Extracting Geometrical Features From Data

Topological Data Analysis

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Topological Data Analysis

Outline:

The Notion of Shape

Simplicial Complexes

Simplicial Homology

From Data to Complexes

Persistent Homology

Visualizing Persistence

Persistence & Stability

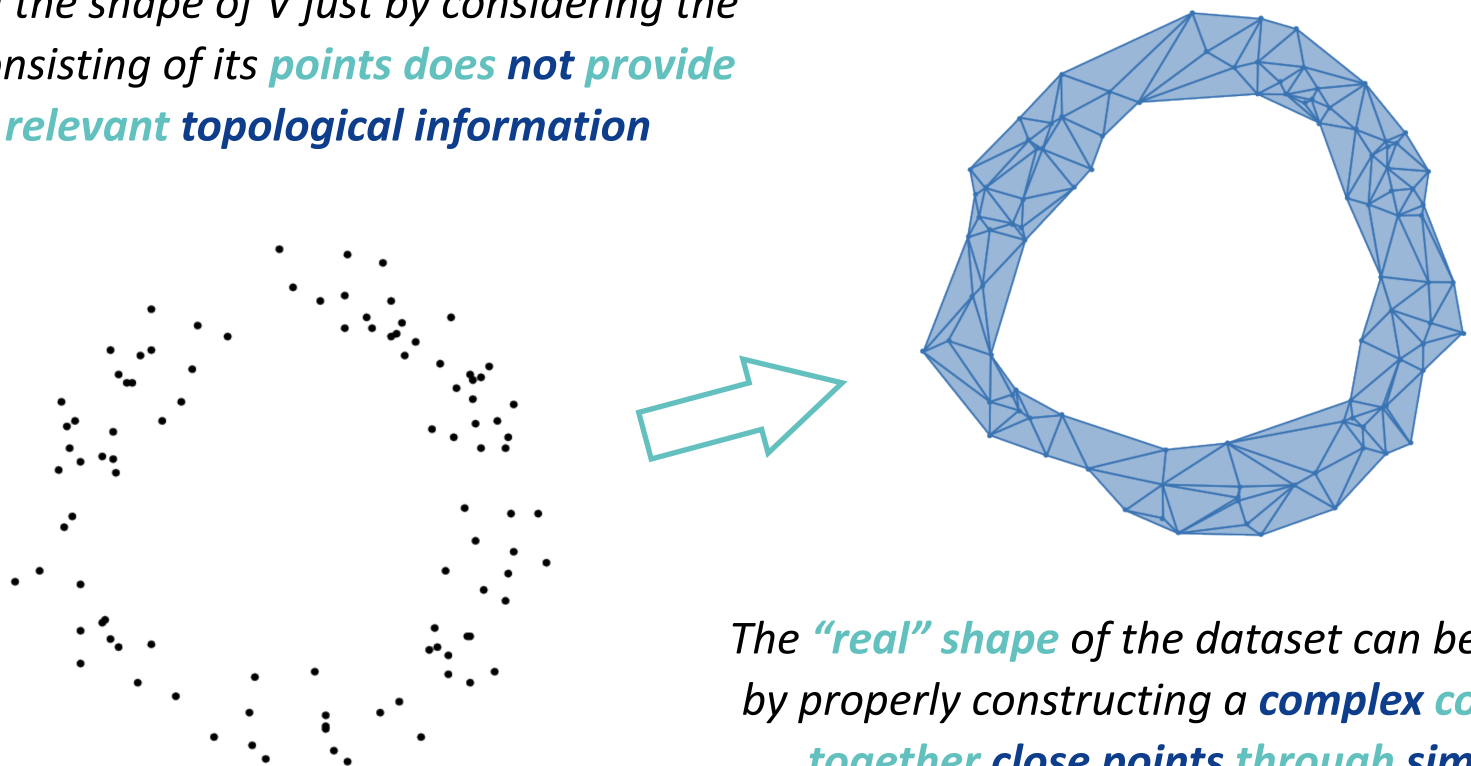
Computing Persistence

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)*	✓
Vietoris-Rips complex	*Abstract*	*Arbitrary (up to |V| - 1)*	✓
Alpha-shapes	*Geometric*	*n*	✓
Witness complexes	*Abstract*	*Arbitrary (up to |V| - 1)*	✓

Nerve Complexes

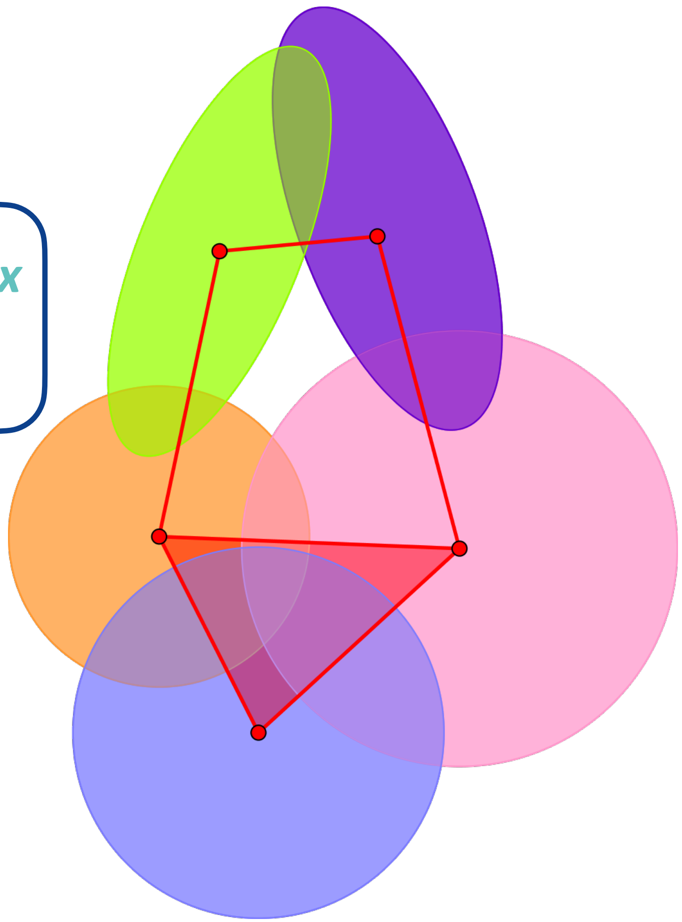
Definition:

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,

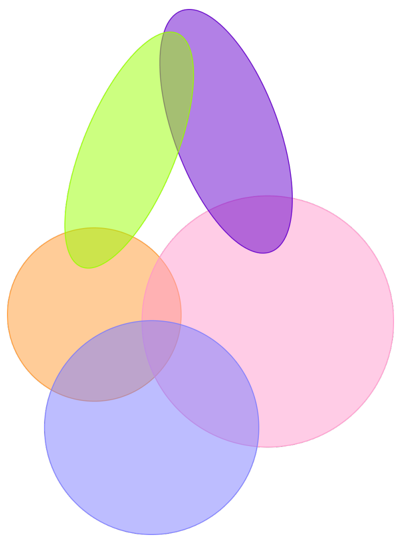
$$Nrv(S) := \{\sigma \subseteq S \mid \bigcap_{s \in \sigma} s \neq \emptyset\}$$



Nerve Complexes

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)*



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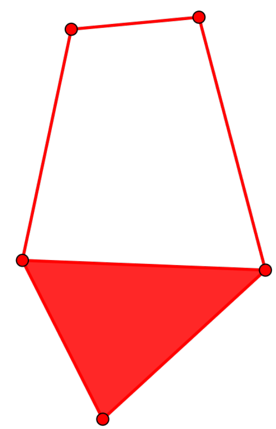


Nerve Complexes

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:

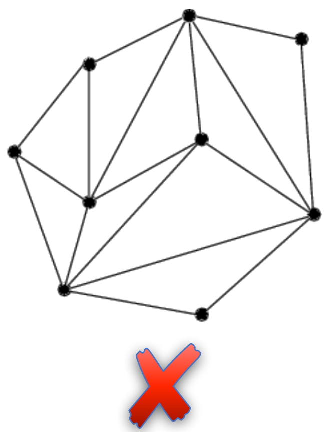
*If S is an open cover of a (para)**compact** space X such that every non-empty intersection of finitely many sets in S is **contractible**, then **X** is **homotopy equivalent** to the nerve **Nrv(S)***

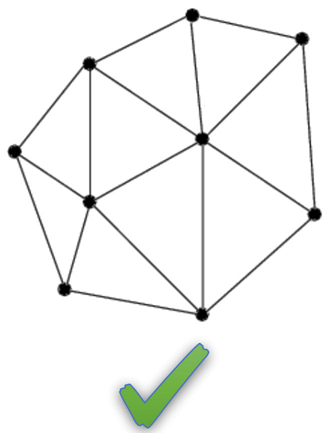
Delaunay Triangulations

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*





Images from [De Floriani 2003]

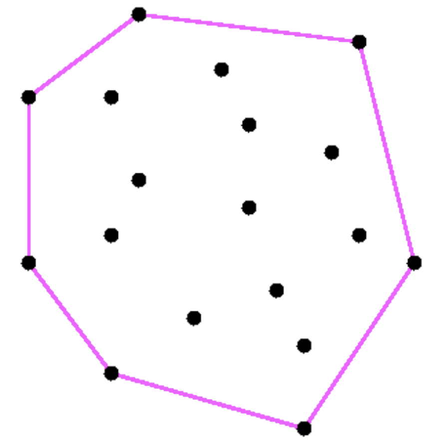
Delaunay Triangulations

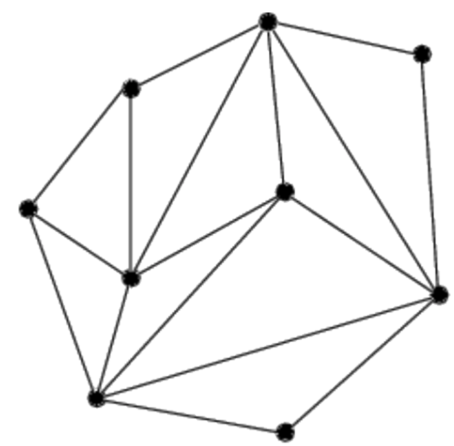
Definitions:

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





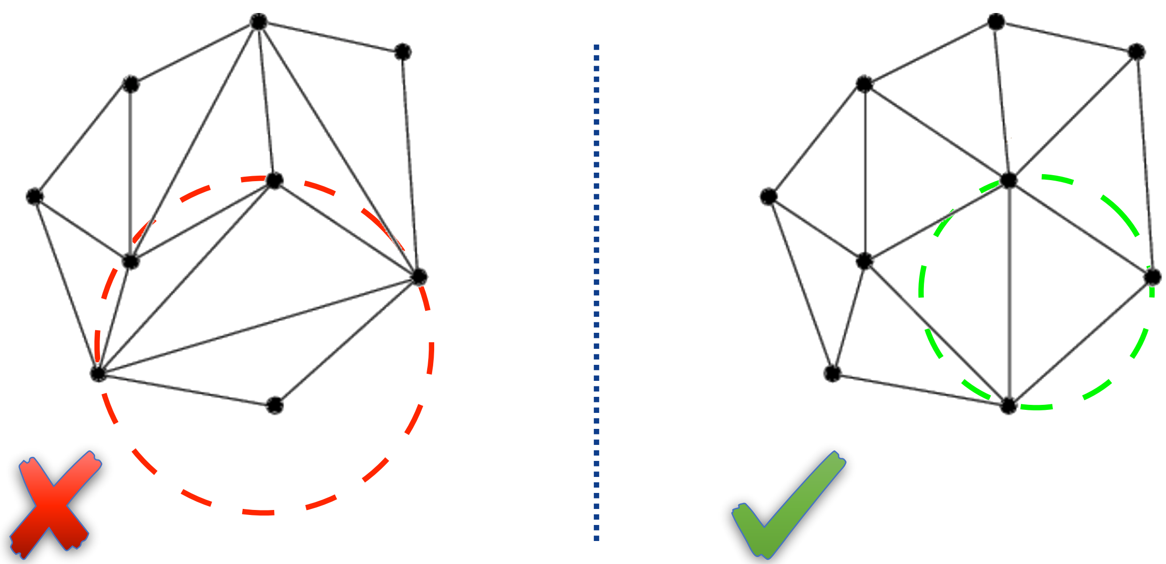
Images from [De Floriani 2003]

Delaunay Triangulations

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]

Delaunay Triangulations

Definition:

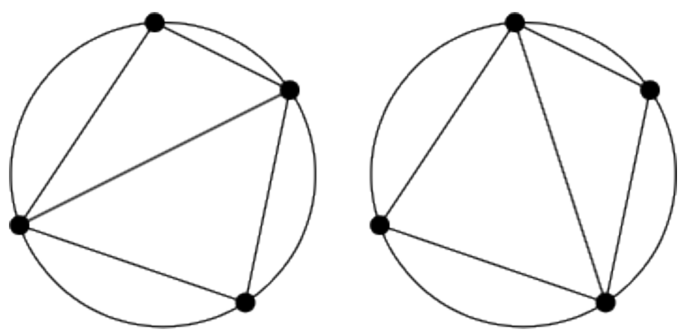
A finite set of points V in $\mathbb{R}^n$ is ***in general position*** if no n + 2 of the points lie on a common (n − 1)-sphere

E.g. , ***for n = 2,***

V in general position — *if and only if* — *No four or more points are co-circular*

Theorem:

If V is in general position, then Del(V) is ***unique***



Images from [De Floriani 2003]

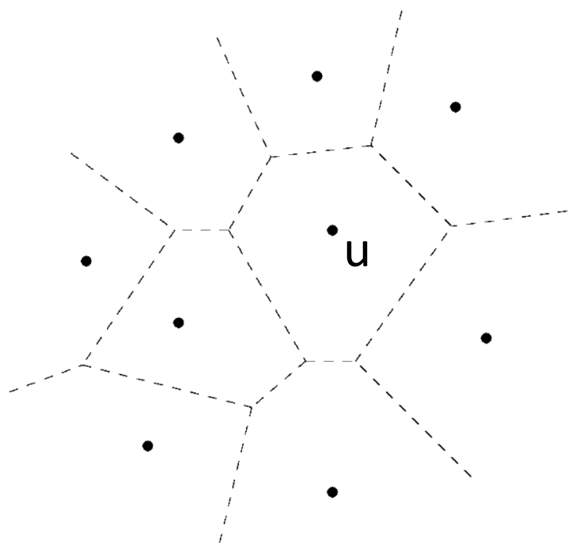
Delaunay Triangulations

Definitions:

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

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

- *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]

Delaunay Triangulations

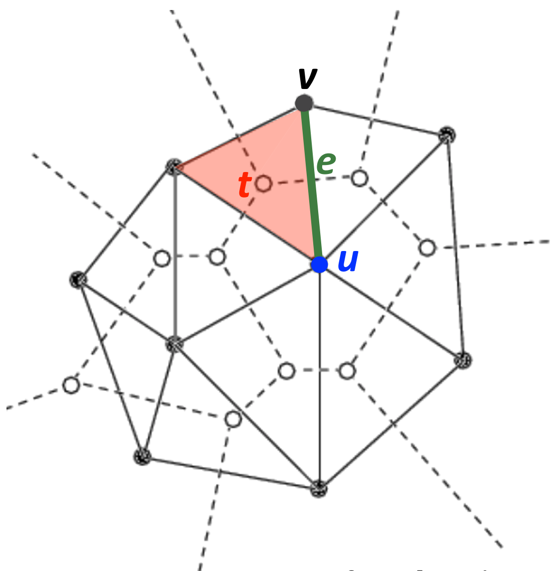
Duality Property:

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 $R_V(u)$*
- *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 $R_V(u)$ and $R_V(v)$*



Images from [De Floriani 2003]

