CS164: Simplicial Complexes, Homology, Persistence

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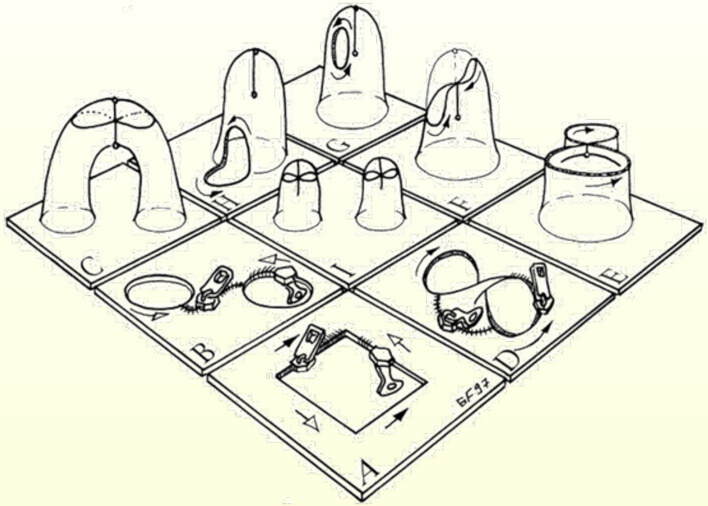
[Most slides: Afra Zomorodian]

Why Topology?

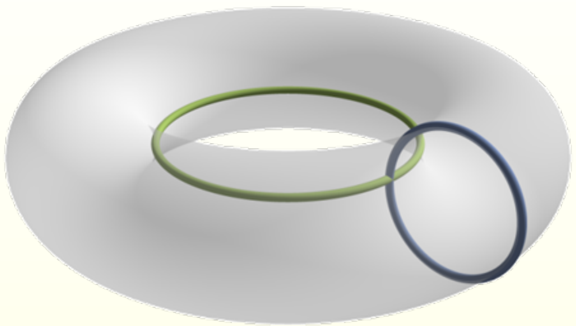
- Topology is the study of connectivity
- It investigates properties of shapes and spaces that are less sensitive to exact metric information
- As a consequence, it produces shape and space invariants that are robust to many kinds of deformation and noise

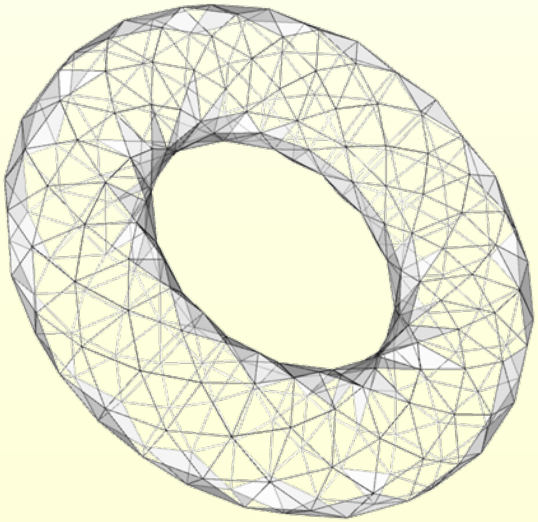


cross-handle = 2 cross-caps

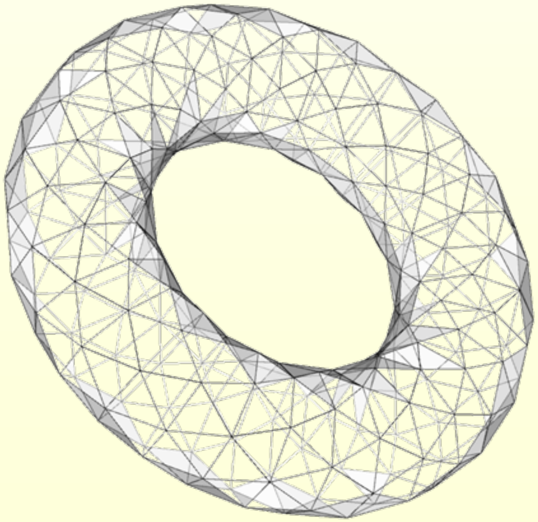
Computational Representations of Topology

- We need to find discrete representations of infinite, continuous topological spaces
- We need to develop efficient algorithms for the manipulation of such representations, as well as for extracting topological information from them



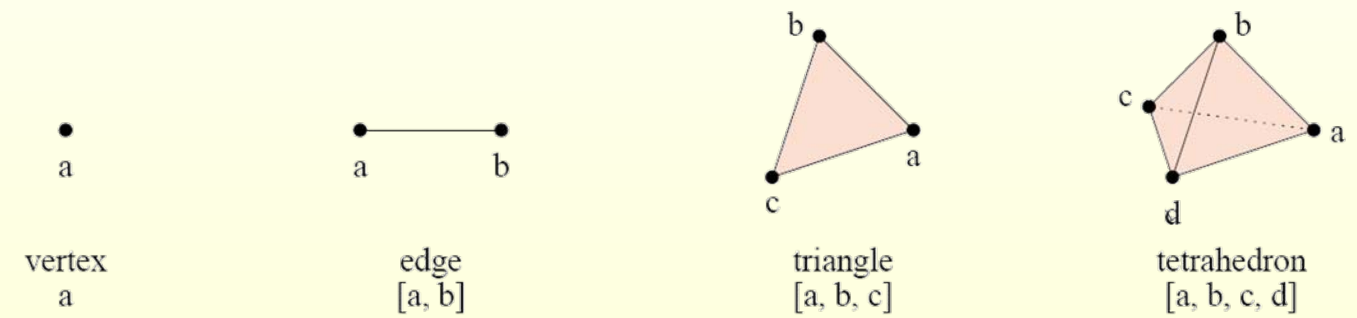


Simplicial Complexes



Simplices

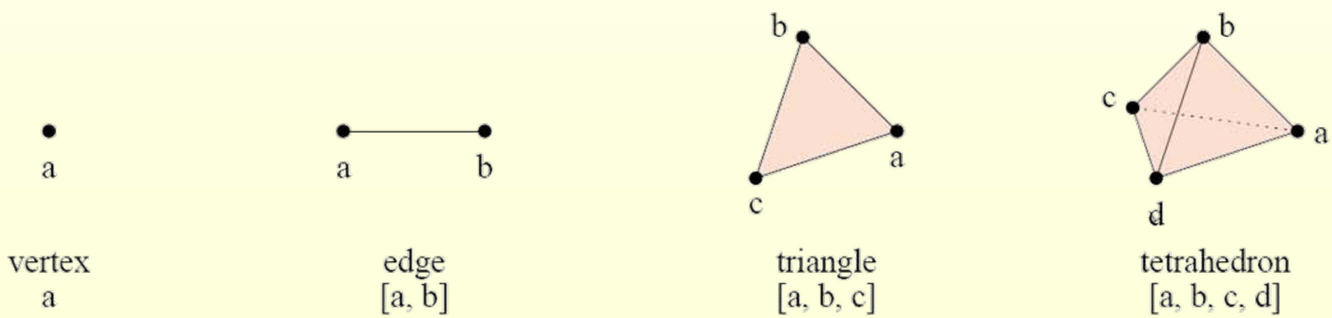
- A k-simplex is the convex hull of $k + 1$ affinely independent points $S = \{v_0, v_1, \ldots, v_k\}$. The points in S are the vertices of the simplex.
- A k-simplex is a k-dimensional subspace of $\mathbb{R}^d$, $\dim \sigma = k$.



0-simplex 1-simplex 2-simplex 3-simplex

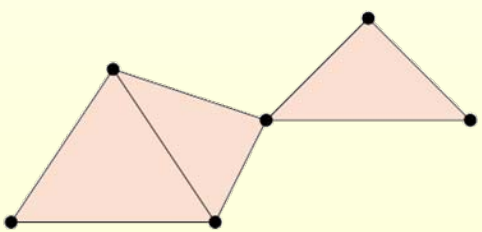
Faces

- σ: a k-simplex defined by $S = \{v_0, v_1, \ldots, v_k\}$.
- τ defined by $T \subseteq S$ is a face of σ
- σ is its coface.
- $\sigma \geq \tau$ and $\tau \leq \sigma$.
- $\sigma \leq \sigma$ and $\sigma \geq \sigma$.

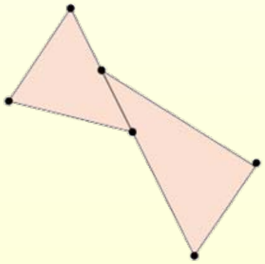


Simplicial Complex

- A simplicial complex K is a finite set of simplices such that
  1. $\sigma \in K, \tau \leq \sigma \Rightarrow \tau \in K$,
  2. $\sigma, \sigma' \in K \Rightarrow \sigma \cap \sigma' \leq \sigma, \sigma'$ or $\sigma \cap \sigma' = \emptyset$.
- The dimension of K is $\dim K = \max\{\dim \sigma \mid \sigma \in K\}$.
- The vertices of K are the zero-simplices in K.
- A simplex is principal if it has no proper coface in K.



Yes



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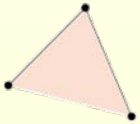

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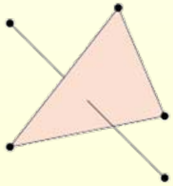
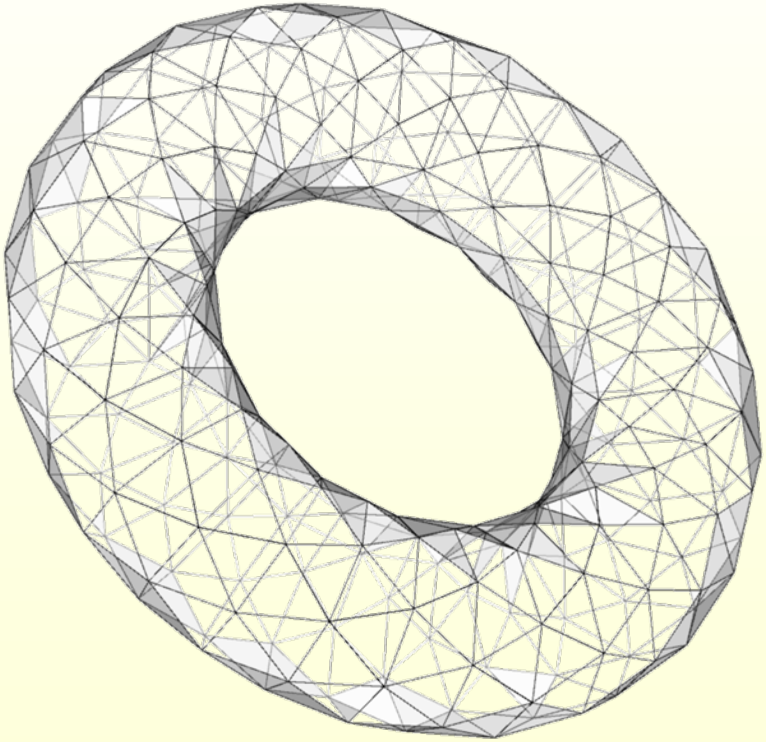


No

A Triangle Mesh is a Simplicial Complex



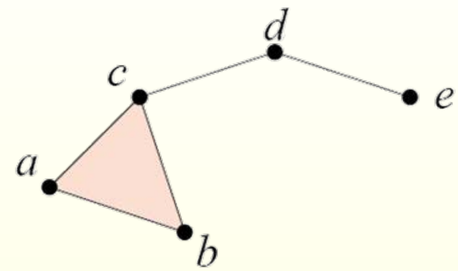
Abstract Simplicial Complex

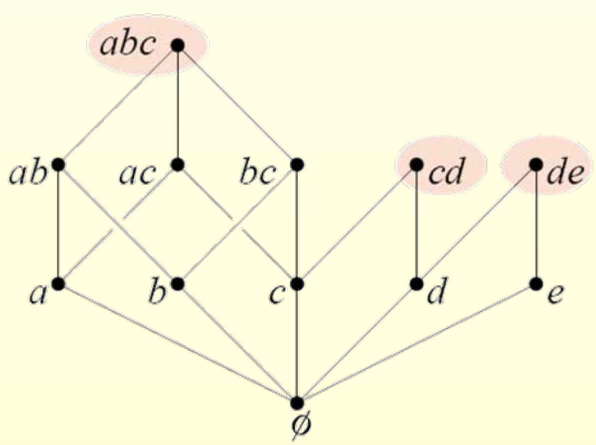
- An abstract simplicial complex is a set K, together with a collection $\mathcal{S}$ of subsets of K called (abstract) simplices such that:
  1. For all $v \in K$, $\{v\} \in \mathcal{S}$. We call the sets $\{v\}$ the vertices of K.
  2. If $\tau \subseteq \sigma \in \mathcal{S}$, then $\tau \in \mathcal{S}$.
- We call $\mathcal{S}$ the complex.

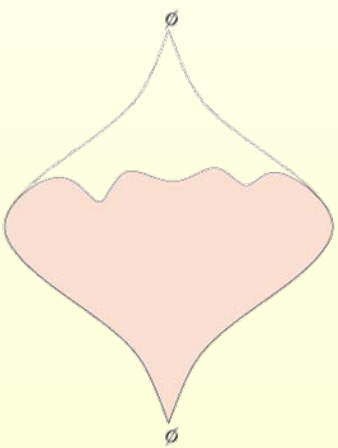
Relationship

- Let K be a simplicial complex with vertices V and let $\mathcal{S}$ be the collection of all subsets $\{v_0, v_1, \ldots, v_k\}$ of V such that the vertices $v_0, v_1, \ldots, v_k$ span a simplex of K. Then, $\mathcal{S}$ is the vertex scheme of K.
- K and $\mathcal{S}$ form an abstract simplicial complex.
- Two abstract simplicial complexes are isomorphic if we can one from the other by renaming vertices.
- (Theorem) Every abstract complex $\mathcal{S}$ is isomorphic to the vertex scheme of some simplicial complex K.
- We call K a geometric realization of $\mathcal{S}$.

An Example

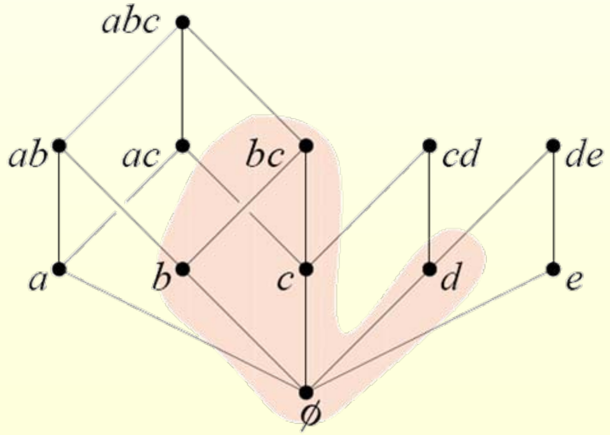






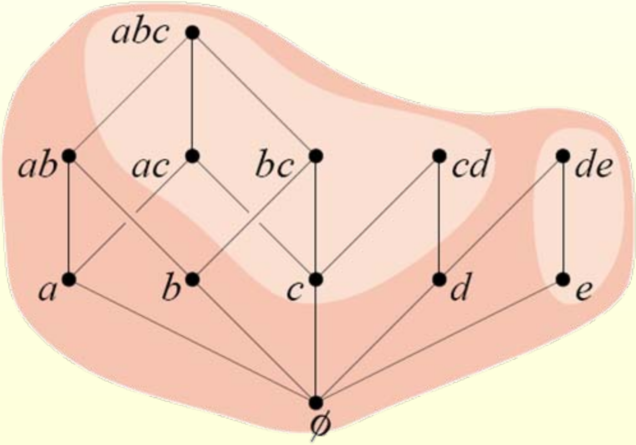
Subcomplex

- A subcomplex is a simplicial complex $L \subseteq K$. The smallest subcomplex containing a subset $L \subseteq K$ is its closure, $\mathrm{Cl}\, L = \{\tau \in K \mid \tau \leq \sigma \in L\}$.
- Everything "below" is included.



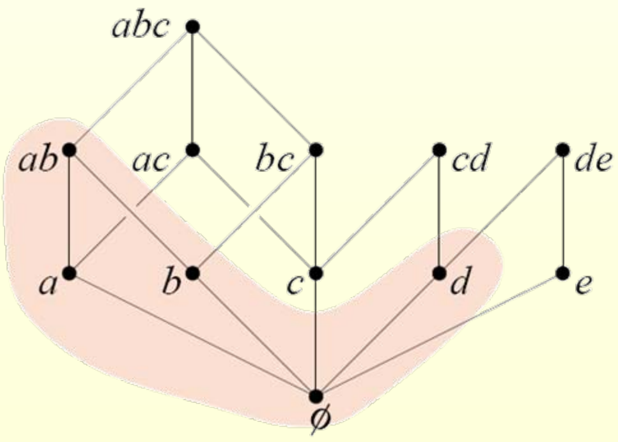
Star

- The star of L contains all of the cofaces of L,
  $\mathrm{St}\, L = \{\sigma \in K \mid \sigma \geq \tau \in L\}$.
- Everything "above" is included.
- Stars are analogs of neighborhoods (open).



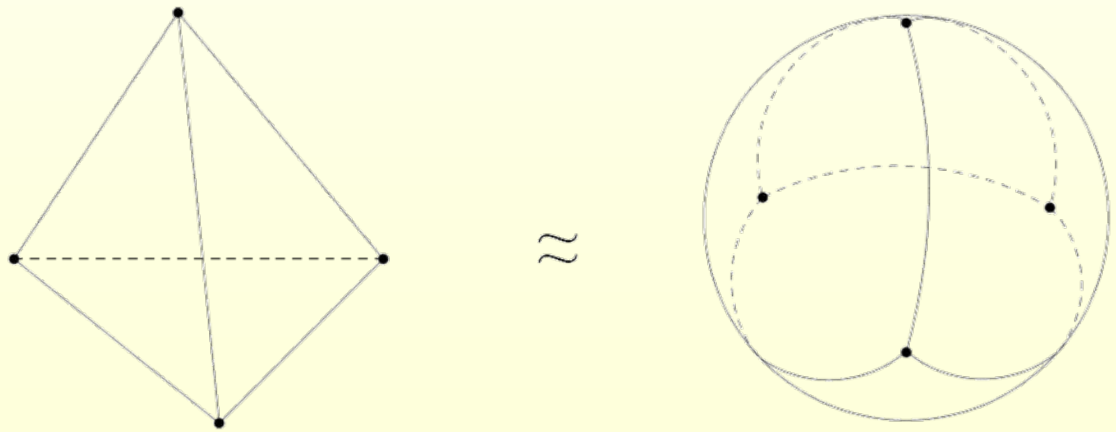
Link

- The link of L is the boundary of its star,
  $\mathrm{Lk}\, L = \mathrm{Cl}\,\mathrm{St}\, L - \mathrm{St}\,(\mathrm{Cl}\, L - \{\emptyset\})$.



Triangulations

- The underlying space $|K|$ of a simplicial complex K is $|K| = \cup_{\sigma \in K} \sigma$.
- $|K|$ is a topological space.
- A triangulation of a topological space $\mathbb{X}$ is a simplicial complex K such that $|K| \approx \mathbb{X}$.



We typically study shapes and spaces via triangulations of them

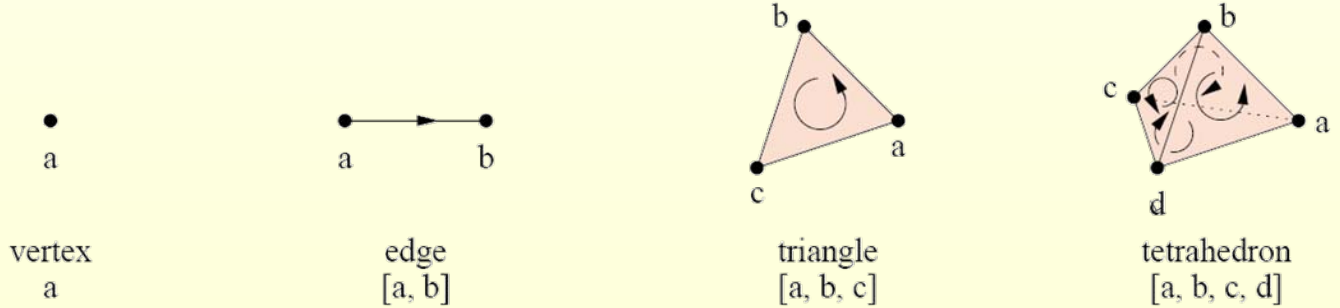
Orientability I

- An orientation of a k-simplex $\sigma \in K, \sigma = \{v_0, v_1, \ldots, v_k\}, v_i \in K$ is an equivalence class of orderings of the vertices of σ, where

$$(v_0, v_1, \ldots, v_k) \sim (v_{\tau(0)}, v_{\tau(1)}, \ldots, v_{\tau(k)})$$

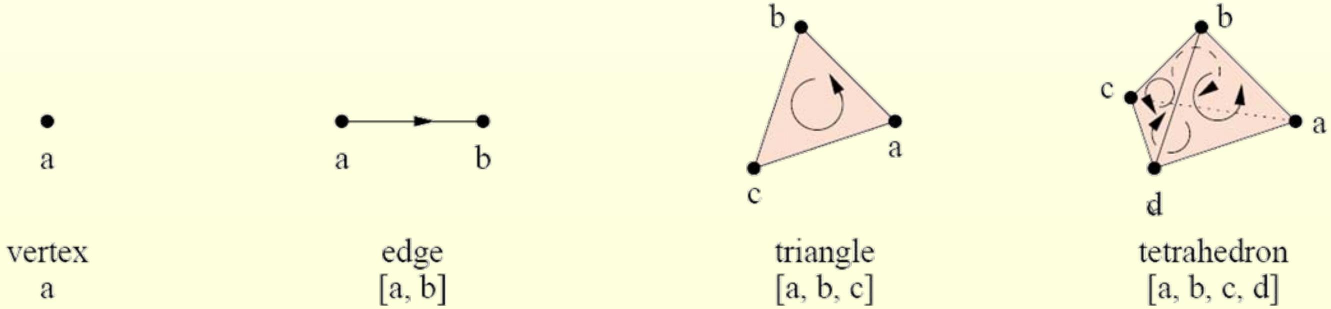
are equivalent orderings if the parity of the permutation τ is even.

- We denote an oriented simplex, a simplex with an equivalence class of orderings, by $[\sigma]$.



Orientability II

- Two k-simplices sharing a $(k-1)$-face σ are consistently oriented if they induce different orientations on σ.
- A triangulable d-manifold is orientable if all d-simplices can be oriented consistently.
- Otherwise, the d-manifold is non-orientable



Invariants

- A (topological) invariant is a map f that assigns the same object to spaces of the same topological type.
- $\mathbb{X} \approx \mathbb{Y} \implies f(\mathbb{X}) = f(\mathbb{Y})$
- $f(\mathbb{X}) \neq f(\mathbb{Y}) \implies \mathbb{X} \not\approx \mathbb{Y}$ (contrapositive)
- $f(\mathbb{X}) = f(\mathbb{Y}) \implies$ nothing
- "coarser" differentiation

Invariants provide partial information about a space

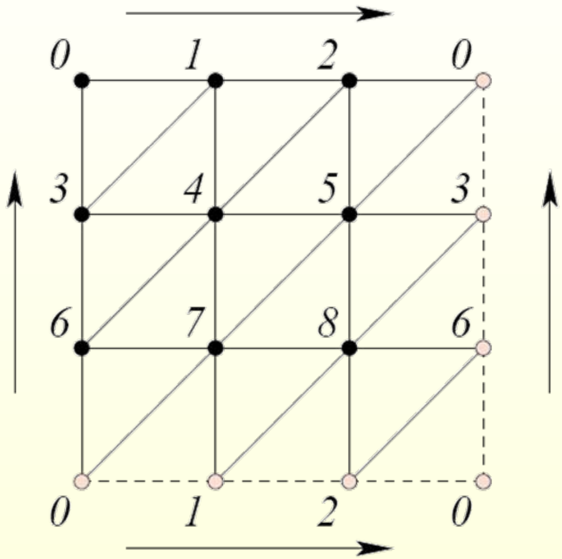
Euler Characteristic

- K a simplicial complex with s_k k-simplices.
- The Euler characteristic $\chi(K)$ is

$$\chi(K) = \sum_{i=0}^{\dim K} (-1)^i s_i = \sum_{\sigma \in K - \{\emptyset\}} (-1)^{\dim \sigma}.$$

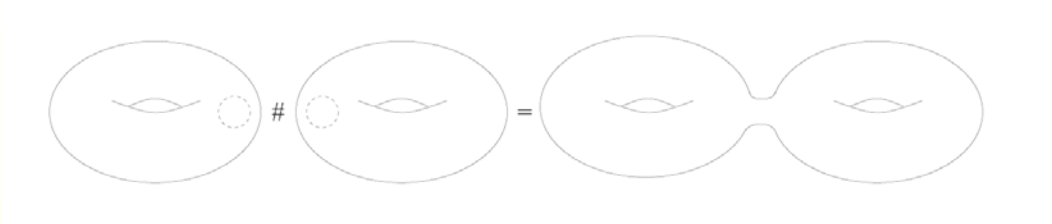
- $v - e + f = 1$ (Graph Theory)
- Invariant for $|K|$
- Any triangulation gives the same answer!
- Intrinsic property

Basic 2-Manifolds

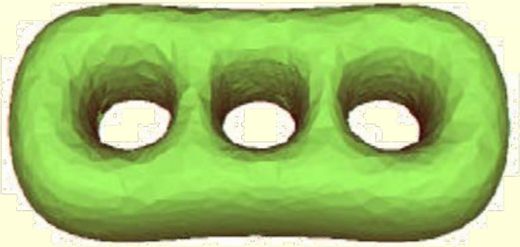


2-Manifold	χ
Sphere $\mathbb{S}^2$	2
Torus $\mathbb{T}^2$	0
Klein bottle $\mathbb{K}^2$	0
Projective plane $\mathbb{R}\mathrm{P}^2$	1

Euler and Connected Sums



- (Theorem) For compact surfaces $\mathbb{M}_1, \mathbb{M}_2$, $\chi(\mathbb{M}_1 \# \mathbb{M}_2) = \chi(\mathbb{M}_1) + \chi(\mathbb{M}_2) - 2.$
- $\chi(g\mathbb{T}^2) = 2 - 2g$
- $\chi(g\mathbb{R}\mathrm{P}^2) = 2 - g$
- The connected sum of g tori is called a surface with genus g.

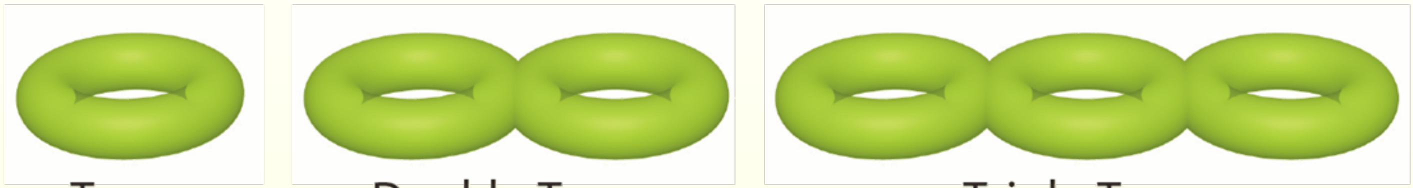


Compact 2-Manifolds

- d = 2: orientable

$\mathbb{S}^2$

add handles



Torus Double Torus Triple Torus . . .

- d = 2: non-orientable

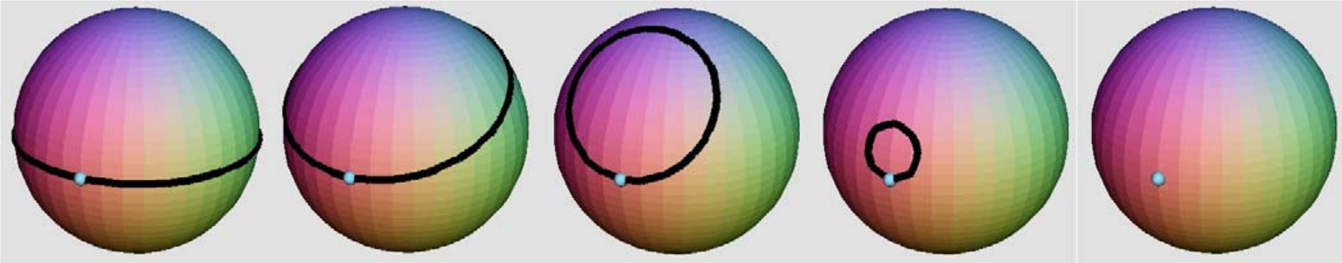
Projective Plane $\mathbb{P}^2$

Klein Bottle

add cross-caps

. . .

Euler characteristic and orientability are two invariants providing a full classification of compact 2-manifolds

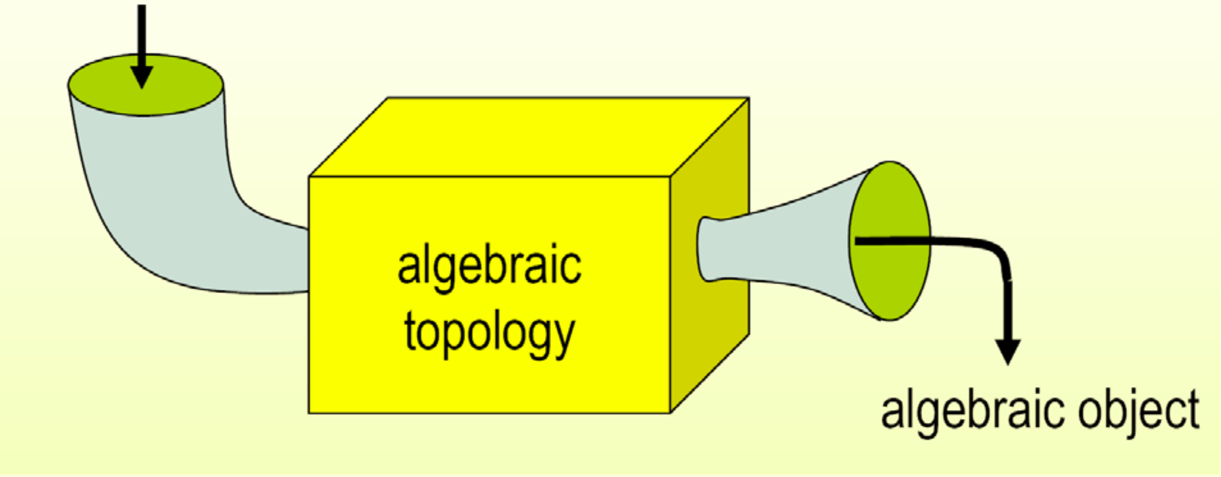


d = 3: Very hard

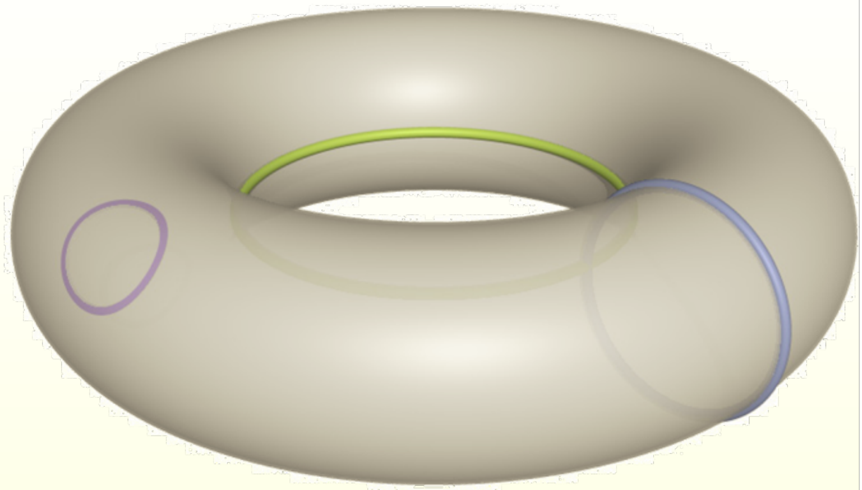
d $\geq$ 4: *Undecidable* [Markov 1958]

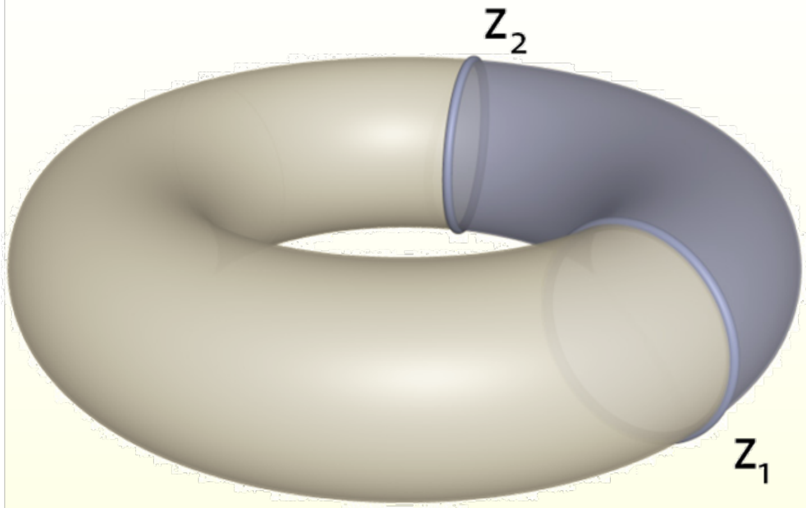
[Grigori Perelman, 2003]

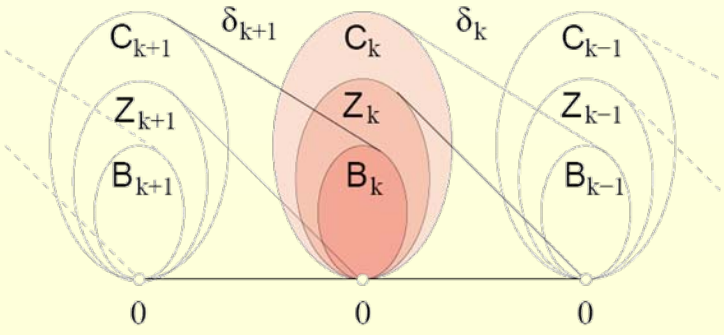
Homology



Homology

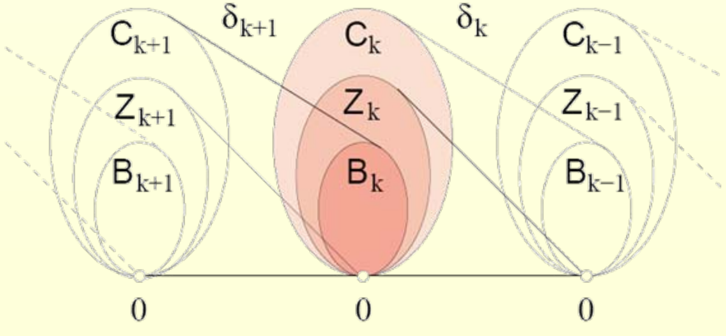






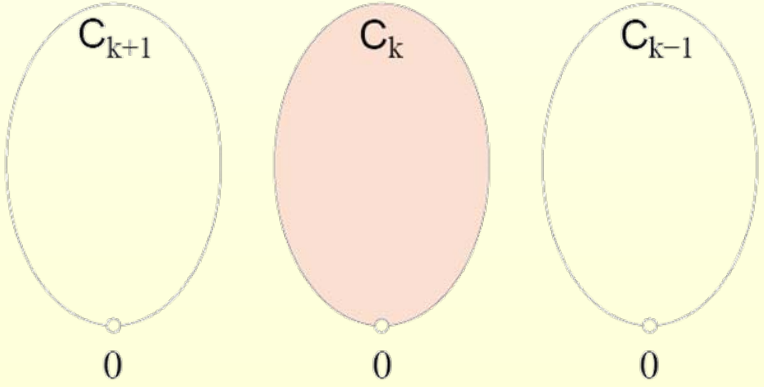
Why Homology?

- Algebraization of first layer of geometry in structures
- How cells of dimension n attach to cells of dimension $n-1$
- Less transparent, more machinery
- Combinatorial
- Finite description
- Computable



Chain Group

- Simplicial complex K
- k-chain: $c = \sum_i n_i[\sigma_i], n_i \in \mathbb{Z}, \sigma_i \in K$ (like a path)
- $[\sigma] = -[\tau]$ if $\sigma = \tau$ and σ and τ have different orientations.
- The kth chain group C_k of K is the free abelian group on its set of oriented k-simplices
- rank C_k =?



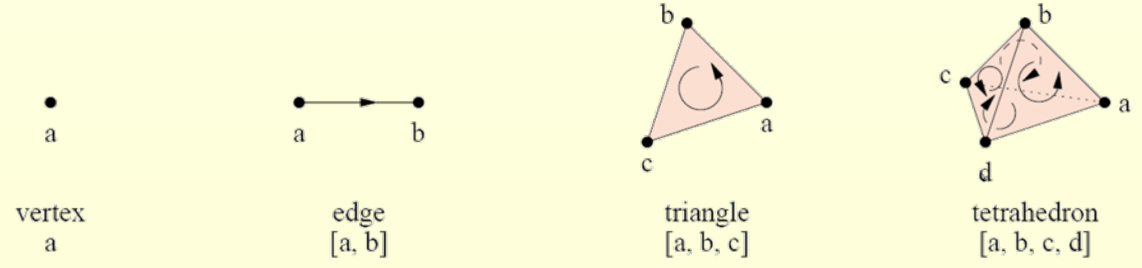
Boundary Operator

- The boundary operator $\partial_k : \mathsf{C}_k \to \mathsf{C}_{k-1}$ is a homomorphism defined linearly on a chain c by its action on any simplex $\sigma = [v_0, v_1, \ldots, v_k] \in c$,

$$\partial_k \sigma = \sum_i (-1)^i [v_0, v_1, \ldots, \hat{v}_i, \ldots, v_k],$$

where $\hat{v}_i$ indicates that v_i is deleted from the sequence.

- $\partial_1 [a, b] = b - a.$
- $\partial_2 [a, b, c] = [b, c] - [a, c] + [a, b] = [b, c] + [c, a] + [a, b].$
- $\partial_3 [a, b, c, d] = [b, c, d] - [a, c, d] + [a, b, d] - [a, b, c].$
- $\partial_1 \partial_2 [a, b, c] = [c] - [b] - [c] + [a] + [b] - [a] = 0.$



Boundary Theorem

- (Theorem) $\partial_{k-1}\partial_k = 0$, for all k.
- Proof:

$\partial_{k-1}\partial_k[v_0, v_1, \ldots, v_k] =$

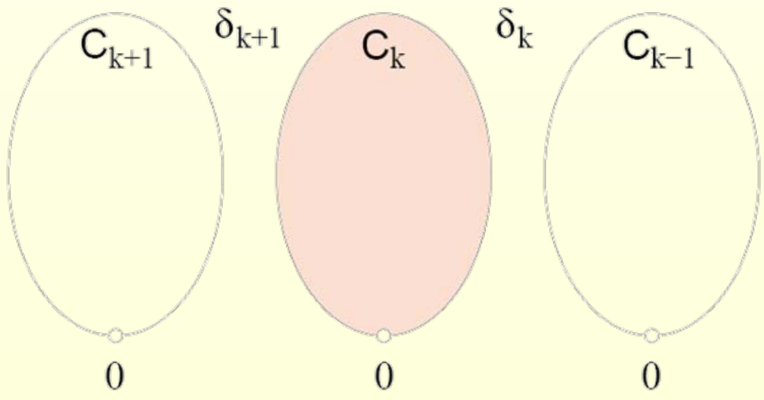
$$\begin{aligned}
&= \partial_{k-1}\sum_i (-1)^i [v_0, v_1, \ldots, \hat{v}_i, \ldots, v_k] \\
&= \sum_{j<i} (-1)^i (-1)^j [v_0, \ldots, \hat{v}_j, \ldots, \hat{v}_i, \ldots, v_k] \\
&\quad + \sum_{j>i} (-1)^i (-1)^{j-1} [v_0, \ldots, \hat{v}_i, \ldots, \hat{v}_j, \ldots, v_k] \\
&= 0,
\end{aligned}$$

as switching i and j in the second sum negates the first sum.

Chain Complex

- The boundary operator connects the chain groups into a chain complex C_*:

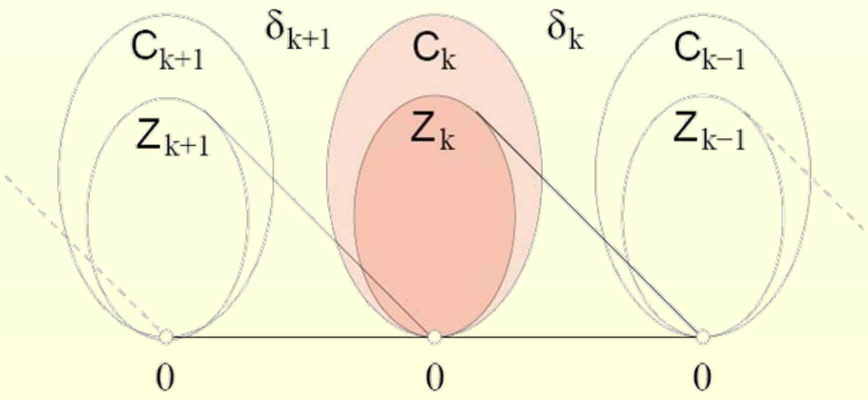
$$\ldots \to C_{k+1} \xrightarrow{\partial_{k+1}} C_k \xrightarrow{\partial_k} C_{k-1} \to \ldots .$$



Cycle Group

- Let c be a k-chain
- If it has no boundary, it is a k-cycle (zycle?)
- $\partial_k c = \emptyset$, so $c \in \ker \partial_k$
- The kth cycle group is

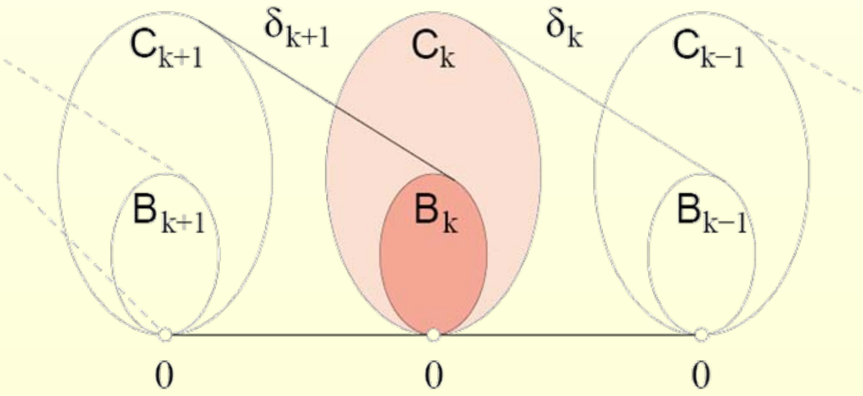
$$\mathsf{Z}_k = \ker \partial_k = \{c \in \mathsf{C}_k \mid \partial_k c = \emptyset\}.$$



Boundary Group

- Let b be a k-chain
- If b is a boundary of something, it is a k-boundary.
- The kth boundary group is

$$\mathsf{B}_k = \operatorname{im} \partial_{k+1} = \{c \in \mathsf{C}_k \mid \exists d \in \mathsf{C}_{k+1} : c = \partial_{k+1} d\}.$$

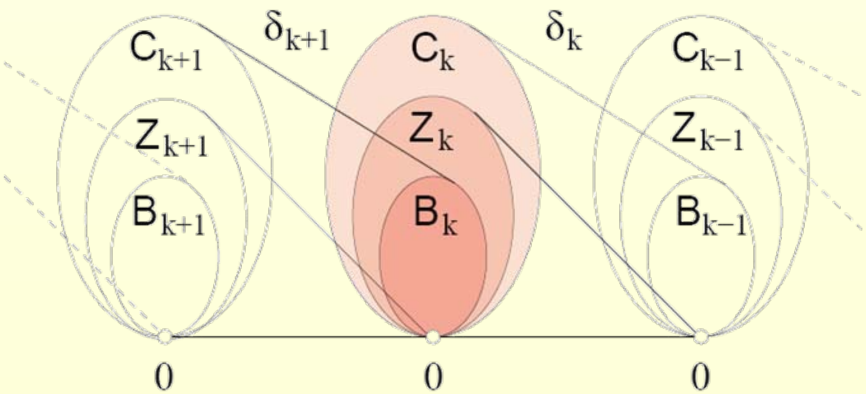


Nesting Property

- Let b be a k-boundary.
- Then, $\exists c \in \mathsf{C}_{k+1}$, such that $b = \partial_{k+1} c$.
- What is the boundary of b?

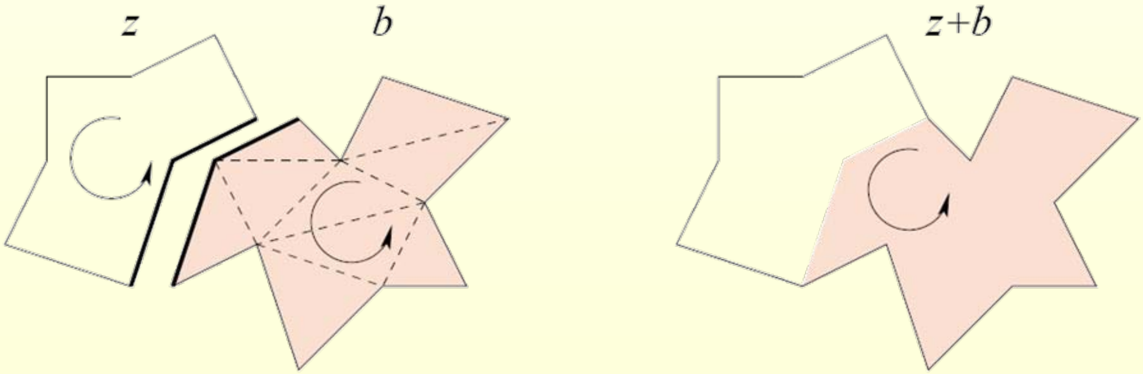
$$\partial_k b = \partial_k \partial_{k+1} c = \emptyset,$$

  by the boundary theorem.
- That is, every boundary is a cycle!
- $\mathsf{B}_k \subseteq \mathsf{Z}_k \subseteq \mathsf{C}_k$



Cycle Equivalence

- z is a k-cycle
- b is a k-boundary
- We would like to have $z + b$ be equivalent to z
- That is, if $z_1 - z_2 = b$ where b is a boundary, then $z_1 \sim z_2$
- Any boundary would do!

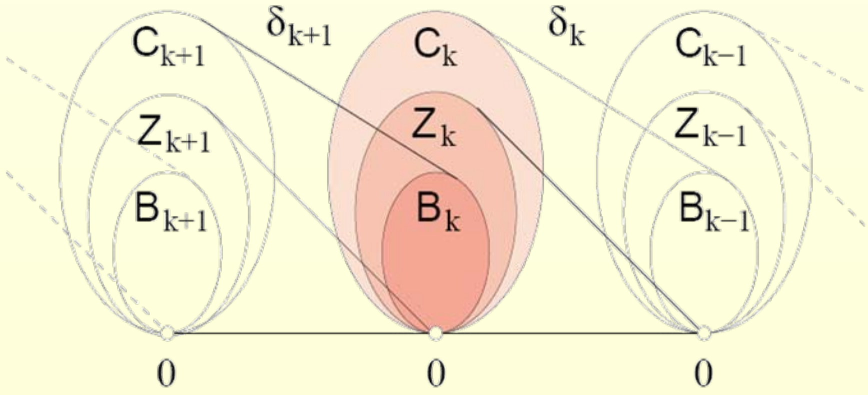


Simplicial Homology

- The kth homology group is

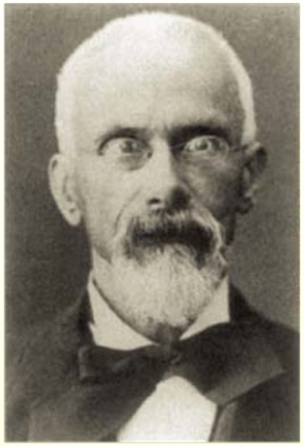
$$\mathsf{H}_k = \mathsf{Z}_k / \mathsf{B}_k = \ker \partial_k / \operatorname{im} \partial_{k+1}.$$

- If $z_1 = z_2 + \mathsf{B}_k$, $z_1, z_2 \in \mathsf{Z}_k$, we say z_1 and z_2 are homologous
- $z_1 \sim z_2$.

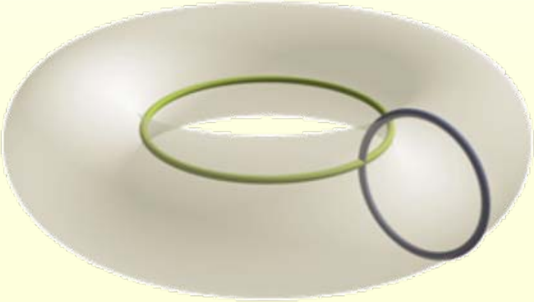


Z_2 Homology

- H_k is a vector space
- kth Betti number β_k = rank H_k
  = rank Z_k – rank B_k



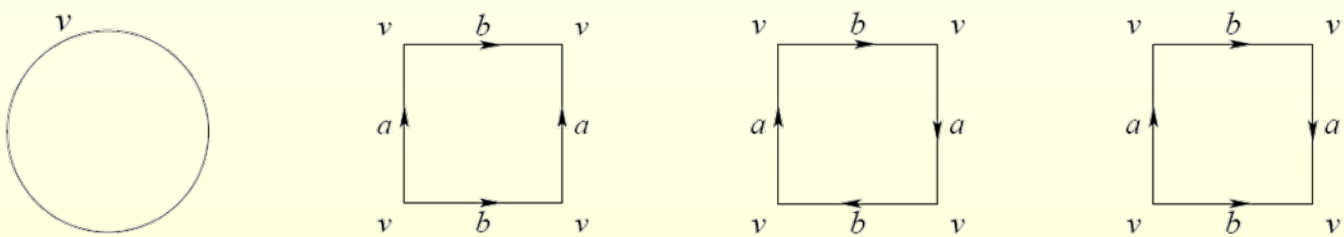
- Enrico Betti (1823 – 1892)
- Geometric interpretation in R^3
  - β_0 is number of components
  - β_1 is rank of a basis for tunnels
  - β_2 is number of voids



1, 2, 1

Homology of 2-Manifolds

2-manifold	H_0	H_1	H_2
sphere	$\mathbb{Z}$	$\{0\}$	$\mathbb{Z}$
torus	$\mathbb{Z}$	$\mathbb{Z} \times \mathbb{Z}$	$\mathbb{Z}$
projective plane	$\mathbb{Z}$	$\mathbb{Z}_2$	$\{0\}$
Klein bottle	$\mathbb{Z}$	$\mathbb{Z} \times \mathbb{Z}_2$	$\{0\}$



(a) Sphere (b) Torus (c) Projective plane (d) Klein bottle

Again, homology is independent of the triangulation

Euler Revisited

- Let K be a simplicial complex and $s_i = |\{\sigma \in K \mid \dim \sigma = i\}|$. The Euler characteristic $\chi(K)$ is

$$\chi(K) = \sum_{i=0}^{\dim K} (-1)^i s_i = \sum_{\sigma \in K - \{\emptyset\}} (-1)^{\dim \sigma}.$$

- We have new language!
- Let C_* be the chain complex on K
- $\operatorname{rank}(\mathsf{C}_i) = |\{\sigma \in K \mid \dim \sigma = i\}|$
- $\chi(K) = \chi(\mathsf{C}_*) = \sum_i (-1)^i \operatorname{rank}(\mathsf{C}_i)$.

Euler-Poincaré

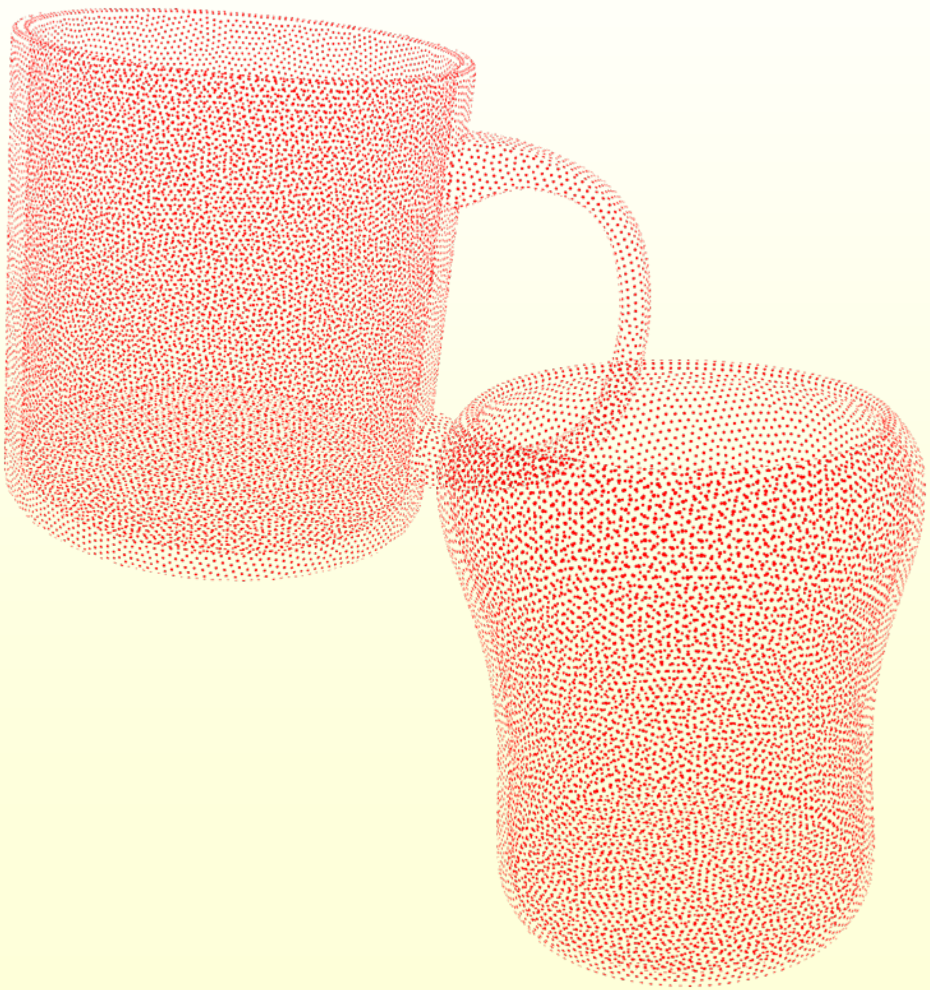
- Homology functors H_*
- $\mathsf{H}_*(\mathsf{C}_*)$ is a chain complex:

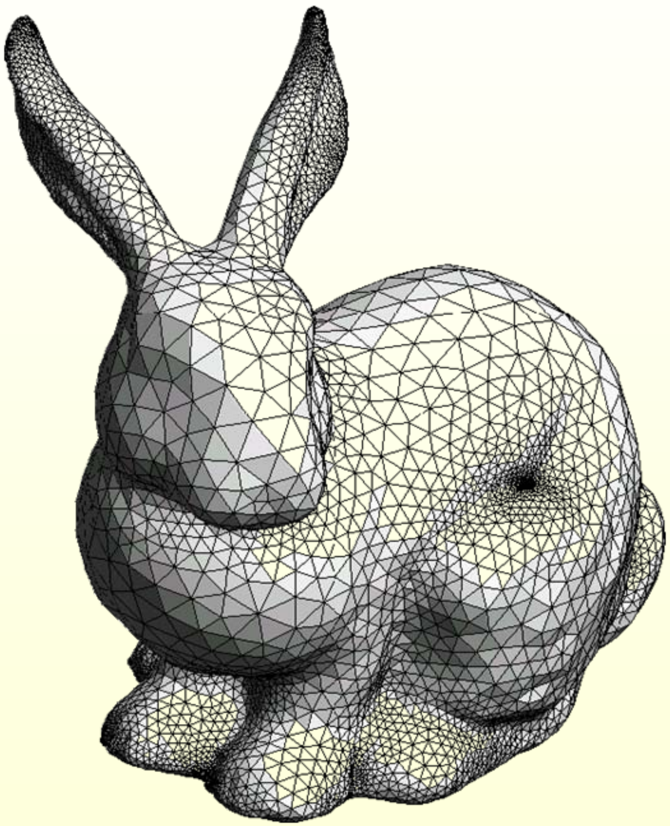
$$\ldots \to \mathsf{H}_{k+1} \xrightarrow{\partial_{k+1}} \mathsf{H}_k \xrightarrow{\partial_k} \mathsf{H}_{k-1} \to \ldots .$$

- What is its Euler characteristic?
- (Theorem) $\chi(K) = \chi(\mathsf{C}_*) = \chi(\mathsf{H}_*(\mathsf{C}_*))$.
- $\sum_i (-1)^i s_i = \sum_i (-1)^i \operatorname{rank}(\mathsf{H}_i) = \sum_i (-1)^i \beta_i$
- Sphere: $2 = 1 - 0 + 1$
- Torus: $0 = 1 - 2 + 1$

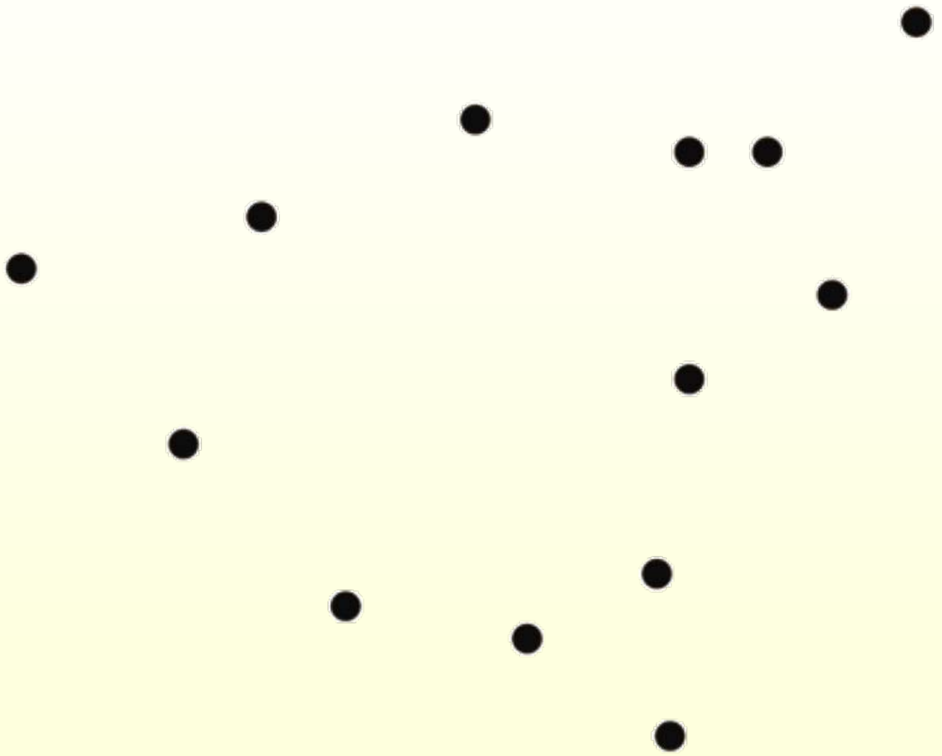
Point Clouds and the Complex Zoo

What Does This All Mean for Point Clouds or Meshes?



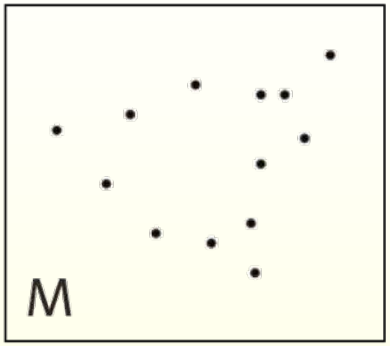


Topology of Points



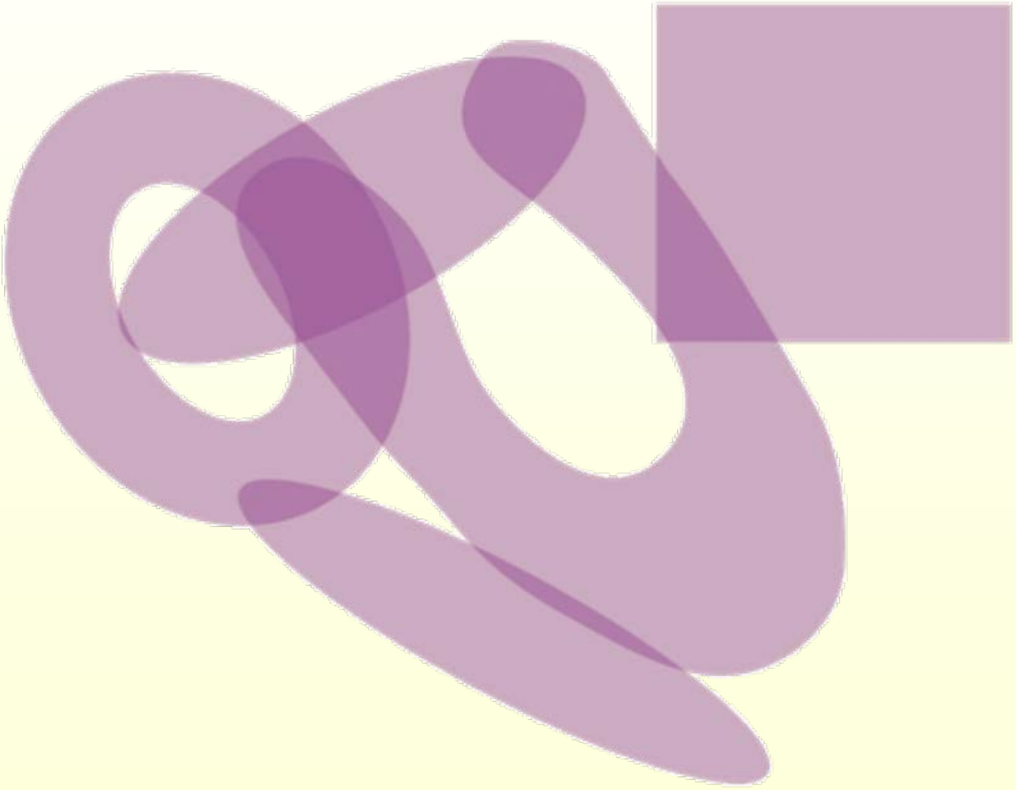
A Hidden Space X

- Topological space $\mathbb{X}$
- Underlying space



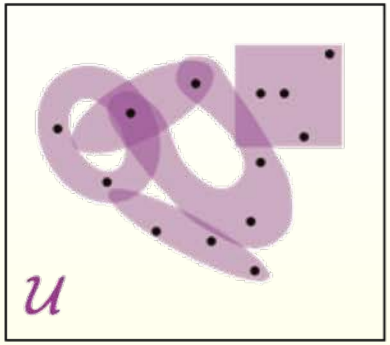
- Given: set of sample points M from $\mathbb{X}$
- Question: How can we recover the topology of $\mathbb{X}$ from M?
- Problem: M has no interesting topology.

Open Cover



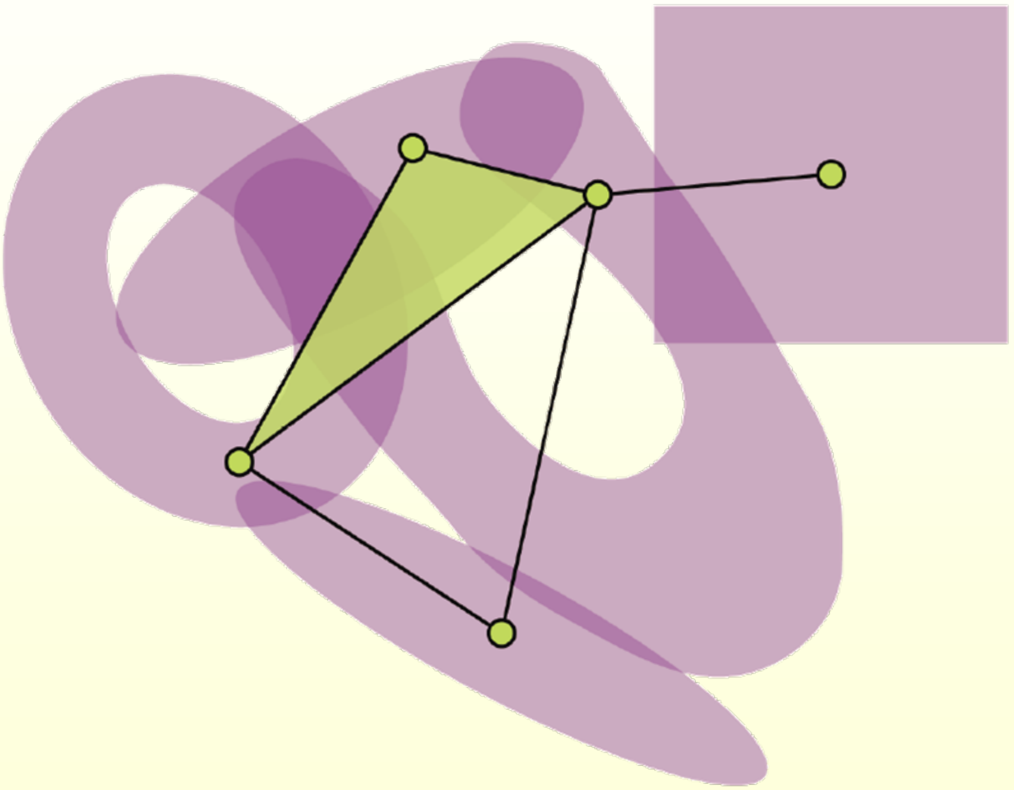
Formally

- Cover $\mathcal{U} = \{U_i\}_{i \in I}$
  - U_i, open
  - $M \subseteq \bigcup_{i \in I} U_i$



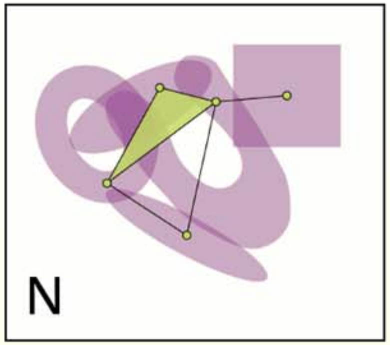
- Idea: The cover approximates the underlying space $\mathbb{X}$
- Question′: What is the topology of $\mathcal{U}$?
- Problem: $\mathcal{U}$ is an infinite point set

The Nerve of the Cover



An abstract simplicial complex

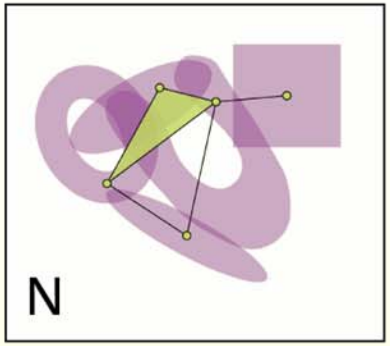
Formally



- $\mathbb{X}$: topological space
- $\mathcal{U} = \bigcup_{i \in I} U_i$: open cover of $\mathbb{X}$
- The nerve N of $\mathcal{U}$ is
  - $\emptyset \in N$
  - If $\cap_{j \in j} U_j \neq \emptyset$ for $J \subseteq I$, then $J \in N$
- Dual structure
- (Abstract) Simplicial complex

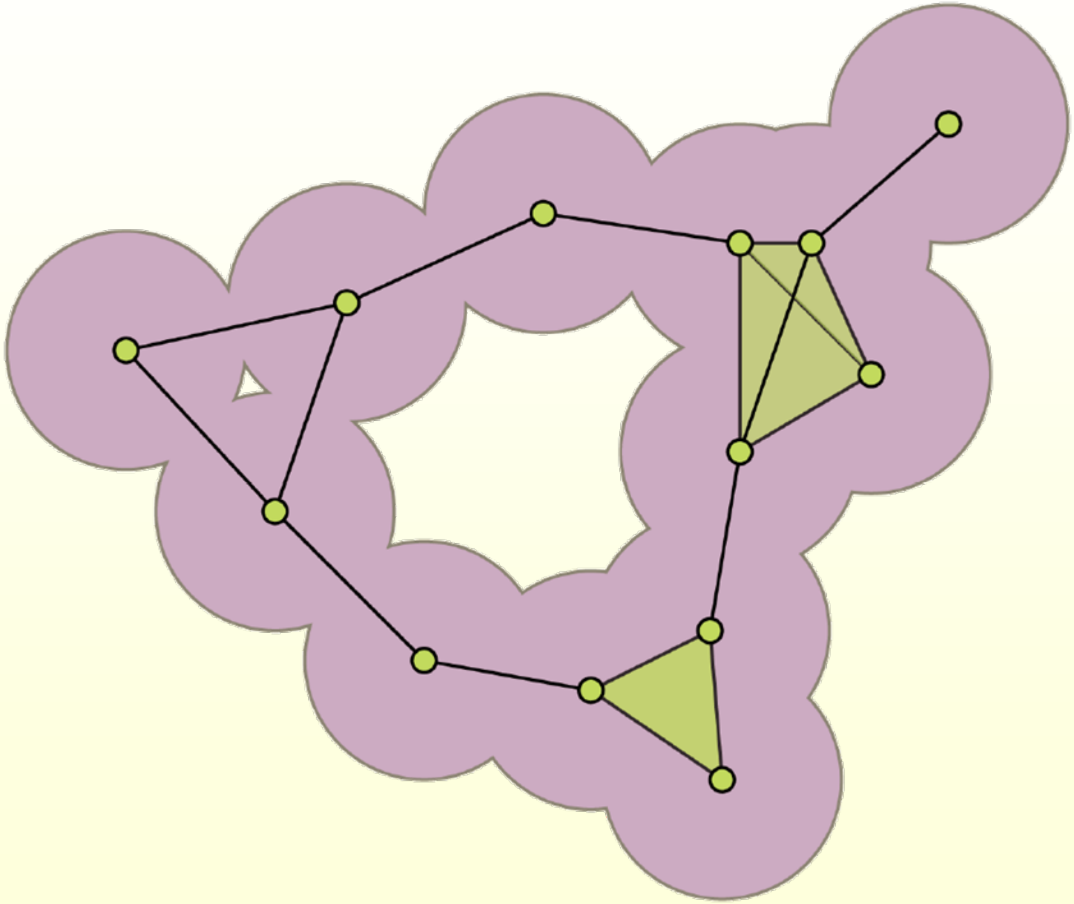
The Nerve Lemma

- **(Lemma [Leray])**
  If sets in the cover are contractible, and their finite ~~unions~~ are contractible, then N $\simeq \mathcal{U}$.   intersections



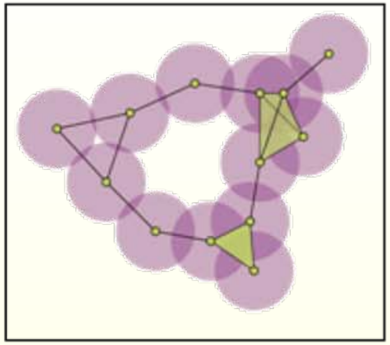
- *The cover should not introduce or eliminate topological structure*
- Idea: Use "nice" sets for covering
  - contractible
  - convex
- Dual (abstract) simplicial complex will be our representation

The Čech Complex



Ball radius is a parameter ε

Formally

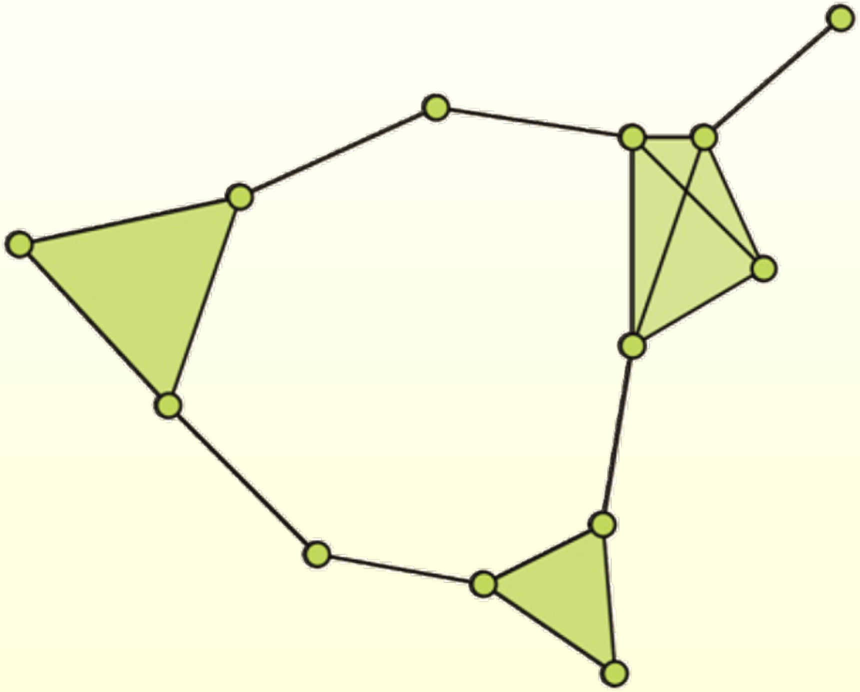


- Set: Ball of radius ε
  $B_\varepsilon(x) = \{ y \mid d(x, y) < \varepsilon\}$
- Cover: B_ε at every point in M
- Cech complex is nerve of the union of ε-balls

$$C_\epsilon(M) = \left\{ \text{conv}\, T \mid T \subseteq M, \bigcup_{m \in T} B_\epsilon(m) \neq \emptyset \right\}$$

- Cover satisfies Nerve Lemma
- Eduard Cech (1893 – 1960)

Vietoris-Rips Complex

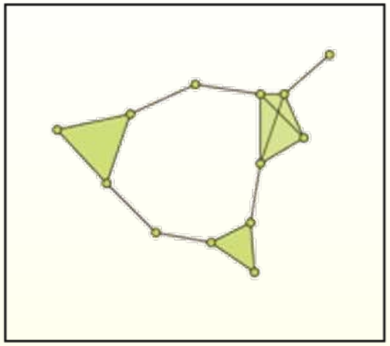


Distance is a parameter ε

Formally

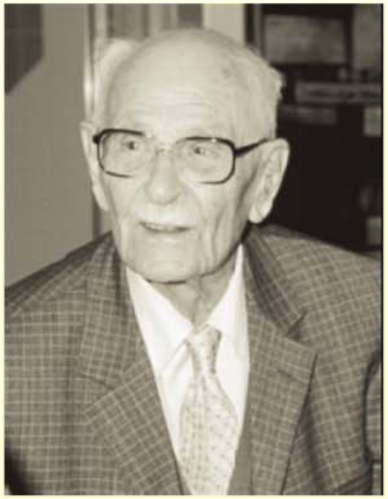
1. Construct ε-graph
2. Expand by add a simplex whenever all its faces are in the complex

- Note: We expand by dimension

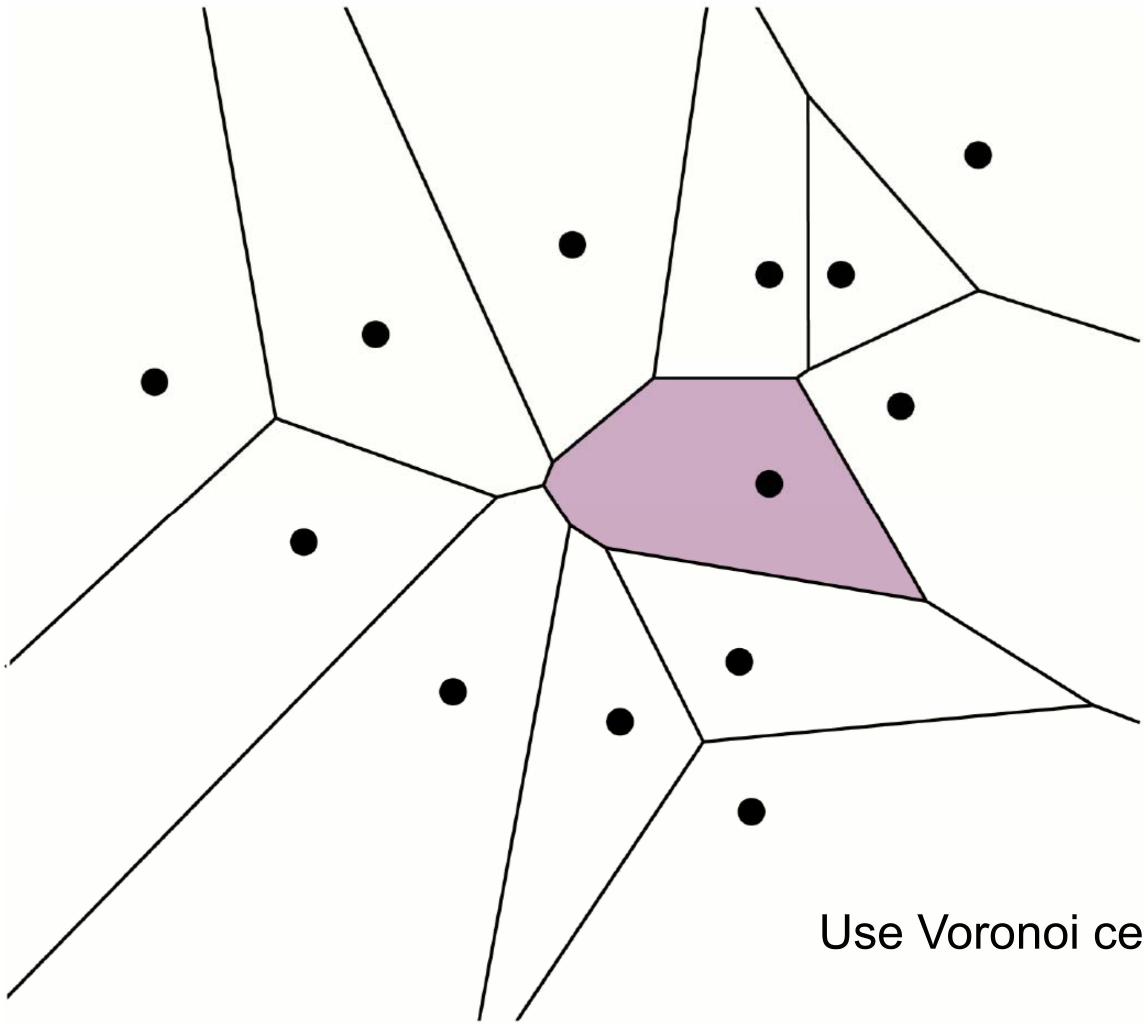


$$V_\epsilon(M) = \{\mathrm{conv}\, T \mid T \subseteq M, \mathrm{d}(x,y) < \epsilon, \forall x,y \in T\}$$

- $V_{2\varepsilon}(M) \supseteq C_\varepsilon(M)$
- Not homotopic to union of balls
- Leopold Vietoris (1891 – 2002)
- Eliyahu Rips (1948 –)

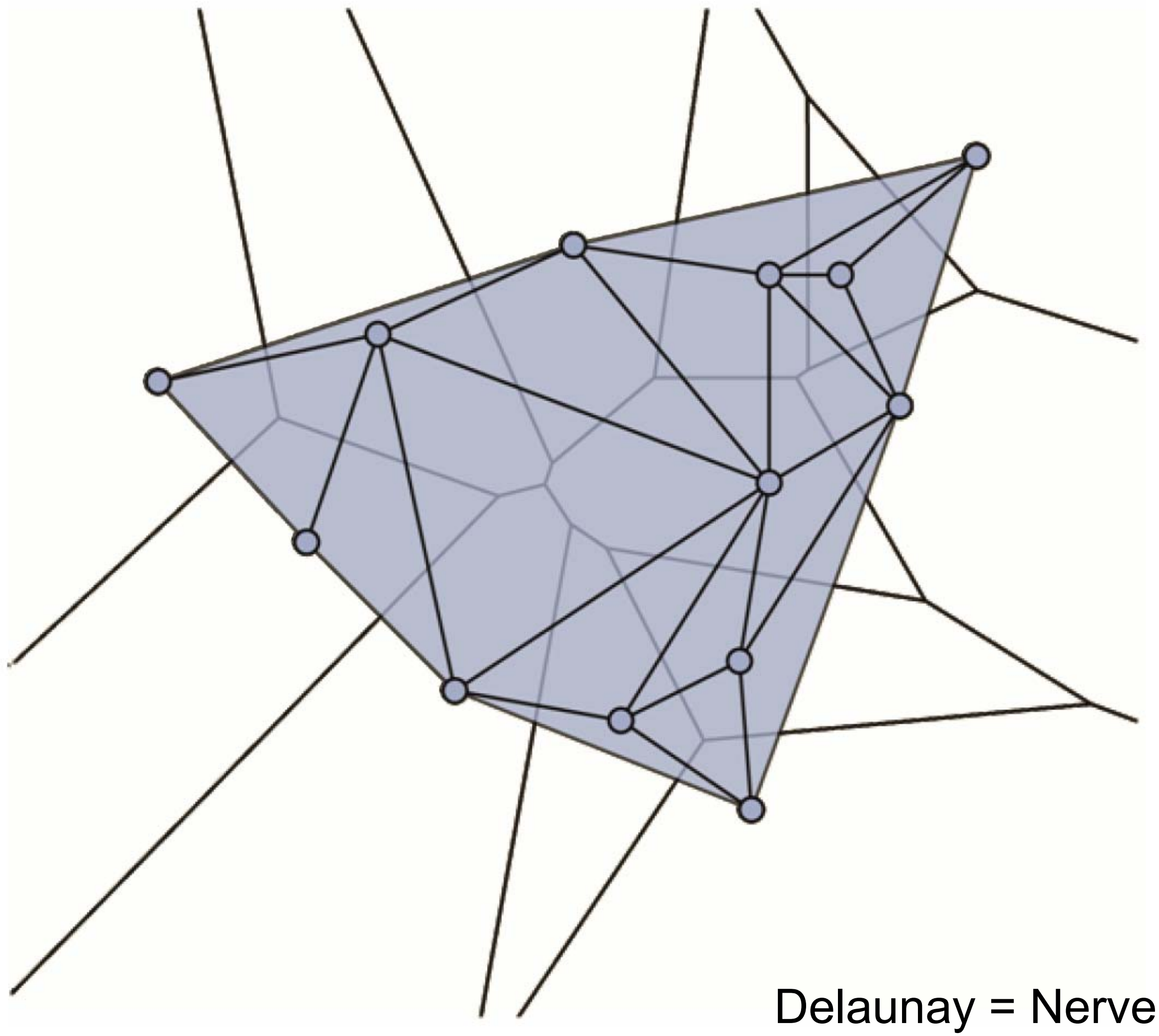


Geometric Complexes: Voronoi



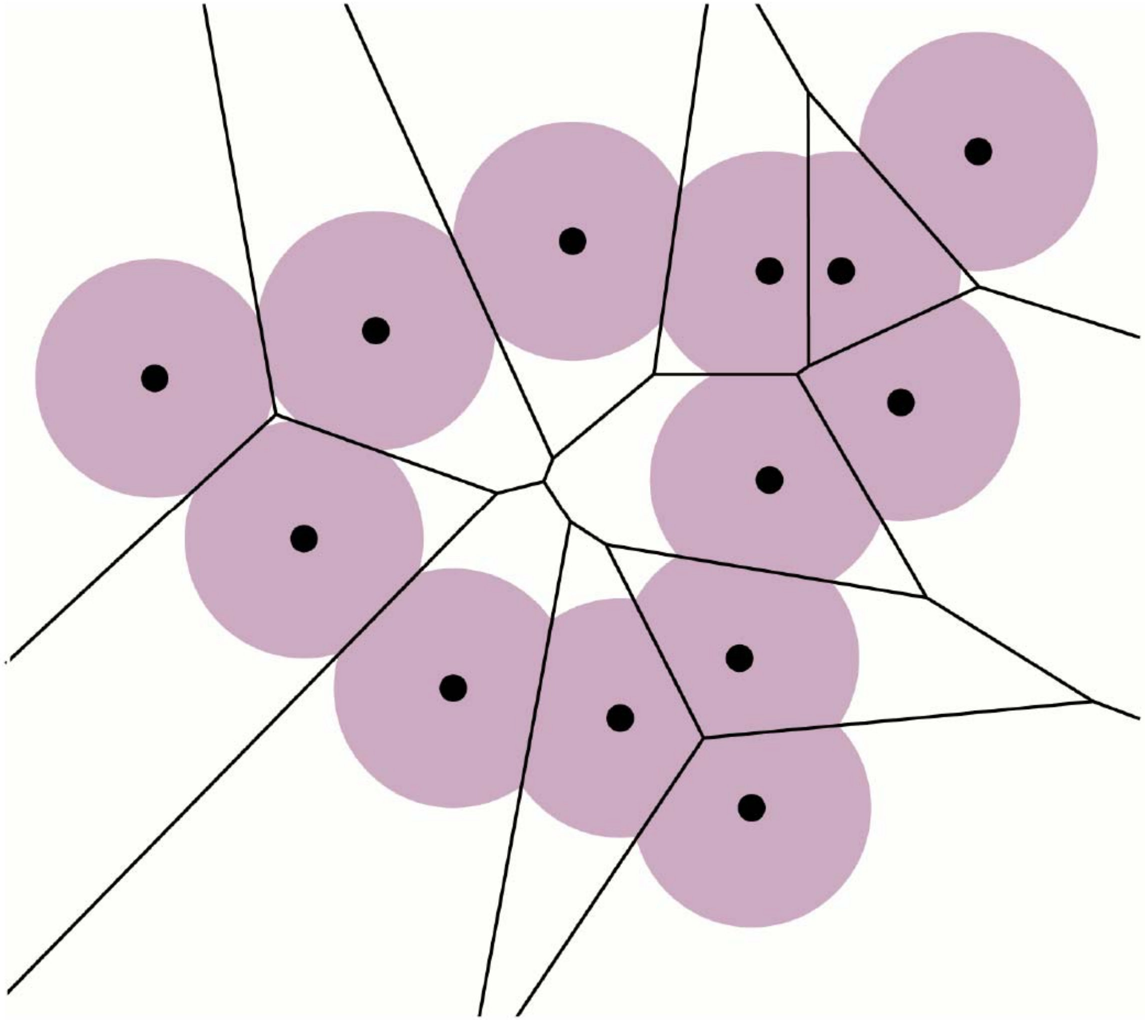
Use Voronoi cells as open cover

Dual Complex: Delaunay



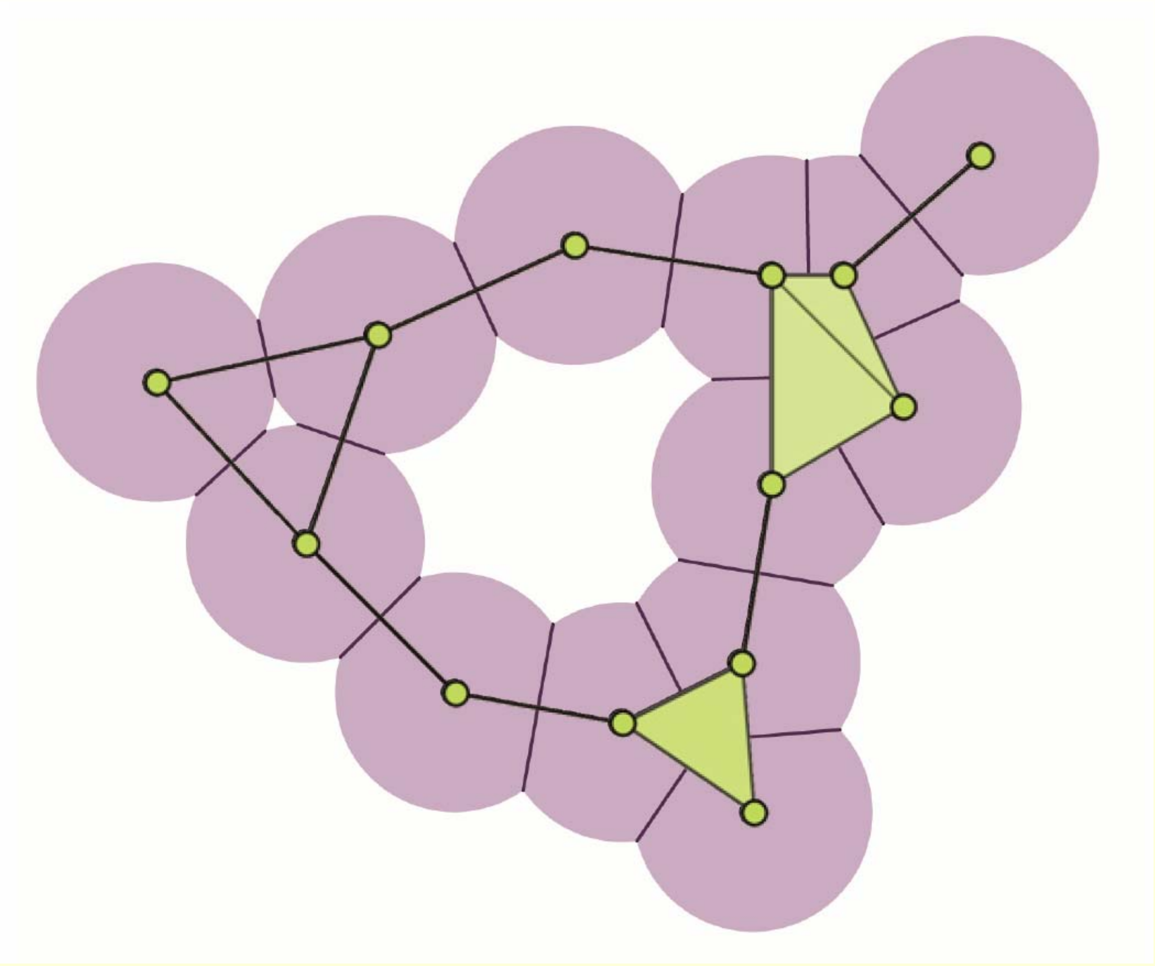
Delaunay = Nerve of Voronoi

Restricted Voronoi



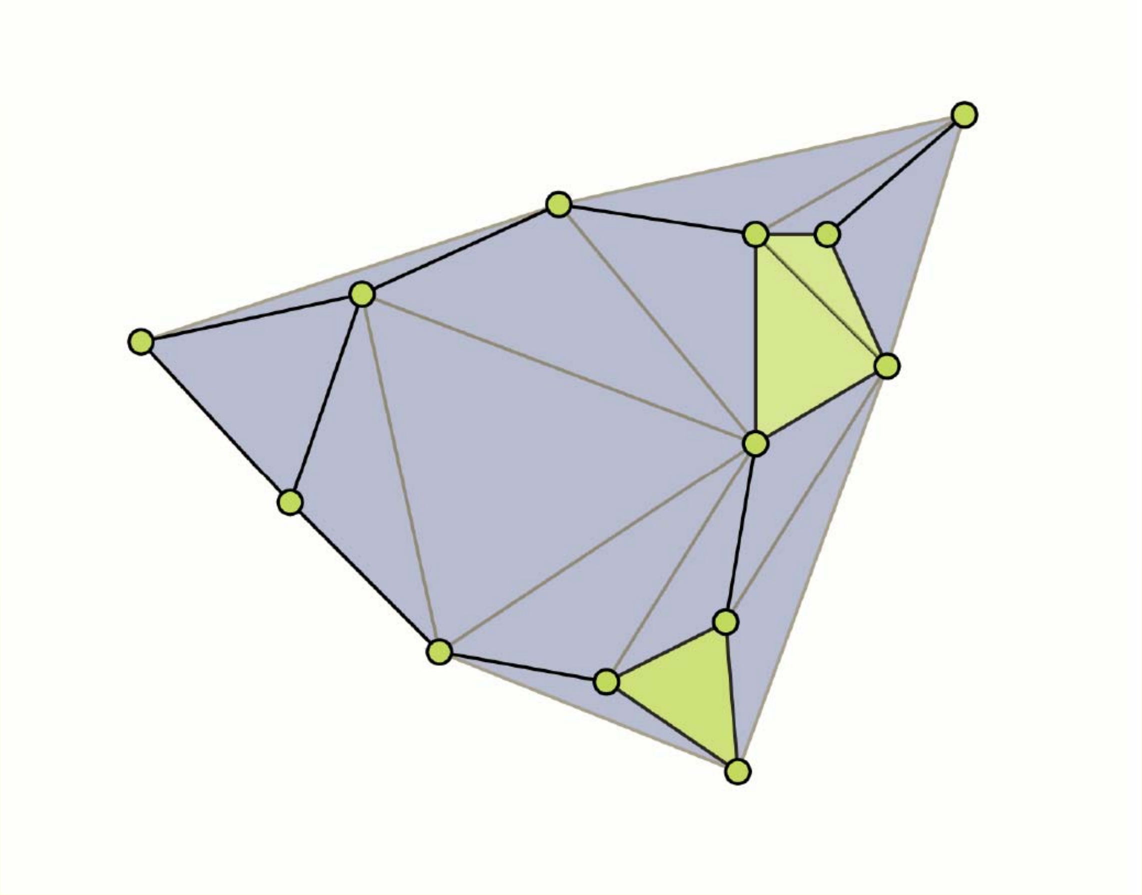
Ball radius is a parameter ε

Alpha Complex



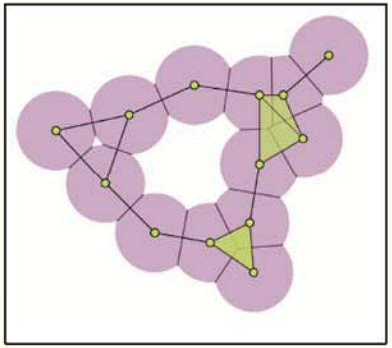
Ball radius is a parameter ε

Subcomplex of Delaunay



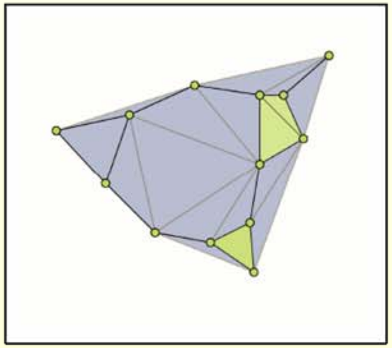
Formally

- Alpha cell: $A_\varepsilon(p) = B_\varepsilon(p) \cap V(p)$
- Alpha shape: union of alpha cells
- Alpha complex: nerve of alpha shape



$$A_\epsilon(M) = \left\{ \operatorname{conv} T \mid T \subseteq M, \bigcap_{p \in T} A_\epsilon(p) \neq \emptyset \right\}$$

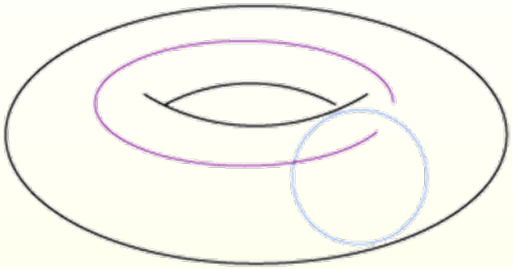
- Let D be the Delaunay triangulation
  - $A_0 = \emptyset$
  - $A_\varepsilon \subseteq D$
  - $A_\infty = D$

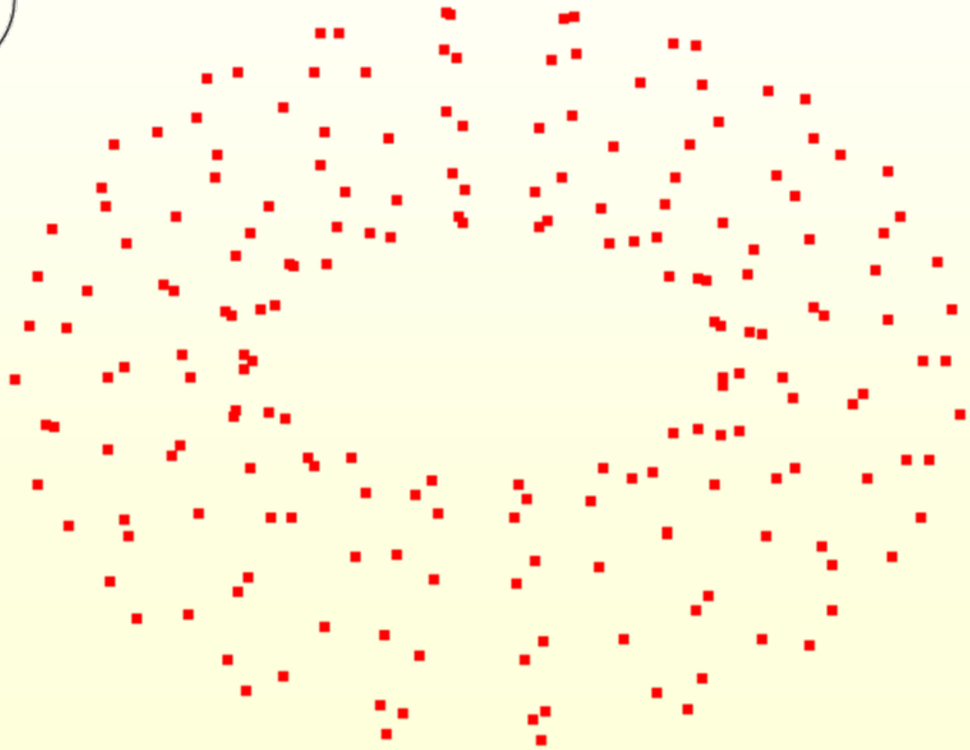


- $A_\varepsilon \simeq C_\varepsilon$
- [Edelsbrunner, Kirkpatrick, and Seidel '83], et al.

Persistent Homology

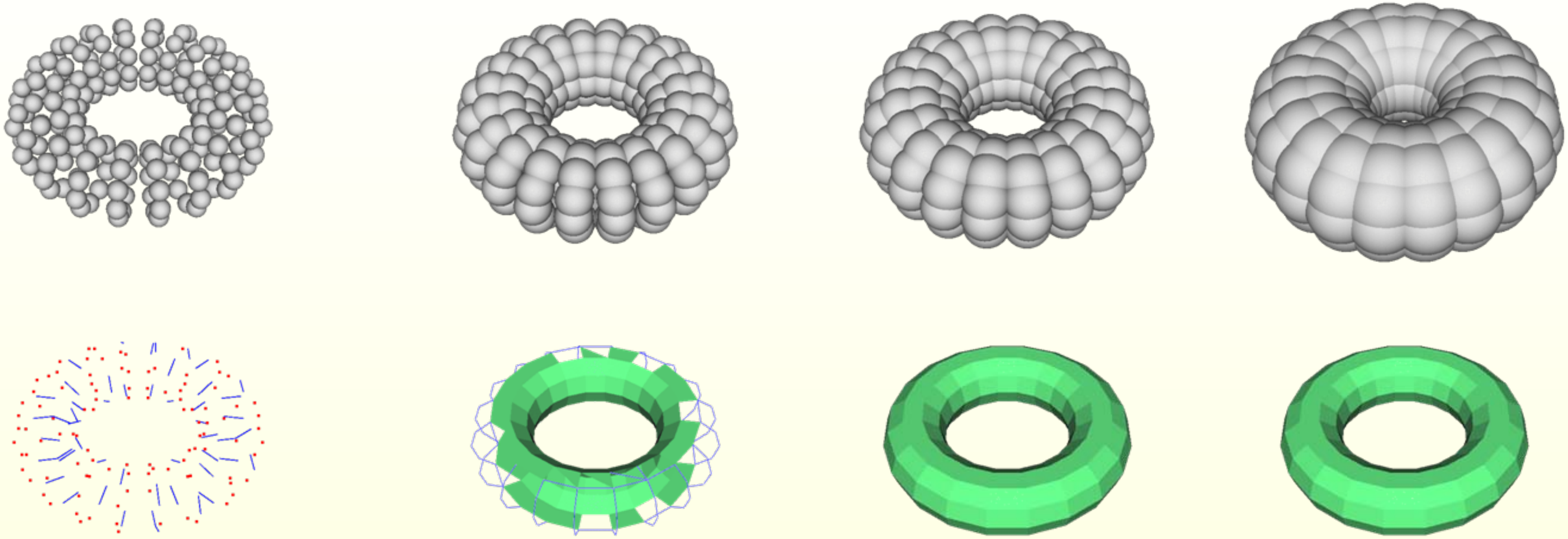
Detecting a Torus





PCD

Question of Scale: A Filtration

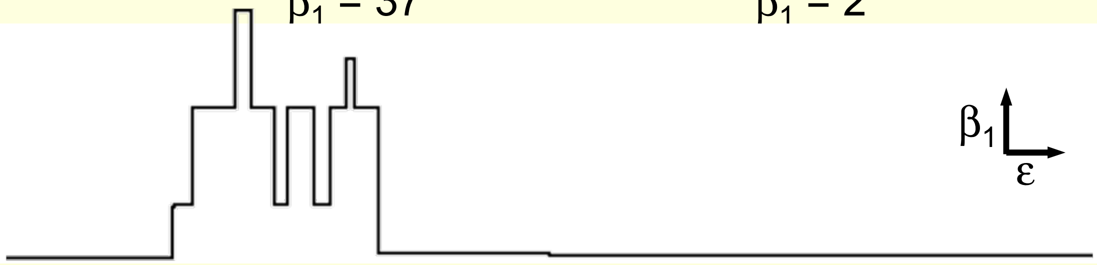


$\beta_0 = 150$, $\beta_1 = 0$

$\beta_0 = 1$, $\beta_1 = 37$

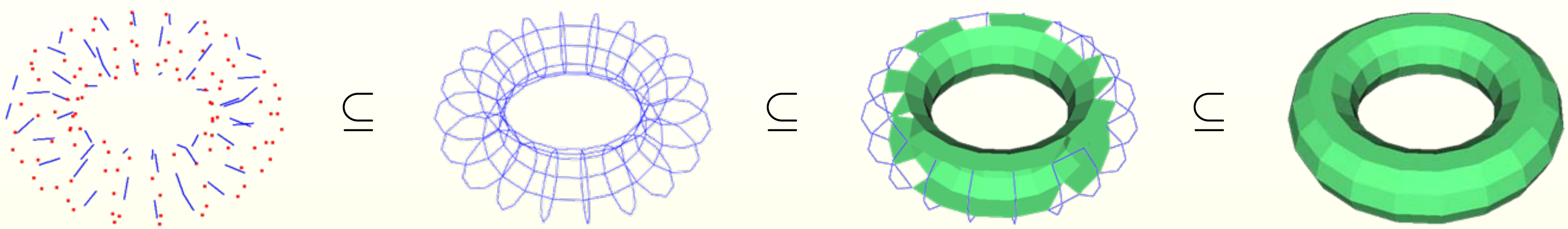
$\beta_0 = 1$, $\beta_1 = 2$

$\beta_0 = 1$, $\beta_1 = 1$



Čech Filtration

Inductive Systems on Complexes



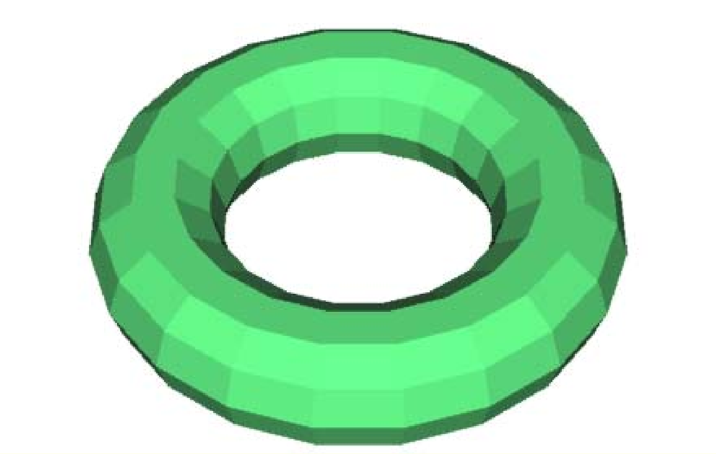
$K^{250} \xrightarrow{\;i\;} K^{500} \longrightarrow K^{994} \longrightarrow K^{1452}$

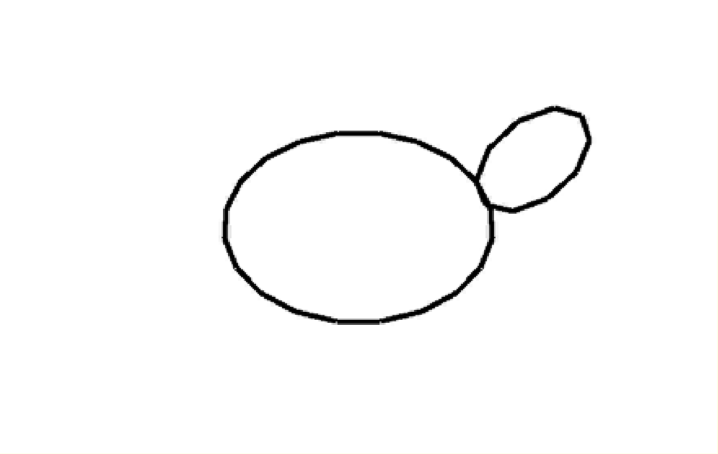
Functoriality ↓

$H_k(K^{25}) \longrightarrow H_k(K^{50}) \longrightarrow H_k(K^{994}) \longrightarrow H_k(K^{1452})$

Idea: Follow basis elements from birth to death
while maintaining compatible bases

Consistent Bases Exist





Persistent Homology

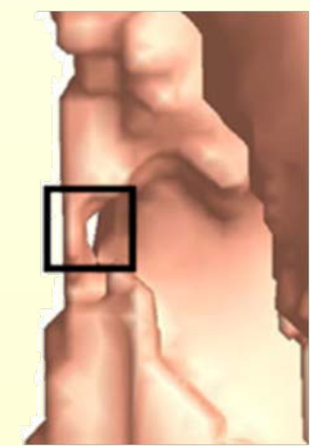
[Zomorodian. Edelsbrunner, Letcher 2002]

- Homology: $H_k(K^l) = Z_k(K^l) / B_k(K^l)$
- The p-persistent k-th Homology group

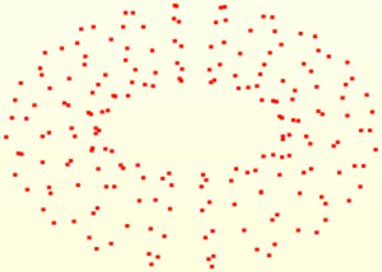
$$H_k^{l,p} = Z_k^l / (B_k^{l+p} \cap Z_k^l)$$

Persistent topological features are part of the shape; transient ones may be noise.

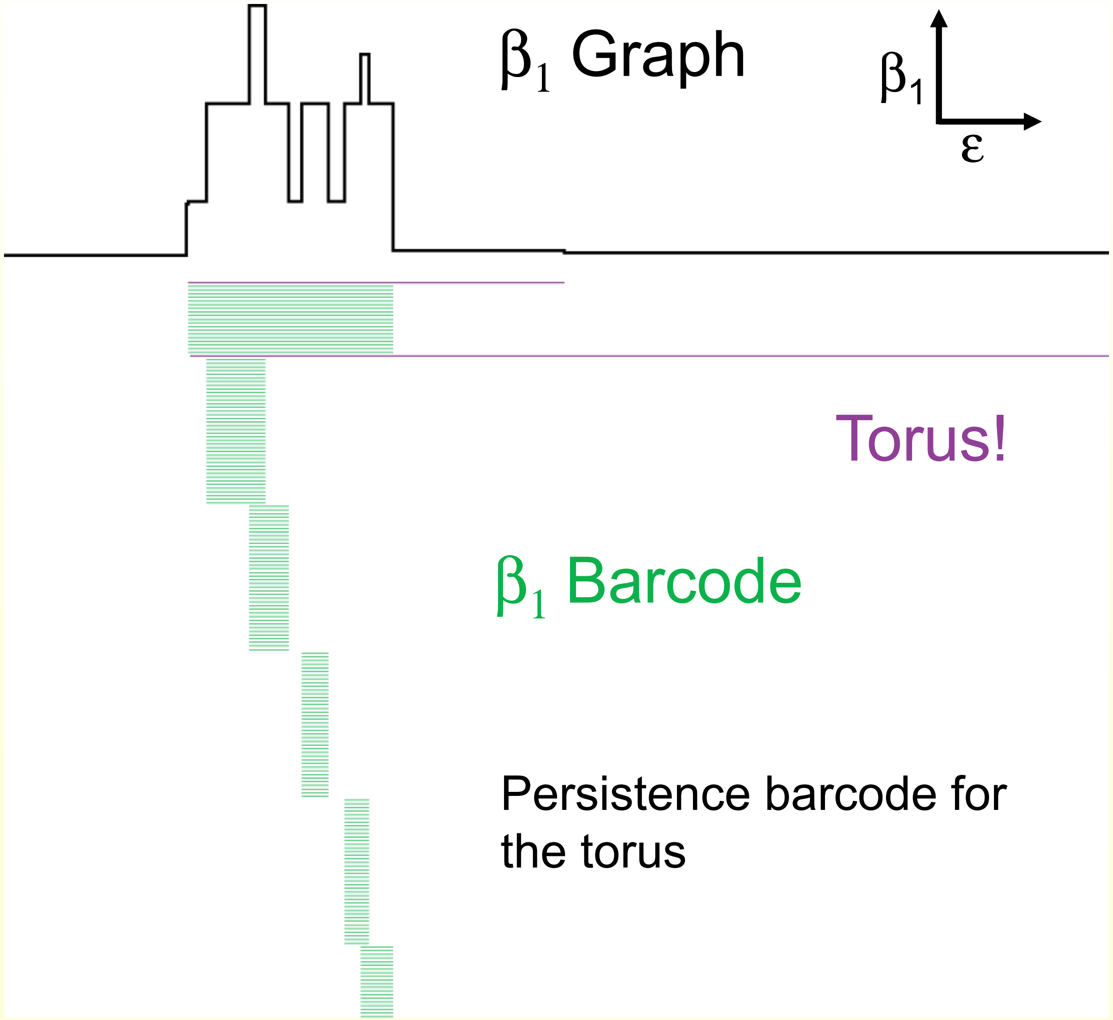
- Persistence Barcode: multiset of intervals



Deconstructing the Graph

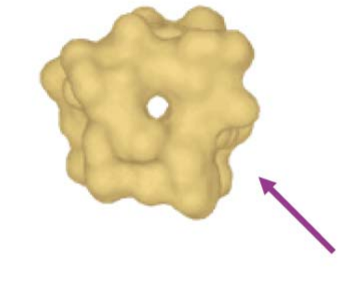


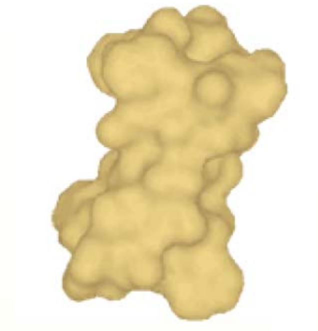
PCD

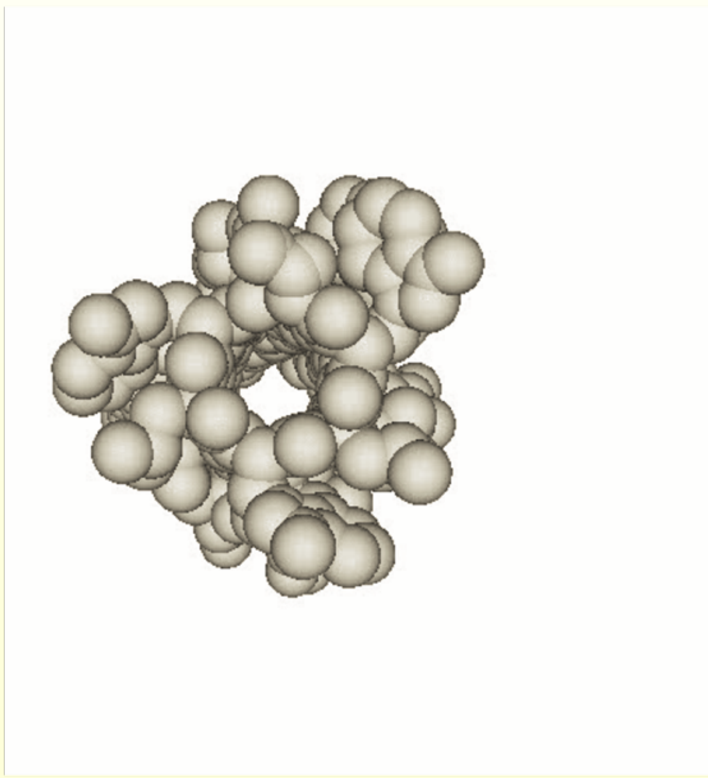


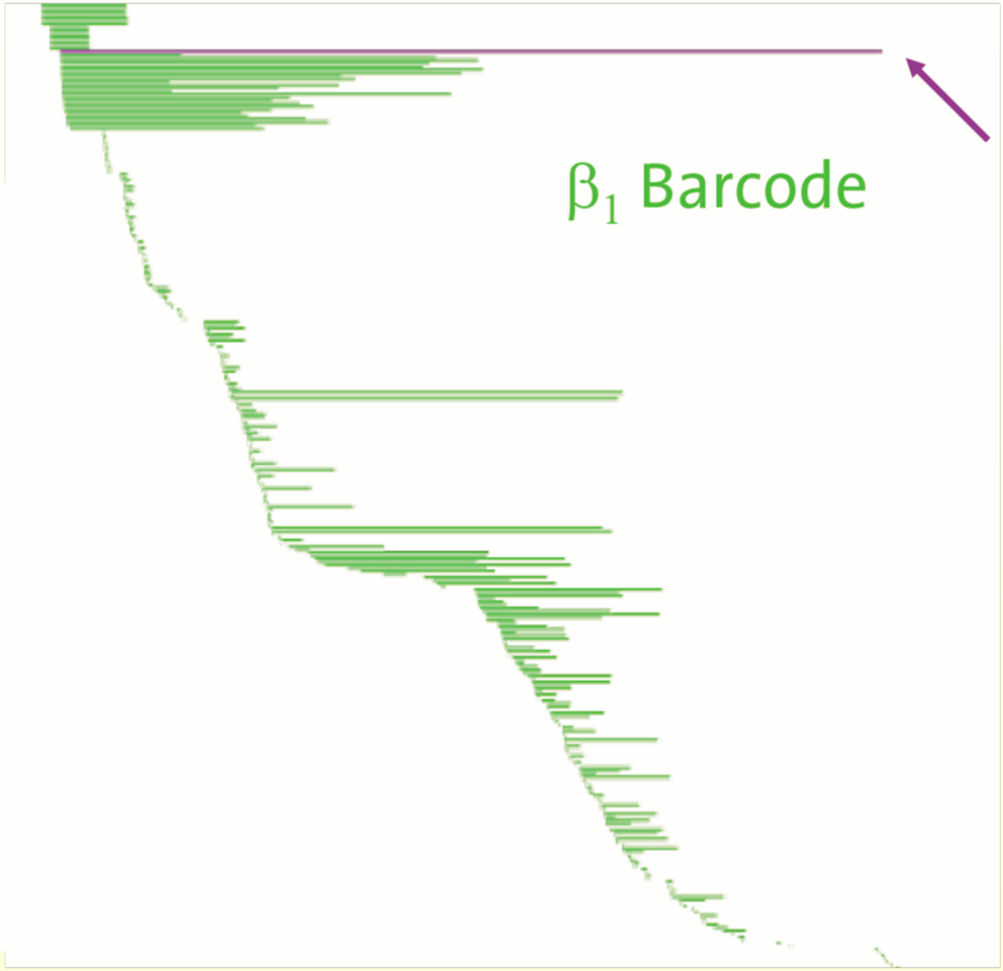
Persistence barcode for the torus

3D Structure Discovery: Gramicidin A









Making Topology a Finer Tool

Geometry discriminating — Topology classifying

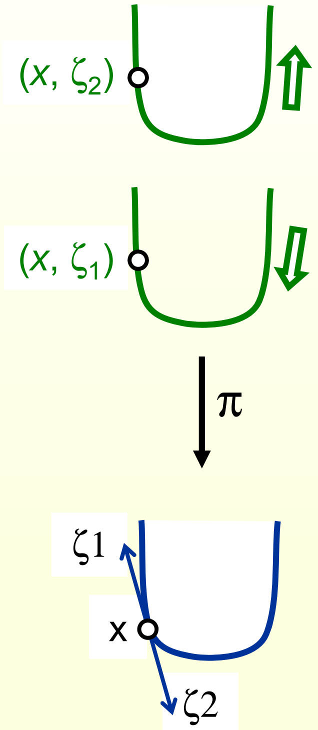
- Topology: connectivity of a space
- Key Idea: no reason to look at the original space only
  - Add geometry $\Rightarrow$ look at derived space(s)
  - **Compute topology of derived space(s)**

    1. Find filtration
    2. Compute persistence

via the tangent complex

Our recipe

2-D Curve Tangent Complex

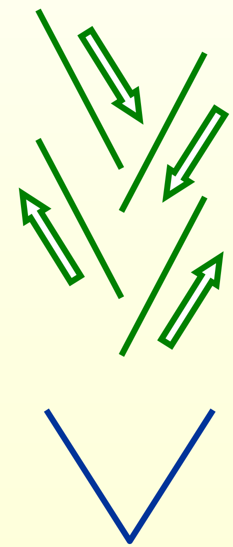


T(X) has two components:
$\beta_0(T(X)) = 2$

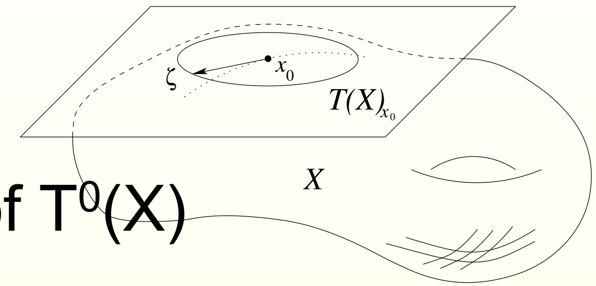
There are two points in its fiber $\pi^{-1}(x)$

Every point x on a smooth curve X has two tangent directions.

