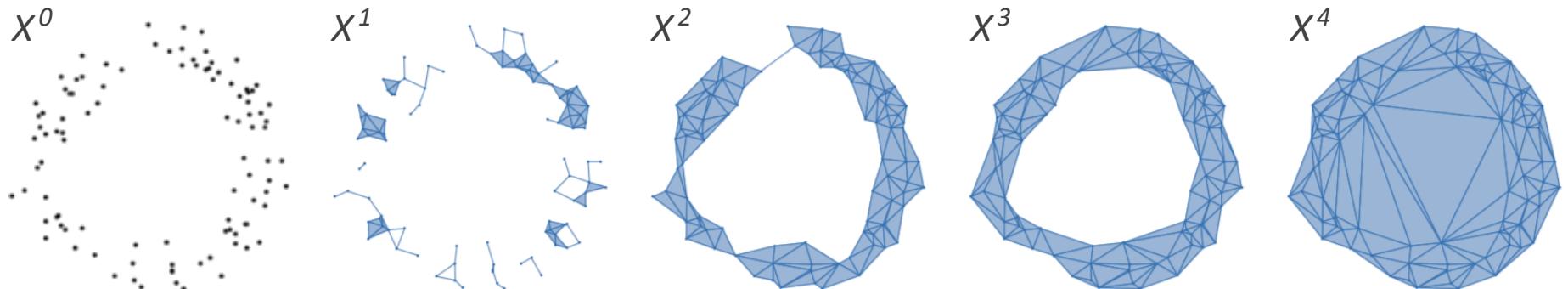


Relevant Homological Information

The Solution? Persistent Homology

In a Nutshell:

*Persistent homology allows for
describing the homology changes of an evolving object*



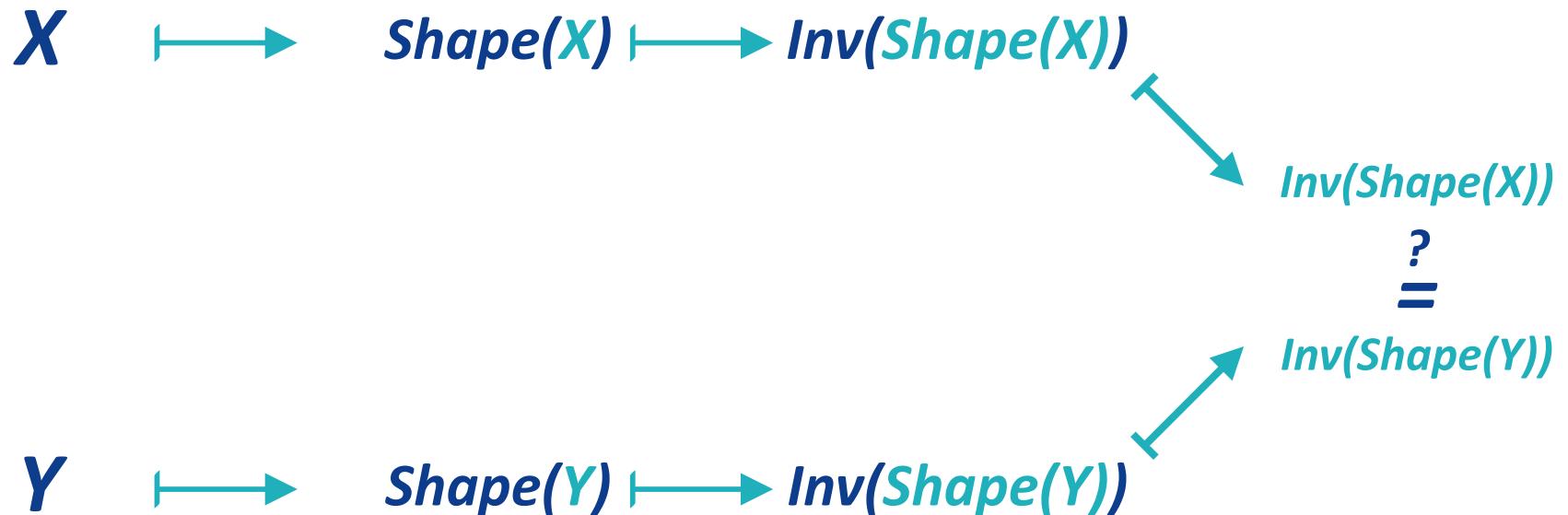
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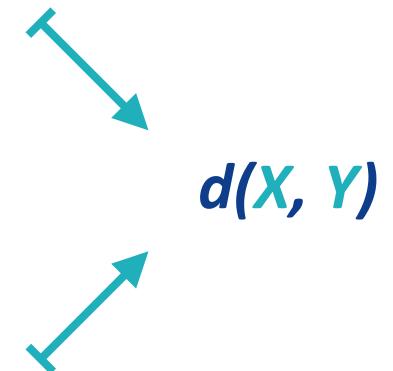
Do X and Y have the same shape?


$$X \xrightarrow{\quad} X' \xrightarrow{\quad} \text{Shape}(X') \xrightarrow{\quad} \text{Inv}(\text{Shape}(X'))$$
$$\begin{matrix} & \xleftarrow{\quad} & \text{Inv}(\text{Shape}(X')) \\ & ? = & \\ & \xrightarrow{\quad} & \text{Inv}(\text{Shape}(Y')) \end{matrix}$$
$$Y \xrightarrow{\quad} Y' \xrightarrow{\quad} \text{Shape}(Y') \xrightarrow{\quad} \text{Inv}(\text{Shape}(Y'))$$

Do X and Y have a *similar* shape?


$$X \xrightarrow{\quad} X' \xrightarrow{\quad} \text{Shape}(X') \xrightarrow{\quad} \text{Inv}(\text{Shape}(X'))$$
$$d(\text{Inv}(\text{Shape}(X')), \text{Inv}(\text{Shape}(Y')))$$
$$Y \xrightarrow{\quad} Y' \xrightarrow{\quad} \text{Shape}(Y') \xrightarrow{\quad} \text{Inv}(\text{Shape}(Y'))$$


Do X and Y have a similar shape?


$$X \xrightarrow{\quad} X' \xrightarrow{\quad} \text{Shape}(X') \xrightarrow{\quad} \text{Inv}(\text{Shape}(X'))$$
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Do X and Y have a similar shape?



$$X \xrightarrow{\quad} X' \xrightarrow{\quad} \text{Shape}(X') \xrightarrow{\quad} \text{Inv}(\text{Shape}(X'))$$

$$Y \xrightarrow{\quad} Y' \xrightarrow{\quad} \text{Shape}(Y') \xrightarrow{\quad} \text{Inv}(\text{Shape}(Y'))$$

$$\begin{array}{c} d(X, Y) \\ \swarrow \quad \searrow \\ \end{array}$$

The entire procedure has to be *stable*
i.e. *robust to noise and small perturbations*

Do X and Y have a similar shape?



$$X \xrightarrow{\quad} X' \xrightarrow{\quad} \text{Shape}(X') \xrightarrow{\quad} \text{Inv}(\text{Shape}(X'))$$

$$Y \xrightarrow{\quad} Y' \xrightarrow{\quad} \text{Shape}(Y') \xrightarrow{\quad} \text{Inv}(\text{Shape}(Y'))$$

$$\begin{array}{c} d(X, Y) \\ \swarrow \quad \searrow \\ \end{array}$$

In other words,
Similar Data \Rightarrow Similar Algebraic Invariants

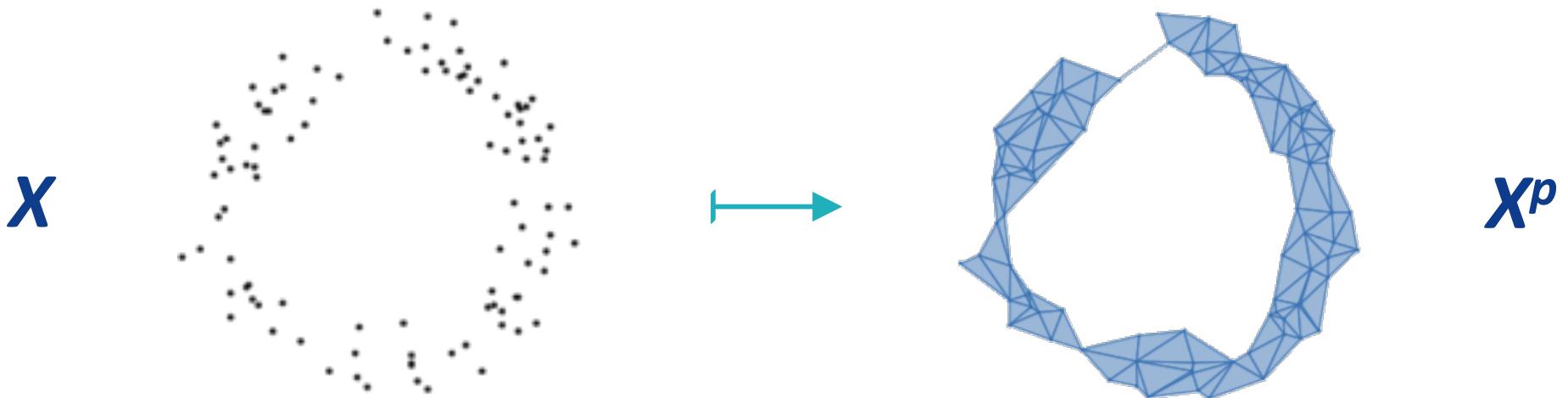
Persistent Homology

From an Input Data X to a Topological Representation X' :

