Introduction to Topological Data Analysis
MATH 491 - Non-Research Independent Study
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Contents

1 Introduction

Topological Data Analysis (TDA) is a field of applied mathematics that is useful in the study and analysis of complex, high-dimensional data. There are numerous approaches to data analytics, of which TDA is a relatively newer framework that uses topology to identify and understand the underlying shape and structure of data. TDA has been applied across a wide range of disciplines, including biology, chemistry, and finance, and there is ongoing research in the field as new techniques continue to be developed.

The purpose of undertaking this independent study was to survey relevant topics to gain an understanding of TDA. To achieve this goal, we have divided our studies into five sections, which we present in this document: Basics of Topology, Complexes, Homology Groups, Persistent Homology, and Applications in Data Analysis. The *Basics of Topology* section serves as a foundation for understanding the key concepts from topology that are used in TDA. In the *Complexes* section, we describe how we can construct topological spaces from data sets. In the *Homology Groups* section we explain how to use vector spaces and linear transformations to study topological spaces. In the *Persistent Homology* section we explain the fundamental tool used in TDA to identify topological features that persist across various constructions of the topological space associated to a data set. Finally, in the *Applications in Data Analysis* section, we present a real-world example of how TDA has been applied to analyze data.

2 Basics of Topology

2.1 Topological Spaces

Definition 2.1. Let X be a set. The collection of all subsets of X is called the *power set of* X, and it is denoted by $\mathcal{P}(X)$ or 2^X. If X is finite with cardinal n, then the cardinal of $\mathcal{P}(X)$ is 2^n.

Example: The power set of the empty set is $\mathcal{P}(\emptyset) = \{\emptyset\}$, and the power set of $\{1, 2, 3\}$ is $\mathcal{P}\big(\{1, 2, 3\}\big) = \big\{\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}\big\}$.

Definition 2.2. Let X be a set, and let $\mathcal{T} \subseteq \mathcal{P}(X)$ be a collection of subsets of X. We say the pair $(X, \mathcal{T})$ is a *topological space* and the collection $\mathcal{T}$ is a *topology on* X if the following axioms are satisfied:

1. $\emptyset, X \in \mathcal{T}$
2. If $\{\mathcal{O}_i\}_{i\in I} \subseteq \mathcal{T}$, then $\bigcup_{i\in I} \mathcal{O}_i \in \mathcal{T}$, i.e. the union of an arbitrary collection of elements in $\mathcal{T}$ is in $\mathcal{T}$.
3. If $\{\mathcal{O}_i\}_{i=1}^n \subseteq \mathcal{T}$ for some $n \in \mathbb{N}$, then $\bigcap_{i=1}^n \mathcal{O}_i \in \mathcal{T}$, i.e. the intersection of a finite collection of elements in $\mathcal{T}$ is in $\mathcal{T}$.

Definition 2.3. Let $(X, \mathcal{T})$ be a topological space. If $\mathcal{O} \in \mathcal{T}$,

- $\mathcal{O}$ is an *open set* for the topology $\mathcal{T}$
- $X \setminus \mathcal{O}$ is a *closed set* for the topology $\mathcal{T}$

A subset A of X is a closed set if and only if its complement, $A^c = X \setminus A$, is open.

Intuition

We want the elements of $\mathcal{T}$ to behave like open intervals in $\mathbb{R}$, where each open set is a set where every point can be through of as having some "wiggle room" within the set in any direction. On the other hand, the complements of the elements of $\mathcal{T}$ should behave like closed intervals in $\mathbb{R}$.

Remark. The collection of closed sets for the topology $\mathcal{T}$ satisfy a dual set of axioms:

1. $\emptyset, X$ are closed sets.
2. If $\{\mathcal{C}_i\}_{i \in I}$ is a collection of closed sets, then $\bigcap_{i \in I} \mathcal{C}_i$ is closed, i.e. the intersection of an arbitrary collection of closed sets is closed.
3. If $\{\mathcal{C}_i\}_{i=1}^{n}$ for some $n \in \mathbb{N}$ is a finite collection of closed sets, then $\bigcup_{i=1}^{n} \mathcal{C}_i$, i.e. the union of a finite collection of closed sets is closed.