A corner point has four tangent directions:
$\beta_0(T(X)) = 4$



3-D Curvature-Filtered Tangent Complex



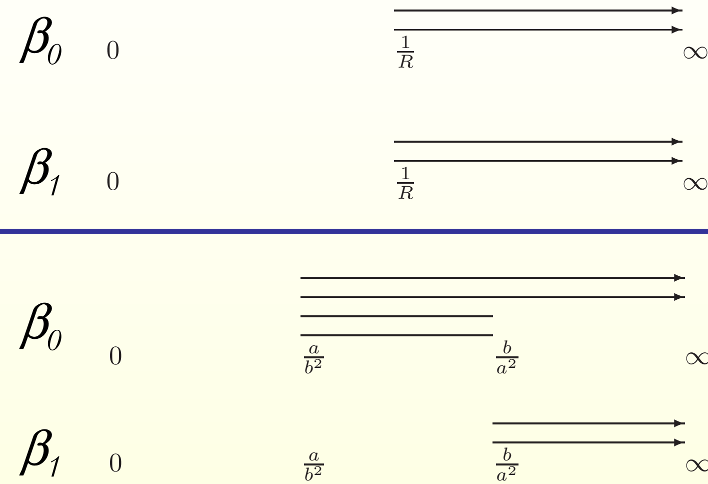
- Derived space
  - $T^0(X)$: space of (point, tangent)
  - Tangent complex $T(X)$: closure of $T^0(X)$
- Filtration by increasing curvature
  - Let $\rho(x, \zeta)$ be the radius of the circle of second order contact
  - $T_\delta^0(X)$: points of $T^0(X)$ with $1/\rho \leq \delta$.
  - $T_\delta(X)$: closure of $T_\delta^0(X)$
- Filtered tangent complex $T^{filt}(X)$ is the family

$$\{T_\delta(X)\}_{\delta \geq 0}$$

Persistence Barcodes: Circle vs. Ellipse

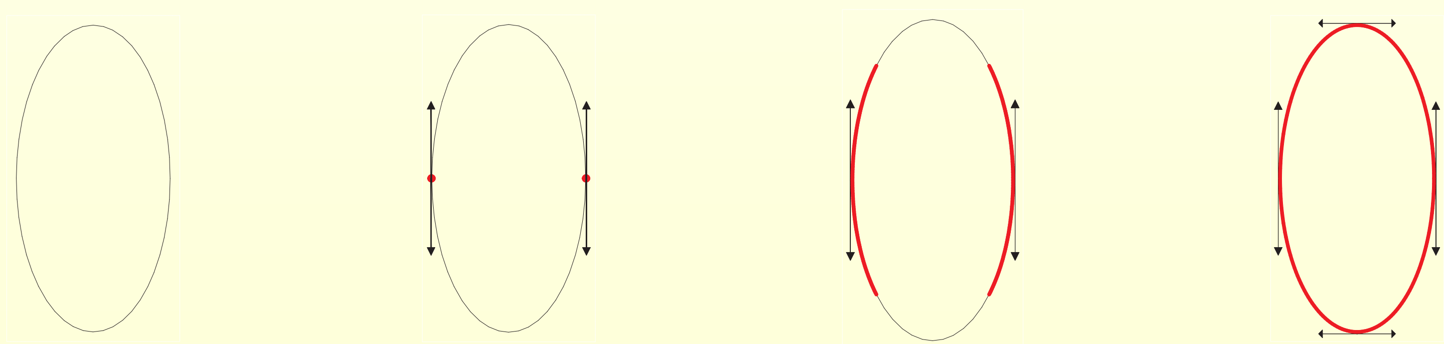
T^{filt}(circle of radius *R*) is simple: the entire complex (2 copies of circle) appears at once, at = 1/*R.*

T^{filt}(ellipse) evolves through four stages: points at *lower* curvature appear earlier.



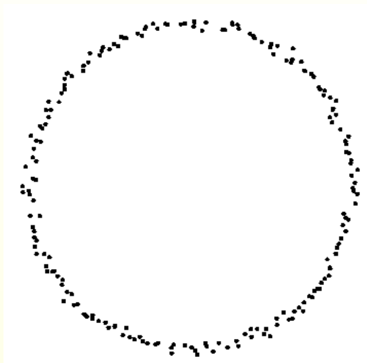
Persistence Barcodes

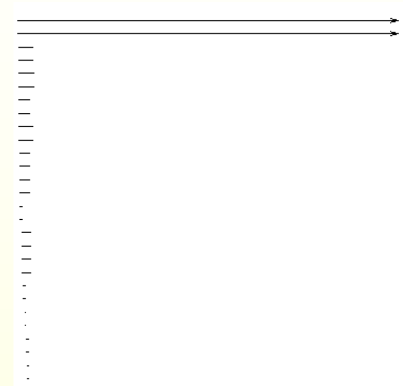
$$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1$$



$0 \leq \delta < \frac{a}{b^2}$ $\quad$ $\delta = \frac{a}{b^2}$ $\quad$ $\frac{a}{b^2} < \delta < \frac{b}{a^2}$ $\quad$ $\delta \geq \frac{b}{a^2}$

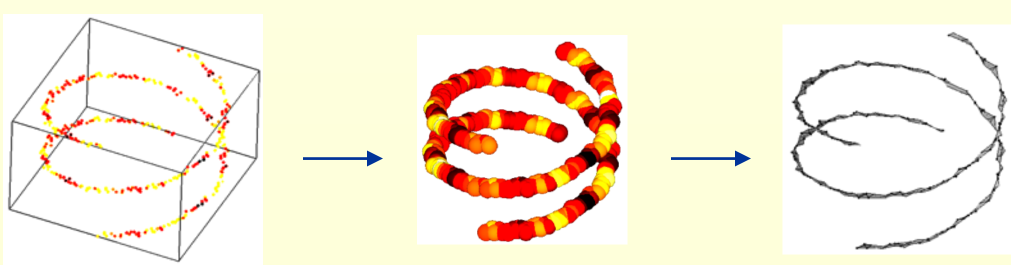
Applying Barcodes to 2D PCDs



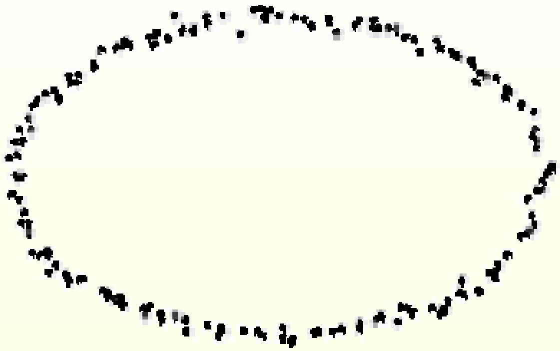


Input: Shape

Output: Descriptor

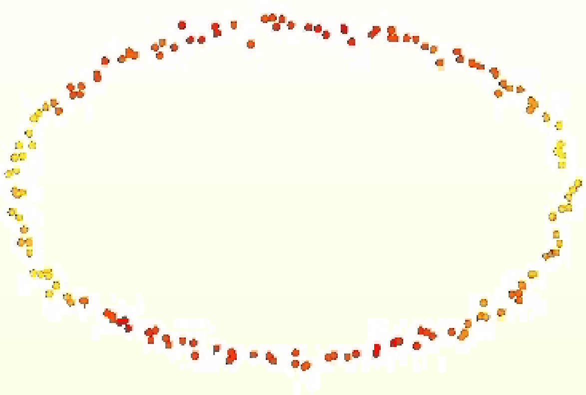


Fibers



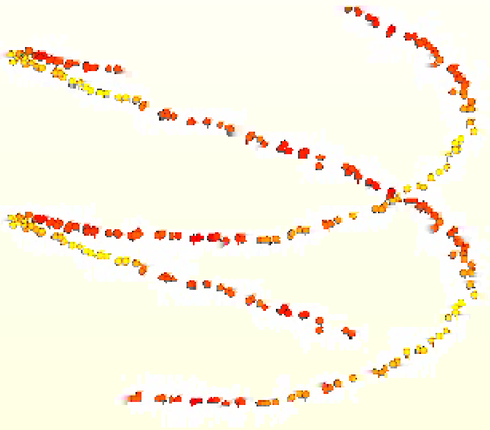
- PCD $P \subset X$, sampled from smooth closed 1-manifold
- We compute tangent fibers $\pi^{-1}(P)$ by normal estimation at each point

Filtering by Curvature



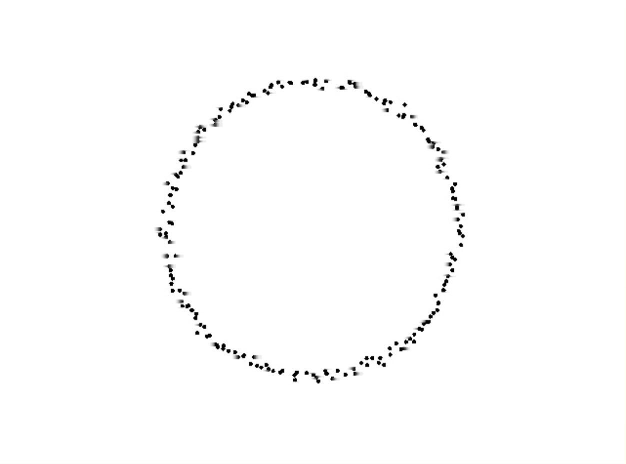
- Construct tangent complex incrementally
- Transform points to coordinate frame provided by tangent computation
- Fit osculating parabola to estimate curvature (more robust integral methods possible)

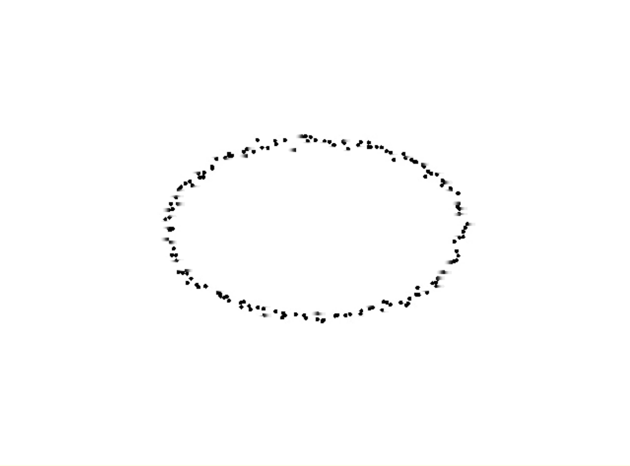
Approximating $T(X)$

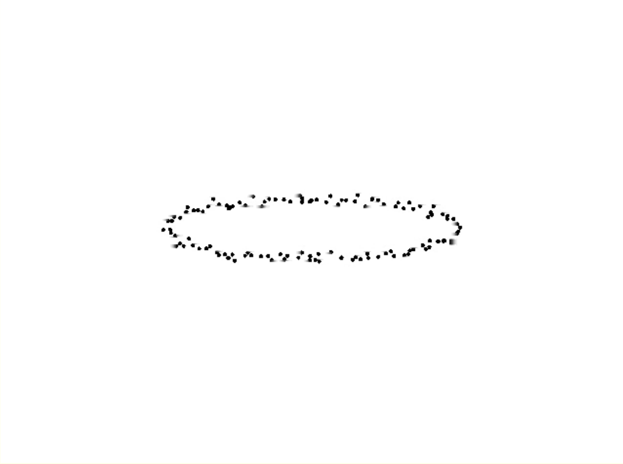


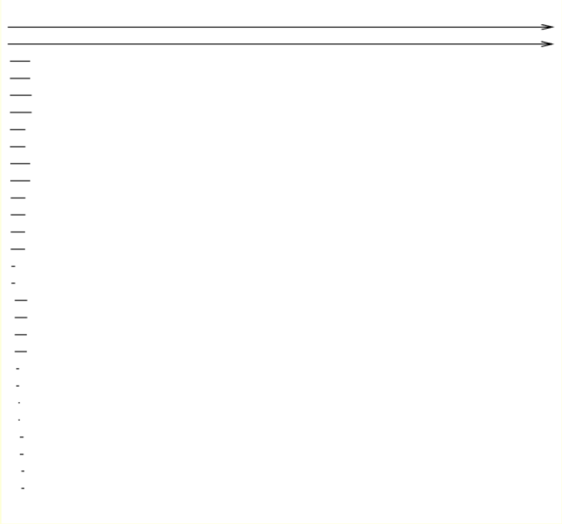
- $\mathbb{R}^n \times \mathbb{S}^{n\text{-}1}$ with $ds^2 = dx^2 + \omega^2\, d\zeta^2$
- $T(X) \approx \bigcup_{p \in \pi^{-1}(P)} B_\varepsilon(p)$

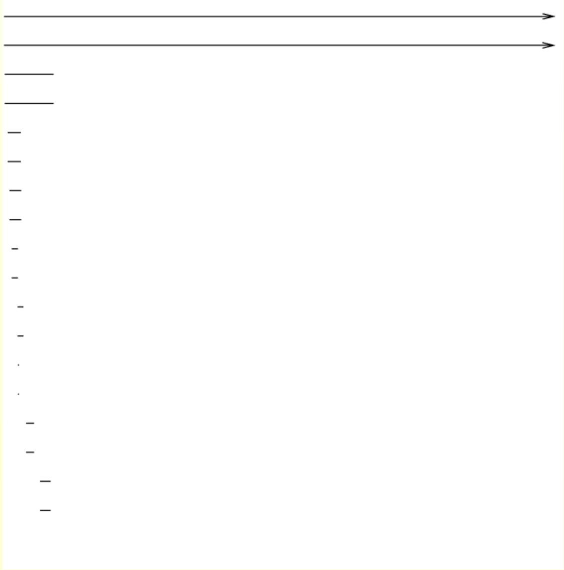
Family of Ellipses

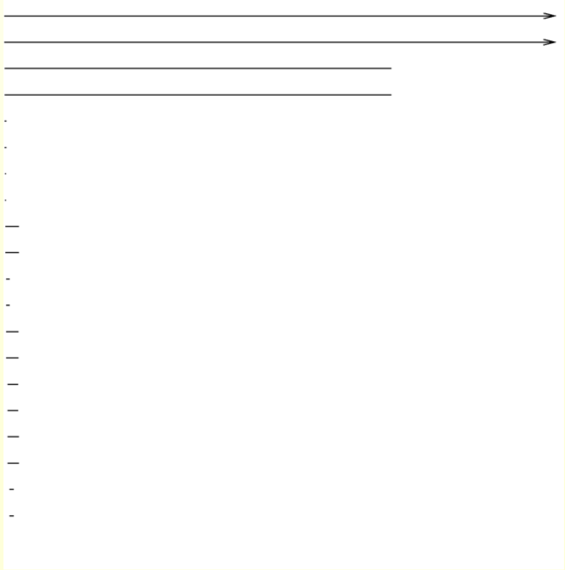




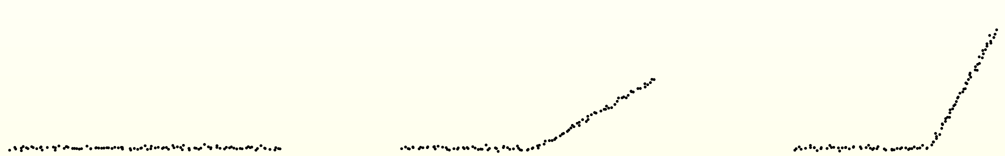








Articulated Arm Parametrization



Summary

- We are flooded by point set *data* and need to find structure in them
- *Topology* studies connectivity of spaces
- *Topological analysis* may be viewed as generalization of clustering
- To analyze point sets, we require a *combinatorial representation* approximating the original space
- *Homology* focuses on the structure of cycles
- *Persistent homology* analyzes the relationship of structures at multiple scales