Let X be a **point cloud** $V \subseteq \mathbb{R}^d$

We set $X' := \{X^p\}_{p \in \mathbb{R}}$, where, chosen a value $p \in \mathbb{R}$, X^p is defined as

$$\{\sigma \subseteq V \mid d(u, v) \leq p, \forall u, v \in \sigma\}$$



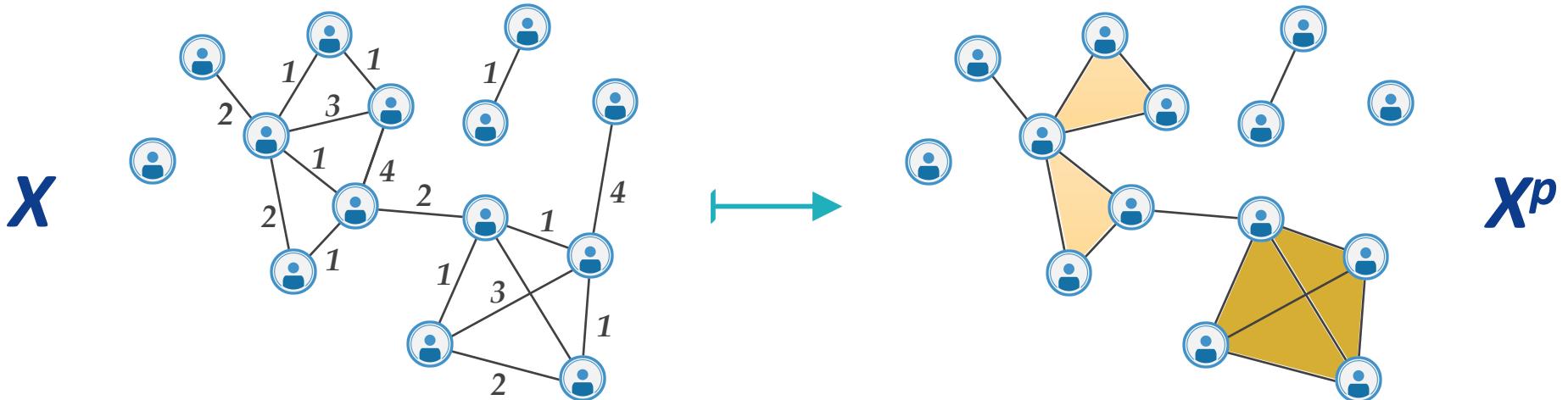
Persistent Homology

From an Input Data X to a Topological Representation X' :

Let X be a **weighted graph** $G := (V, E, w: E \rightarrow \mathbb{R})$

We set $X' := \{X^p\}_{p \in \mathbb{R}}$, where, chosen a value $p \in \mathbb{R}$, X^p is defined as

$$\{\sigma \subseteq V \mid w(u, v) \leq p, \forall u, v \in \sigma\}$$



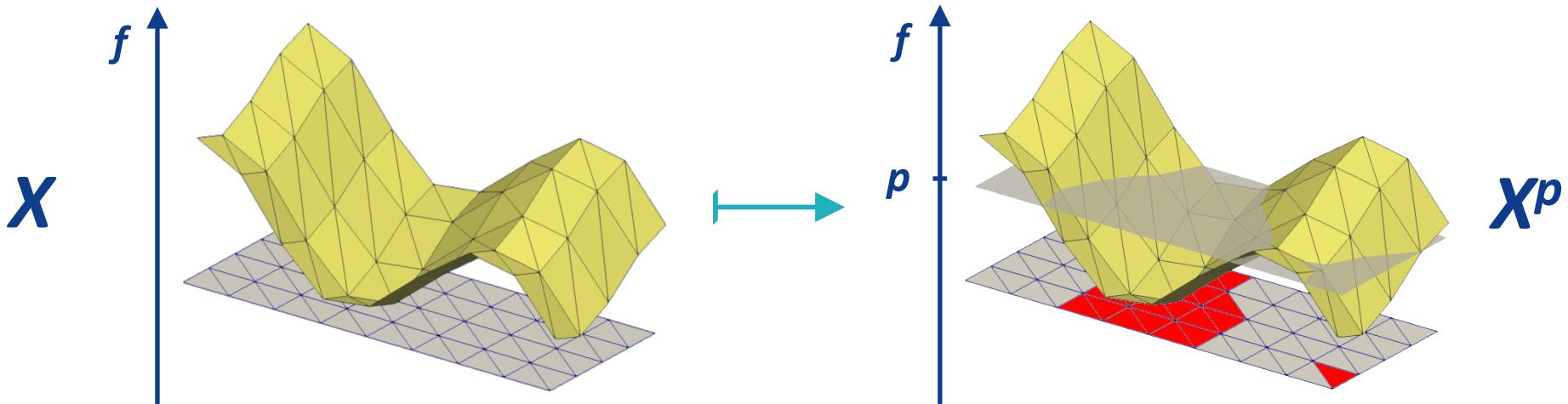
Persistent Homology

From an Input Data X to a Topological Representation X' :

Let X be a **function** $f: D \rightarrow \mathbb{R}$

We set $X' := \{X^p\}_{p \in \mathbb{R}}$, where, chosen a value $p \in \mathbb{R}$, X^p is defined as

$$\{ \sigma \in D \mid f(\sigma) \leq p \}$$



Persistent Homology

From an Input Data X to a Topological Representation X' :

*Independently from the construction procedure,
the collection of topological spaces $\{X^p\}_{p \in \mathbb{R}}$, called **filtration** of X ,
satisfies that, for any $p, q \in \mathbb{R}$ such that $p \leq q$,*

$$X^p \subseteq X^q$$

Working Assumption:

We can always pretend that parameter p varies over \mathbb{N}

Persistent Homology

From a Topological Representation X' to an Algebraic Structure $\text{Shape}(X')$:

Given a filtration $X' := \{X^p\}_{p \in \mathbb{N}}$, a value $i \in \mathbb{N}$, and a field \mathbb{F} , the i^{th} persistence module M of X' over \mathbb{F} is defined as the **finitely generated graded $\mathbb{F}[x]$ -module**

$$M := \bigoplus_{p \in \mathbb{N}} M_p$$

where:

- ◆ $M_p := H_i(X^p; \mathbb{F})$, the set of **homogeneous elements of grade p**
- ◆ The **action $x^{q-p} h$ over an element h of grade p** is defined as $\mu_{i,p,q}(h)$, where:
 - ❖ $\mu_{i,p,q}(h) : H_i(X^p; \mathbb{F}) \rightarrow H_i(X^q; \mathbb{F})$ is the linear map induced by the inclusion $X^p \subseteq X^q$

Persistent Homology

From an Algebraic Structure $\text{Shape}(X')$ to an Algebraic Invariant $\text{Inv}(\text{Shape}(X'))$:

Theorem (structure for finitely generated graded modules over a PID):

Any persistence module M can be expressed as

$$M \cong \bigoplus_{k=1}^n \mathbb{F}[x](-r_k) \oplus \bigoplus_{j=1}^m \left(\mathbb{F}[x]/(x^{q_j-p_j}) \right) (-p_j)$$

So, M is completely determined by the collection of values r_k and of pairs (p_j, q_j)

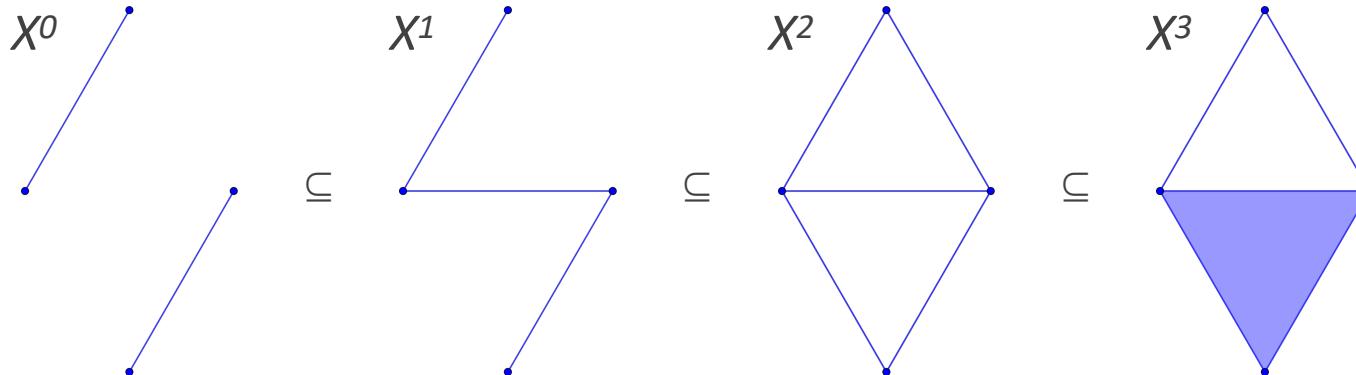
Such descriptors are typically expressed as pairs, called **persistence pairs** of M , of

the kind (r_k, ∞) and (p_j, q_j)

