

Topological Data Analysis

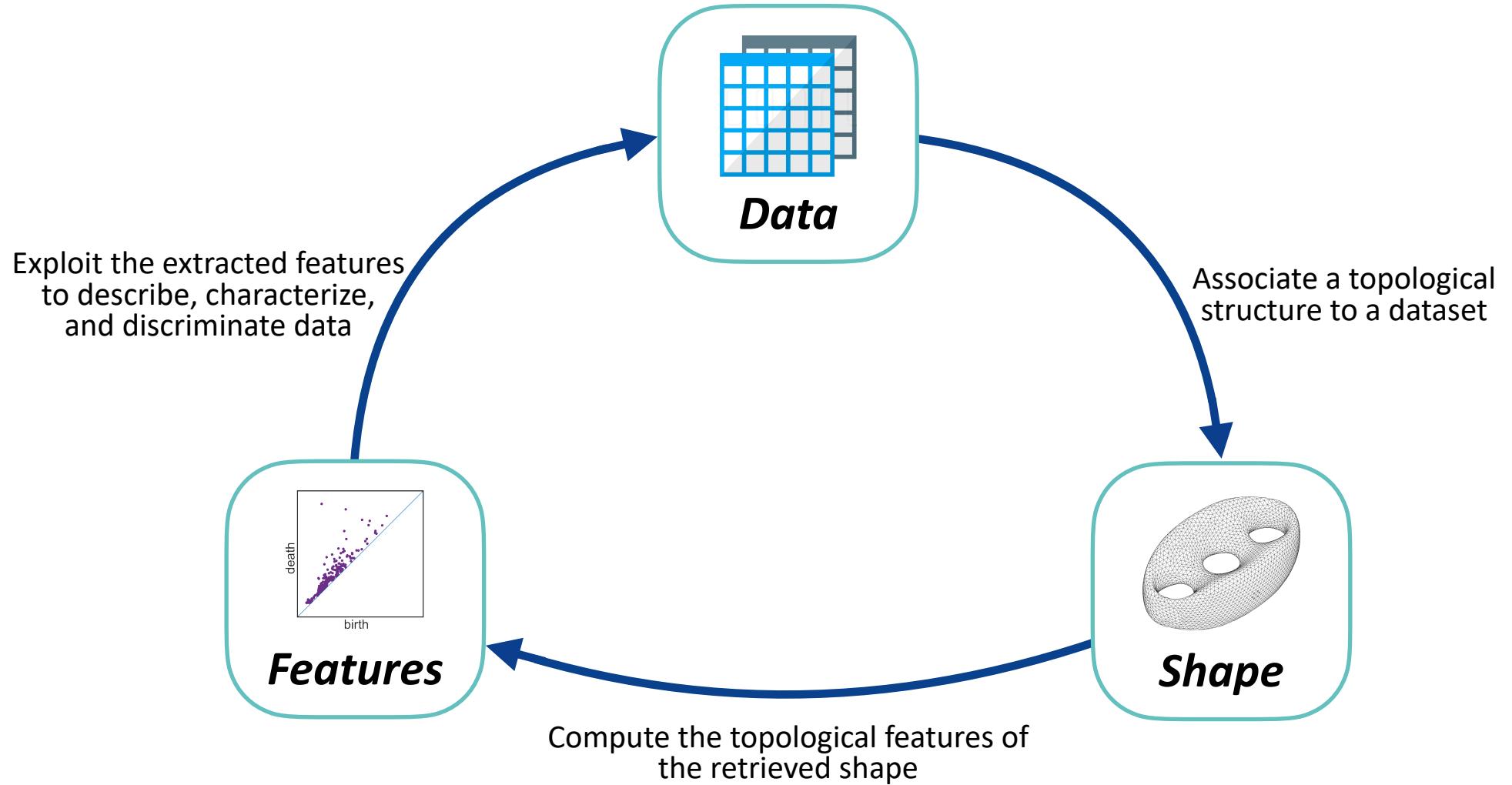
Complexes & Data

Ulderico Fugacci

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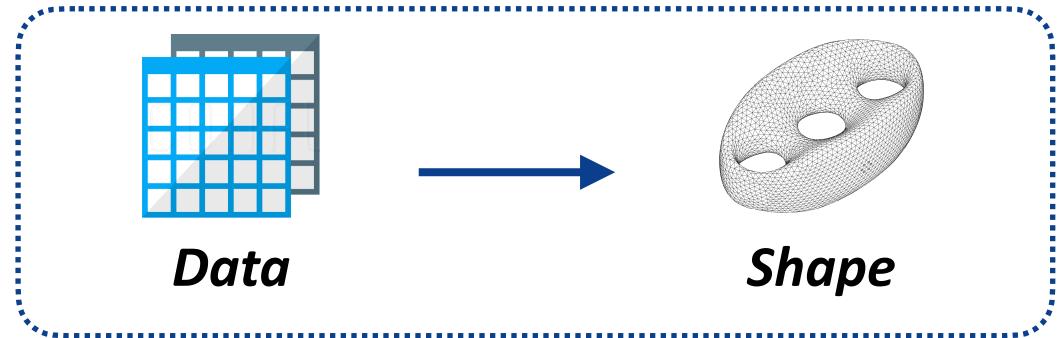
Topological Data Analysis



Complexes & Data

Goal:

We want to associate a topological structure to a given dataset

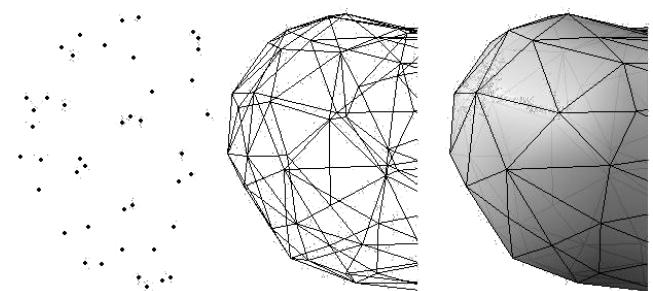


Due to the nature of data and to our computational ambitions, datasets will be represented by "**discrete**" structures

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

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)



Complexes & Data

- ◆ *Simplicial Complexes* (and other discrete representations)
- ◆ *From Data to Complexes*

Complexes & Data

- ◆ *Simplicial Complexes (and other discrete representations)*
- ◆ *From Data to Complexes*

Simplicial Complexes

Definitions:

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

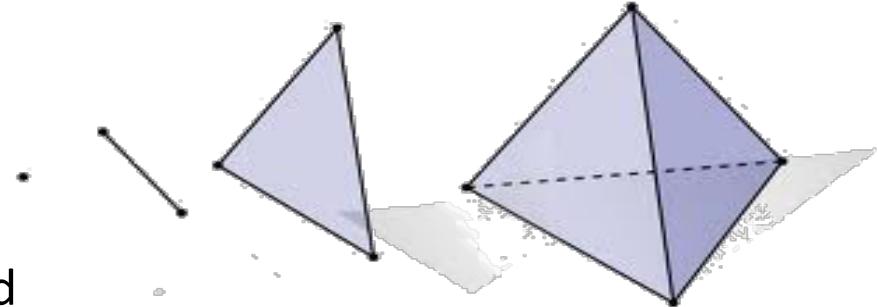
geometrically independent if vectors $v_1 - v_0, \dots, v_k - v_0$ are **linearly independent** over \mathbb{R}

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

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

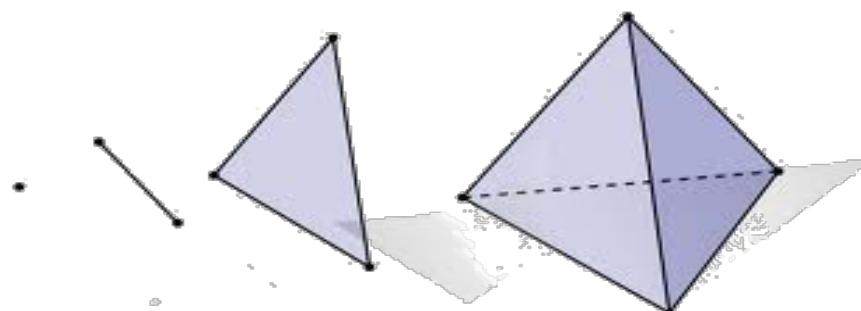
The numbers t_i are uniquely determined by x and are called **barycentric coordinates** of x
E.g. a 0-simplex is a vertex, a 1-simplex is an edge, a 2-simplex is a triangle, a 3-simplex is a tetrahedron



Simplicial Complexes

Definitions:

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

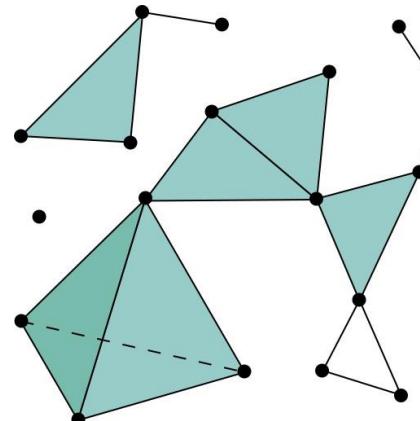


Simplicial Complexes

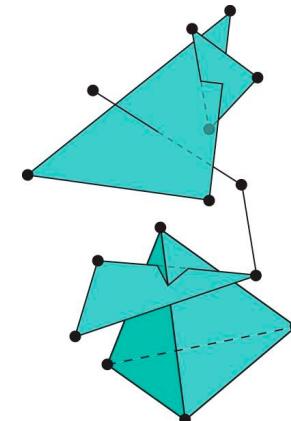
Definition:

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 complex



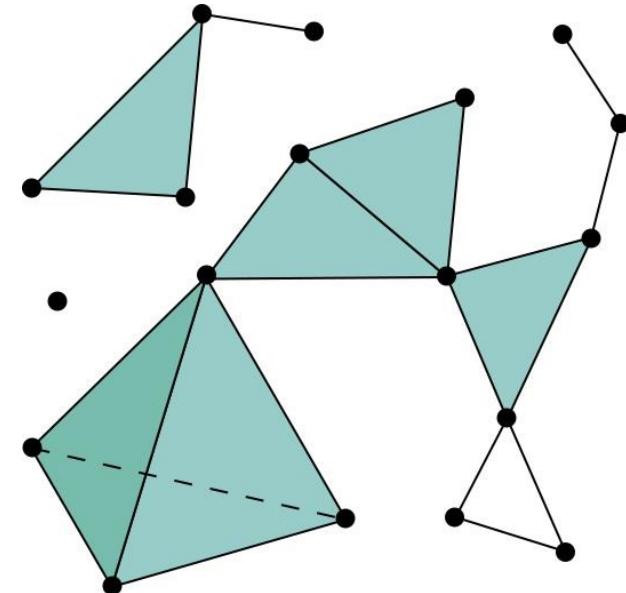
non-simplicial complex

Simplicial Complexes

Definitions:

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

- ◆ The **dimension** of a simplicial complex K in \mathbb{R}^n , denoted as $\dim(K)$, is the supremum of the dimensions of the simplices of K
- ◆ A simplex σ of K such that $\dim(\sigma) = \dim(K)$ is called **maximal**
- ◆ A simplex σ 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

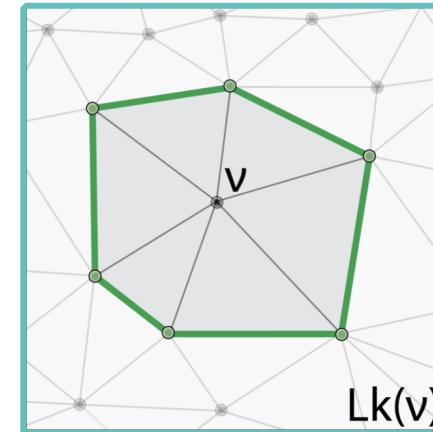
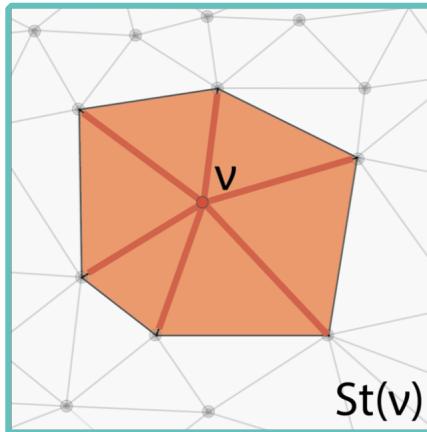


Simplicial Complexes

Definitions:

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

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

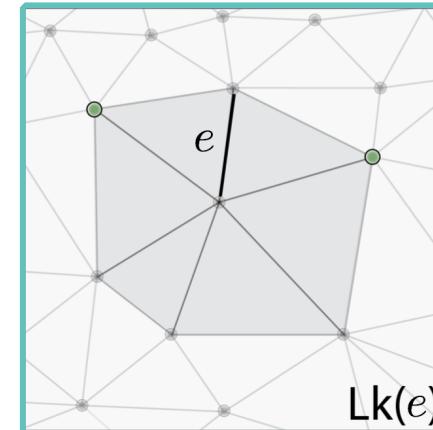
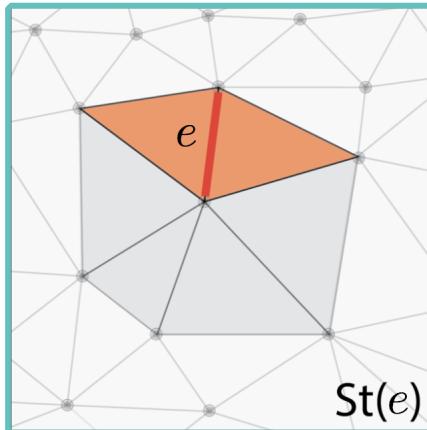


Simplicial Complexes

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Simplicial Complexes

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_1 and T_2 :

- ◆ **T_1** : A subset F of $|K|$ is a closed set of $(|K|, T_1)$ if and only if $F \cap \sigma$ is a closed set of (σ, T_σ) for each σ in K where T_σ is the subspace topology induced on σ by \mathbb{E}^n
- ◆ **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

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 $f: K \rightarrow K'$ is called a **simplicial map** if for every simplex $\sigma = v_0v_1 \dots v_k$ in K , $f(\sigma) = f(v_0)f(v_1)\dots f(v_k)$ is a simplex in K'
- ◆ The restriction f_V of f to the set of vertices V of K is called the **vertex map** of f

Simplicial Complexes

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 σ 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 $\sigma \in K$ 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

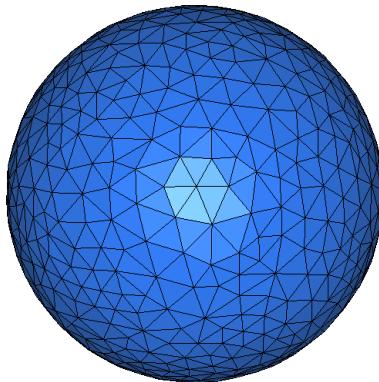
Simplicial Complexes

Definition:

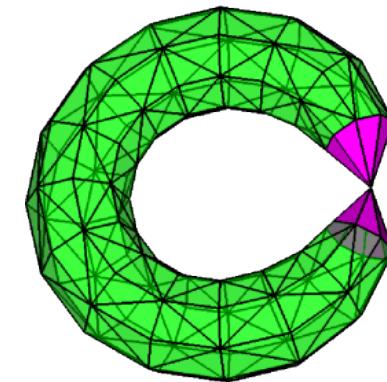
A simplicial complex K is called

- ◆ ***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^{n-1} [or to the $(n - 1)$ -disk $D^{n-1} := \{x \in \mathbb{R}^{n-1} : |x| \leq 1\}$]

*combinatorial
manifold*



*non-combinatorial
manifold*



Proposition:

If K is a combinatorial n -manifold [with boundary], then K is a n -manifold [with boundary]

The converse is:

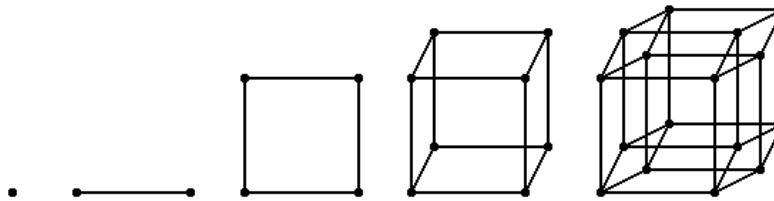
True for $n \leq 3$

Open for $n = 4$

False for $n > 4$

Regular Grids

Hyper-Cube:

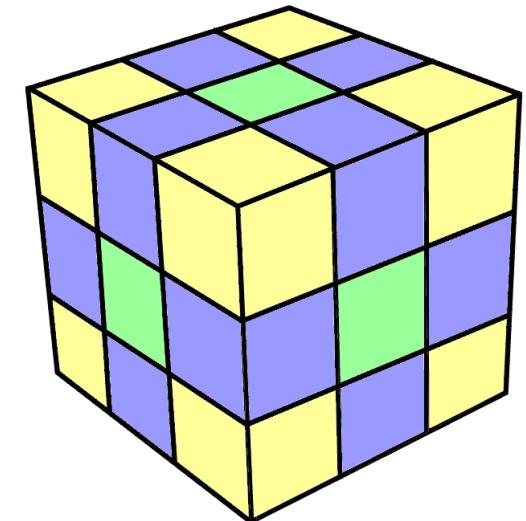


A k -hyper-cube η is the *Cartesian product of k closed intervals* of equal length

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*

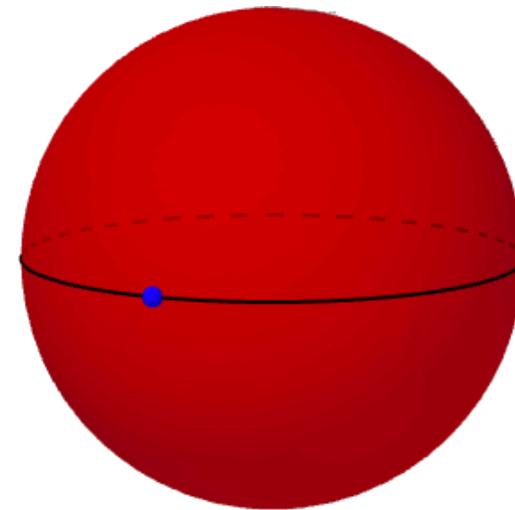
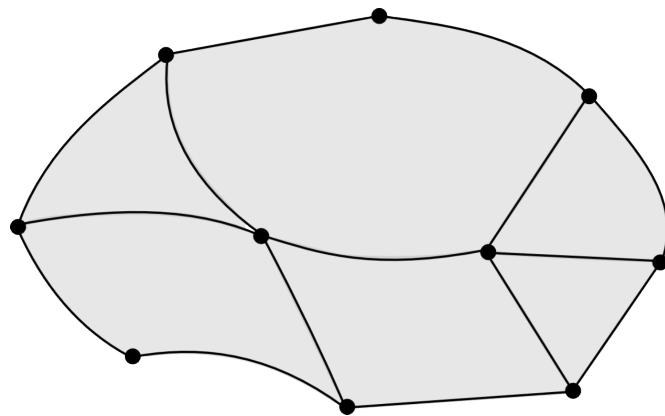


Cell Complexes

Intuitively:

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 $i(D^k)$**

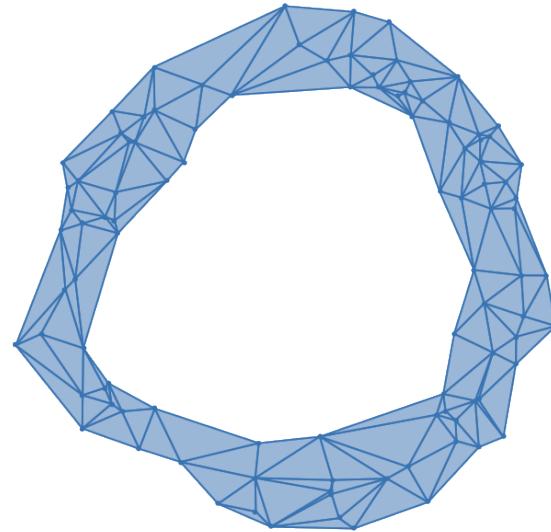
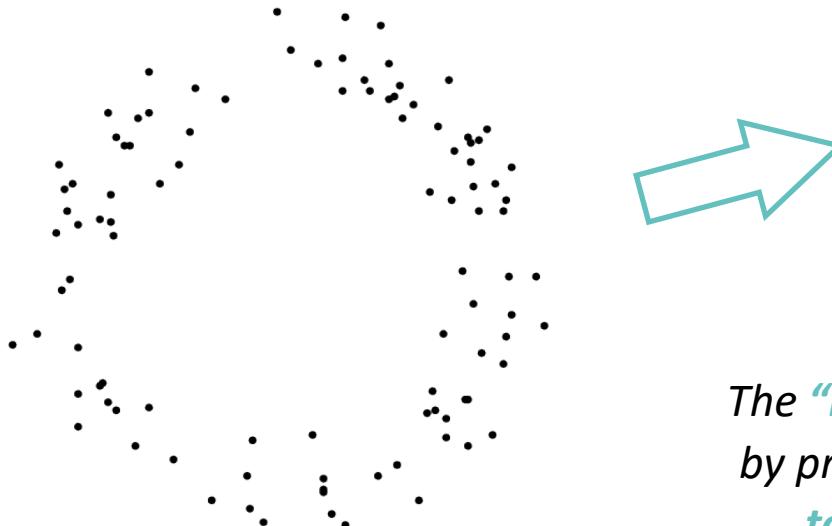
Complexes & Data

- ◆ *Simplicial Complexes (and other discrete representations)*
- ◆ **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	<i>Geometric</i>	n	
Čech complex	<i>Abstract</i>	<i>Arbitrary (up to $V - 1$)</i>	
Vietoris-Rips complex	<i>Abstract</i>	<i>Arbitrary (up to $V - 1$)</i>	
Alpha-shapes	<i>Geometric</i>	n	
Witness complexes	<i>Abstract</i>	<i>Arbitrary (up to $V - 1$)</i>	

Nerve Complexes

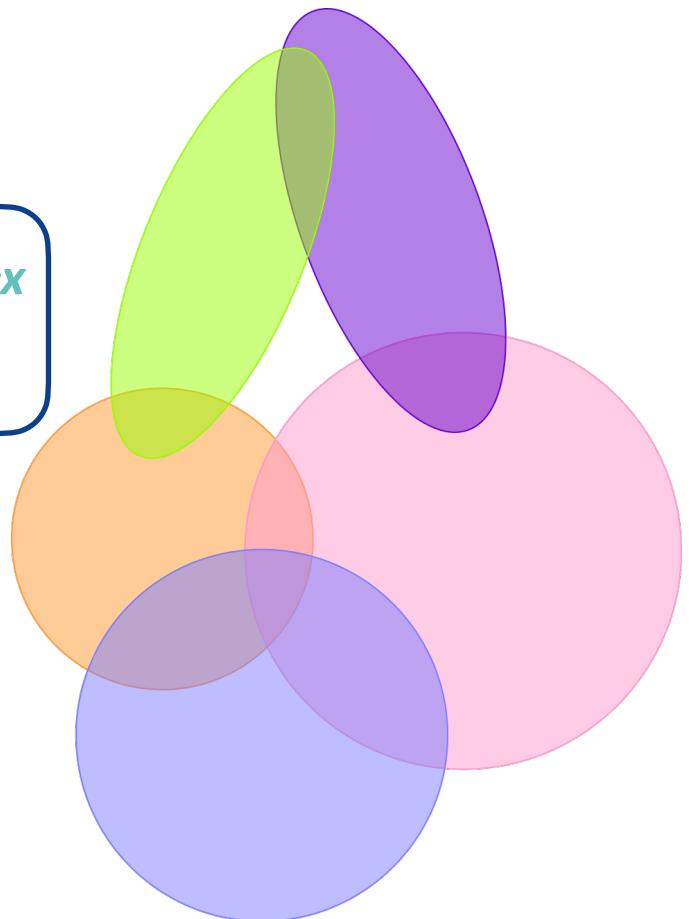
Definition:

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

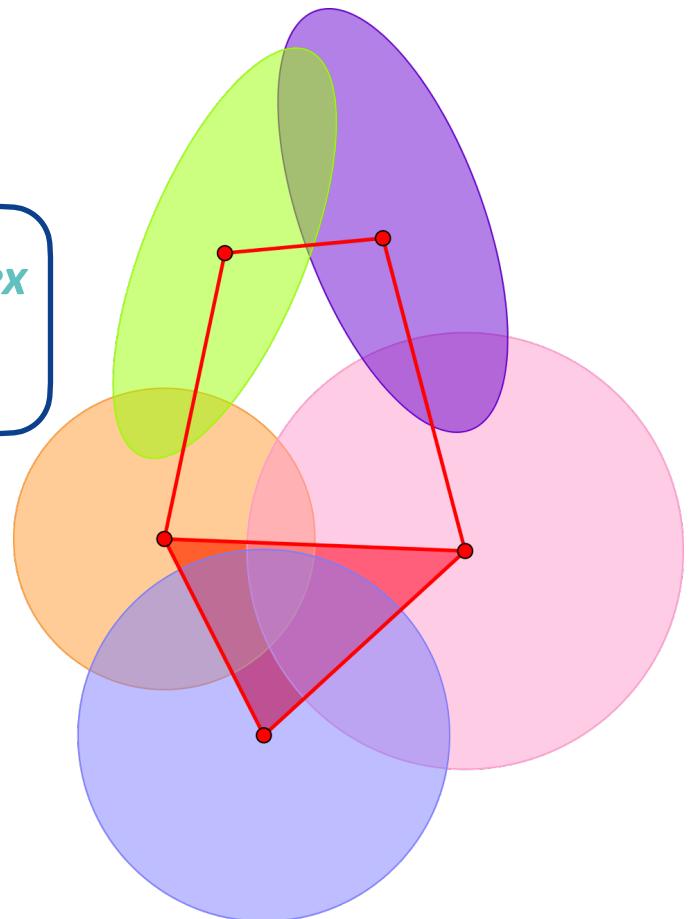
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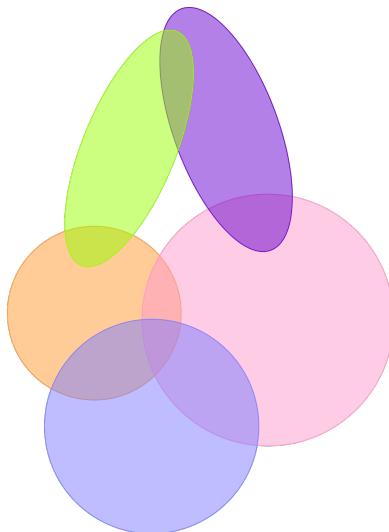
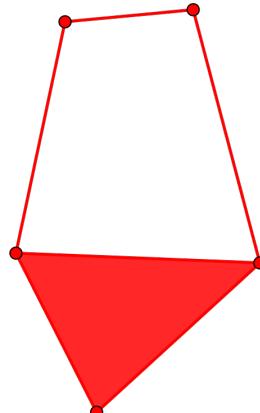
$$Nrv(S) := \{\sigma \subseteq S \mid \bigcap_{s \in \sigma} s \neq \emptyset\}$$



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)

 \approx 

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:

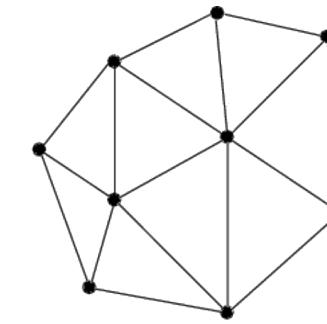
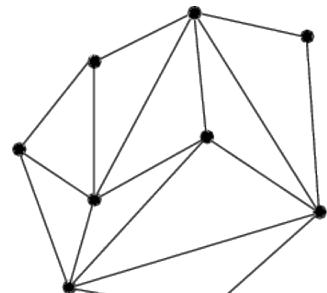
If S is an open cover of a (para)**compact** space X such that every non-empty intersection of finitely many sets in S is **contractible**, then X is **homotopy equivalent** to the nerve $\text{Nrv}(S)$

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



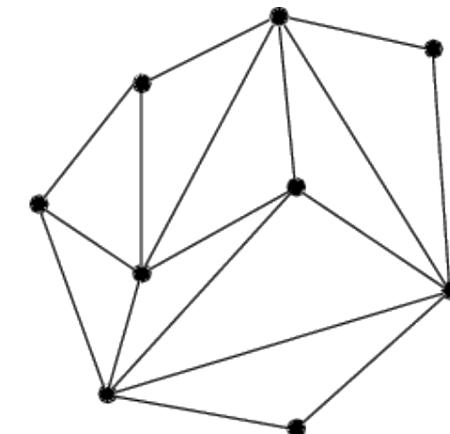
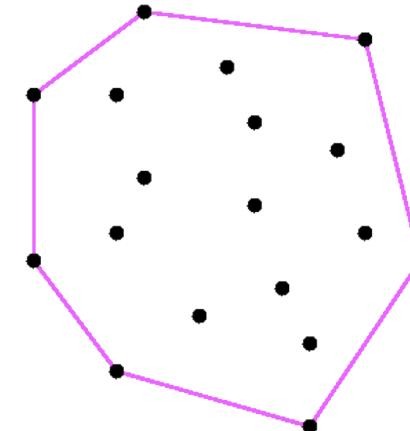
Images from [De Floriani 2003]

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



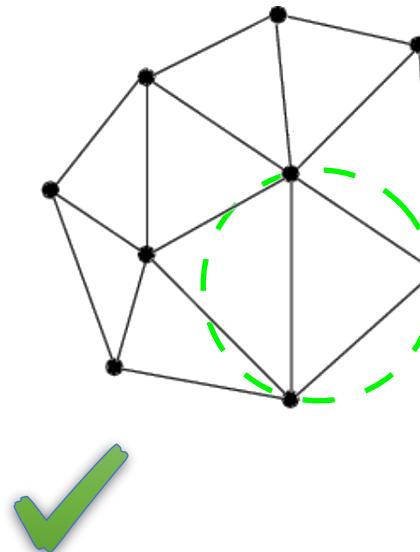
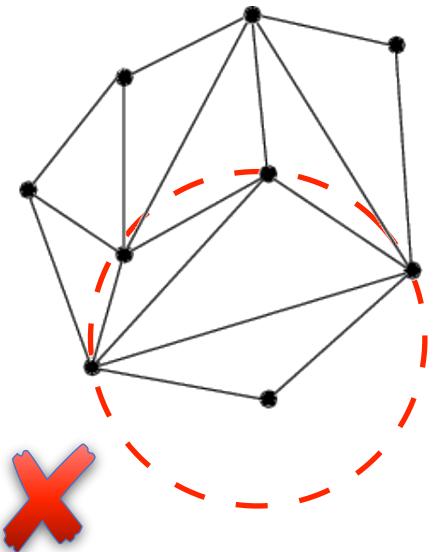
Images from [De Floriani 2003]

Delaunay Triangulations

Definition:

A **Delaunay triangulation** is a triangulation $\text{Del}(V)$ of V such that:

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



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 $n = 2$,

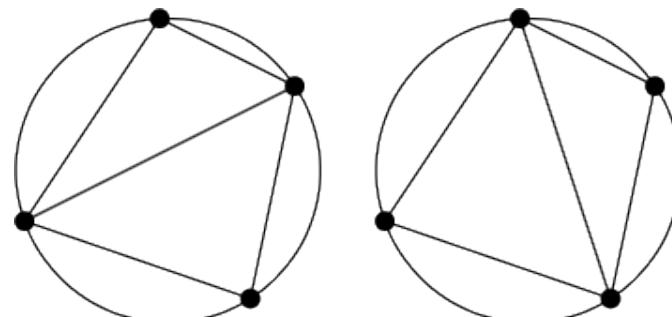
V in general position



No four or more points are co-circular

Theorem:

If V is in general position, then $\text{Del}(V)$ is *unique*



Images from [De Floriani 2003]

Delaunay Triangulations

Definitions:

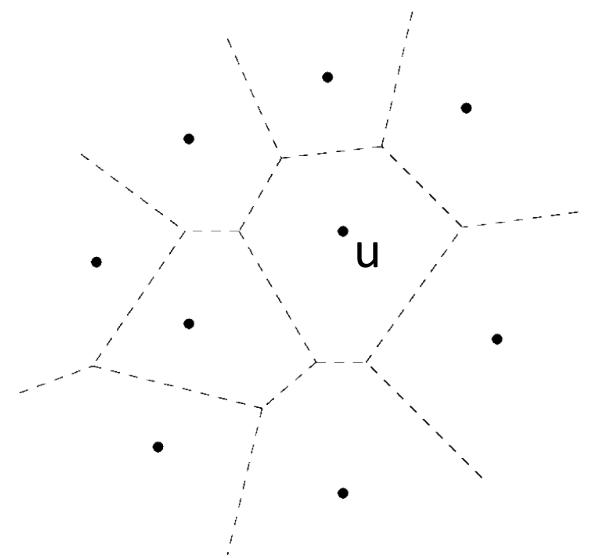
The **Voronoi region** of u in V is the set of points of \mathbb{R}^2 for which u is the closest

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

- ◆ 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

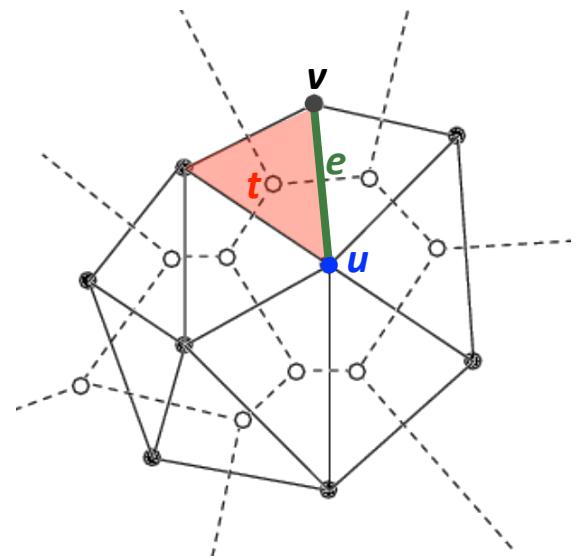
Duality Property:

If V is in general position, then

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

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

- ◆ Each **point u** of V corresponds to a Voronoi region $R_V(u)$
- ◆ Each **triangle t** of $\text{Del}(V)$ corresponds to a vertex in $\text{Vor}(V)$
- ◆ Each **edge $e=(u,v)$** in $\text{Del}(V)$ 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

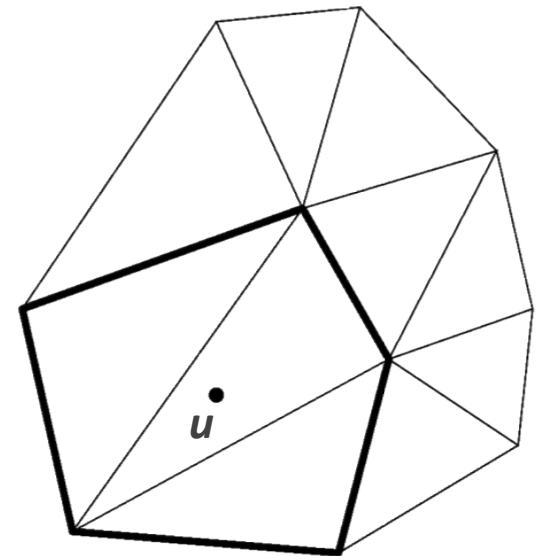
Let V_i be a subset of V and let u be a point in $V \setminus V_i$,

Input:

$\text{Del}(V_i)$, a Delaunay triangulation of V_i

Output:

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



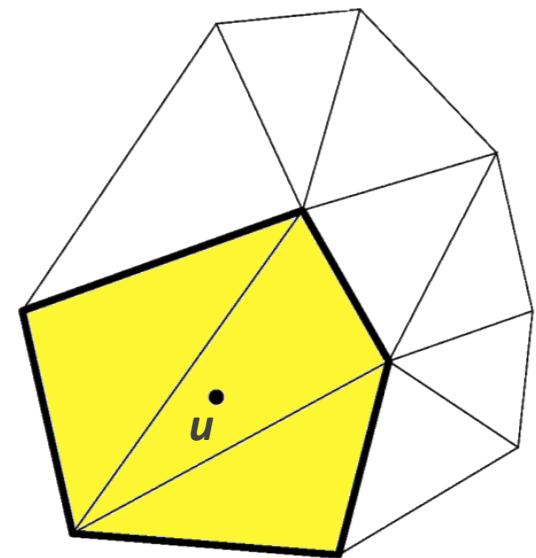
Images from [De Floriani 2003]

Delaunay Triangulations

Watson's Algorithm:

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

- ◆ The **influence region R_u** of a point u is the region in the plane formed by the union of the triangles in $\text{Del}(V_i)$ 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 $\text{Del}(V_i)$ which bound R_u



Delaunay Triangulations

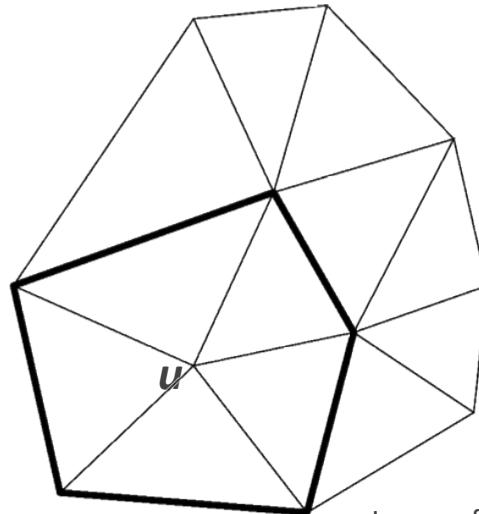
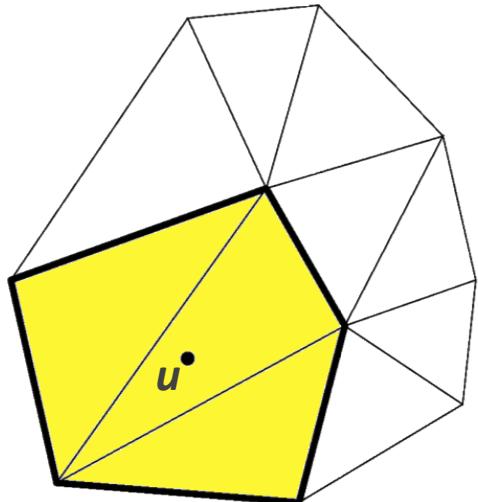
Watson's Algorithm:

- ◆ Step 1:

Deletion of the triangles of $\text{Del}(V_i)$ 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:

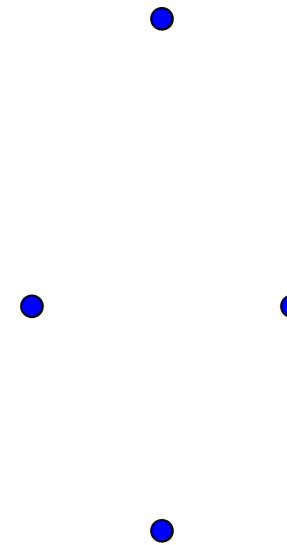
Let $N_i = |V_i|$

- ◆ *Detection of a triangle of $\text{Del}(V_i)$ 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:

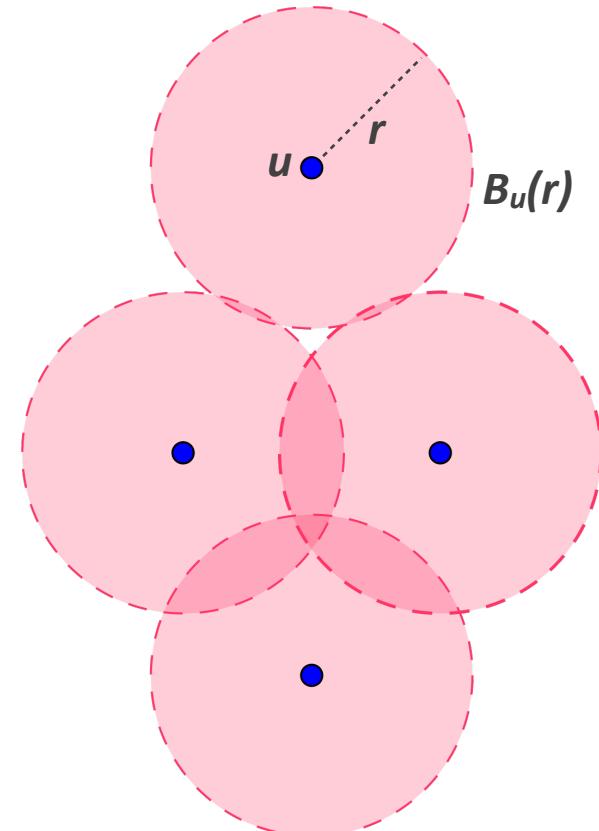


Čech Complexes

Definition:

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

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



Čech Complexes

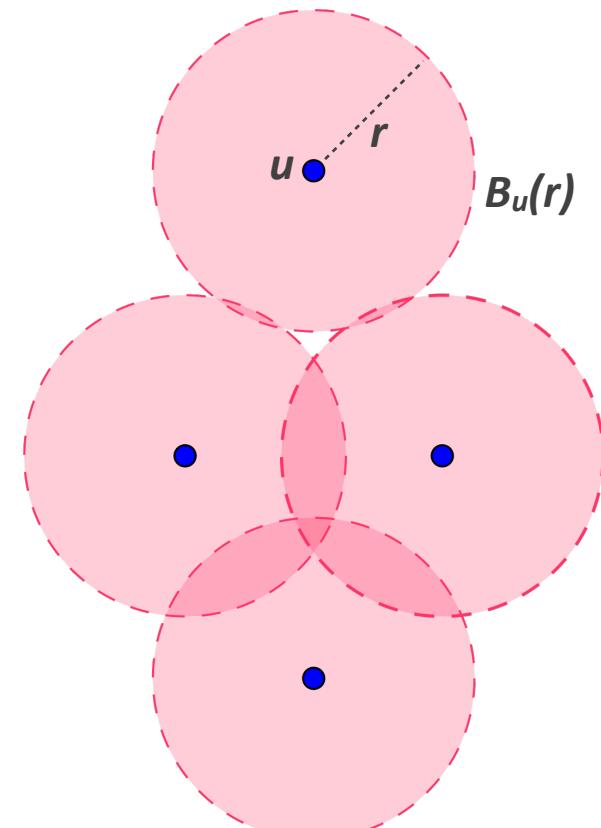
Definition:

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

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

The **Čech complex** $\check{C}ech(r)$ 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

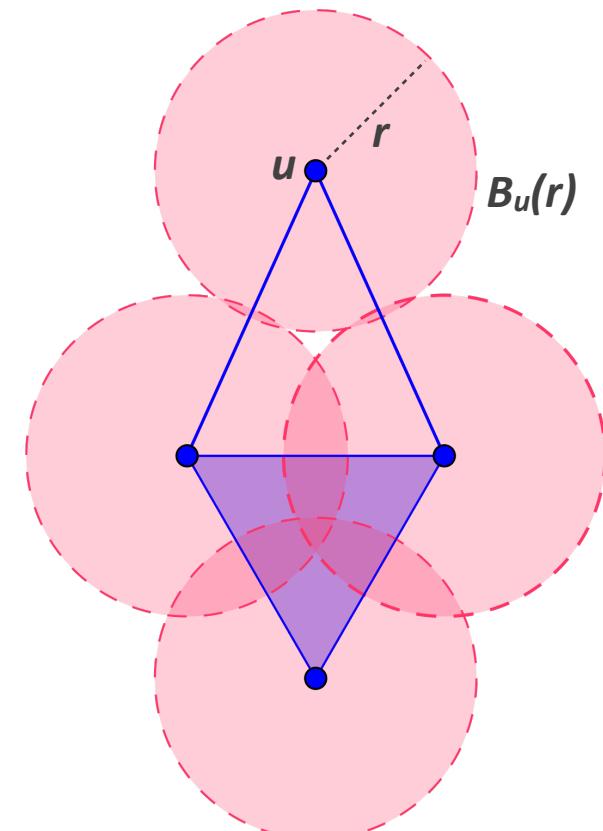
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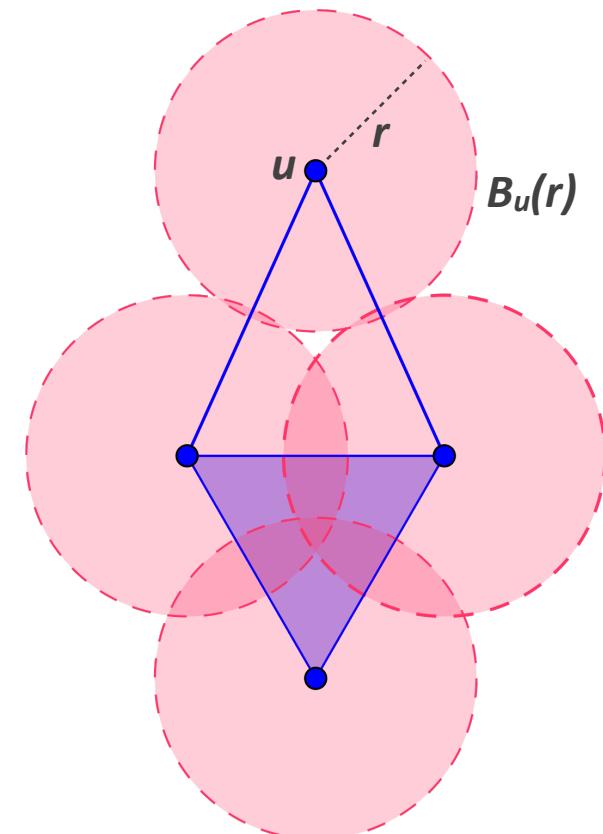
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In practice, **infeasible construction**



Vietoris-Rips Complexes

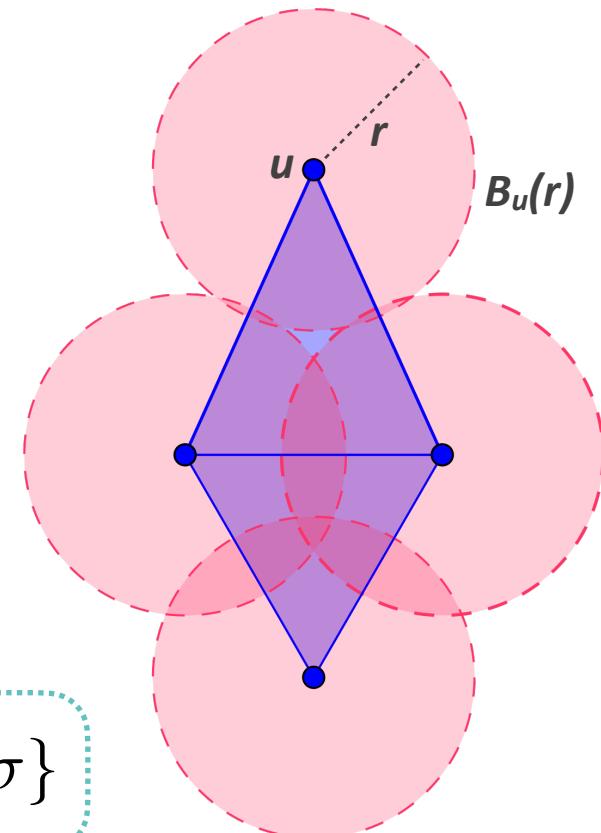
Definition:

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,

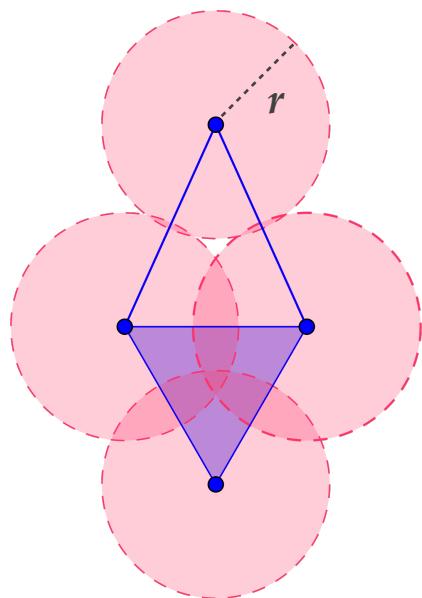
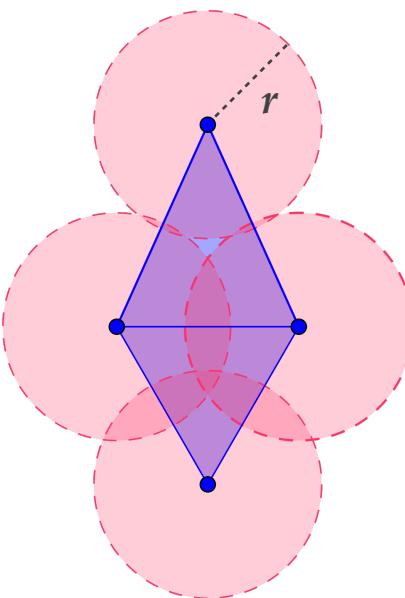
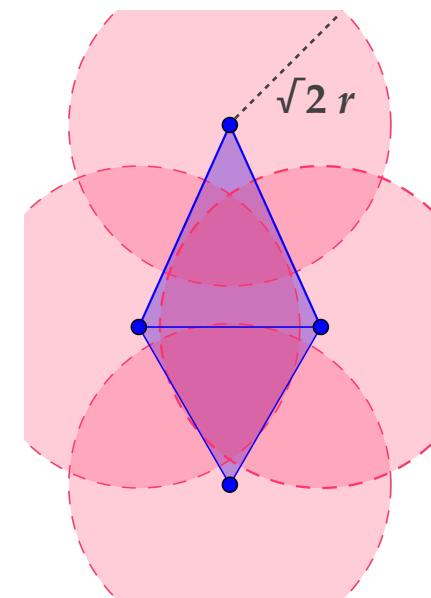
$$VR(r) := \{\sigma \subseteq V \mid d(u, v) \leq 2r, \forall u, v \in \sigma\}$$



Vietoris-Rips Complexes

Properties:

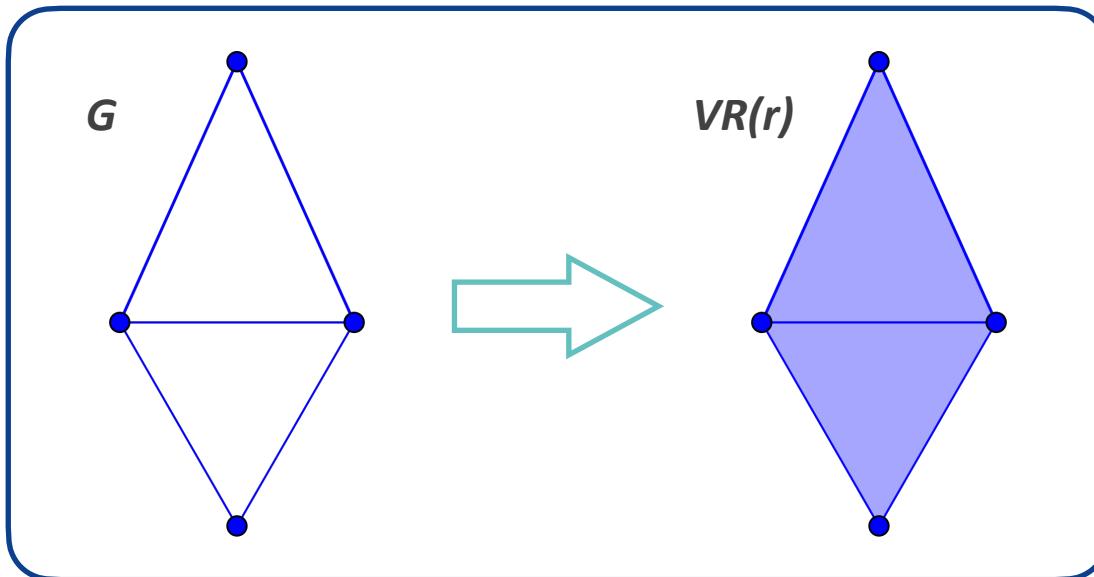
- $\check{\text{C}}\text{ech}(r) \subseteq VR(r) \subseteq \check{\text{C}}\text{ech}(\sqrt{2}r)$

 \subseteq  \subseteq 

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:

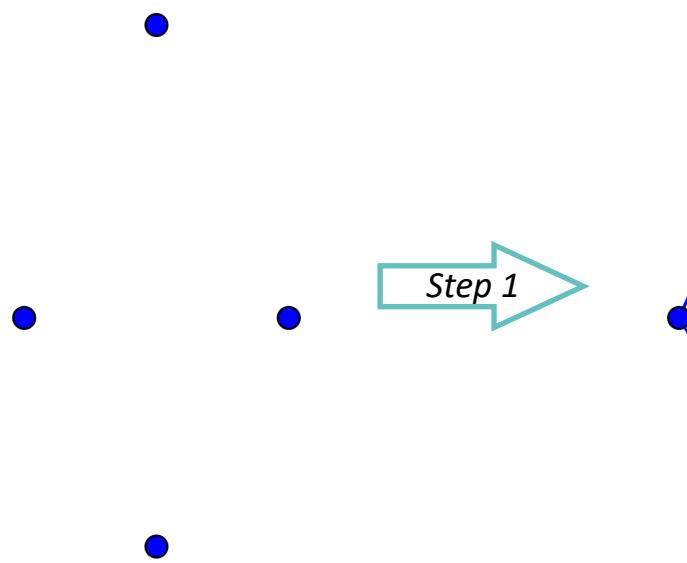
Input: A finite set of points V in \mathbb{R}^n and a real positive number r

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*

Vietoris-Rips Complexes

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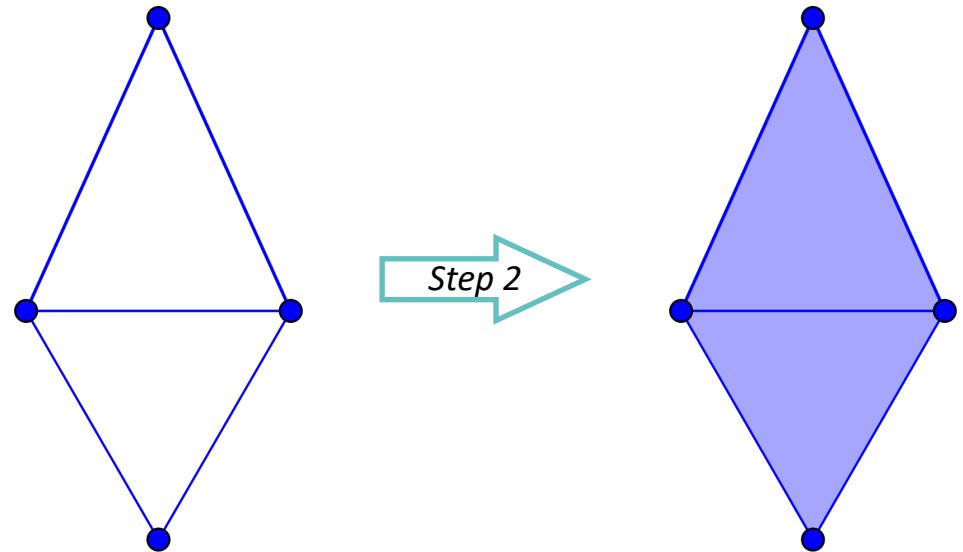
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- ❖ *Incremental*
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Vietoris-Rips Complexes

