Topological Data Analysis

# **Complexes & Data**

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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)



Simplicial Complexes (and other discrete representations)



#### Simplicial Complexes (and other discrete representations)

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* 



- 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





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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<sub>2</sub>: 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



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>)* 



#### ◆ Simplicial Complexes (and other discrete representations)

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* 

#### 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* 

#### 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	n	$\checkmark$
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)** 

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



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



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In practice, infeasible construction

 $u \in \sigma$ 

 $B_u(r)$ 

## **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

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#### 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)

return \{v \in V \mid v < u, (u, v) \in E\}
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LOWER-NBRS(G, u)

return \{v \in V \mid v < u, (u, v) \in E\}
```





#### **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

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

#### 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







Flag Complex of a Weighted Network:

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











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

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

+ <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  $F(\tau) \leq F(\sigma)$ 







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