Persistent Homology

Intuitively:

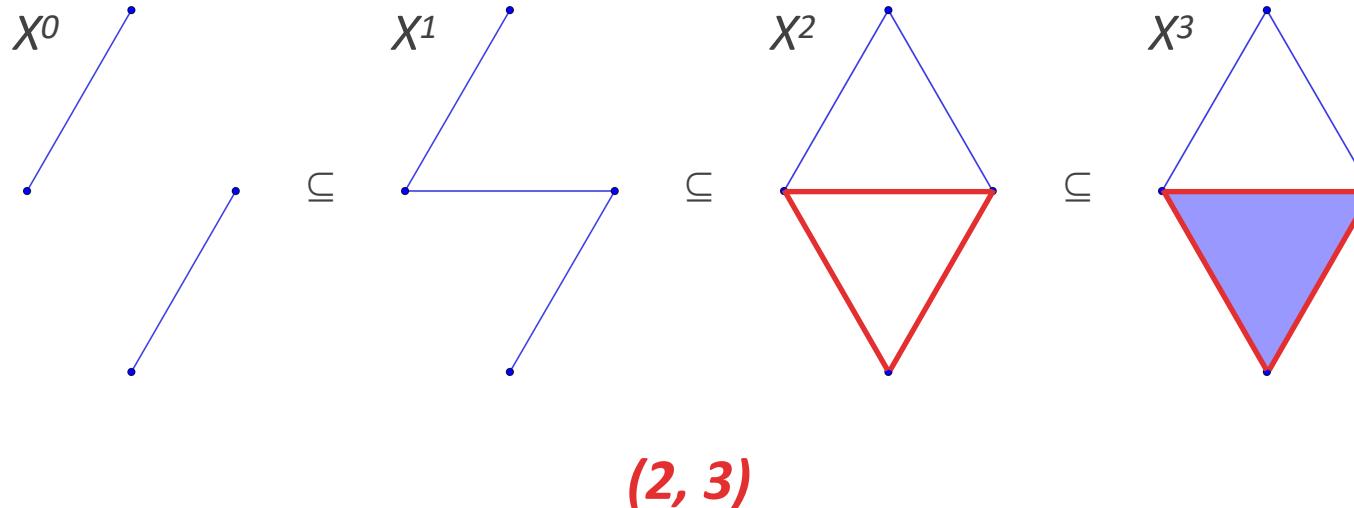
Given a filtration $X' := \{X^p\}_{p \in \mathbb{N}}$, a **persistence pair** $(p, q) \in \mathbb{N} \times (\mathbb{N} \cup \{\infty\})$ with $p < q$ represents a **homological class** that is **born at step p** and **dies at step q**



Persistent Homology

Intuitively:

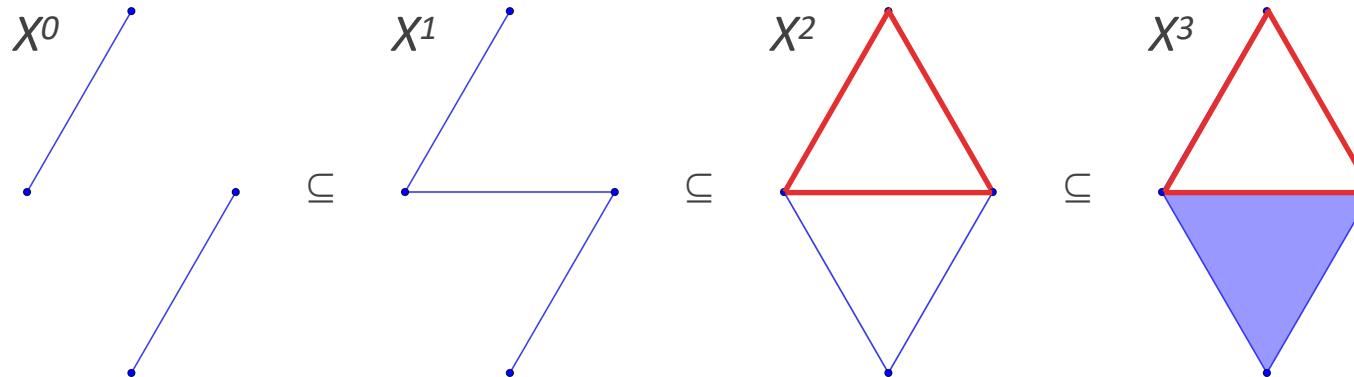
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Persistent Homology

Intuitively:

Given a filtration $X' := \{X^p\}_{p \in \mathbb{N}}$, a **persistence pair** $(p, q) \in \mathbb{N} \times (\mathbb{N} \cup \{\infty\})$ with $p < q$ represents a **homological class** that is **born at step p** and **dies at step q**

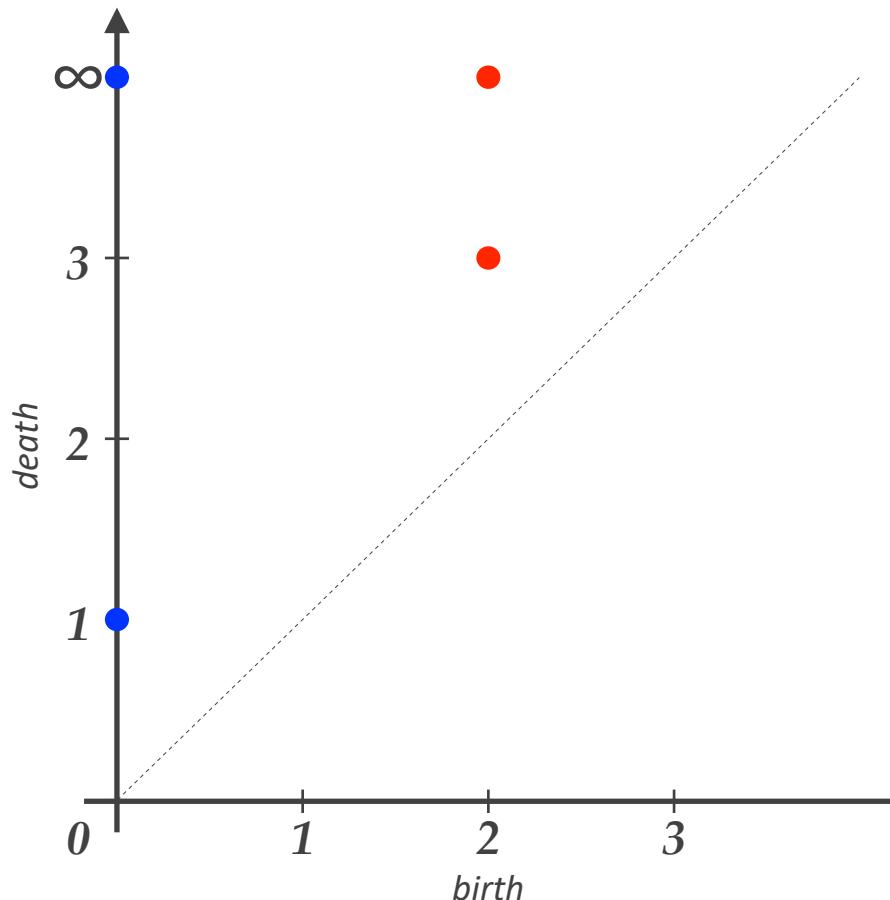


(2, ∞) essential pair

Persistent Homology

Persistence Diagrams:

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



H_0	(0, 1)	H_1	(2, 3)
	(0, ∞)		(2, ∞)

Formally, a persistence diagram is a *multi-set*
i.e. points are endowed with *multiplicity*