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 $\sigma \in K$

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

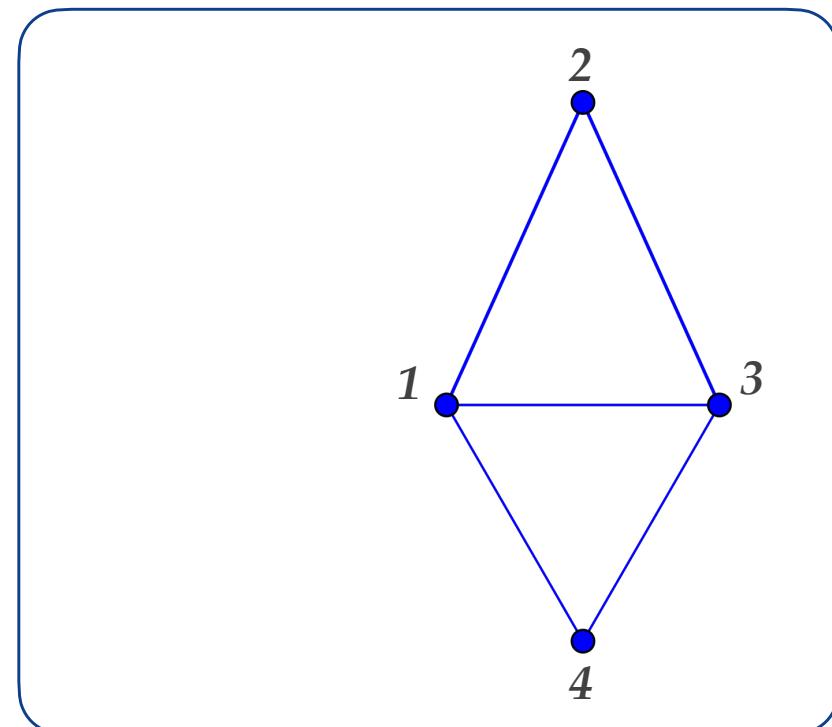
foreach $v \in N$

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

return K

LOWER-NBRS(G, u)

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



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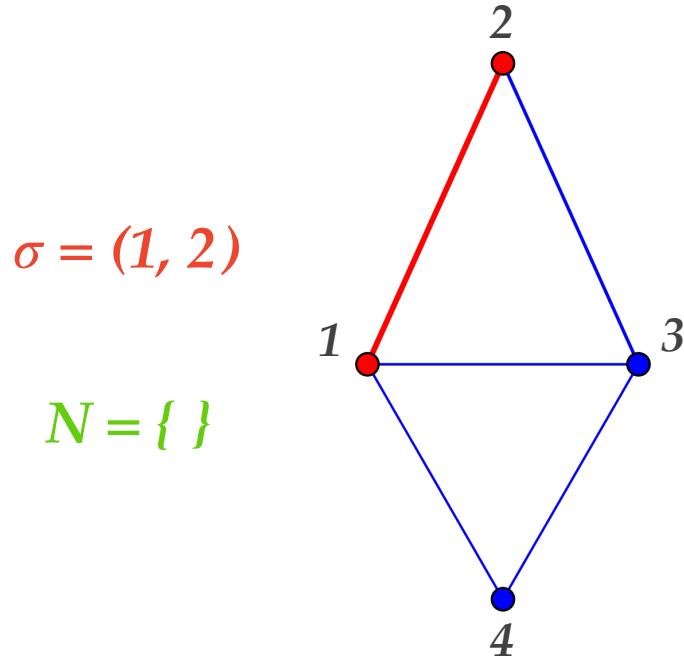
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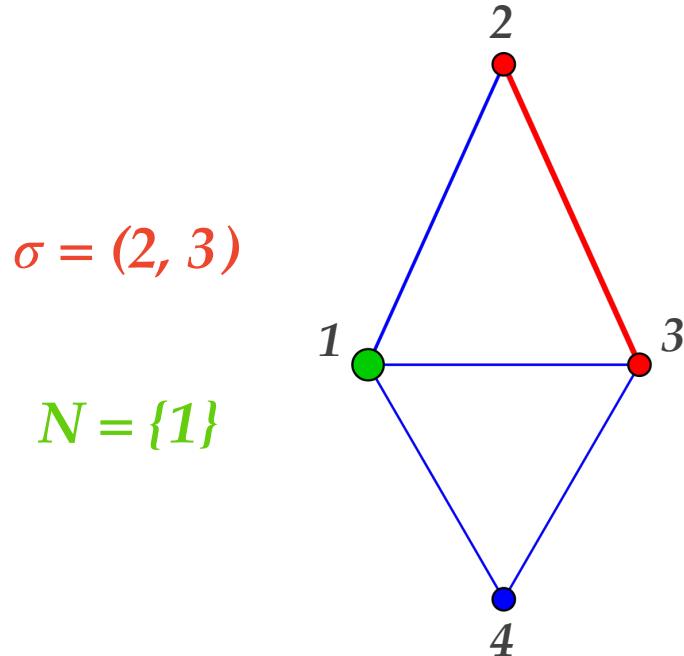
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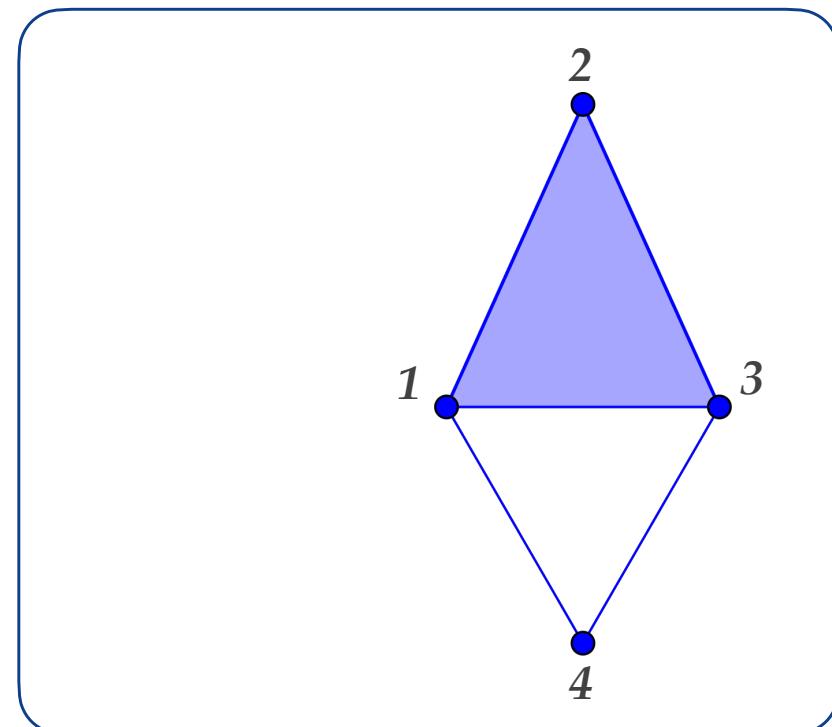
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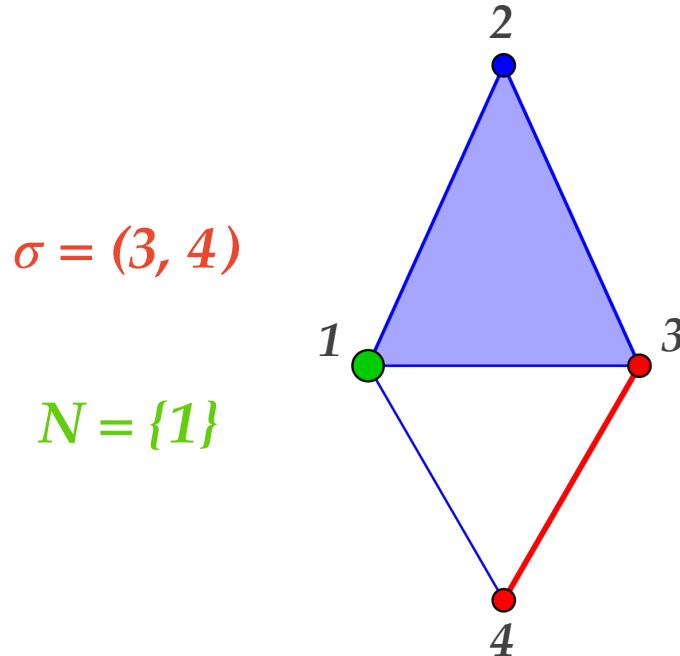
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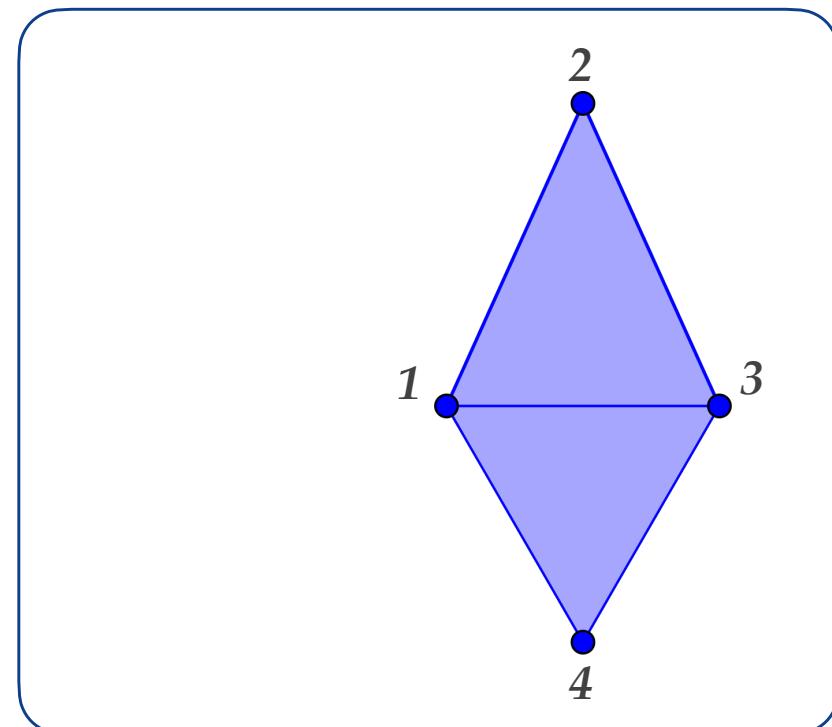
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From Data to Complexes

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,

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

$$A_u(r) \subseteq B_u(r) \quad \rightarrow \quad \text{Alpha}(r) \subseteq \check{\text{C}}ech(r)$$

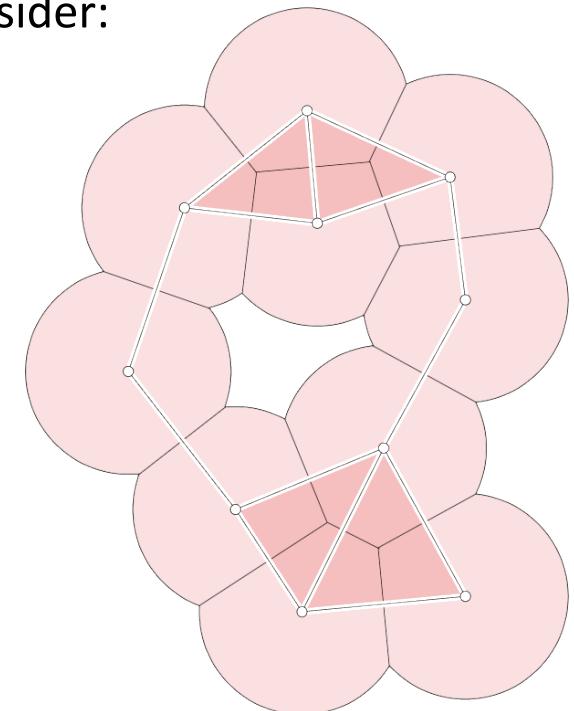


Image from [Edelsbrunner, Harer 2010]

Witness Complexes

Motivation:

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

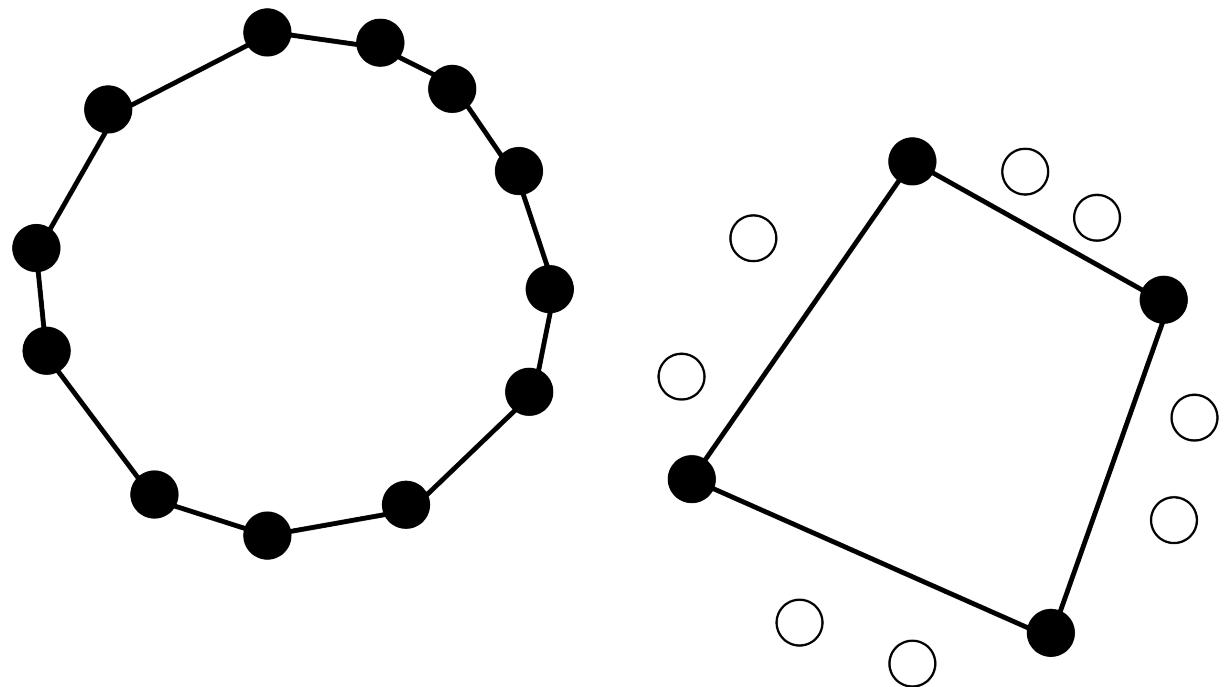
Definitions:

◆ 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

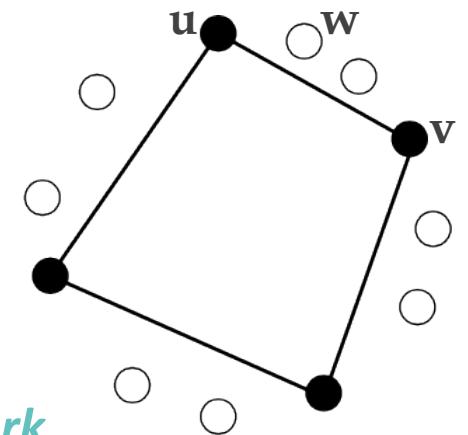
$$\max\{d(u, w), d(v, w)\} \leq m_w + r$$

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

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

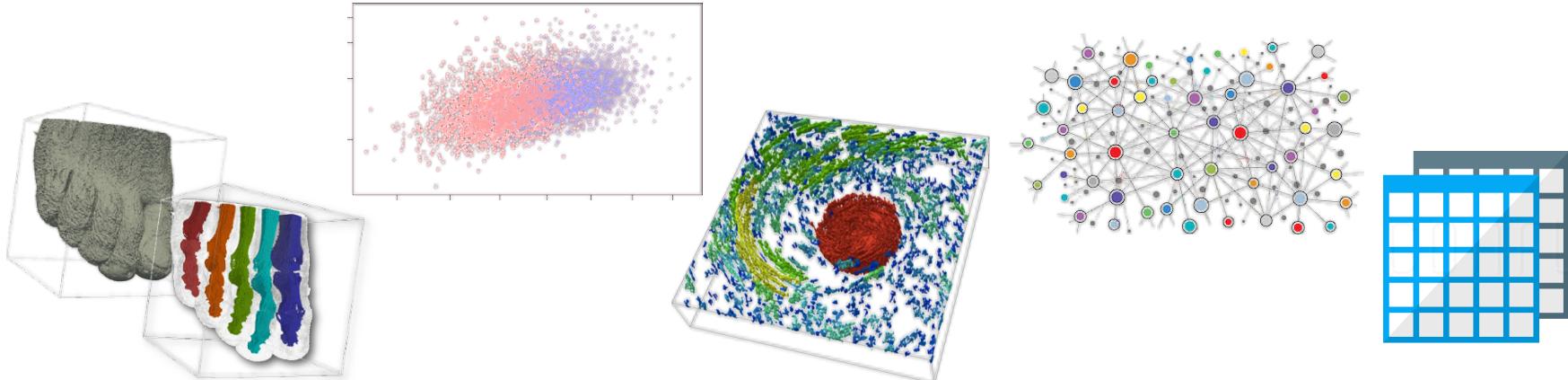


From Data to Complexes

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*

E.g. complex networks, weighted graphs, multivariate functions, matrices, tensors, etc.

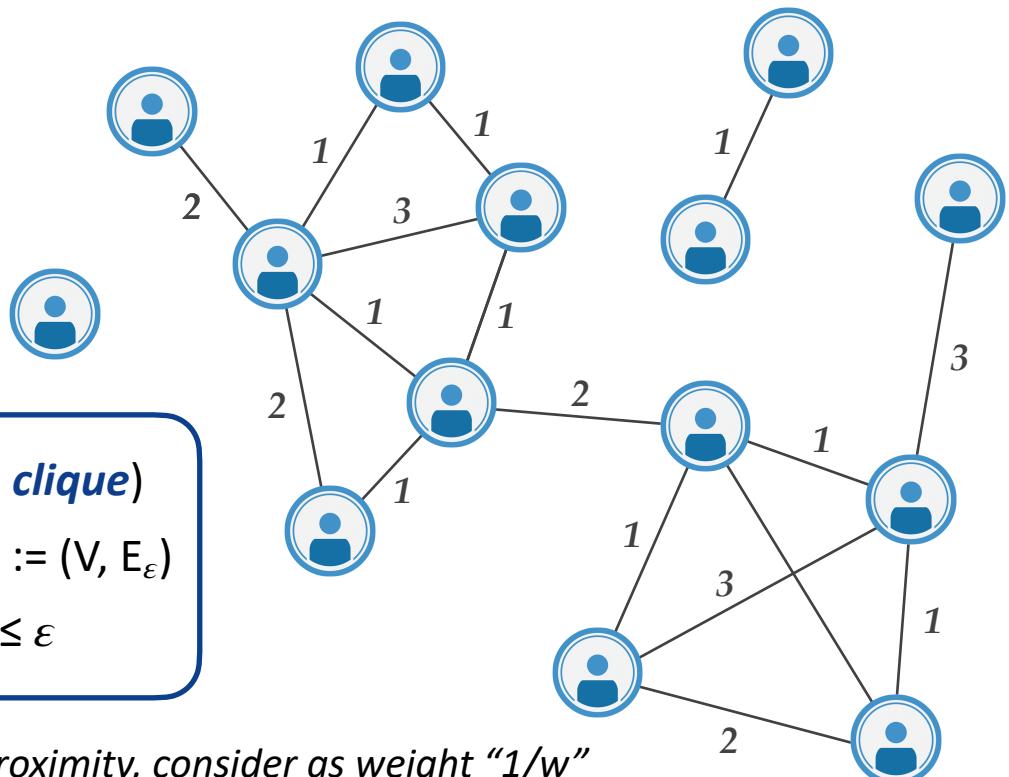
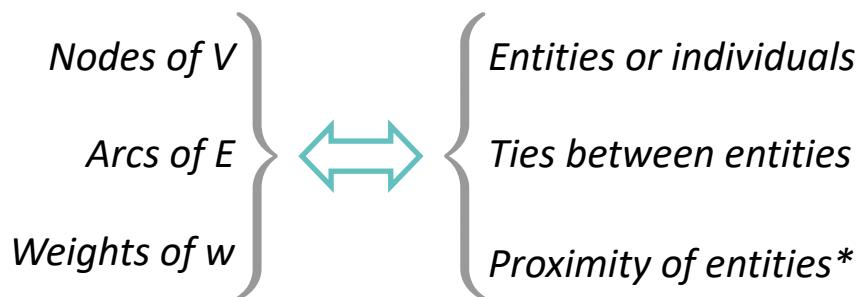


*More properly, a *semi-metric*, i.e. a distance not necessarily satisfying the triangle inequality

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*:

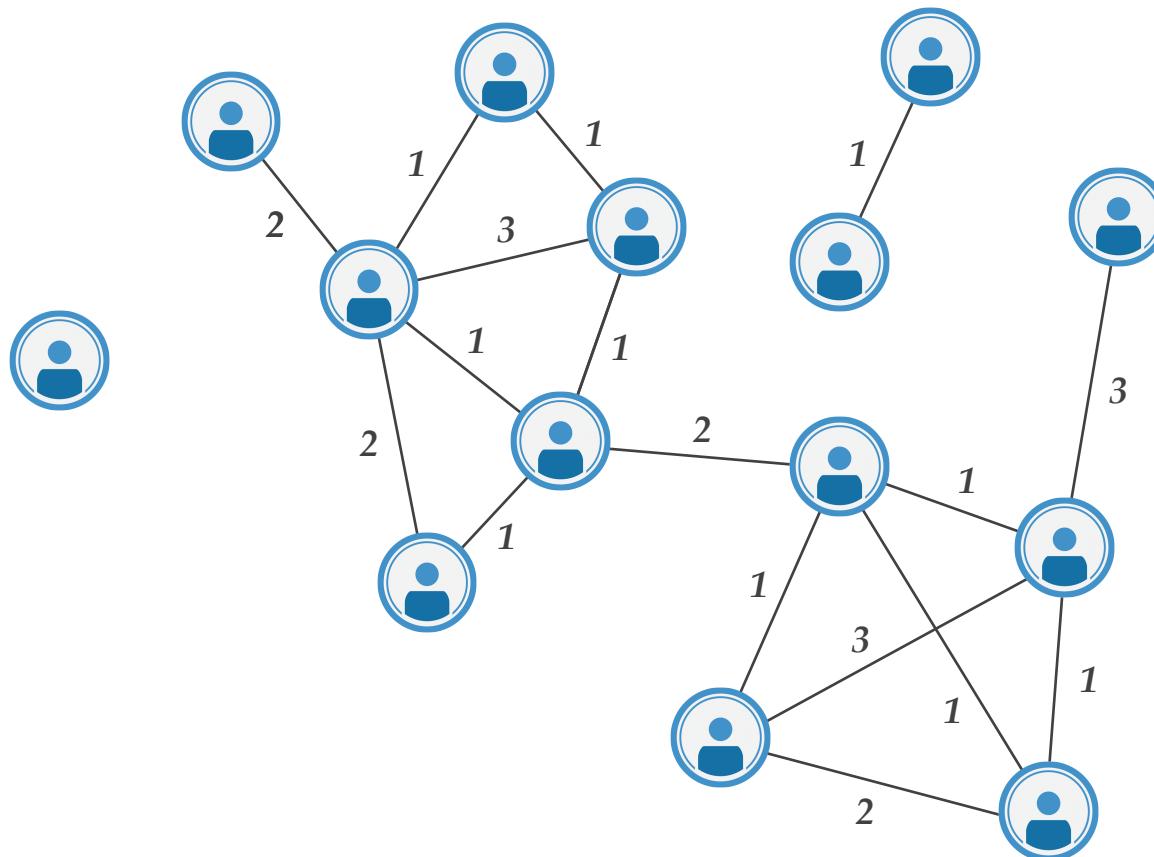


Fixed a *weight threshold* ε , the *flag* (or the *clique*) **complex** is the *VR expansion* of the graph $G_\varepsilon := (V, E_\varepsilon)$ where E_ε are the arcs of E with weight $\leq \varepsilon$

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

From Data to Complexes

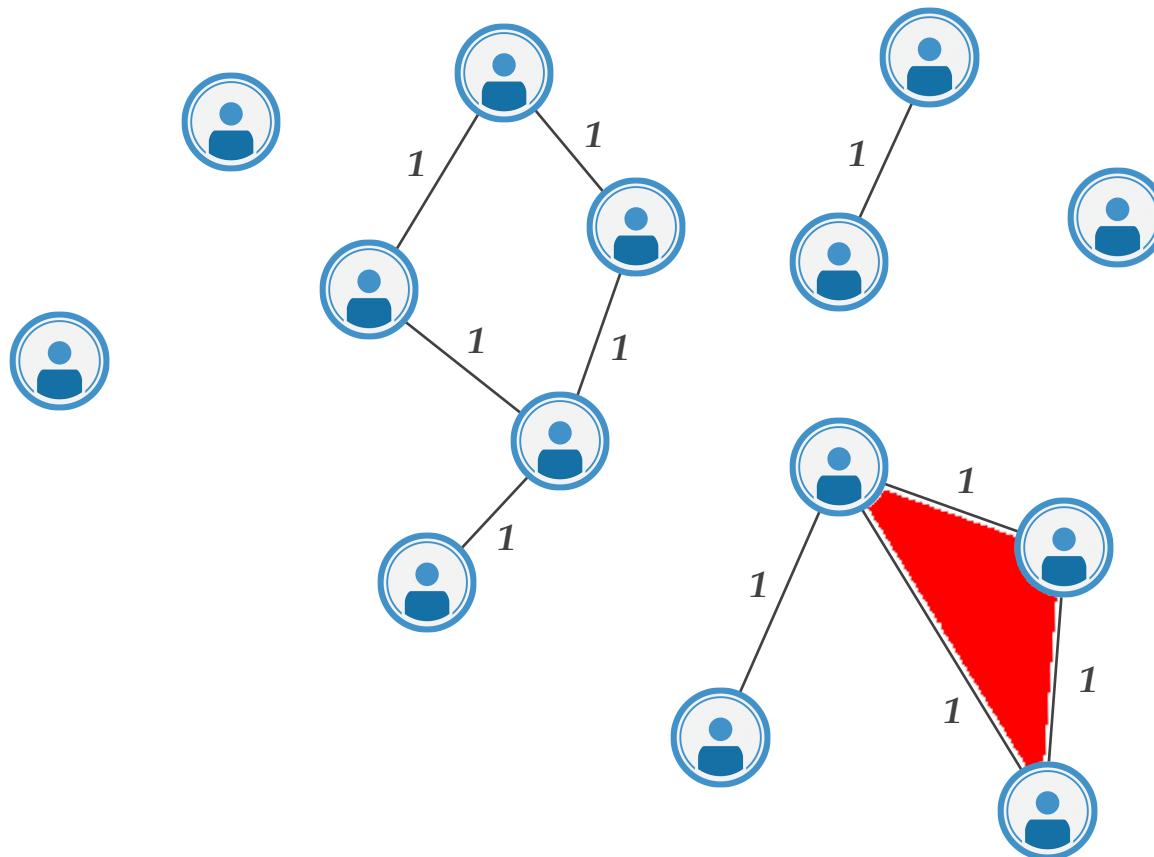
Flag Complex of a Weighted Network:



From Data to Complexes

Flag Complex of a Weighted Network:

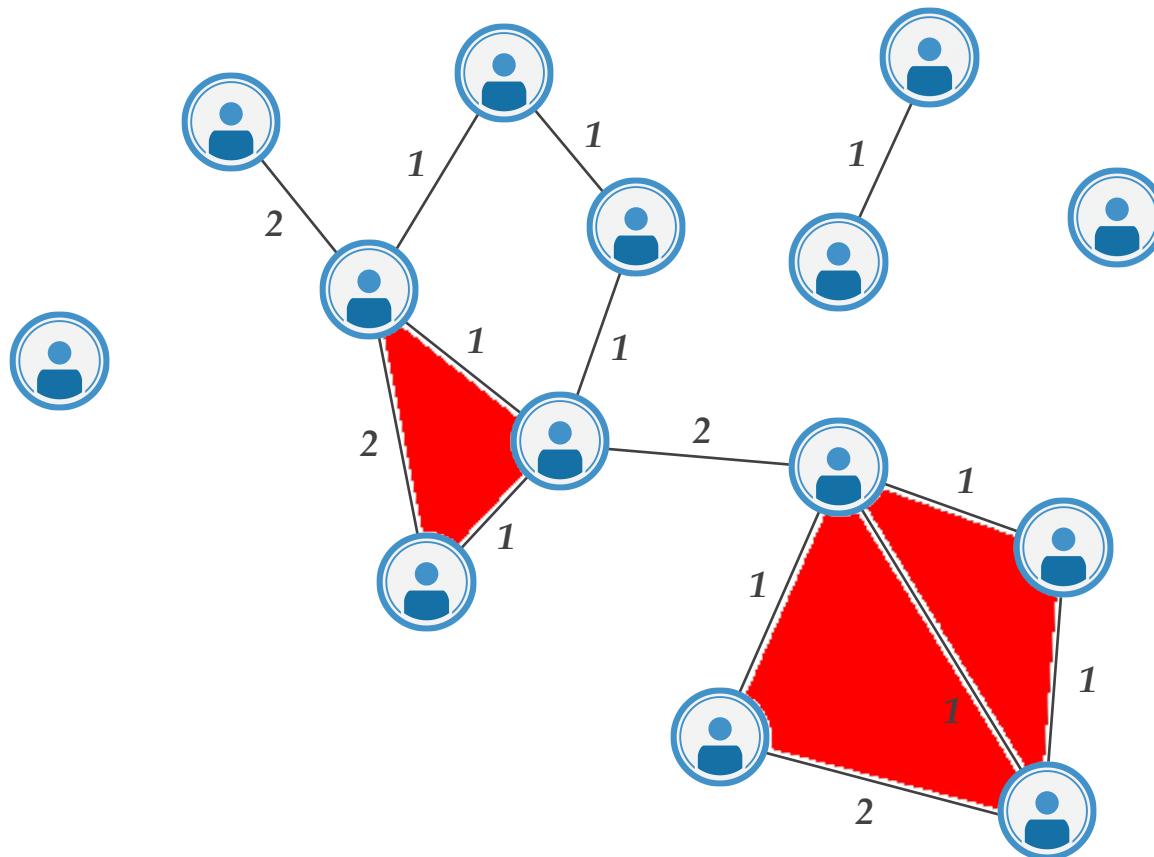
$$\varepsilon = 1$$



From Data to Complexes

Flag Complex of a Weighted Network:

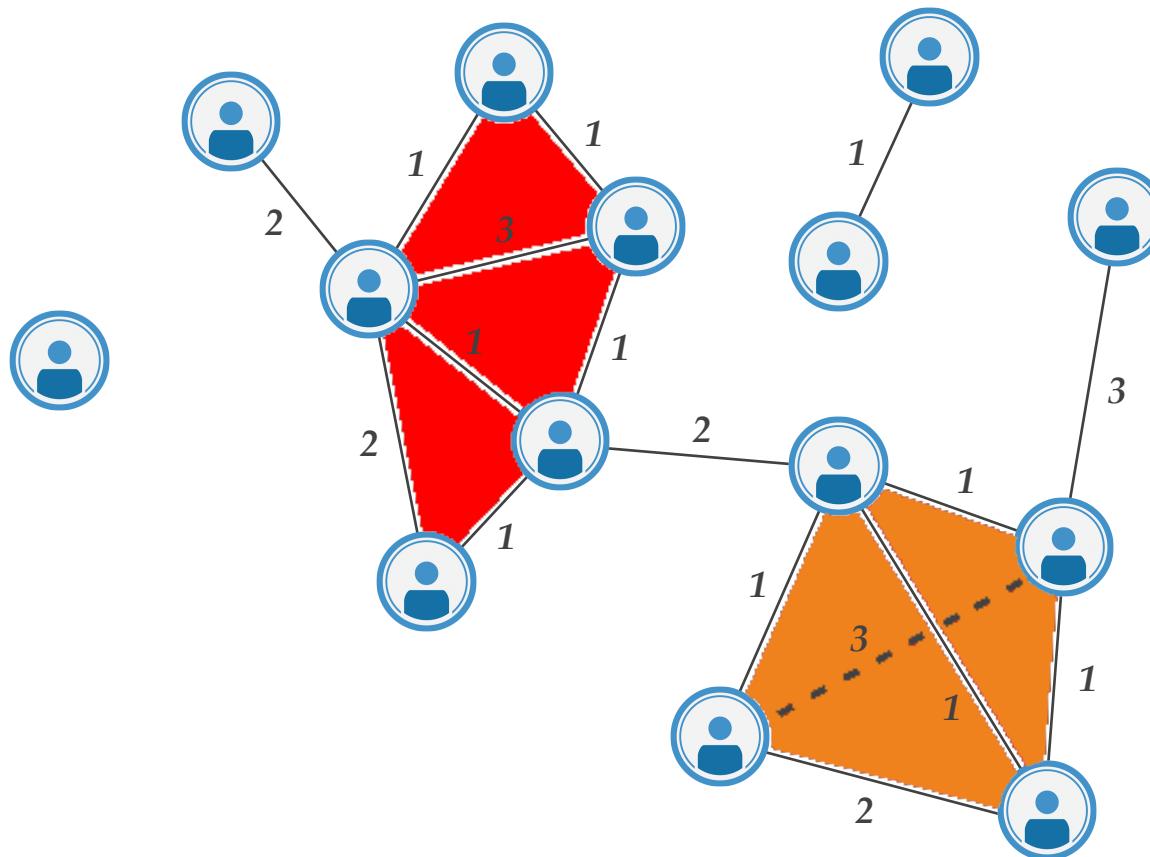
$$\varepsilon = 2$$



From Data to Complexes

Flag Complex of a Weighted Network:

$$\varepsilon = 3$$



Bibliography

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- ◆ **From Data to Complexes:**
 - ❖ H. Edelsbrunner, *Geometry and Topology for Mesh Generation*. Cambridge University Press, 2001.
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