Delaunay Triangulations

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*

Delaunay Triangulations

Watson's Algorithm:

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

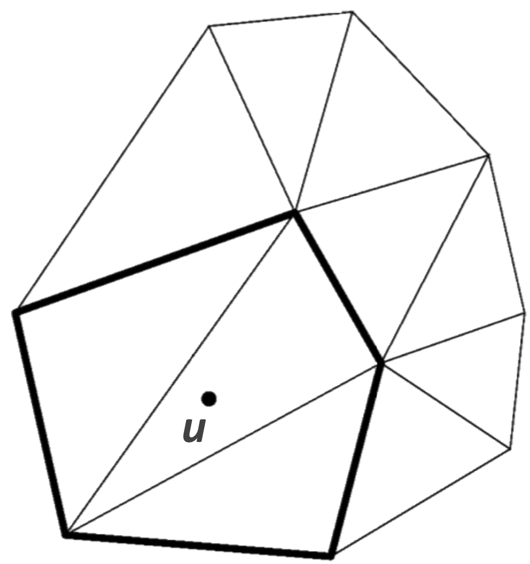
Let V_i be a subset of V and let u be a point in $V \setminus V_i$,

Input:

Del(V_i), a Delaunay triangulation of V_i

Output:

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



Images from [De Floriani 2003]

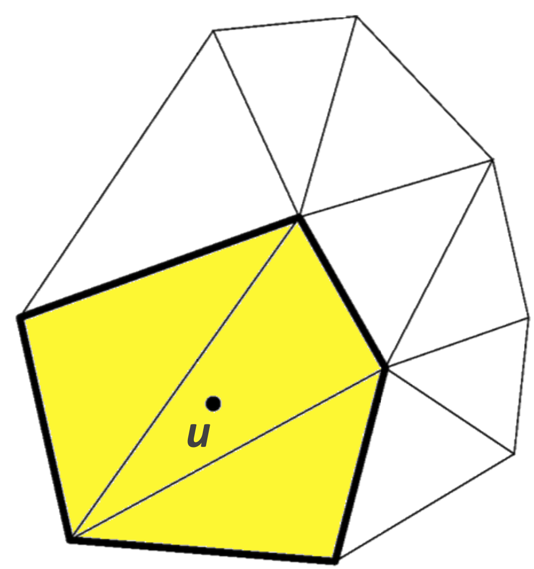
Delaunay Triangulations

Watson's Algorithm:

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

- *The **influence region R_u** of a point u is the region in the plane formed by the union of the triangles in Del(V_i) whose circumcircle contains u in its interior*

- *The **influence polygon P_u** of u is the polygon formed by the edges of the triangles of Del(V_i) which bound R_u*

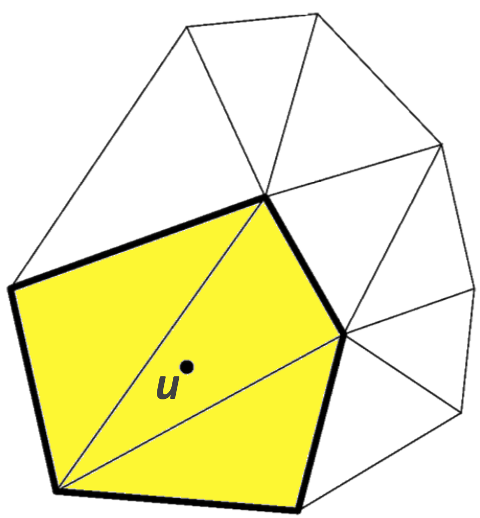


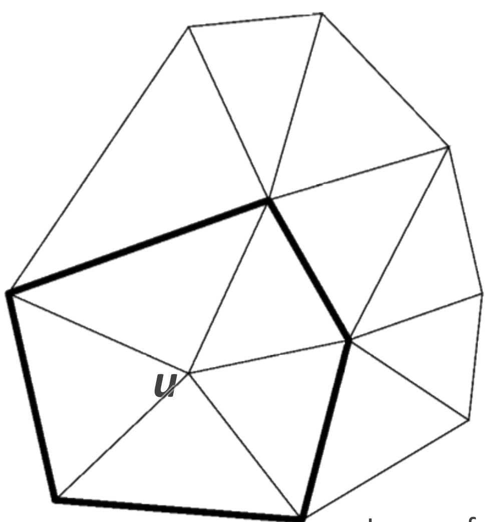
Images from [De Floriani 2003]

Delaunay Triangulations

Watson's Algorithm:

- **Step 1:**
  Deletion of the triangles of Del(V_i) forming the ***influence region R_u***
- **Step 2:**
  Re-triangulation of R_u by joining u to the vertices of the influence polygon P_u





Images from [De Floriani 2003]

Delaunay Triangulations

Watson's Algorithm:

Let $N_i = |V_i|$

- *Detection of a triangle of Del(V_i) containing the new point u: O(N_i) in the worst case*
- *Detection of the triangles forming the region of influence through a breadth-first search: O($|R_u|$)*
- *Re-triangulation of P_u is in O($|P_u|$)*

- ***Inserting a point*** *u in a triangulation with N_i vertices:* ***O(N_i)*** *in the worst case*
- ***Inserting all points*** *of V:* ***O(N^2)*** *in the worst case, where N =|V|*

Čech Complexes

Definition:

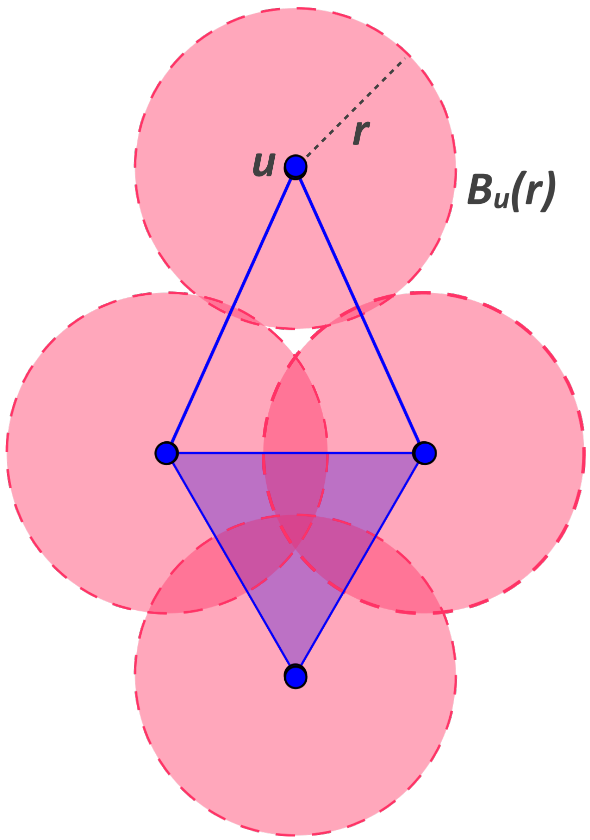
Given a finite set of points V in $\mathbb{R}^n$, let us consider:

- ***$B_u(r)$***, *the* ***closed ball*** *with* ***center u*** *∈ 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***

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

In practice, **infeasible construction**

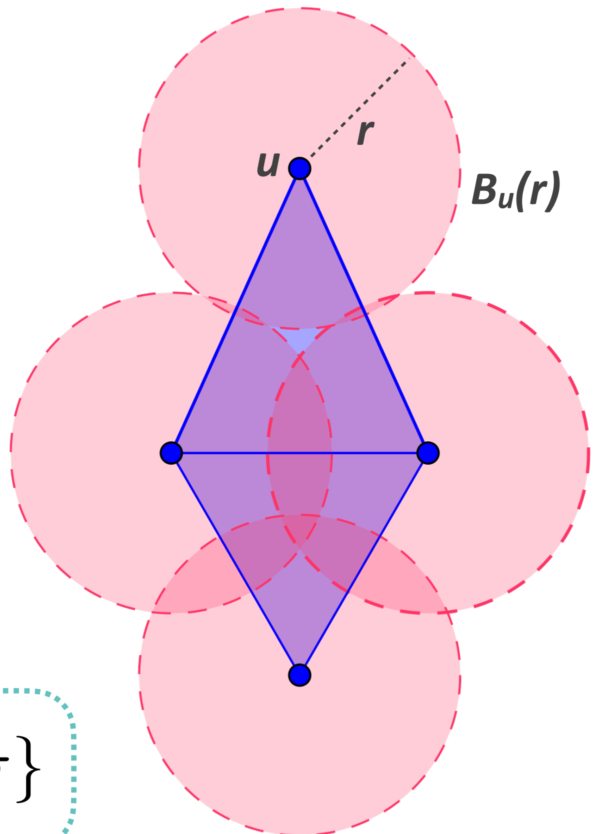


Vietoris-Rips Complexes

Definition:

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***



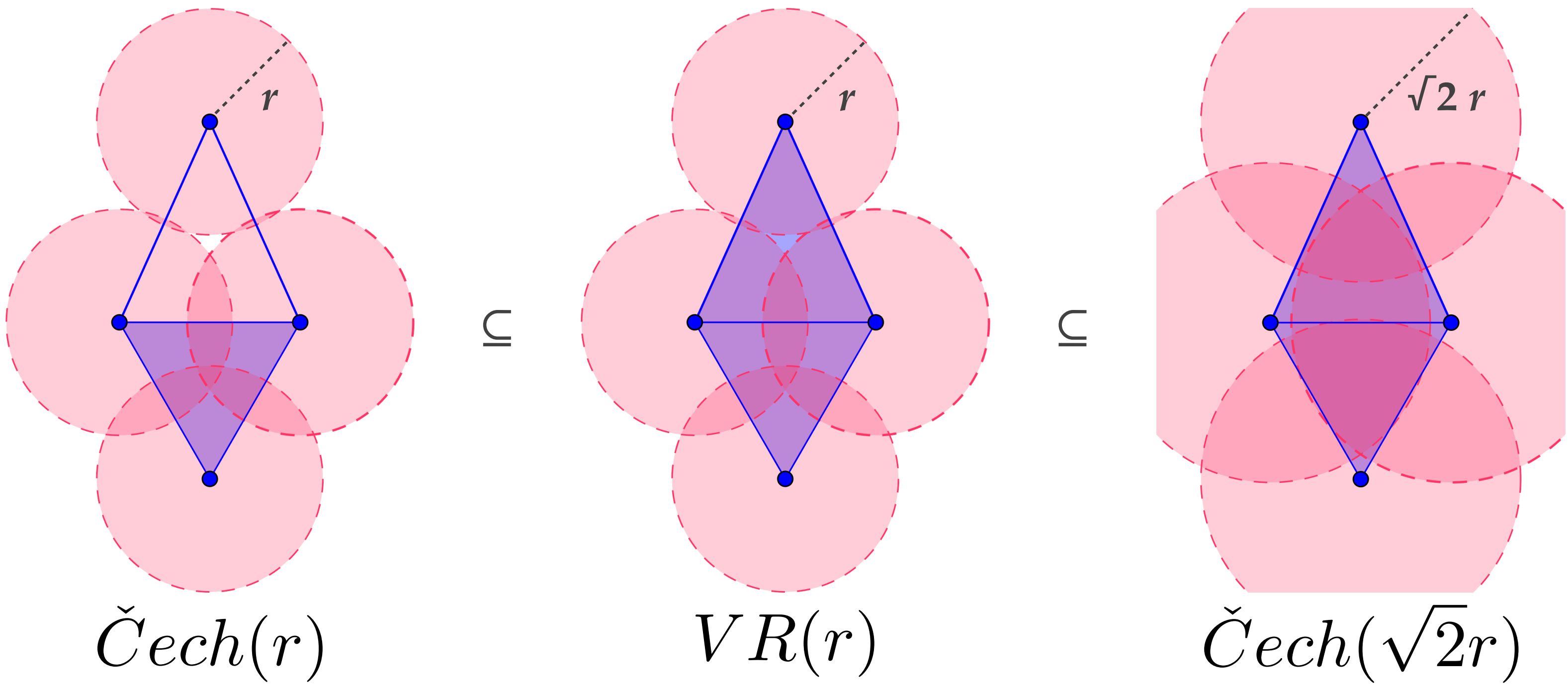
Formally,

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

Vietoris-Rips Complexes

Properties:

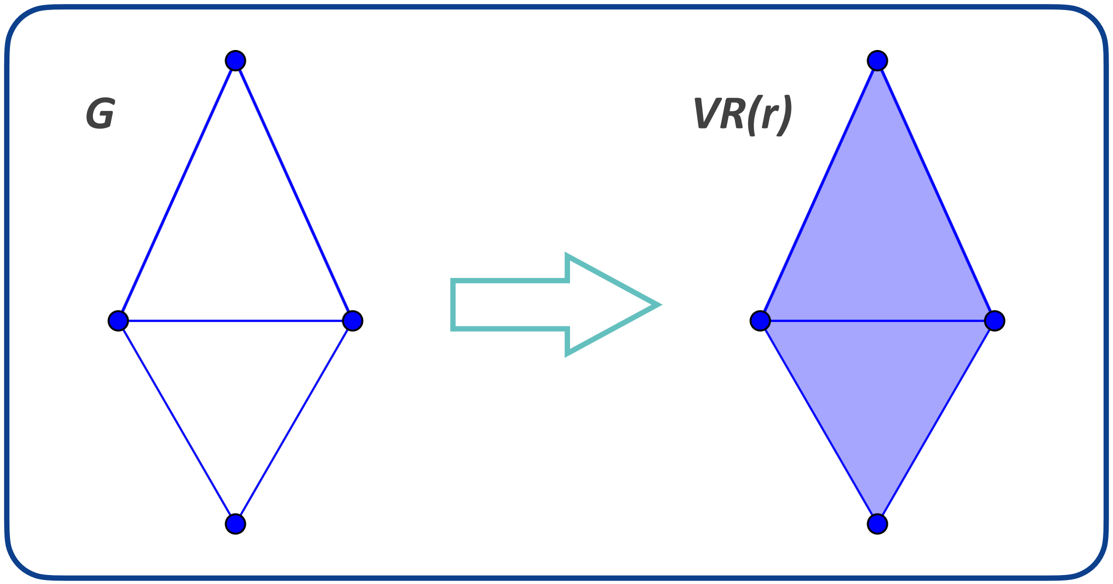
- $\check{C}ech(r) \subseteq VR(r) \subseteq \check{C}ech(\sqrt{2}r)$



Vietoris-Rips Complexes

Properties:

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



Vietoris-Rips Complexes

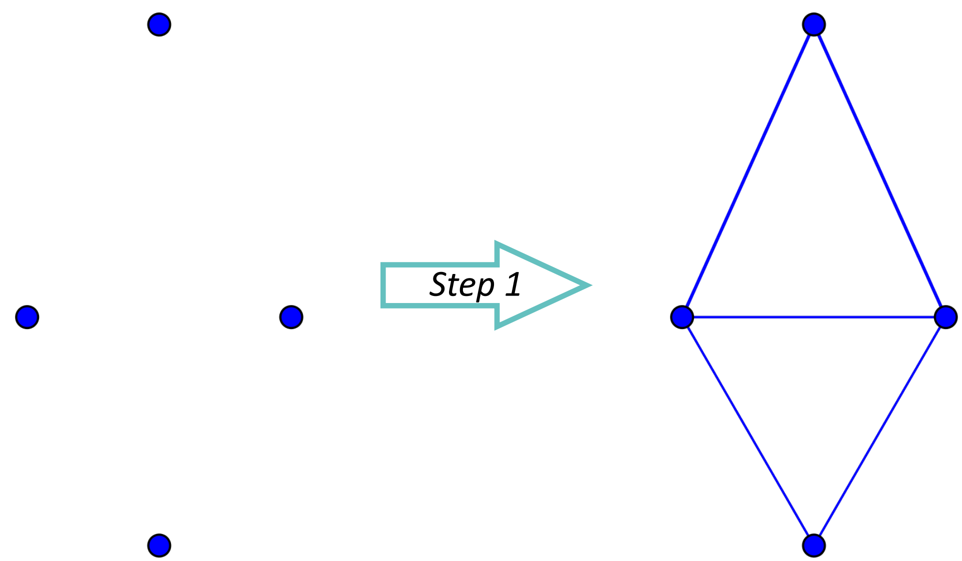
Algorithms:

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 ($O(|V|^2)$ time complexity)*
  - *Approximate*
  - *Randomized*
  - *Landmarking*
- ***Step 2 - Vietoris-Rips Expansion:***
  - *Inductive*
  - *Incremental*
  - *Maximal*



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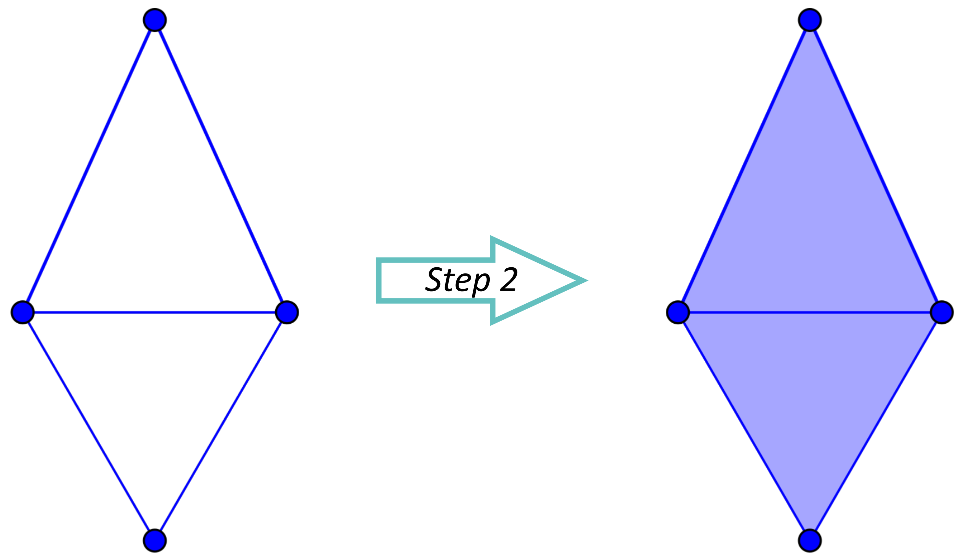


Vietoris-Rips Complexes

Inductive VR expansion:

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

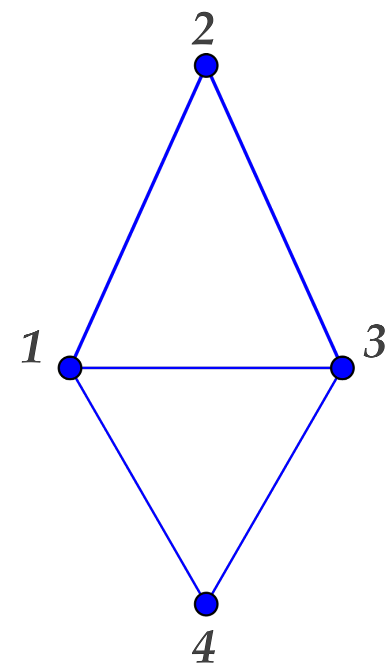
Output: The k-skeleton K of the Vietoris-Rips complex VR(r)

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)

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



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```
INDUCTIVE-VR(G, k)
   K = V ∪ E
   for i = 1 to k
      foreach i-simplex σ ∈ K
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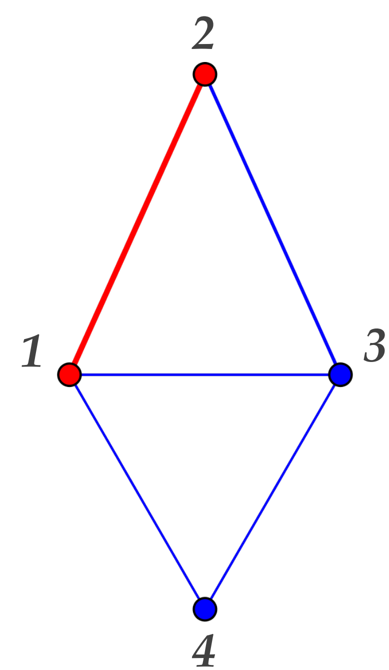
            foreach v ∈ N
               K = K ∪ { σ ∪ {v}}
      return K

LOWER-NBRS(G, u)
      return {v ∈ V | v < u , (u, v) ∈ E}
```

$\sigma = (1, 2)$

$N = \{\ \}$



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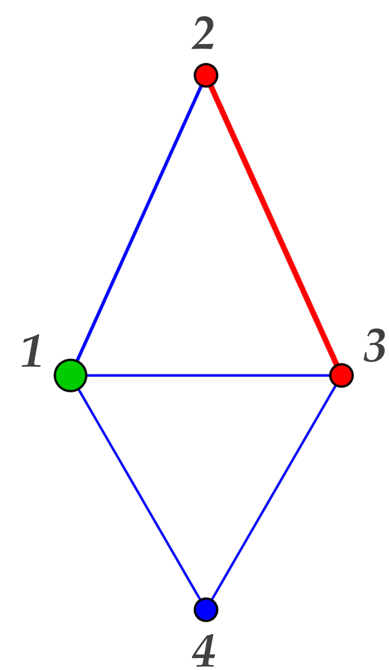
  return K

LOWER-NBRS(G, u)

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

$\sigma = (2, 3)$

$N = \{1\}$



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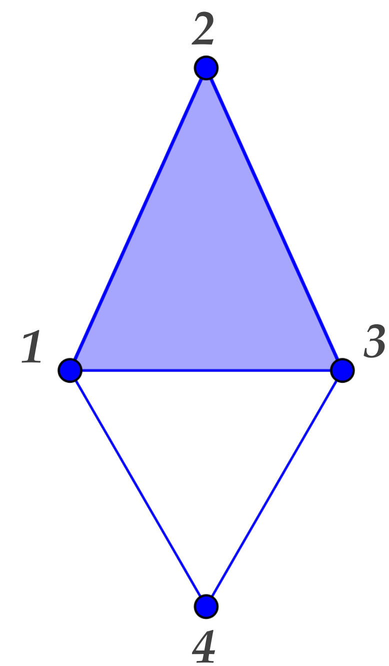
for $i = 1$ ***to*** k
foreach *i-simplex* $\sigma \in K$
$N = \cap_{u \in \sigma}$ *LOWER-NBRS(G, u)*
foreach $v \in N$
$K = K \cup \{ \sigma \cup \{v\}\}$
return *K*

LOWER-NBRS(G, u)

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



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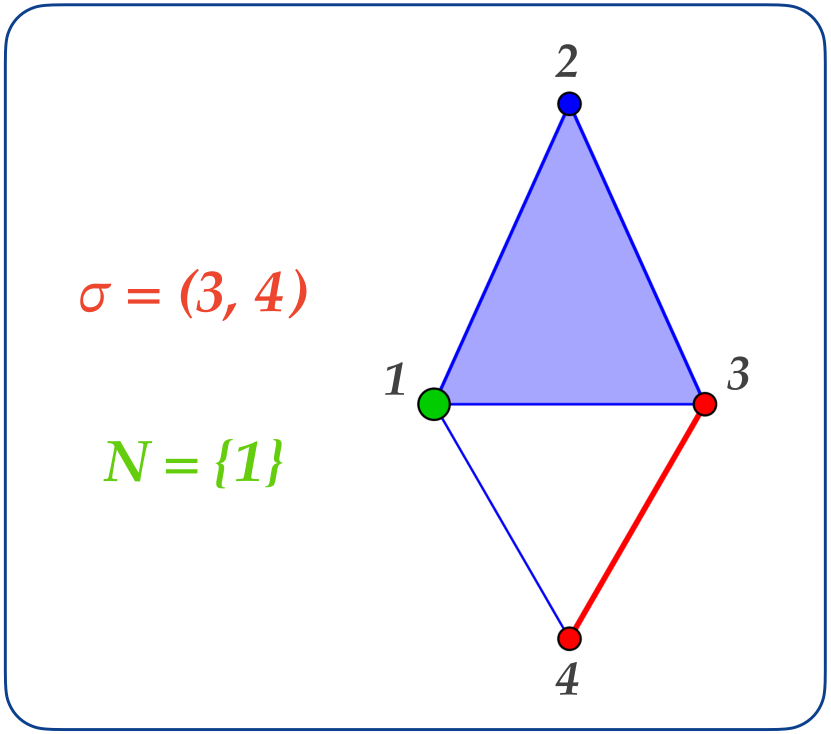
    return K
```