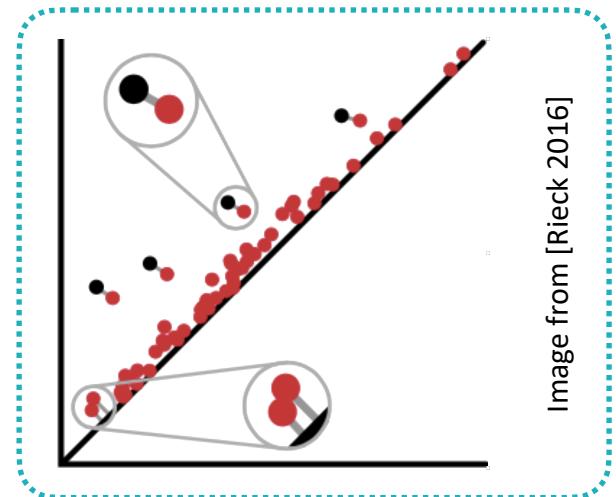
Persistent Homology

From an Algebraic Invariant $\text{Inv}(\text{Shape}(X'))$ to a Similarity Check $d(X, Y)$:

Given two persistence diagrams D_X and D_Y , their **bottleneck distance** d_B is defined as

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

where γ ranges over all bijections from D_X to D_Y



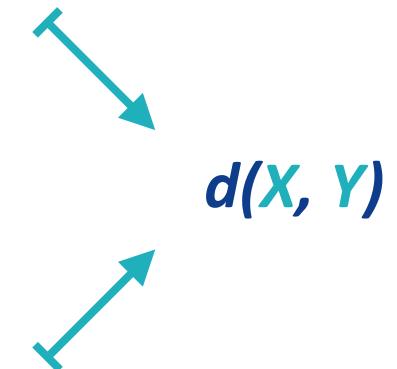
Do X and Y have a similar shape?

Persistent Homology Pipeline:



$X \longleftrightarrow X' \longleftrightarrow Shape(X') \longleftrightarrow Inv(Shape(X'))$

$Y \longleftrightarrow Y' \longleftrightarrow Shape(Y') \longleftrightarrow Inv(Shape(Y'))$

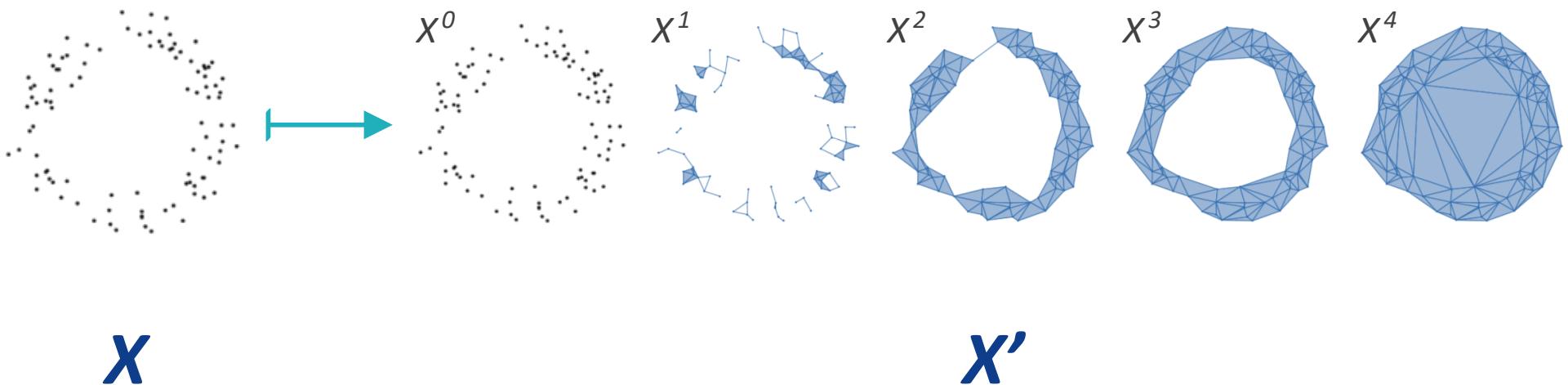


Do X and Y have a similar shape?

Persistent Homology Pipeline:

*Input
Data*

*Topological
Representation*

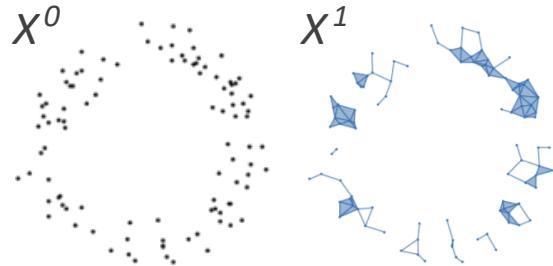


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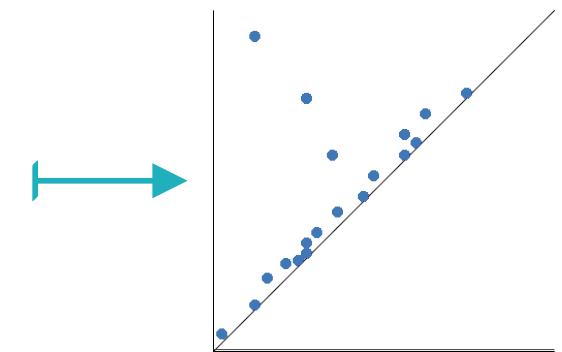
Persistent Homology Pipeline:

**Topological
Representation**

**Algebraic
Invariant**



X'



$\text{Inv}(\text{Shape}(X'))$

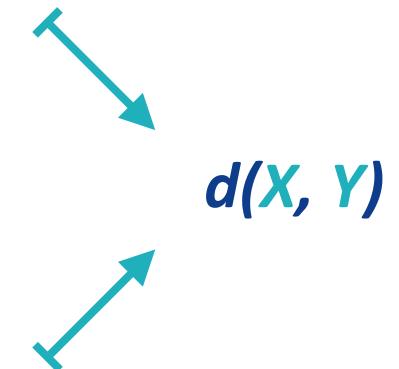
Do X and Y have a similar shape?

Persistent Homology Pipeline:



$X \longleftrightarrow X' \longleftrightarrow Shape(X') \longleftrightarrow Inv(Shape(X'))$

$Y \longleftrightarrow Y' \longleftrightarrow Shape(Y') \longleftrightarrow Inv(Shape(Y'))$



Do X and Y have a similar shape?

AI-Oriented Alternative:

*Input
Data*

*Topological
Representation*

*Algebraic
Structure*

*Feature
Vector*

*Learning
Process*

$$X \longleftrightarrow X' \longleftrightarrow \text{Shape}(X') \longleftrightarrow \phi(\text{Shape}(X'))$$

$$Y \longleftrightarrow Y' \longleftrightarrow \text{Shape}(Y') \longleftrightarrow \phi(\text{Shape}(Y'))$$

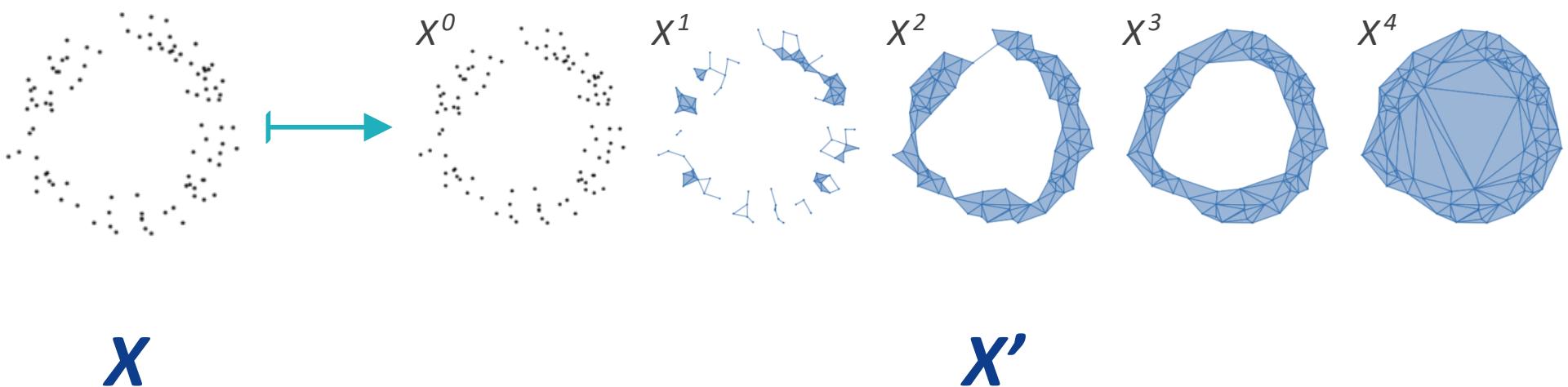
$$k(X, Y)$$

Do X and Y have a similar shape?