Examples:

1. Let X be a set. If $\mathcal{T} = \{\emptyset, X\}$, we call $\mathcal{T}$ the *indiscrete/trivial topology*. If $\mathcal{T} = \mathcal{P}(X)$, we call $\mathcal{T}$ the *discrete topology*.
2. The set of real numbers, $\mathbb{R}$, with the collection of open intervals and arbitrary unions of open intervals is known as $\mathbb{R}$ *with the usual topology* or $\mathbb{R}$ *with the Euclidean topology*.
3. The adjectives "open" and "closed" are not mutually exclusive. Some open sets are also closed sets, and some sets are neither open sets nor closed sets. In fact, let $X = \{1, 2, 3, 4, 5, 6\}$ and $\mathcal{T} = \{\emptyset, X, \{1\}, \{3, 4\}, \{1, 3, 4\}, \{2, 3, 4, 5, 6\}\}$. Then,
   - The point sets $\emptyset$ and X are both open and closed (this is true in every space $(X, \mathcal{T})$)
   - $\{1\}$ and $\{2, 3, 4, 5, 6\}$ are both open and closed
   - $\{3, 4\}, \{1, 3, 4\}$ are open but not closed
   - $\{2, 3\}$ is neither open nor closed
   - $\{1, 5, 6\}$ is closed but not open

Usually, it is difficult to specify the topology on a set by describing the entire collection of open sets. One can instead specify a smaller collection of subsets, and define the topology in terms of that.

Definition 2.4. Let X be a set. A *basis* for a topology on X is a collection $\mathcal{B} \subset \mathcal{P}(X)$ (elements of $\mathcal{B}$ are called *basis elements*) such that

1. For each $x \in X$, there is at least one basis element $B \in \mathcal{B}$ containing x.
2. If $x \in X$ belongs to the intersection of two basis elements B_1 and B_2, then there exists a basis element B_3, containing x, such that $B_3 \subseteq B_1 \cap B_2$.

The *topology* $\mathcal{T}$ *generated by* $\mathcal{B}$ is formed as follows: Let $\mathcal{O} \subseteq X$, then
$\mathcal{O} \in \mathcal{T}$ if and only if for each $x \in \mathcal{O}$, there is a $B \in \mathcal{B}$ such that $x \in B$ and $B \subseteq \mathcal{O}$.

Examples:

1. For any set X with the indiscrete topology, the collection of singletons
$$\mathcal{B} = \Big\{ \{x\} : \ x \in X \Big\}$$
is a basis. When $X = \mathbb{N}$, then this basis has a countable number of elements.
2. Consider $\mathbb{R}$ with the usual topology. The collection of open intervals
$$\mathcal{B} = \Big\{ (a,b) \subset \mathbb{R} : \ a, b \in \mathbb{R} \text{ and } a < b \Big\}$$
is a basis for the usual topology. This basis has an uncountable number of elements.
3. Let $\mathcal{C}$ be the collections of all interiors of circles in the plane, and let $\mathcal{R}$ be the collections of all interior of rectangles (with sides parallel to the coordinate axes) in the plane. These collections generate the same topology in $\mathbb{R}^2$.

Definition 2.5. Let $(X, \mathcal{T})$ be a topological space, and let $Y \subseteq X$ be a non-empty subset of X. The collection $\mathcal{T}_Y := \{\mathcal{O} \cap Y \ : \ \mathcal{O} \in \mathcal{T}\} \subseteq \mathcal{P}(Y)$ is called the *subspace topology on* Y *induced by* $\mathcal{T}$, and $(Y, \mathcal{T}_Y)$ is said to be a *subspace of* $(X, \mathcal{T})$.

Example: Consider $\mathbb{R}$ with the usual topology and $[0,1] \subseteq \mathbb{R}$. Some elements of $\mu_{[0,1]}$ are $\{(a,b) : 0 < a < b < 1\}$, $\{[0,b) : 0 < b < 1\}$, and $\{(a,1] : 0 < a < 1\}$.

As we saw in a previous example, subsets of a topological space are not necessarily open or closed. However, the definition below tells us how to find open and closed sets related to arbitrary subsets of a topological space.

Definition 2.6. