Matematica Discreta e Applicazioni

## **Topological Data Analysis**

**Ulderico Fugacci** 

**CNR - IMATI** 



## **Topological Data Analysis**

**Topology** *describes, characterizes,* and *discriminates shapes* by studying their properties that are preserved under *continuous deformations*, such as *stretching* and *bending*, but *not tearing* or *gluing* 



## **Topological Data Analysis**

Assumption in TDA: *Any data* can be endowed with a *shape*. So, any data can be studied in terms of its *topological features* 





### **Topological Data Analysis**

Outline:

The Notion of Shape Simplicial Complexes Simplicial Homology From Data to Complexes Persistent Homology Visualizing Persistence *Persistence & Stability* **Computing Persistence Data Structures** 

# The Notion of Shape

### **Geometry or Topology?**

#### Which of these domains look similar?



#### **Geometry or Topology?**

And what about these ones?



## Geometry or Topology?

#### The answer depends on the *point of view* we adopt



Geometry cares about those properties which change when an object is continuously deformed E.g. length, area, volume, angles, curvature, ...

## Geometry or Topology?

#### The answer depends on the point of view we adopt



Topology Georetry cares about those properties which change when an object is continuously deformed E.g. connectivity, orientation, manifoldness, ...

#### Homeomorphisms



Given two topological spaces (X, T) and (X', T'), a function f:  $X \rightarrow X'$  is called *homeomorphism* if:

- f is a *bijection*
- f is continuous
- f<sup>-1</sup> is continuous



Two topological spaces (X, T) and (X', T') are *homeomorphic* and denoted  $X \cong X'$  if there exists a homeomorphism f:  $X \rightarrow X'$ 

Homeomorphisms induce an *equivalence relation* of topological spaces partitioning them into equivalence classes

#### Homeomorphisms



The notion of homeomorphism captures the idea of continuous deformation

















#### Definition:

*I* is a *topological invariant* if, given two topological spaces (X, T) and (X', T'),

X is homeomorphic to X'



Some classical topological invariants:

- Connectedness
- Compactness
- Manifoldness

\$<u>.</u>.....

X and X' have the same

topological invariant

I(X) = I(X')

- Orientability
- Euler characteristic
- Homology
- Homotopy

Is there a "perfect" topological invariant I such that  $X \cong X'$  if and only if I(X) = I(X')?

**Question:** 



#### Is there a "perfect" topological invariant I such that $X \cong X'$ if and only if I(X) = I(X')?

Let us **simplify the question** and let focus on:

- Considering a specific topological invariant I (e.g. the homology)
- Completely characterizing just the **spheres**  $S^n := \{x \in \mathbb{R}^n : |x| = 1\}$

The above question turns into the following:

If X and S<sup>n</sup> have the same homology, then  $X \cong S^n$ ?



#### Is there a "perfect" topological invariant I such that $X \cong X'$ if and only if I(X) = I(X')?

Let us **simplify the question** and let focus on:

- Considering a specific topological invariant I (e.g. the homology)
- Completely characterizing just the **spheres**  $S^n := \{x \in \mathbb{R}^n : |x| = 1\}$

The above question turns into the following:

If X and S<sup>n</sup> have the same homology, then  $X \cong S^n$ ?



Replacing homology with homotopy, the answer is positive!

But:

Replacing homology with homotopy, the answer is positive!

**Poincaré Conjecture** (3rd Millennium Prize Problem):

But:

If X is a closed n-manifold homotopy equivalent to  $S^n$ , then  $X \cong S^n$ 



Proven by Grigori Perelman in 2003

Replacing homology with homotopy, the answer is positive!

**Poincaré Conjecture** (3rd Millennium Prize Problem):

But:

If X is a closed n-manifold homotopy equivalent to  $S^n$ , then  $X \cong S^n$ 



Proven by Grigori Perelman in 2003

Replacing homology with homotopy, the answer is positive!

**Poincaré Conjecture** (3rd Millennium Prize Problem):

If X is a closed n-manifold homotopy equivalent to  $S^n$ , then  $X \cong S^n$ 



Proven by Grigori Perelman in 2003

So:

But:

Why we will mainly focus on homology rather than homotopy?

Replacing homology with homotopy, the answer is positive!

**Poincaré Conjecture** (3rd Millennium Prize Problem):

If X is a closed n-manifold homotopy equivalent to  $S^n$ , then  $X \cong S^n$ 



Proven by Grigori Perelman in 2003

So:

**But:** 

Why we will mainly focus on homology rather than homotopy?

Because, in practice, computing homotopy groups is nearly impossible!

## Bibliography

#### Some References:

- Books on TDA:
  - A. J. Zomorodian. *Topology for computing*. Cambridge University Press, 2005.
  - H. Edelsbrunner, J. Harer. Computational topology: an introduction. American Mathematical Society, 2010.
  - R. W. Ghrist. *Elementary applied topology*. Seattle: Createspace, 2014.
- Papers on TDA:
  - G. Carlsson. *Topology and data*. Bulletin of the American Mathematical Society 46.2, pages 255-308, 2009.
- Intro to (Algebraic) Topology:
  - E. Sernesi. *Geometria 2*. Bollati Boringhieri, Torino, 1994.
  - A. Hatcher. *Algebraic topology.* Cambridge University Press, 2002.

# **Simplicial Complexes**

Data



We want to associate a topological structure to a given dataset

Goal:

Due to the nature of data and to

our computational ambitions, datasets will be represented by "discrete" structures

Among various possibilities, *simplicial complexes* represent the most suitable choice

Shape

In fact, simplicial complexes are able to deal with data:

- of *large size* (e.g. consisting of a huge number of samples)
- of *high dimension* (e.g. involving a large number of variables or parameters)
- unorganized (e.g. not arranged in a regular grid)

Definitions:

A set V := {  $v_0$ ,  $v_1$ , ...,  $v_k$  } of points in  $\mathbb{R}^n$  is called

*geometrically independent* if vectors  $v_1 - v_0$ , ...,  $v_k - v_0$  are *linearly independent* over  $\mathbb{R}$ 

E.g. two distinct points, three non-collinear points, four non-coplanar points

The *k-simplex*  $\sigma = v_0 v_1 \dots v_k$  spanned by a geometrically independent set V = { $v_0, v_1, \dots, v_k$ } of in  $\mathbb{R}^n$  is the *convex hull* of V, i.e. the set of all points  $x \in \mathbb{R}^n$  such that

$$x = \sum_{i=0}^{k} t_i v_i$$
 where  $\sum_{i=0}^{k} t_i = 1$  and  $t_i \ge 0$  for all i

The numbers t<sub>i</sub> are uniquely determined by x and are called *barycentric coordinates* of x *E.g. a 0-simplex is a vertex, a 1-simplex is an edge, a 2-simplex is a triangle, a 3-simplex is a tetrahedron* 

#### Definitions:

- The points  $v_0$ ,  $v_1$ , ...,  $v_k$  spanning a k-simplex  $\sigma$  are called the *vertices* of  $\sigma$
- k is called the *dimension* of  $\sigma$  and denoted as dim( $\sigma$ )
- Any simplex au spanned by a non-empty subset of V is called a *face* of  $\sigma$
- + Conversely,  $\sigma$  is called a *coface* of  $\tau$



Definition:

A (geometric) simplicial complex K in  $\mathbb{R}^n$  is a collection of simplices in  $\mathbb{R}^n$  such that

- Every face of a simplex of K is in K
- The non-empty intersection of any two simplices of K is a face of each of them



#### **Simplicial Complexes**

#### Definitions:

Given a (geometric) simplicial complex K in  $\mathbb{R}^n$ ,

 The *dimension* of a simplicial complex K in ℝ<sup>n</sup>, denoted as dim(K), is the supremum of the dimensions of the simplices of K



- A simplex  $\sigma$  of K such that dim( $\sigma$ ) = dim(K) is called *maximal*
- A simplex  $\sigma$  of K which is not a proper face of any simplex of K is called *top*
- A subcollection of K that is itself a simplicial complex is called a *subcomplex* of K

Definitions:

Given a simplex  $\sigma$  of a (geometric) simplicial complex K in  $\mathbb{R}^n$ ,

- The *star* of  $\sigma$  is the set *St(\sigma)* of the cofaces of  $\sigma$
- The *link* of σ is the set *Lk(σ)* of the faces of the simplices in St(σ) such that do not intersect σ




Definitions:

Given a simplex  $\sigma$  of a (geometric) simplicial complex K in  $\mathbb{R}^n$ ,

- The *star* of  $\sigma$  is the set *St(\sigma)* of the cofaces of  $\sigma$
- The *link* of σ is the set *Lk(σ)* of the faces of the simplices in St(σ) such that do not intersect σ





Given a (geometric) simplicial complex K in  $\mathbb{R}^n$ ,

its **polytope** |K| is the subset of  $\mathbb{R}^n$  defined as the union of the simplices of K

The polytope |K| can be endowed with *two possible topologies* T<sub>1</sub> and T<sub>2</sub>:

- *T*<sub>1</sub>: A subset F of |K| is a closed set of (|K|, T<sub>1</sub>) if and only if F ∩ σ is a closed set of (σ, T<sub>σ</sub>) for each σ in K where T<sub>σ</sub> is the subspace topology induced on σ by E<sup>n</sup>
- ←  $T_2$ : The subspace topology induced on |K| by  $\mathbb{E}^n$

In general, the two topologies  $T_1$ ,  $T_2$  are *different*, but

**Proposition:** If K is a **finite** simplicial complex,  $T_1 = T_2$ 

From now on, if not differently specified, we consider only *finite* simplicial complexes

#### Proposition:

Given a simplicial complex K and a topological space (X, T), a function f from  $(|K|, T_1)$  to (X, T) is **continuous** if and only if  $f|_{\sigma}$  is continuous for each  $\sigma \in K$ 

#### Definition:

Given two simplicial complexes K and K',

- A function f: K → K' is called a *simplicial map* if for every simplex σ = v₀v₁... v<sub>k</sub> in K,
   f(σ) = f(v₀)f(v₁)... f(v<sub>k</sub>) is a simplex in K'
- The restriction f<sub>v</sub> of f to the set of vertices V of K is called the vertex map of f

#### Definition:

An *abstract simplicial complex* K on a set V is a collection of finite non-empty subsets of V, called *simplices*, such that if  $\sigma \in K$  and  $\tau \subseteq \sigma$ , then  $\tau \in K$ 

Analogously to the case of a geometric simplicial complex,

- The elements of V are called *vertices* of K
- The *dimension* of a simplex  $\sigma$  is one less than the number of its elements
- The supremum of the dimensions of the simplices in K is called *dimension* of K
- ► Each non-empty subset τ of a simplex σ ∈ K is called a *face* of σ and σ is called a *coface* of τ

*The notions of geometric simplicial complex and abstract simplicial complex are equivalent.* More properly, it is always possible,

- Given an abstract simplicial complex, to endow it with a **geometric realization**
- Given a geometric simplicial complex, to forget its geometry thus obtaining an abstract simplicial complex

**Definition:** A simplicial complex K is called

- *n-manifold [with boundary]* if its polytope |K| is a (topological) n-manifold [with boundary]
- Combinatorial n-manifold [with boundary] if, for every vertex v, the link Lk(v) is homeomorphic to the (n − 1)-sphere S<sup>n-1</sup> [or to the (n − 1)-disk D<sup>n-1</sup>:={x ∈ ℝ<sup>n-1</sup> : |x|≤1}]



#### **Regular Grids**



A *regular grid H* is a (finite) collection of hyper-cubes such that:

- Each face of a hyper-cube of H is in H
- Each non-empty intersection of two hyper-cubes in H is a face of both
- The domain of H is a hyper-cube



## **Cell Complexes**



Similarly to simplicial complexes and regular grids,

A *cell complex* Γ is a collection of cells *"suitably glued together"* 





Where a *k-cell* is a topological space homeomorphic to the *k-dimensional open disk i(D<sup>k</sup>)* 

#### Bibliography

Some References:

- Simplicial Complexes:
  - J. R. Munkres. *Elements of algebraic topology*. CRC Press, 1984.

# **Simplicial Homology**

Given a topological space X, the *homology of X* is a *topological invariant* 

intuition

detecting the "holes" of X

capturing the independent non-bounding cycles of X

formalism

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

#### Simplicial Homology



Given a simplicial complex K,

\* a *k-chain* is a formal sum (with  $\mathbb{Z}_2$  coefficients) of k-simplices of K



#### Examples:

- a + b + e is a 0-chain
- fg + dg + de + eg is a 1-chain
- *abg* + *afg* is a 2-chain

The *chain complex* C<sub>\*</sub>(K) associated with K consists of:

- A collection {∂<sub>k</sub>}<sub>k∈ℤ</sub> of linear maps where the *boundary map* ∂<sub>k</sub>: C<sub>k</sub>(K) → C<sub>k-1</sub>(K) is defined by



#### Simplicial Homology



- ◆ ð₁( ab ) = a + b
- ◆  $∂_1(ab + bc) = a + 2b + c = a + c$
- $\partial_2(afg + efg) = af + ag + 2fg + ef + eg =$ = af + ag + ef + eg
- ★  $\partial_1(af + ag + ef + eg) =$  = 2a + 2f + 2g + 2e = 0

#### **Simplicial Homology**



### Simplicial Homology



#### Definition:

- A k-chain c is called:
- ★ k-cycle if c ∈ Ker( $∂_k$ )
- ◆ *k*-*boundary* if c ∈ Im( $\partial_{k+1}$ )

#### Each k-boundary is a k-cycle

Given a 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<sub>k</sub>(K) is the group of k-cycles of K
- B<sub>k</sub>(K) is the group of k-boundaries of K



 $H_k(K)$  partitions the k-cycles into equivalence classes called *homology classes* 



#### Definition:

Two k-cycles are said *homologous* if they belong to the same homology class or, equivalently, *if their difference is a k-boundary* 

ab+ag+bc+cg is homologous to bc+bg+cd+dg

### Simplicial Homology



#### Simplicial Homology



Homology groups can be defined *in a more general way* by choosing coefficients in  $\mathbb Z$ 

Theorem:

Each homology group can be expressed as

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

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

We call:

+  $\beta_k$ , the *k*<sup>th</sup> *Betti number* of K

\*  $\lambda_1,\ldots,\lambda_{p_k}$ , the *torsion coefficients* of K

+  $c_1, \ldots, c_{eta_k}, c'_1, \ldots, c'_{p_k}$ , the *homology generators* of K



Image from [Dey et al. 2008]

#### Working with coefficients in $\mathbb Z$ :

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]

#### Simplicial Homology

The Klein bottle K is a non-orientable 2-dimensional

**Example:** 

manifold embeddable in  $\mathbb{R}^4$  which can be built from

a unit square by the following construction





By considering  $\mathbb Z$  as coefficient group,

K has the following homology groups

Example:

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

So, it can be distinguished from a torus T

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



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

**Example:** 

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



#### Bibliography

Some References:

- Simplicial Homology:
  - J. R. Munkres. *Elements of algebraic topology*. CRC Press, 1984.

# From Data to Complexes

#### From Data to Complexes

Let us consider a dataset represented by a *finite point cloud V in*  $\mathbb{R}^n$ 

Studying the shape of V just by considering the space consisting of its **points does not provide any relevant topological information** 



The *"real" shape* of the dataset can be captured by properly constructing a *complex connecting together close points through simplices* 

#### From Data to Complexes

#### Standard Constructions:

A number of possible choices have been introduced in the literature:

#### Delaunay triangulations

- \* Voronoi diagrams
- Čech complexes
- Vietoris-Rips complexes
- Alpha-shapes
- Witness complexes

Most of the above constructions are based on the notion of *Nerve complex* 

#### From Data to Complexes

#### A First Classification:

Given a finite point cloud V in  $\mathbb{R}^n$ ,

	Output Complex	Dimension	Dependence on a Parameter
Delaunay triangulation	Geometric	n	×
Čech complex	Abstract	Arbitrary (up to  V  - 1)	$\checkmark$
Vietoris-Rips complex	Abstract	Arbitrary (up to  V  - 1)	
Alpha-shapes	Geometric	п	$\checkmark$
Witness complexes	Abstract	Arbitrary (up to  V  - 1)	



Given a finite collection S of sets in  $\mathbb{R}^n$ ,

The *nerve Nrv(S)* of S is the *abstract simplicial complex* generated by the *non-empty common intersections* 

#### Formally,

$$Nrv(S) := \{ \sigma \subseteq S \mid \bigcap_{s \in \sigma} s \neq \emptyset \}$$



Nerve Theorem:

If S is a finite collection of **convex** sets in  $\mathbb{R}^n$ , then the **nerve of S** and the **union** 

of the sets in S are homotopy equivalent (and so they have the same homology)



Nerve Theorem can be *generalized* by replacing the *convexity* of sets in S with the request that all non-empty common intersections are *contractible* (*i.e. that can be continuously shrunk to a point*)

#### **Original Nerve Theorem:**

If S is an open cover of a (para)**compact** space X such that every non-empty intersection of finitely many sets in S is **contractible**, then **X** is **homotopy equivalent** to the nerve **Nrv(S)** 

# **Delaunay Triangulations**

Given a finite point cloud V in  $\mathbb{R}^n$ ,

The *Delaunay triangulation* of V is a classic notion in Computational Geometry:

- Producing a "nice" triangulation of V
  - free of long and skinny triangles
- Named after **Boris Delaunay** for his work on this topic from 1934
- \* Originally defined for sets of points in  $\mathbb{R}^2$  but generalizable to arbitrary dimensions



# **Delaunay Triangulations**

Definitions:

Given a finite point cloud V in  $\mathbb{R}^2$ ,

- ★ The convex hull of V is the smallest convex subset
  CH(V) of  $\mathbb{R}^2$  containing all the points of V
- A triangulation of V is A 2-dimensional simplicial complex K such that:
  - The domain of K is CH(V)
  - The 0-simplices of K are the points in V



Images from [De Floriani 2003]
Definition:

A **Delaunay triangulation** is a triangulation **Del(V)** of V such that:

the *circumcircle of any triangle* does *not contain any point* of V in its interior





Images from [De Floriani 2003]

#### Definition:

A finite set of points V in  $\mathbb{R}^n$  is *in general position* if no n + 2 of the points lie on a common (n – 1)-sphere

*E.g.* , *for n = 2*, V in general *No four or more points* if and only if are co-circular position Theorem: If V is in general position, then Del(V) is **unique** Images from [De Floriani 2003]



The *Voronoi region* of u in V is the set of points of  $\mathbb{R}^2$  for which u is the closest

$$R_V(u) := \{ x \in \mathbb{R}^2 \mid \forall v \in V, d(x, u) \le d(x, v) \}$$

- \* Any Voronoi region is a convex closed subset of  $\mathbb{R}^2$
- + A Voronoi region is not necessarily bounded

The Voronoi diagram is the collection Vor(V)

of the Voronoi regions of the points of V



Images from [De Floriani 2003]

Duality Property:

If V is in general position, then

the **Delaunay triangulation coincides** with the **nerve of the Voronoi diagram** 

$$Del(V) = \{ \sigma \subseteq V \mid \bigcap_{u \in \sigma} R_V(u) \neq \emptyset \}$$

- Each point u of V corresponds to a Voronoi region R<sub>V</sub>(u)
- Each triangle t of Del(V) correspond to a vertex in Vor(V)
- Each edge e=(u,v) in Del(V) corresponds to an edge shared by the two Voronoi regions R<sub>V</sub>(u) and R<sub>V</sub>(v)



### Algorithms:

- Two-step algorithms:
  - Computation of an arbitrary triangulation K'
  - Optimization of K' to produce a Delaunay triangulation
- Incremental algorithms [Guibas, Stolfi 1983; Watson 1981]:
  - \* Modification of an existing Delaunay triangulation while adding a new vertex at a time
- Divide-and-conquer algorithms [Shamos 1978; Lee, Schacter 1980]:
  - Recursive partition of the point set into two halves
  - Merging of the computed partial solutions
- Sweep-line algorithms [Fortune 1989]:
  - \* Step-wise construction of a Delaunay triangulation while moving a sweep-line in the plane

#### Watson's Algorithm:

A Delaunay triangulation is computed by **incrementally adding a single point** to an existing Delaunay triangulation