AI-Oriented Alternative:

*Input
Data*

*Topological
Representation*

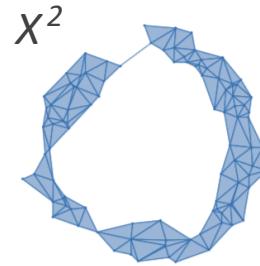
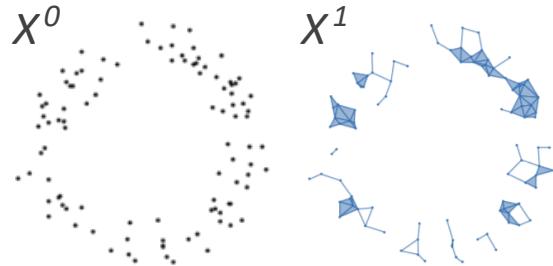


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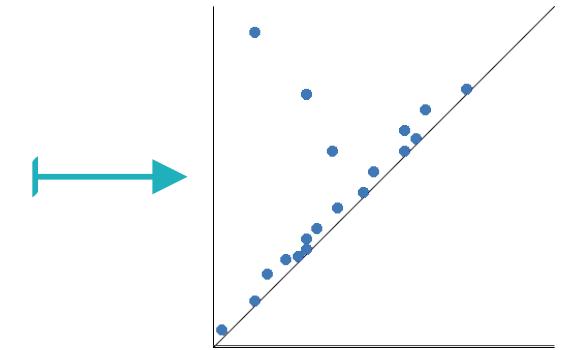
AI-Oriented Alternative:

Topological
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X'



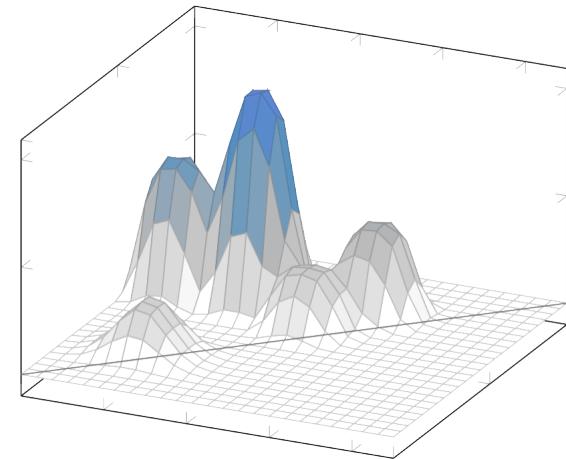
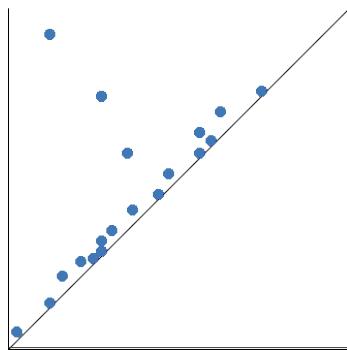
$\text{Inv}(\text{Shape}(X'))$

Do X and Y have a similar shape?

AI-Oriented Alternative:

*Algebraic
Invariant*

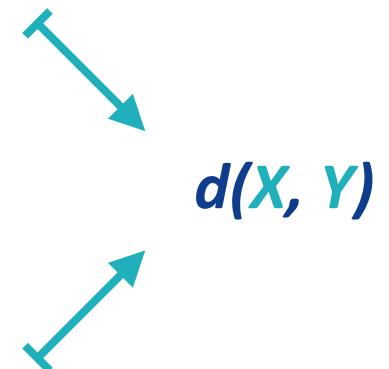
*Feature
Vector*



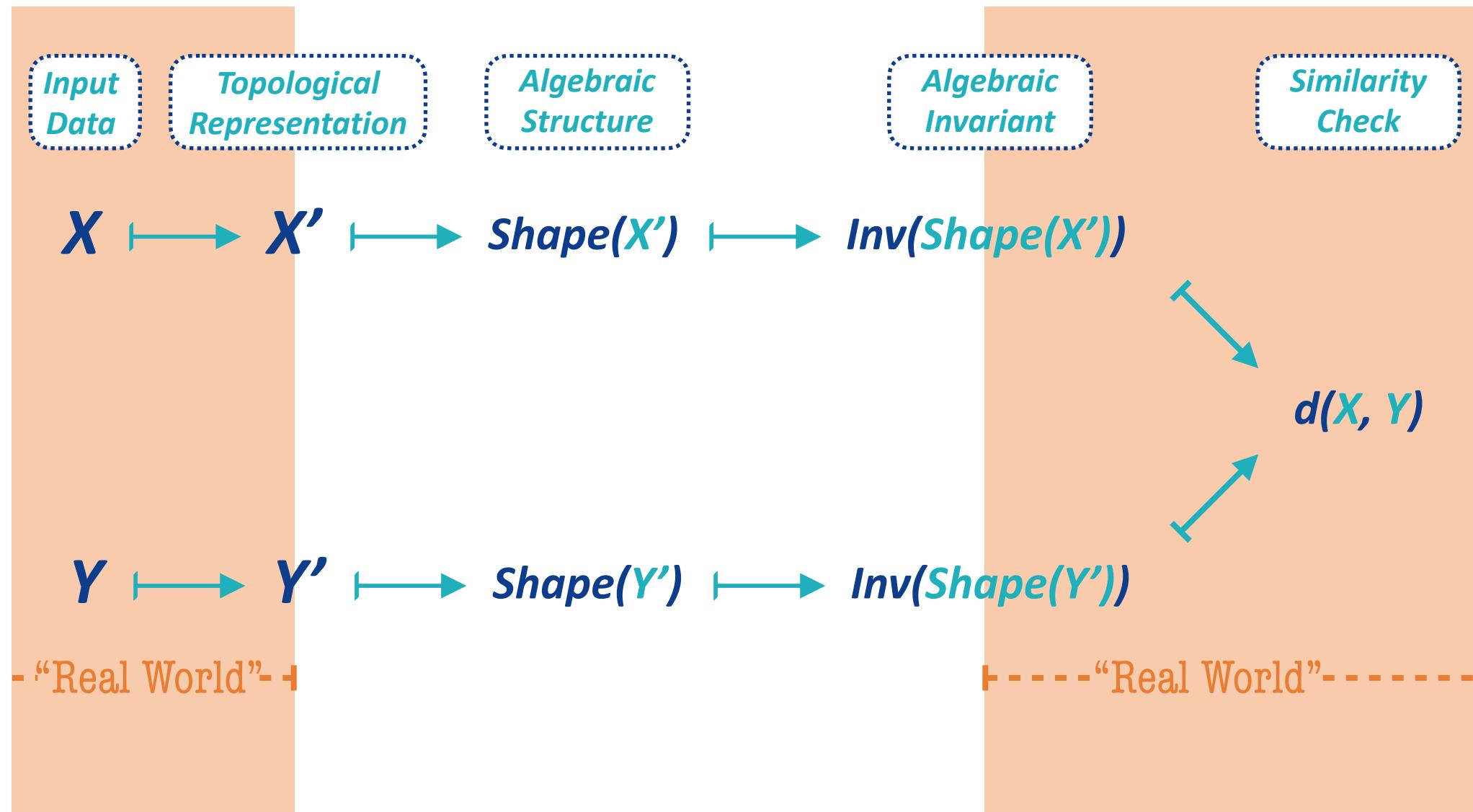
$\text{Inv}(\text{Shape}(X'))$

$\phi(\text{Shape}(X'))$

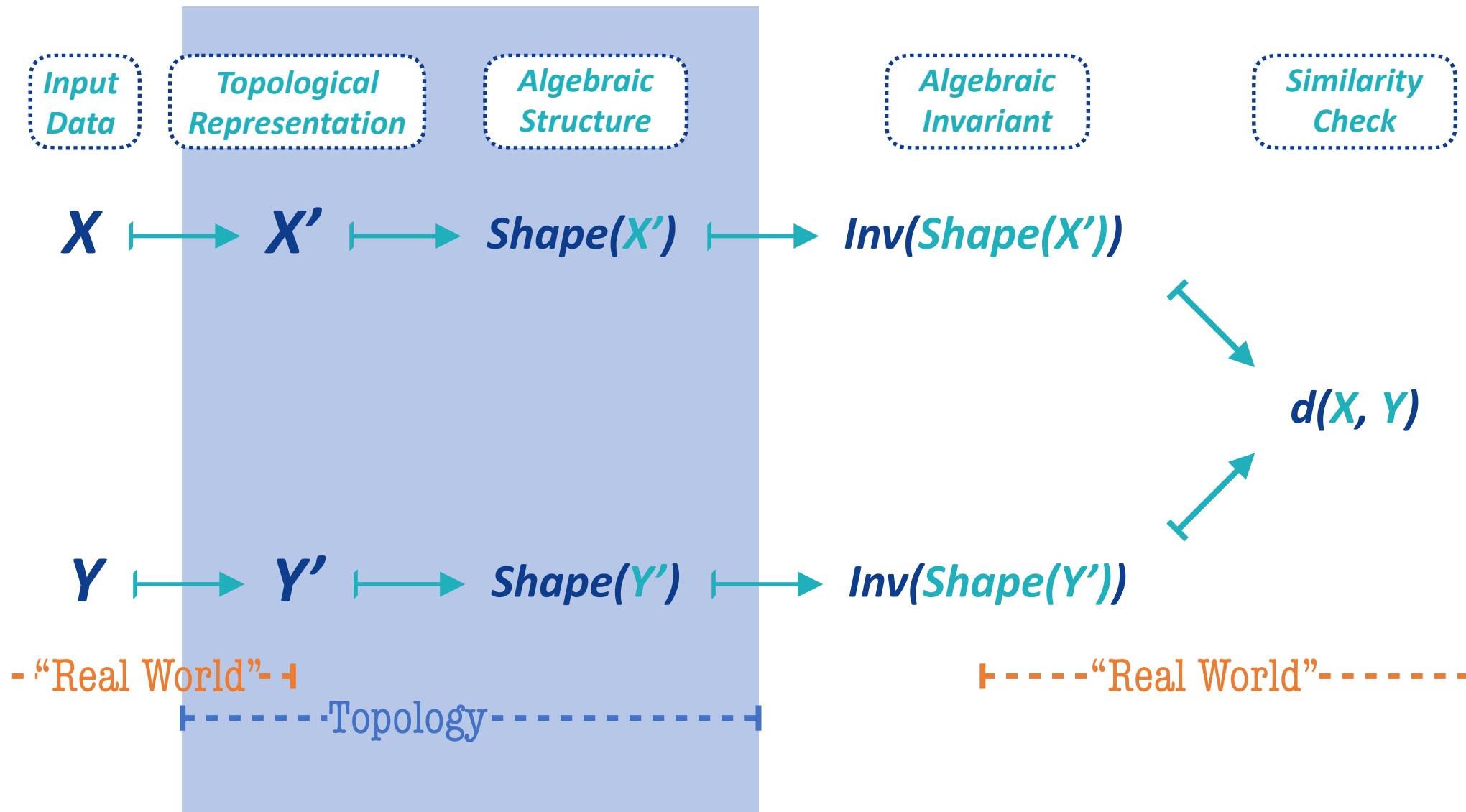
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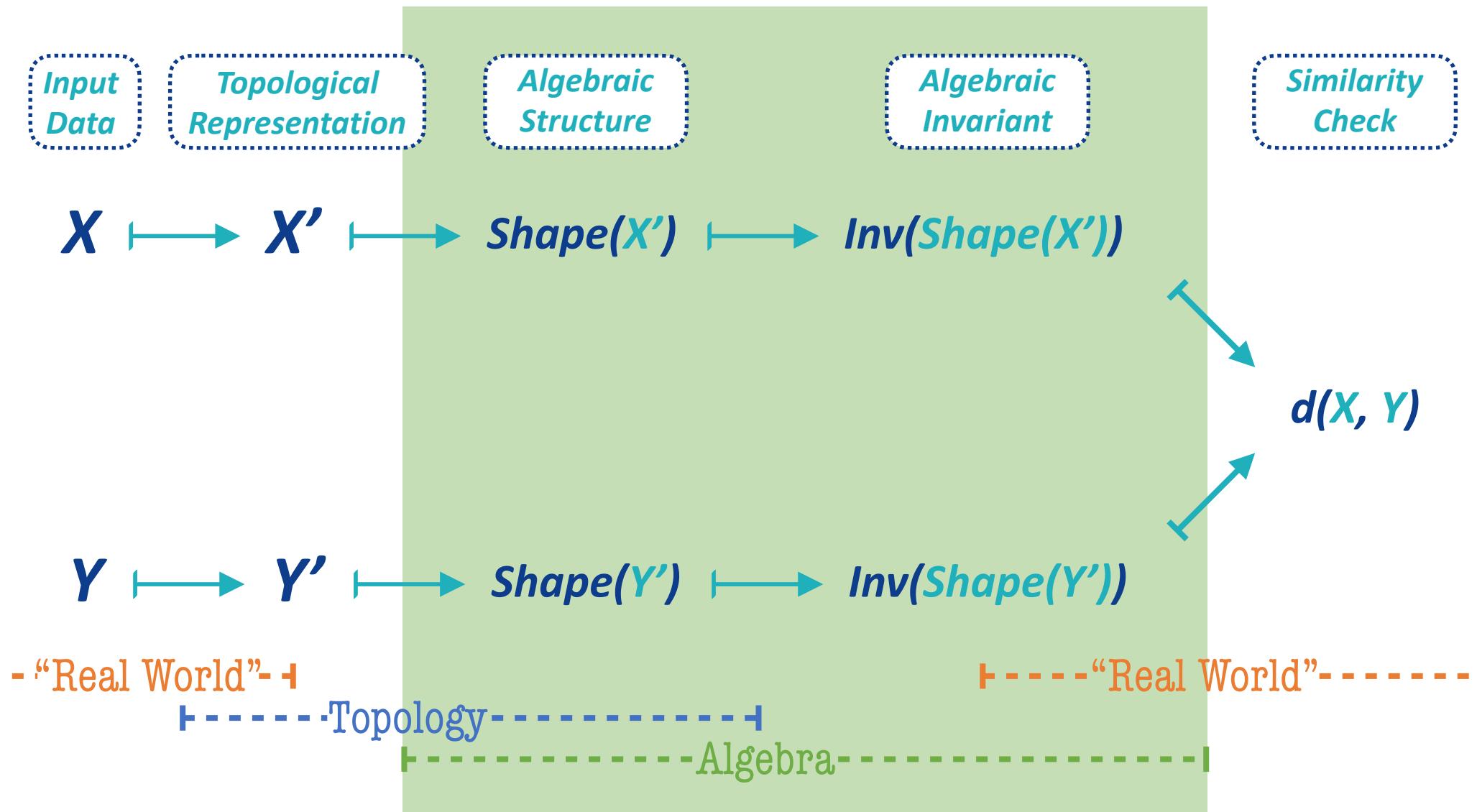
Do X and Y have a similar shape?



Do X and Y have a similar shape?



Do X and Y have a similar shape?



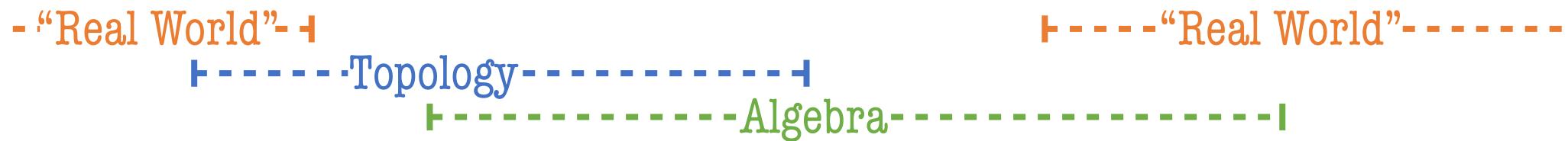
Do X and Y have a similar shape?



$$X \xrightarrow{\quad} X' \xrightarrow{\quad} \text{Shape}(X') \xrightarrow{\quad} \text{Inv}(\text{Shape}(X'))$$

$$\begin{array}{c} d(X, Y) \\ \longleftrightarrow \\ d(\text{Shape}(X'), \text{Shape}(Y')) \end{array}$$

$$Y \xrightarrow{\quad} Y' \xrightarrow{\quad} \text{Shape}(Y') \xrightarrow{\quad} \text{Inv}(\text{Shape}(Y'))$$



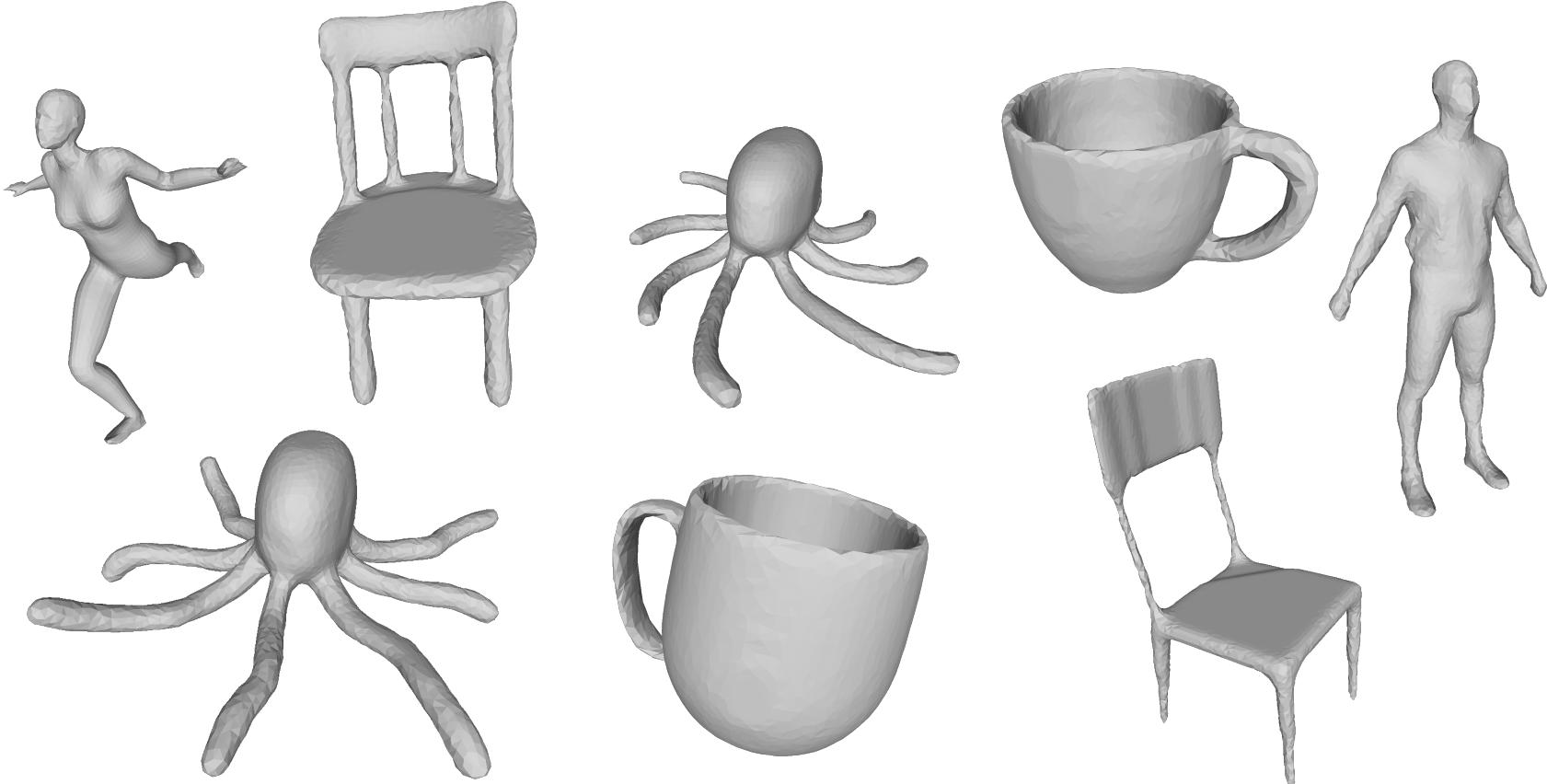
Persistent Homology for Shape Comparison

- ◆ Quick Overview on TDA
- ◆ **Case Study**

Case Study

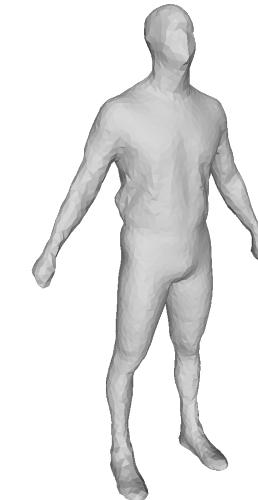
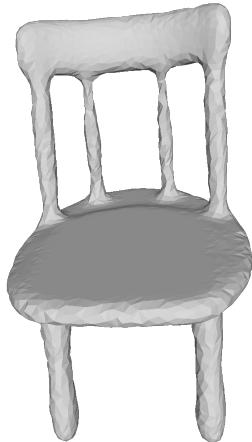
Goal:

Given a dataset of 80 surfaces, classify them on the basis of their shape



Case Study

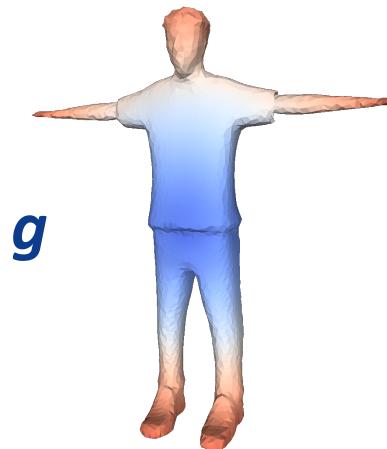
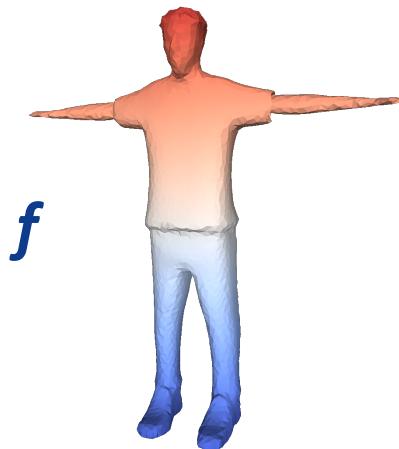
Homology is not enough



Case Study

*In order to adopt **persistent homology**,
we need to filter each surface through a function:*

- ◆ $f(x, y, z) := z$
- ◆ $g(x, y, z) := \text{distance of } (x, y, z) \text{ from the model barycentre}$



Software Packages

Several software packages for computing persistent homology have been developed:

- ◆ *javaPlex*
 - ◆ *jHoles*
 - ◆ *Dionysus*
 - ◆ *Perseus*
 - ◆ *PHAT*
 - ◆ *DIPHA*
 - ◆ *Gudhi*
 - ◆ *SimpPers*
 - ◆ *Ripser*
 - ◆ *giotto-tda*
 - ◆ *TDAstats*
- ◆ ...

Software Packages

PHAT:

- ◆ **Language:**
 - ❖ C++ (with Python bindings)
- ◆ **Algorithms:**
 - ❖ Standard, Dual, Twist, Chunk, Spectral Sequences
- ◆ **Coefficient Fields:**
 - ❖ \mathbb{Z}_2
- ◆ **Homology:**
 - ❖ Simplicial, Cubical
- ◆ **Accepted Inputs:**
 - ❖ Boundary Matrices
- ◆ **Computed Filtrations:**
 - ❖ -
- ◆ **Visualizations:**
 - ❖ -
- ◆ **Additional Features:**
 - ❖ -

Software Packages

Ripser:

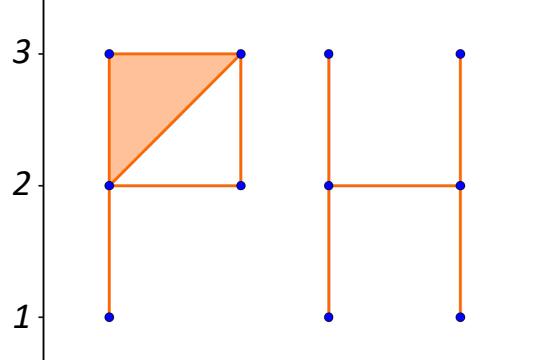
- ◆ **Language:**
 - ❖ C++ (with Python bindings)
- ◆ **Algorithms:**
 - ❖ Dual, Twist
- ◆ **Coefficient Fields:**
 - ❖ \mathbb{Z}_p
- ◆ **Homology:**
 - ❖ Simplicial
- ◆ **Accepted Inputs:**
 - ❖ Point Clouds, Distance Matrices

- ◆ **Computed Filtrations:**
 - ❖ Vietoris-Rips and Čech complexes, Alpha-Shapes, Lower Star of Cubical complexes
- ◆ **Visualizations:**
 - ❖ Persistence Diagrams (through Persim: Persistence Images)
- ◆ **Additional Features:**
 - ❖ Representative Cocycles (through Persim: Bottleneck distance, modified Gromov–Hausdorff distance, Sliced Wasserstein kernel, Heat kernel)

Persistent Homology Computation

Standard Algorithm:

From:



[Zomorodian & Carlsson 2005]

To:

[1, 2]

H₀

[1, ∞)

H_1 [3, ∞)

<i>i</i> \ <i>j</i>	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
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<i>low</i>								4	6	7	5	3						13	14		15	16		22

Compute a *reduced boundary matrix* for K^f from which easily read the persistence pairs

Persistent Homology Computation

Given a filtered simplicial complex, let us consider its *filtering function* f :

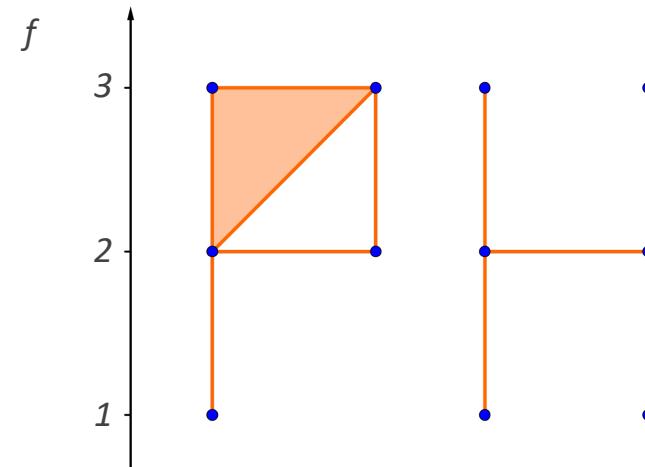
$$f(\sigma) := \min \{ p \mid \sigma \in K^p \}$$