LOWER-NBRS(G, u)

```
    return {v ∈ V | v < u , (u, v) ∈ E}
```



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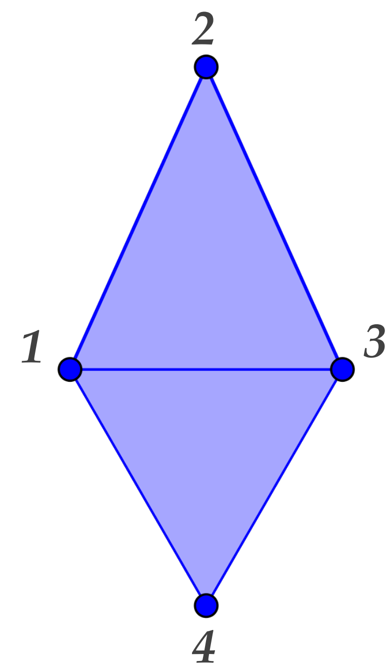


From Data to Complexes

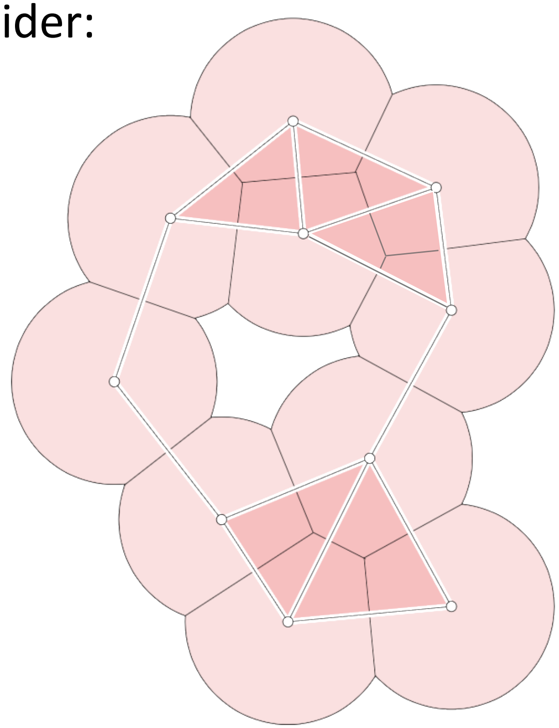
		
Delaunay triangulation	Bounded Dimension	Trivial Homology
Čech/VR complex	“Real” Homology	High Dimension Large Size

Alpha-Shapes

Definition:

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

- ***$A_u(r) := B_u(r) \cap R_V(u)$***, *the* ***intersection*** *of the* ***closed ball*** *with* ***center u*** *$\in$ 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,

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

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

Image from [Edelsbrunner, Harer 2010]

Witness Complexes

Motivation:

The “shape” of a point cloud can be captured ***without considering all the input points***

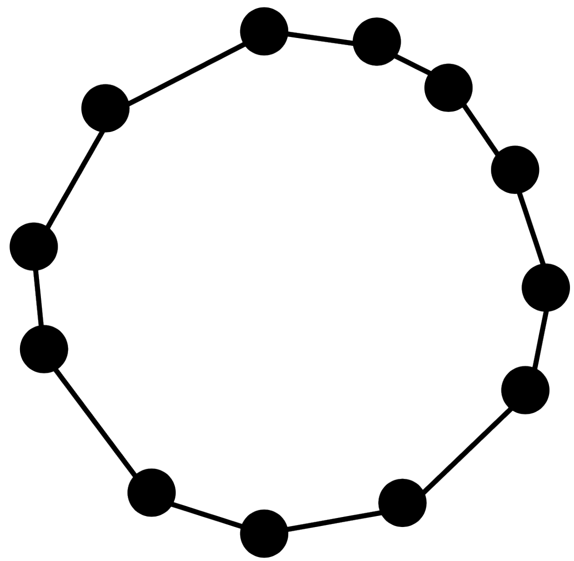
Definitions:

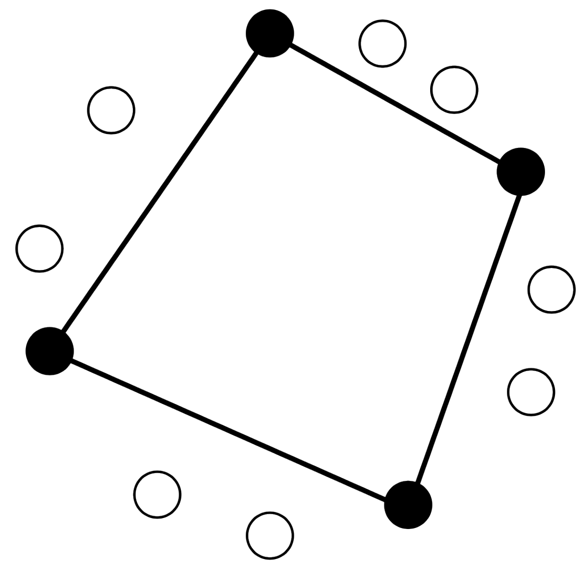
- ***Landmarks:***

  Selected points

- ***Witnesses:***

  Remaining points





Images from [de Silva, Carlsson 2004]

Witness Complexes

Definition:

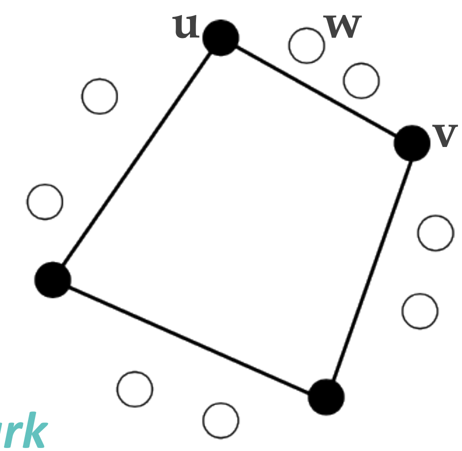
The ***witness complex W(r)*** of radius *r* is defined by:

- *u is in W(r) if u is a landmark*
- *(u, v) is in W(r) if there exists a witness w such that*

$$max\{d(u,w), d(v,w)\} \leq m_w + r$$

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

- *the i-simplex σ 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

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

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*

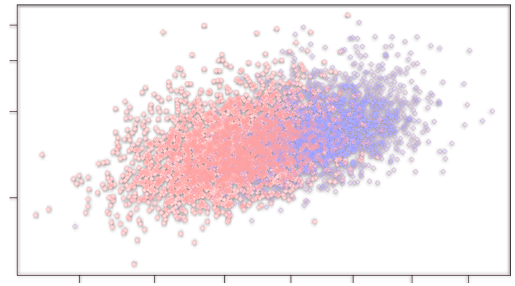
enabling to cover a **wide plethora of datasets**