Let  $V_i$  be a subset of V and let u be a point in  $V \setminus V_i$  ,

#### <u>Input:</u>

**Del(V**<sub>i</sub>), a Delaunay triangulation of V<sub>i</sub>

#### Output:

**Del(V**<sub>i+1</sub>), a Delaunay triangulation of  $V_{i+1} := V_i \cup \{u\}$ 



Images from [De Floriani 2003]

#### Watson's Algorithm:

Given a Delaunay triangulation  $Del(V_i)$  of  $V_i$  and a point u in  $V \setminus V_i$ ,

- The influence region R<sub>u</sub> of a point u is the region in the plane formed by the union of the triangles in Del(V<sub>i</sub>) whose circumcircle contains u in its interior
- The influence polygon P<sub>u</sub> of u is the polygon formed by the edges of the triangles of Del(V<sub>i</sub>) which bound R<sub>u</sub>



Images from [De Floriani 2003]

#### Watson's Algorithm:

+ <u>Step 1:</u>

Deletion of the triangles of Del(V<sub>i</sub>) forming the *influence region* R<sub>u</sub>

+ <u>Step 2</u>:

**Re-triangulation of R**<sub>u</sub> by joining u to the vertices of the influence polygon P<sub>u</sub>





#### Watson's Algorithm:

Let  $N_i = |V_i|$ 

- ◆ Detection of a triangle of Del(V<sub>i</sub>) containing the new point u: O(N<sub>i</sub>) in the worst case
- Detection of the triangles forming the region of influence through a breadth-first search: O(|R<sub>u</sub>|)
- Re-triangulation of P<sub>u</sub> is in O(|P<sub>u</sub>|)
- Inserting a point u in a triangulation with N<sub>i</sub> vertices: O(N<sub>i</sub>) in the worst case
- Inserting all points of V: O(N<sup>2</sup>) in the worst case, where N = |V|

## Čech Complexes



Given a finite set of points V in  $\mathbb{R}^n$ , let us consider:

# Čech Complexes



Given a finite set of points V in  $\mathbb{R}^n$ , let us consider:

- +  $B_u(r)$ , the closed ball with center  $u \in V$  and radius r
- *S*, the collection of these balls



# Čech Complexes



Given a finite set of points V in  $\mathbb{R}^n$ , let us consider:

- +  $B_u(r)$ , the closed ball with center  $u \in V$  and radius r
- *S,* the collection of these balls

The Čech complex Čech(r) of V of radius r is the nerve of S  $\check{C}ech(r) := \{ \sigma \subseteq V \mid \bigcap_{u \in \sigma} B_u(r) \neq \emptyset \}$ 



# Čech Complexes



Given a finite set of points V in  $\mathbb{R}^n$ , let us consider:

- +  $B_u(r)$ , the closed ball with center  $u \in V$  and radius r
- S, the collection of these balls

The Čech complex Čech(r) of V of radius r is the nerve of S  $\check{C}ech(r) := \{ \sigma \subseteq V \mid \bigcap_{u \in \sigma} B_u(r) \neq \emptyset \}$ 



# Čech Complexes



Given a finite set of points V in  $\mathbb{R}^n$ , let us consider:

- +  $B_u(r)$ , the closed ball with center  $u \in V$  and radius r
- S, the collection of these balls

The *Čech complex Čech(r)* of V of radius r is the *nerve of S*  $ch(r):=\{\sigma \subseteq V \mid igcap B_u(r) 
eq$ 

$$\check{C}ech(r) := \{ \sigma \subseteq V \mid \bigcap_{u \in \sigma} B_u(r) \neq \emptyset \}$$

In practice, infeasible construction



 $B_u(r)$ 

## **Vietoris-Rips Complexes**



Given a finite set of points V in  $\mathbb{R}^n$ ,

The Vietoris-Rips complex VR(r) of V and r is the abstract simplicial complex consisting of all subsets of diameter at most 2r

#### Formally,

 $VR(r) := \{ \sigma \subseteq V \mid d(u, v) \le 2r, \forall u, v \in \sigma \}$ 

### **Vietoris-Rips Complexes**



#### Properties:

- $\star \check{C}ech(r) \subseteq VR(r) \subseteq \check{C}ech(\sqrt{2}r)$
- VR(r) is completely determined by its 1-skeleton
  - ✤ I.e. the graph G of its vertices and its edges



Step 1

# **Vietoris-Rips Complexes**

#### Algorithms:

**Input:** A finite set of points V in  $\mathbb{R}^n$  and a real positive number r

**Output:** The Vietoris-Rips complex VR(r)

A *two-step* approach is typically adopted:

- + Step 1 Skeleton Computation:
  - Exact (O(|V|<sup>2</sup>) time complexity )
  - Approximate
  - \* Randomized
  - Landmarking
- + Step 2 Vietoris-Rips Expansion:
  - Inductive
  - Incremental
  - Maximal

#### Algorithms:

**Input:** A finite set of points V in  $\mathbb{R}^n$  and a real positive number r

**Output:** The Vietoris-Rips complex VR(r)

A *two-step* approach is typically adopted:

- + Step 1 Skeleton Computation:
  - Exact (O(|V|<sup>2</sup>) time complexity )
  - Approximate
  - \* Randomized
  - Landmarking
- + Step 2 Vietoris-Rips Expansion:
  - Inductive
  - Incremental
  - Maximal



#### Inductive VR expansion:

<u>Input:</u> The 1-skeleton G = (V, E) of VR(r)

**Output:** The k-skeleton K of the Vietoris-Rips complex VR(r)

#### INDUCTIVE-VR(G, k)

```
K = V \cup E
for i = 1 to k
foreach i-simplex \sigma \in K
N = \cap_{u \in \sigma} LOWER-NBRS(G, u)
foreach v \in N
K = K \cup \{ \sigma \cup \{v\} \}
return K
LOWER-NBRS(G, u)
```



#### Inductive VR expansion:

<u>Input:</u> The 1-skeleton G = (V, E) of VR(r)

**Output:** The k-skeleton K of the Vietoris-Rips complex VR(r)

#### INDUCTIVE-VR(G, k)

```
K = V \cup E

for i = 1 to k

foreach i-simplex \sigma \in K

N = \bigcap_{u \in \sigma} LOWER-NBRS(G, u)

foreach v \in N

K = K \cup \{ \sigma \cup \{v\} \}

return K

LOWER-NBRS(G, u)
```



#### Inductive VR expansion:

<u>Input:</u> The 1-skeleton G = (V, E) of VR(r)

**Output:** The k-skeleton K of the Vietoris-Rips complex VR(r)

```
INDUCTIVE-VR(G, k)
```

```
K = V \cup E

for i = 1 to k

foreach i-simplex \sigma \in K

N = \bigcap_{u \in \sigma} LOWER-NBRS(G, u)

foreach v \in N

K = K \cup \{ \sigma \cup \{v\} \}

return K

LOWER-NBRS(G, u)
```