Conversely, $K^p := \{ \sigma \in K \mid f(\sigma) \leq p \}$

Total Ordering on K^f :

A sequence $\sigma_1, \sigma_2, \dots, \sigma_n$ of the simplices of K^f such that:

- ◆ if $f(\sigma_i) < f(\sigma_j)$, then $i < j$
- ◆ if σ_i is a proper face of σ_j , then $i < j$



Persistent Homology Computation

Given a filtered simplicial complex, let us consider its *filtering function* f :

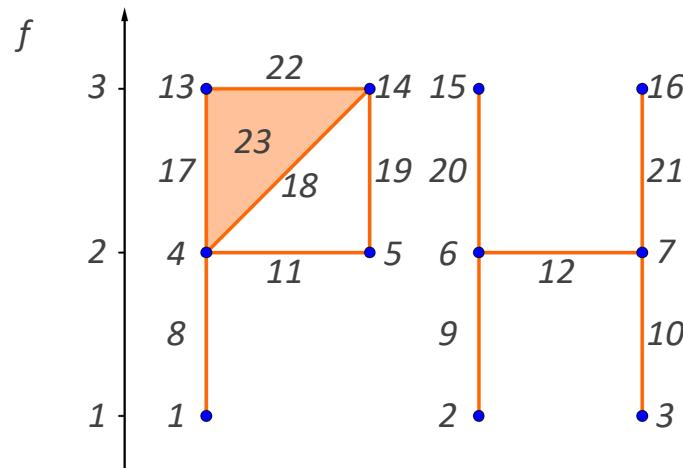
$$f(\sigma) := \min \{ p \mid \sigma \in K^p \}$$

Conversely, $K^p := \{ \sigma \in K \mid f(\sigma) \leq p \}$

A Possible Choice:

Set $\sigma < \sigma'$ if:

- ◆ $f(\sigma) < f(\sigma')$
- ◆ $f(\sigma) = f(\sigma')$ and $\dim(\sigma) < \dim(\sigma')$
- ◆ $f(\sigma) = f(\sigma')$, $\dim(\sigma) = \dim(\sigma')$, and σ precedes σ' w.r.t. the *lexicographic order* of their vertices

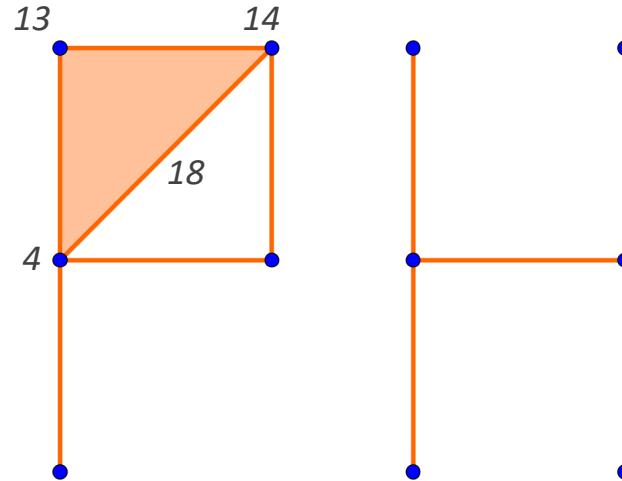


Persistent Homology Computation

Boundary Matrix:

A square matrix \mathbf{M} of size $n \times n$ defined by

$$M_{i,j} := \begin{cases} 1 & \text{if } \sigma_i \text{ is a face of } \sigma_j \text{ s.t. } \dim(\sigma_i) = \dim(\sigma_j) - 1 \\ 0 & \text{otherwise} \end{cases}$$



E.g.

- ◆ $M_{4,18} = 1$
- ◆ $M_{14,18} = 1$
- ◆ $M_{13,18} = 0$

Persistent Homology Computation

Reduced Matrix:

Given a non-null column j of a boundary matrix M ,

$$\text{low}(j) := \max \{ i \mid M_{i,j} \neq 0 \}$$

A matrix R is called **reduced** if, for each pair of non-null columns j_1, j_2 ,

$$\text{low}(j_1) \neq \text{low}(j_2)$$

Equivalently, if low function is **injective** on its domain of definition

Persistent Homology Computation

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
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22																							1	
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low								4	6	7	5	7						13	14	14	15	16	14	22

$low(10) = 7 = low(12)$



M is not reduced

Persistent Homology Computation

Reduction Algorithm:

```
Matrix  $R = M$ 
for  $j = 1, \dots, n$  do
    while  $\exists j' < j$  with  $\text{low}(j') = \text{low}(j)$  do
         $R.\text{column}(j) = R.\text{column}(j) + R.\text{column}(j')$ 
    endwhile
endfor
return  $R$ 
```

Time Complexity:

At most n^2 column additions



$O(n^3)$ in the worst case

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
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23																								
low								4	6	7	5	7						13	14	14	15	16	14	22

Initialize \mathbf{R} to \mathbf{M} , where

\mathbf{M} is the **boundary matrix** of K^f

expressed according with a **total ordering** of its simplices

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1				1											
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low									4	6	7	5	3						13	14		15	16	22

The algorithm returns the above **reduced matrix R**

Persistent Homology Computation

Retrieving Persistence Pairs:

- ◆ For each $i = 1, \dots, n$,
if there exists j such that $\text{low}(j) = i$  $[i, j]$ is a pair for R
- ◆ Once every i has been parsed,
if i is an **unpaired** value  $[i, \infty)$ is a pair for R

From pairs of R to the “**actual**” persistence pairs of K^f :

$[i, j]$ corresponds to $[f(\sigma_i), f(\sigma_j)]$

(homological degree = $\dim(\sigma_i)$)

$[i, \infty)$ corresponds to $[f(\sigma_i), \infty)$

Persistent Homology Computation

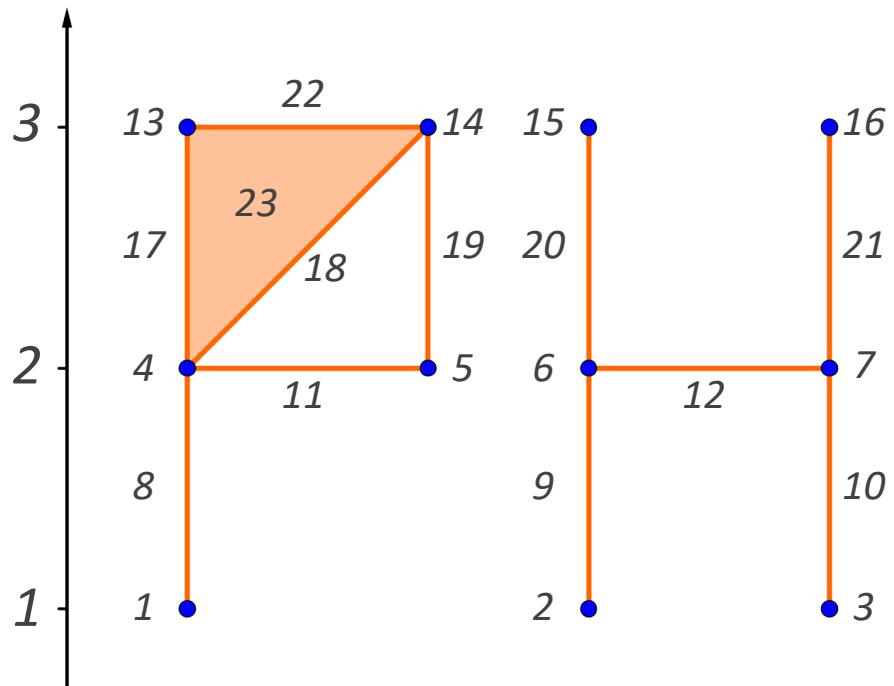
H_0
 $[1, \infty)$
 $[2, \infty)$
 $[3, 12]$
 $[4, 8]$
 $[5, 11]$
 $[6, 9]$
 $[7, 10]$
 $[13, 17]$
 $[14, 18]$
 $[15, 20]$
 $[16, 21]$

 H_1
 $[19, \infty)$
 $[22, 23]$

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1								1																	
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Persistent Homology Computation

	H_0
$[1, \infty)$	$[1, \infty)$
$[2, \infty)$	$[1, \infty)$
$[3, 12]$	$[1, 2]$
$[4, 8]$	$[2, 2]$
$[5, 11]$	$[2, 2]$
$[6, 9]$	$[2, 2]$
$[7, 10]$	$[2, 2]$
$[13, 17]$	$[3, 3]$
$[14, 18]$	$[3, 3]$
$[15, 20]$	$[3, 3]$
$[16, 21]$	$[3, 3]$



H_1 $[19, \infty)$ $[3, \infty)$
 $[22, 23]$ $[3, 3]$