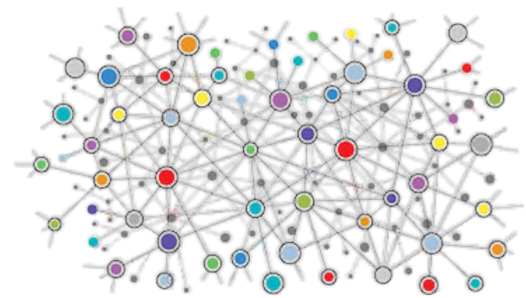
More properly, a* ***semi-metric**, i.e. a distance not necessarily satisfying the triangle inequality*

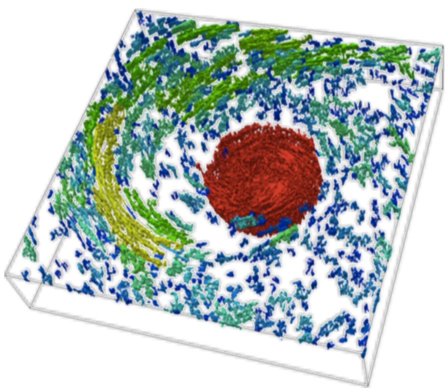
From Data to Complexes

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*





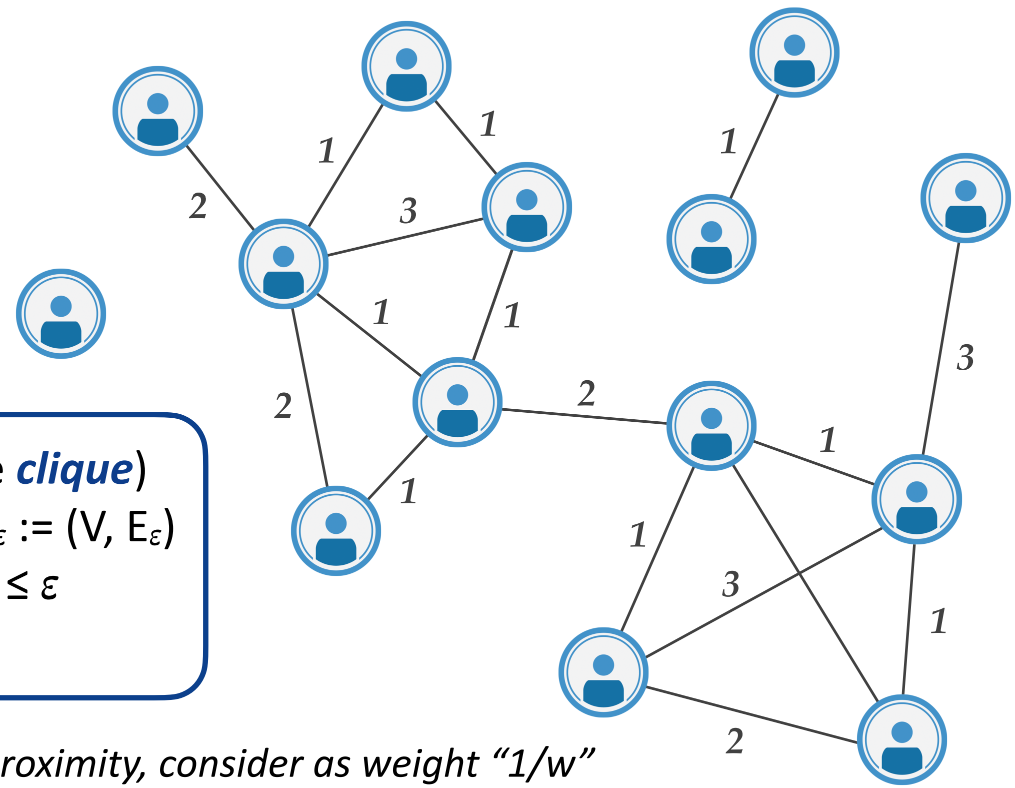


From Data to Complexes

Flag Complex of a Weighted Network:

Let G := (V, E, w: E ⟶ ℝ) be a ***weighted undirected graph*** representing a ***network***:

Nodes of V	⇔	*Entities or individuals*
Arcs of E		*Ties between entities*
Weights of w		*Proximity of entities**



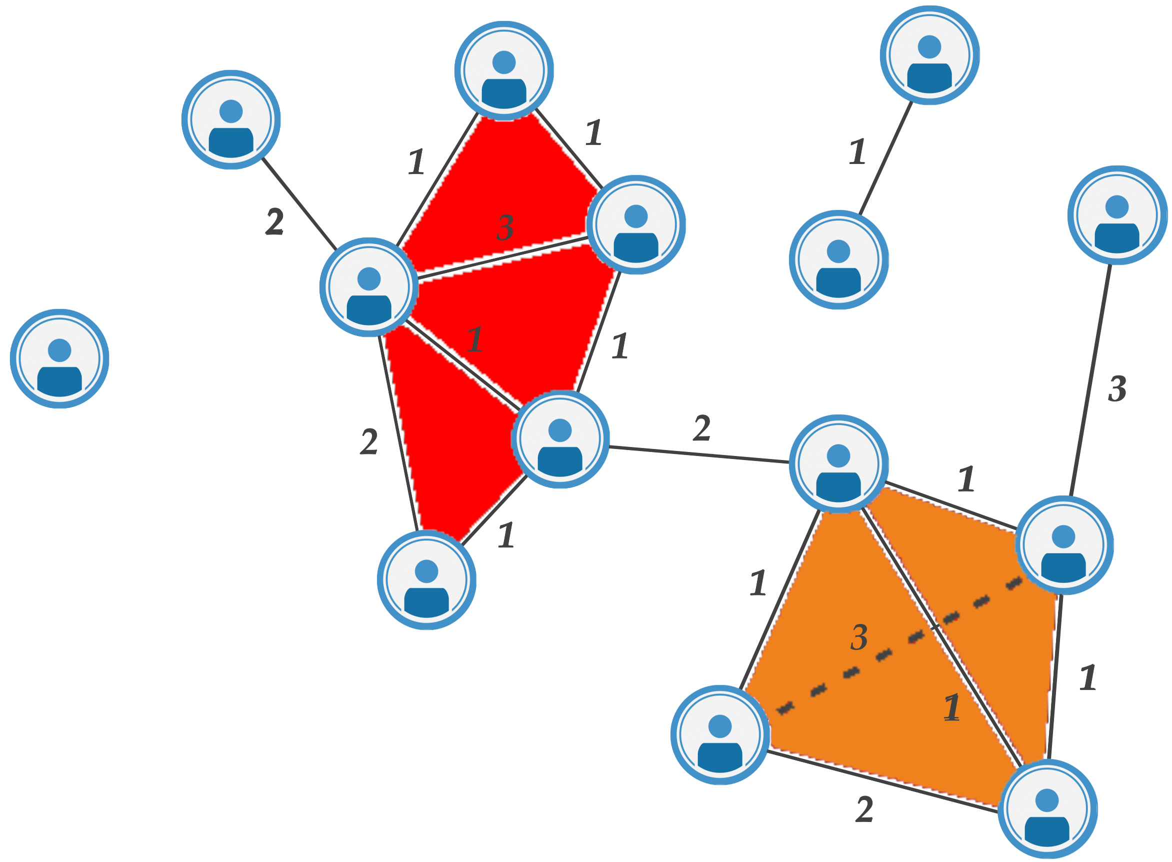
Fixed a ***weight threshold*** ε, the ***flag*** (or the ***clique***) ***complex*** is the ***VR expansion*** of the graph $G_\varepsilon := (V, E_\varepsilon)$ where E_ε are the arcs of E with weight $\leq \varepsilon$

**If w represents tie strengths rather than node proximity, consider as weight "1/w"*

From Data to Complexes

Flag Complex of a Weighted Network:

$\varepsilon = 3$



From Data to Complexes

Sublevel Sets of Functions

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

- ***Step 1:***

  Transform f: D $\longrightarrow \mathbb{R}$ into a function **F: K** $\longrightarrow \mathbb{R}$ ***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