#### Inductive VR expansion:

<u>Input:</u> The 1-skeleton G = (V, E) of VR(r)

**Output:** The k-skeleton K of the Vietoris-Rips complex VR(r)

#### INDUCTIVE-VR(G, k)

```
K = V \cup E
for i = 1 to k
foreach i-simplex \sigma \in K
N = \cap_{u \in \sigma} LOWER-NBRS(G, u)
foreach v \in N
K = K \cup \{ \sigma \cup \{v\} \}
return K
LOWER-NBRS(G, u)
```



#### Inductive VR expansion:

<u>Input:</u> The 1-skeleton G = (V, E) of VR(r)

**Output:** The k-skeleton K of the Vietoris-Rips complex VR(r)

```
INDUCTIVE-VR(G, k)
```

```
K = V \cup E

for i = 1 to k

foreach i-simplex \sigma \in K

N = \bigcap_{u \in \sigma} LOWER-NBRS(G, u)

foreach v \in N

K = K \cup \{ \sigma \cup \{v\} \}

return K

LOWER-NBRS(G, u)
```



#### Inductive VR expansion:

<u>Input:</u> The 1-skeleton G = (V, E) of VR(r)

**Output:** The k-skeleton K of the Vietoris-Rips complex VR(r)

#### INDUCTIVE-VR(G, k)

```
K = V \cup E

for i = 1 to k

foreach i-simplex \sigma \in K

N = \bigcap_{u \in \sigma} LOWER-NBRS(G, u)

foreach v \in N

K = K \cup \{ \sigma \cup \{v\} \}

return K

LOWER-NBRS(G, u)
```





### **Alpha-Shapes**

#### Definition:

Given a finite set of points V in general position of  $\mathbb{R}^n$ , let us consider:

- A<sub>u</sub>(r) := B<sub>u</sub>(r) ∩ R<sub>V</sub>(u), the intersection of the closed ball with center u ∈ V and radius r and the Voronoi region of u
- *S*, the collection of these convex sets

The *alpha-shape Alpha(r)* of V of radius r is the *nerve of S* 

Formally,

$$Alpha(r) := \{ \sigma \subseteq V \mid \bigcap_{u \in \sigma} A_u(r) \neq \emptyset \}$$

 $A_u(r) \subseteq B_u(r) \square Alpha(r) \subseteq \check{C}ech(r)$ 

Image from [Edelsbrunner, Harer 2010]

### Witness Complexes

#### Motivation:

The "shape" of a point cloud can be captured without considering all the input points



- + Landmarks:
  - Selected points
- + Witnesses:

Remaining points



Images from [de Silva, Carlsson 2004]

### Witness Complexes

 $W_0(r) \subset VR(r) \subset W_0(2r)$ 

#### Definition:

The *witness complex W(r)* of radius *r* is defined by:

- u is in W(r) if u is a landmark
- ◆ (u, v) is in W(r) if there exists a witness w such that
    $max{d(u, w), d(v, w)} ≤ m_w + r$

where  $m_w$  : = the distance of w from the **2nd closest landmark** 

• the i-simplex  $\sigma$  is in W(r) if all its edges belong to W(r)

 $W_0(r)$  is defined by setting  $m_w = 0$  for any witness w

### From Data to Complexes

Not Only Point Clouds in  $\mathbb{R}^n$ 

Most of the presented constructions can be *generalized/adapted* to the case of

a finite collection of elements endowed with a notion of proximity\*

enabling to cover a wide plethora of datasets

\*More properly, a **semi-metric**, i.e. a distance not necessarily satisfying the triangle inequality

### From Data to Complexes

#### Not Only Point Clouds in $\mathbb{R}^n$

- + Point Clouds:
  - Delaunay triangulation
  - \* Čech complexes
  - Vietoris-Rips complexes
  - Alpha-shapes
  - Witness complexes complexes
- Graphs and Complex Networks:
  - Flag complexes
- + Functions:
  - Sublevel sets







### From Data to Complexes

Flag Complex of a Weighted Network:

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










#### From Data to Complexes

Sublevel Sets of Functions

Given a *function* f:  $D \rightarrow \mathbb{R}$ ,

+ <u>Step 1:</u>

Transform f:  $D \rightarrow \mathbb{R}$  into a function **F:**  $K \rightarrow \mathbb{R}$  *defined on a simplicial complex K* 

E.g. if D is a point cloud, construct from it a simplicial complex K and define F as

 $F(\sigma) := \max\{f(v) \mid v \text{ is a vertex of } \sigma\}$ 

+ <u>Step 2</u>:

Build the collection  $\{K^r\}_{r\in\mathbb{R}}$  of the *sublevel sets of F* defined as

$$K^r := \{ \sigma \in K \,|\, F(\sigma) \le r \}$$

Notice that K<sup>r</sup> is a simplicial complex whenever: if  $\tau$  is a face of  $\sigma$  then F( $\tau$ )  $\leq$  F( $\sigma$ )

#### From Data to Complexes



#### From Data to Complexes



#### From Data to Complexes



## Bibliography

#### Some References:

- From Data to Complexes:
  - + H. Edelsbrunner, *Geometry and Topology for Mesh Generation*. Cambridge University Press, 2001.
  - V. de Silva, G. Carlsson. Topological estimation using witness complexes. SPBG 4, pages 157-166, 2004.
  - A. Zomorodian, *Fast construction of the Vietoris-Rips complex*. Computers & Graphics 34.3, pages 263-271, 2010.
  - + H. Edelsbrunner. *Algorithms in Combinatorial Geometry*. Springer Science & Business Media, 2012.

# **Persistent Homology**

#### Persistent Homology





#### Persistent Homology



#### Persistent Homology



#### **Persistent Homology**





#### Persistent Homology



#### Persistent Homology



Which is the shape of a given data?

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



Which is the shape of a given data?

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



#### Persistent Homology



Image from [Ghrist 2008]

#### Persistent Homology



#### 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



#### Incremental Algorithm for Betti Numbers:

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



Image from [Delfinado, Edelsbrunner 1995]

#### Persistent Homology



#### Persistent Homology



#### **Topological Persistence:**

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





Most of the techniques transforming a dataset into a simplicial complex depending on the choice of a parameter actually produce a filtration  $\{K^p\}_{p \in \mathbb{R}}$ 



Working Assumption:

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



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

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

where:

- + M<sub>p</sub> := H<sub>i</sub> (K<sup>p</sup>; 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:
  - \*  $\mu_i^{p,q}(h)$ :  $H_i(K^p; \mathbb{F}) \longrightarrow H_i(K^q; \mathbb{F})$  is the linear map induced by the inclusion  $K^p \subseteq K^q$

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  $(r_k, \infty)$  and  $(p_j, q_j)$ 



Intuitively:

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





Intuitively:

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





Intuitively:

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



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* 

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 hor persistence pairs persistence aps

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 *hop* **PERSISTENCE PAIR** 

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*

### Bibliography

Some References:

- Persistent Homology:
  - U. Fugacci, S. Scaramuccia, F. Iuricich, L. De Floriani. *Persistent homology: a step-by-step introduction for newcomers*. Eurographics Italian Chapter Conference, pages 1-10, 2016.



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



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?

## **Visualizing Persistence**

 $\subseteq$ 

 $\subseteq$ 

#### Given a filtration ${\cal F}$ ,

Persistent pairs of  $\mathcal{F}$  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**



### **Visualizing Persistence**



### **Visualizing Persistence**

#### 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**



### **Visualizing Persistence**



### Bibliography

Some References:

- Persistent Homology:
  - U. Fugacci, S. Scaramuccia, F. Iuricich, L. De Floriani. *Persistent homology: a step-by-step introduction for newcomers*. Eurographics Italian Chapter Conference, pages 1-10, 2016.

# **Persistence & Stability**



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

persistent homology is not affected by noisy data and small perturbations



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

### Distances:

- + For the Data in Input:
  - \* Natural pseudo-distance of shapes
  - ✤ L<sub>∞</sub>-distance of filtering functions
  - \* Gromov-Hausdorff distance of metric spaces/point clouds
- For the Retrieved Persistent Homology Information:
  - Interleaving distance of persistence modules
  - \* Bottleneck (a.k.a. Matching) distance of persistence diagrams
  - Hausdorff distance of persistence diagrams
  - Wasserstein distances of persistence diagrams

Distances for Input Data:

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

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

### 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

### Distances for Input Data:

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



Image from [Rieck 2016]

### Distances for Input Data:

Given two *finite metric spaces* (X, d<sub>x</sub>), (Y, d<sub>Y</sub>) (e.g. two finite point clouds in  $\mathbb{R}^n$ ),

Definitions:

A correspondence C:  $X \Rightarrow Y$  from X to Y is a subset of  $X \times Y$  such that the canonical projections  $\pi_X: C \rightarrow X$  and  $\pi_Y: C \rightarrow Y$  are both surjective

The distortion dis(C) of a correspondence C:  $X \Rightarrow Y$  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:

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

Distances for Persistent Homology Information:

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



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  $\gamma$  ranges over all bijections from  $D_1$  to  $D_2$ 

Distances for Persistent Homology Information:



#### **Definitions:**

Given two persistence diagrams D<sub>1</sub> and D<sub>2</sub>,

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  $\gamma$  ranges over all bijections from  $D_1$  to  $D_2$ 

### 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<sup>th</sup> persistence modules and let D<sub>1</sub>, D<sub>2</sub> be the corresponding persistence diagrams

• 
$$d_H(D_1, D_2) \le d_B(D_1, D_2)$$

$$\bullet \quad d_I(M,N) = d_B(D_1,D_2)$$

#### Theorem:

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

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

### **Stability of Persistence**



### 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,

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

# Bibliography

Some References:

- Stability Results:
  - D. Cohen-Steiner, H. Edelsbrunner, J. Harer. *Stability of persistence diagrams*. Discrete & Computational Geometry 37.1, pages 103-120, 2007.
  - F. Chazal, D. Cohen-Steiner, M. Glisse, L. J. Guibas, S. Y. Oudot. *Proximity of persistence modules and their diagrams*. Proc. of the 35 annual symposium on Computational Geometry, pages 237-246, 2009.
  - F. Chazal, D. Cohen-Steiner, L. J. Guibas, F. Mémoli, S. Y. Oudot. Gromov-Hausdorff stable signatures for shapes using persistence. Computer Graphics Forum 28.5, pages 1393-1403, 2009.

# **Computing Persistence**

*Topological Data Analysis* allows for assigning to (almost) *any dataset* a collection of features representing a *topological summary* of the input data





- How to efficiently compute (persistent) homology?
- + How to compactly encode simplicial complexes of high dimension and large size?

### **Persistent Homology Computation**



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



A sequence  $\sigma_1$ ,  $\sigma_2$ , ...,  $\sigma_n$  of the simplices of K such that:

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

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



**Boundary Matrix:** 

A square matrix **D** of size *n* x *n* defined by

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



Reduced Matrix:

Given a non-null column *j* of a boundary matrix *D*,

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

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

 $low(j_1) \neq low(j_2)$ 

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

### **Persistent Homology Computation**







j < 12  $i \setminus j$ lowFor each *j* < 12, there is **no** *j* **' '** *s* uch that *low(j') = low(j)* So, increase j by 1











Istituto di Matematica Applicata e Tecnologie Informatiche «Enrico Magenes»
12 < j < 19  $i \setminus j$  $\mathbf{2}$ lowFor each *12 < j < 19*, there is **no** *j* **' '** *s* uch that low(j') = low(j)So, increase j by 1



Istituto di Matematica Applicata e Tecnologie Informatiche «Enrico Magenes»





Istituto di Matematica Applicata e Tecnologie Informatiche «Enrico Magenes»





19 < j < 22  $i \setminus j$  $\mathbf{2}$ lowFor each *19 < j < 22*, there is **no** *j* **' '** *s* uch that low(j') = low(j)So, increase j by 1















### **Retrieving Persistence Pairs:**

For each *i* = 1, ..., n,

if there exists *j* such that *low(j) = i* [*i, j*] is a pair for *R* 

Once every i has been parsed,

if *i* is an **unpaired** value



From pairs of R to the "actual" persistence pairs of  $\{K^p\}_p$ :

[*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 <sub>0</sub>	i i	1	2	3	Δ	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
<b>[1,</b> ∞)	$1^{\iota \setminus j}$	1		0	Т	0	0	1	1	5	10	11	14	10	11	10	10	11	10	10	20	21		20
	2									1			1											
[ <b>2</b> , ∞)	3										1		1											
[0 (0]	4								1			1						1	1					
[3, 12]	5											1												
[1 8]	6									1	1										1	1		
[+, 0]	( 0										1											1		
[5, 11]	9																							
	10																							
[0, 9]	11																							
[7, 10]	12																							
	13																	1						
[13, 17]	14																		1					
[14 18]	15																				1			
[14, 10]	10																					1		1
[15, 20]	11																							1
[16 21]	10																							
[10, 21]	$\frac{10}{20}$																							
H1	21																							
[10]	22																							1
[ <b>⊥</b> 3, ∞]	23																							
[22, 23]	low								4	6	7	5	3					13	14		15	16		22

### **Persistent Homology Computation**

H <sub>0</sub>		f 🛉		22			
<i>[1,</i> ∞)	<b>[1, ∞)</b>	3 -	13	22	14 1	15 •	•16
[ <b>2</b> , ∞)	<b>[1, ∞)</b>		17	23	<i>19 2</i>	20	21
[3, 12]	[1, 2]	2		10			7
[4, 8]	[2, 2] [2, 2]	Ζ -	4 -	11	• 5	12	
[6, 9]	[2, 2]		8			9	10
[7, 10]	[2, 2]	1 -	1			2 •	• 3
[13, 17]	[3, 3]						
[14, 18]	[3, 3]						
[15, 20]	[3, 3]		Ц.	<i>[19,</i> ∞)		<b>[3, ∞)</b>	
[16, 21]	[3, 3]		<b>Π</b> 1	[22, 23]	4	[3, 3]	

#### *Standard algorithm* to compute (persistent) homology [Zomorodian & Carlsson 2005]:

- Based on a matrix reduction
- Linear complexity in practical cases
- Cubic complexity in the worst case

### Several different strategies:

#### **Direct approaches:**

- Zigzag persistent homology [Milosavljević et al. '05]
- *Computation with a twist* [Chen, Kerber '11]
- **Dual algorithm** [De Silvia et al. '11]
- *Output-sensitive algorithm* [Chen, Kerber '13]
- Multi-field algorithm [Boissonnat, Maria '14]
- Annotation-based methods [Boissonnat et al. '13; Dey et al. '14]
   Distributed persistent computation [Bauer et al. '14b]

#### **Distributed approaches:**

- Spectral sequences [Edelsbrunner, Harer '08; Lipsky et al. '11]
- Constructive Mayer-Vietoris [Boltcheva et al. '11]
- Multicore coreductions [Murty et al. '13]
- Multicore homology [Lewis, Zomorodian '14]
- Persistent homology in chunks [Bauer et al. '14a]

#### *Coarsening approaches:*

- **Topological operators and simplifications** [Mrozek, Wanner '10; Dłotko, Wagner '14]
- Morse-based approaches [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]

### Direct Approaches:

- Zigzag persistent homology [Milosavljević et al. '05]
- *Computation with a twist* [Chen, Kerber '11]
- Dual algorithm [De Silvia et al. '11]
- Output-sensitive algorithm [Chen, Kerber '13]
- *Multi-field algorithm* [Boissonnat, Maria '14]
- Annotation-based methods [Boissonnat et al. '13; Dey et al. '14]

### Distributed Approaches:

- Spectral sequences [Edelsbrunner, Harer '08; Lipsky et al. '11]
- Constructive Mayer-Vietoris [Boltcheva et al. '11]
- Multicore coreductions [Murty et al. '13]
- Multicore homology [Lewis, Zomorodian '14]
- **Persistent homology in chunks** [Bauer et al. '14a]
- Distributed persistent computation [Bauer et al. '14b]

### Coarsening Approaches:

### • **Topological operators and simplifications** [Dłotko, Wagner '14]

- Acyclic subcomplexes [Mrozek et al. '08]
- ✤ Reductions and coreductions [Mrozek et al. '10]
- ✤ Edge contractions [Attali et al. '11]



### Coarsening Approaches:

### • **Topological operators and simplifications** [Dłotko, Wagner '14]

- \* Acyclic subcomplexes [Mrozek et al. '08]
- ✤ Reductions and coreductions [Mrozek et al. '10]
- ✤ Edge contractions [Attali et al. '11]



### Coarsening Approaches:

#### • **Topological operators and simplifications** [Dłotko, Wagner '14]

- Acyclic subcomplexes [Mrozek et al. '08]
- \* Reductions and coreductions [Mrozek et al. '10]
- ✤ Edge contractions [Attali et al. '11]



### Coarsening Approaches:

### Topological operators and simplifications [Dłotko, Wagner '14]

- Acyclic subcomplexes [Mrozek et al. '08]
- ✤ Reductions and coreductions [Mrozek et al. '10]
- \* Edge contractions [Attali et al. '11]



### Coarsening Approaches:

### • **Topological operators and simplifications** [Dłotko, Wagner '14]

- Acyclic subcomplexes [Mrozek et al. '08]
- ✤ Reductions and coreductions [Mrozek et al. '10]
- ✤ Edge contractions [Attali et al. '11]



## Bibliography

Some References:

- Persistent Homology Computation:
  - A. Zomorodian, G. Carlsson. *Computing persistent homology*. Discrete & Computational Geometry, 33.2, pages 249-274, 2005.
  - N. Otter, M.A. Porter, U. Tillmann, P. Grindrod, H.A. Harrington. A roadmap for the computation of persistent homology. EPJ Data Science, 6.1, 2017.

# **Data Structures**

# **Encoding Simplicial Complexes**

It is enough to have a point cloud consisting of at least **30 points** for having to deal with an associated filtered simplicial complex of more than a **billion** of simplices



Solution:

Issue:

Development of compact and efficient data structures for encoding arbitrary simplicial complexes

# **Encoding Simplicial Complexes**

### Outline:

- Which info to be stored?
- Data Structures
  - \* Simplex-based representations
  - \* Top-based representations
  - \* **Operator-driven** representations
- Comparisons
- Issues and solutions in adopting top-based representations

Out Of Scope:

- Data structures for specific classes of complexes
  - \* E.g. manifold or complexes of low dimension

# **Encoding Simplicial Complexes**

### Data Structure:

The *entities* which a simplicial complex consists of are:

its simplices

 $\mathsf{K} = \mathsf{K}_0 \cup \mathsf{K}_1 \cup \ldots \cup \mathsf{K}_d$ 

where  $K_{i}\xspace$  is the collection of the i-simplices of K

the topological relations

 $\mathsf{R}_{i,j} \subseteq \mathsf{K}_i \times \mathsf{K}_j$ 



between the simplices of K encoding the (co-)boundary of each simplex

A data structure for K has to explicitly store a portion of the above information and to (efficiently) retrieve the remaining part



Store all the entities	Efficiency	
		Compactness
<ul> <li>Simplex-based representations</li> <li>Top-based representations</li> <li>Operator-driven representations</li> </ul>		Store only the top simplices

Store all the entities Incidence Graph	Efficiency	
		Compactness
Simplex-based representations		
<ul> <li>Top-based representations</li> </ul>		Store only the top simplices
Operator-driven representations		top simplices






## **Encoding Simplicial Complexes**



## Simplex-based Representations



All the relations between simplices can be immediately retrieved The representation *size exponentially increases* with the complex dimension

## Simplex-based Representations



where  $I(\sigma)$  denotes the maximum value taken by the vertices of  $\sigma$  w.r.t. a total order on K<sub>0</sub>

Graph is **not uniquely determined** but it depends on the chosen vertex order

## Simplex-based Representations



where  $I(\sigma)$  denotes the maximum value taken by the vertices of  $\sigma$  w.r.t. a total order on K<sub>0</sub>