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

- ***Step 2:***

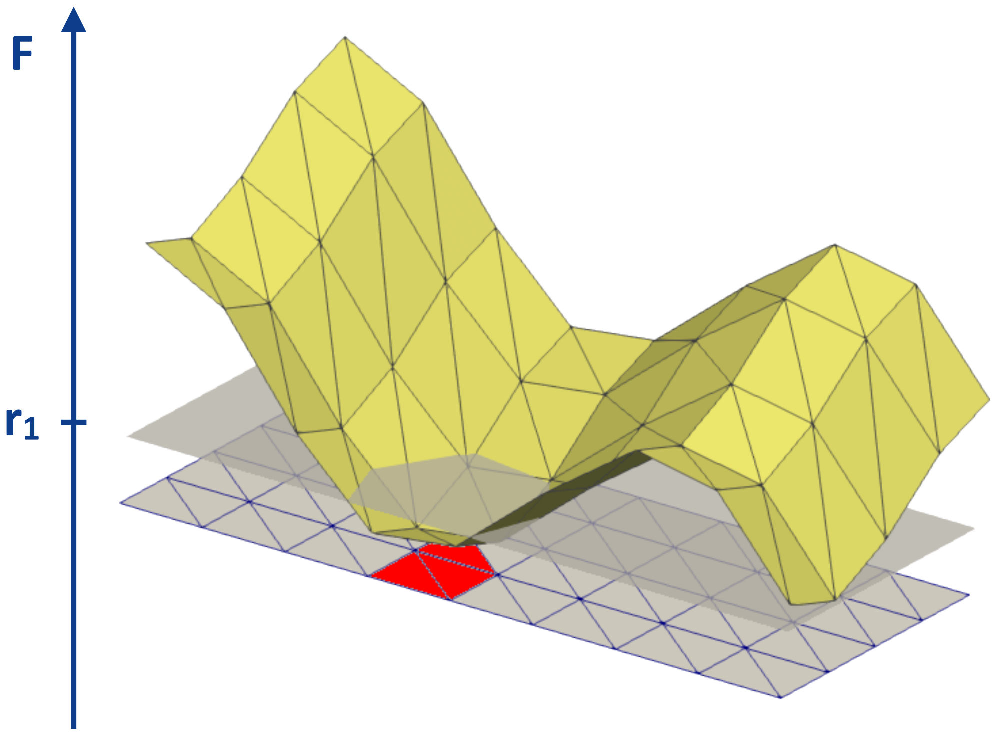
  Build the collection $\{ K^r \}_{r \in \mathbb{R}}$ of the ***sublevel sets of F*** defined as

$$K^r := \{\sigma \in K \mid F(\sigma) \leq r\}$$

  Notice that K^r is a simplicial complex whenever: if τ is a face of σ then $F(\tau) \leq F(\sigma)$

From Data to Complexes

Sublevel Sets of Functions

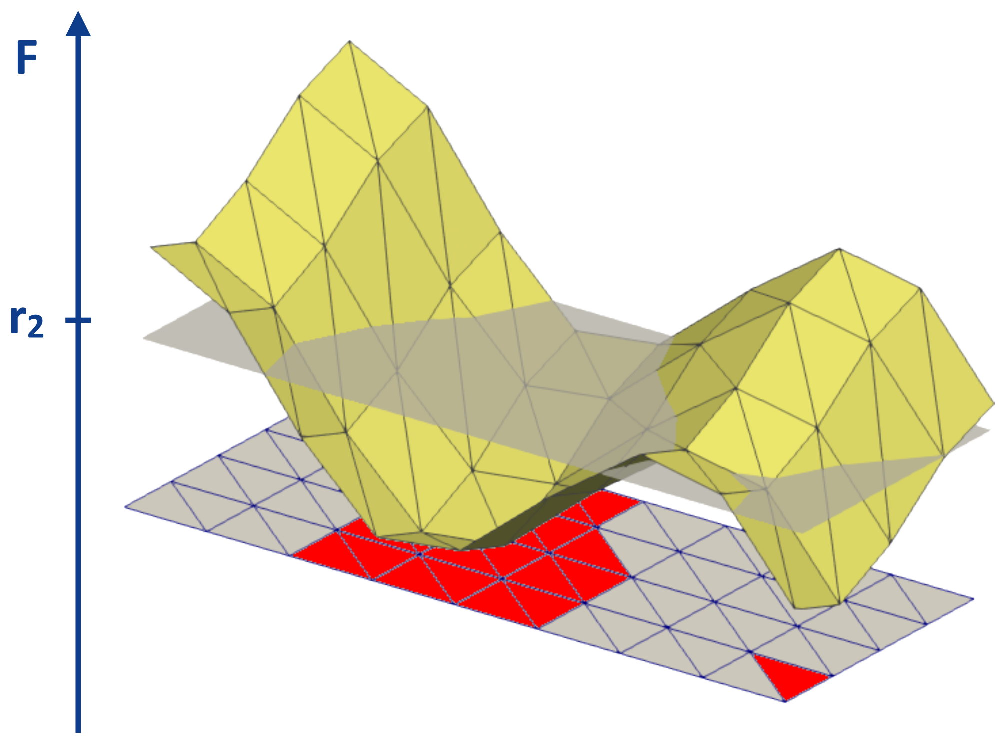


Given a function F: K $\longrightarrow \mathbb{R}$,

$$K^r := \{\sigma \in K \mid F(\sigma) \leq r\}$$

From Data to Complexes

Sublevel Sets of Functions

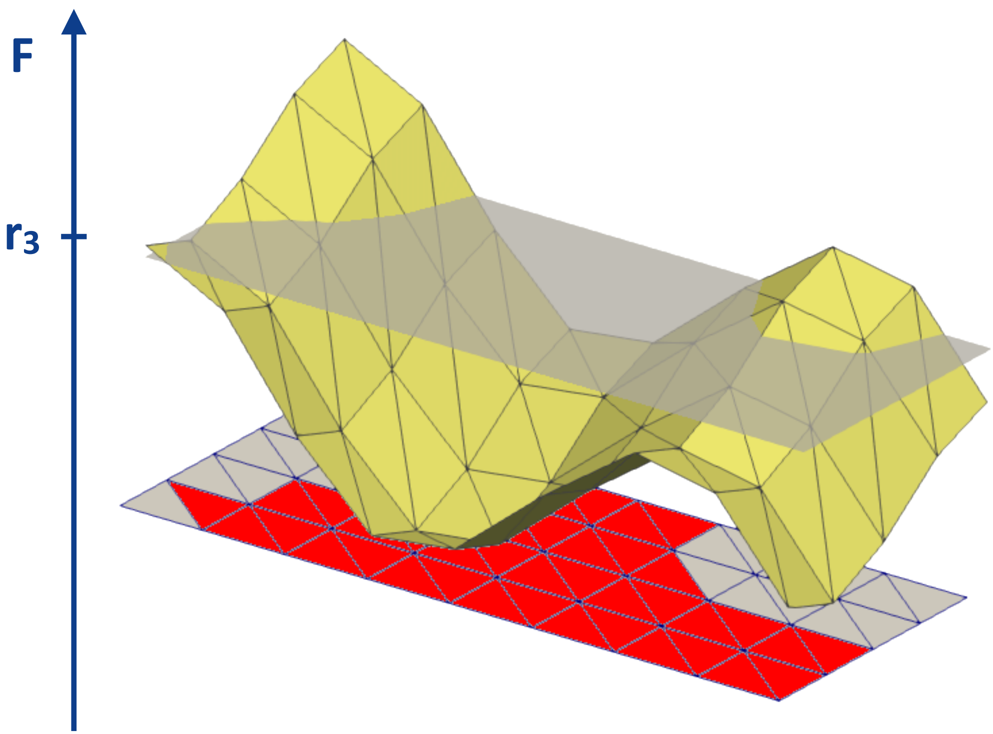


Given a function F: K $\longrightarrow \mathbb{R}$,

$$K^r := \{\sigma \in K \mid F(\sigma) \leq r\}$$

From Data to Complexes

Sublevel Sets of Functions



Given a function F: K ⟶ ℝ,

$$K^r := \{\sigma \in K \mid F(\sigma) \leq r\}$$

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.
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