Graph is **not uniquely determined** but it depends on the chosen vertex order

## **Top-based Representations**



## **Top-based Representations**



$$N \longleftrightarrow (K_0 = V_1 \cup V_2 \cup \ldots \cup V_n) \cup K_{top}$$

 $(\sigma, \tau) \in \mathbf{A} \leftrightarrow \sigma \in \mathbf{K}_{top} \text{ and } (\sigma, \tau) \in \mathbf{R}_{i,0}$ 

plus a map returning, for each j, the vertices of K in V<sub>j</sub> and the top simplices with at least one vertex in V<sub>j</sub>

**Compact and highly adjustable** (e.g. choice of the decomposition, of the maximum number of vertices in each region)

Not all the relations between simplices are immediately available

## **Operator-driven Representations**



The simplicial complex K is encoded by storing its *1-skeleton* (i.e. the graph consisting of the 0- and the 1-simplices) and a *map* returning, for each 1-simplex  $\sigma$ , the blockers of K containing  $\sigma$ , where:

A simplex  $\tau$  is a **blocker** if  $\tau$  does not belong to K but all its faces do



**Designed for** flag complexes (e.g. **VR complexes**) and edge contraction Too specific: **inefficient in any other task** 

# **Encoding Simplicial Complexes**

#### Top-based vs Simplex-based:

Dataset	d	$ \Sigma_0 $	$ \Sigma_{top} $	$ \Sigma $	Storage Cost		
					$IA^*$	IG	ST
DTI-SCAN	3	$0.9\mathrm{M}$	$5.5\mathrm{M}$	$24\mathrm{M}$	0.97	11.9	2.4
VISMALE	3	4.6M	$26\mathrm{M}$	118M	4.7	-	9.7
Ackley4	4	$1.5\mathrm{M}$	$32\mathrm{M}$	$204 \mathrm{M}$	6.8	-	12.8
Amazon01	6	0.2M	0.4M	$2.2\mathrm{M}$	0.12	1.6	0.3
Amazon02	7	0.4M	1.0M	$18.4\mathrm{M}$	0.28	9.8	1.5
Roadnet	3	$1.9\mathrm{M}$	$2.5\mathrm{M}$	$4.8\mathrm{M}$	0.8	3.3	1.0
Sphere-1.0	16	100	224	0.6M	0.003	0.9	0.04
$\operatorname{Sphere-1.2}$	21	100	285	$26\mathrm{M}$	0.0032	-	1.5
Sphere- $1.3$	23	100	382	$197 \mathrm{M}$	0.0034	-	11.01

# **Encoding Simplicial Complexes**



## **Encoding Simplicial Complexes**

### Top-based vs Operator-driven:

data	Ø		contr.	timings			memory peak	
			edges	check	contr.	tot	gen.	simpl.
CHICAGO CHICAGO 28 CHICAGO 56		weak		9.15h	2.27 <i>m</i>	9.19h	5.6	57.2K
	28	top	6.38K	0.01s	0.02s	0.09s	5.0	7.6
		Skel.		0.00s	0.15s	0.15s	7.8	7.8
		weak		out-of-memory			( )	_
	56	top	7.99K	0.04 <i>s</i>	0.06s	0.23s	6.2	10.8
	Skel.		0.00s	0.71 <i>s</i>	0.71 <i>s</i>	14.1	14.1	
S 63 HLV 126		weak		out-of-memory			11.6	_
	63	top	27.9K	0.08s	0.11s	0.38s	11.6	14.9
	Skel.		0.00s	0.74 <i>s</i>	0.75s	26.4	26.8	
		weak	out-of-m			ory	10.0	_
	126	top	31.2K	0.40s	0.49s	1.36s	10.0	25.9
		Skel.		0.01s	7.73s	7.74 <i>s</i>	66.1	66.7
AISMALE 3.5		weak	4.23M	34.3 <i>m</i>	1.28m	40.4m	1.0K	2.0K
	3.5	top		4.34m	0.89m	7.20m		2.0K
		Skel.		0.76 <i>m</i>	3.34h	3.35h	8.0K	8.0K
LOO <sub>4</sub> .5		weak		killed	after 25	hours	7.5K	_
	4.5	top	4.69M	2.89h	26.0m	3.32h		10.7K
		Skel.		killed after 25 hours			19.4K	-
логодина. 1.5		weak		killed after 25 hours			7 5V	_
	1.5	top	14.0M	11.9m	14.8 <i>m</i>	32.0m	/.5K	15.4K
		Skel.		23.19 <i>s</i>	14.6h	14.6 <i>h</i>	50.9K	52.1K

# **Encoding Simplicial Complexes**

Possible Issues in Top-based Representations:

Top-based representations are promising data structures for encoding a simplicial complex K

but, how to ...

Store information associated to each simplex of K (e.g. labels, gradient, ...)?

Attach information to the top simplices only



Efficiently perform operators having explicitly stored a fraction of the entities of K?

Re-define the algorithms performing the operators trying to extract the lowest possible amount of non-explicitly stored entities

# Bibliography

#### Some References:

- Data Structures for Arbitrary Simplicial Complexes:
  - D. Canino, L. De Floriani, K. Weiss. IA\*: an adjacency-based representation for non-manifold simplicial shapes in arbitrary dimensions. Computers & Graphics, 35.3, pages 747-753, 2011.
  - D. Attali, A. Lieutier, D. Salinas. Efficient data structure for representing and simplifying simplicial complexes in high dimensions. International Journal of Computational Geometry & Applications, 22.4, pages 279-303, 2012.
  - J.D. Boissonnat, C. Maria. *The simplex tree: An efficient data structure for general simplicial complexes.* Algorithmica, 70.3, pages 406-427, 2014.
  - R. Fellegara, K. Weiss, L. De Floriani. The Stellar tree: a compact representation for simplicial complexes and beyond. arXiv preprint:1707.02211, 2017.
  - U. Fugacci, F. Iuricich, L. De Floriani. Computing discrete Morse complexes from simplicial complexes.
    Graphical models, 103, 101023, 2019.
  - R. Fellegara, F. Iuricich, L. De Floriani, U. Fugacci. *Efficient Homology-Preserving Simplification of High- Dimensional Simplicial Shapes.* Computer Graphics Forum, 39.1, pages 244-259, 2020.

## **Possible Topics for Seminars**



#### **Discrete Morse Theory**

Study the shape of a space by studying the behavior of a function defined on it

### **Possible Topics for Seminars**



Image courtesy of [Carlsson & Zomorodian 2009]

#### Multi-Parameter Persistent Homology

What if we consider multiple filtering functions?

## **Possible Topics for Seminars**



#### Persistent Homology & Networks

Homological Scaffolds: Topological summaries of weighted graphs
 Clique Community Persistence: Tracking the evolution of network communities

## **Possible Topics for Seminars**



#### **Algorithms & Implementation**

- Efficient computation of Vietoris-Rips complexes and other data-to-complex strategies
- Focus on a specific algorithm for speed-up persistent homology computation
- Use of available **software tools** for testing persistent homology on various datasets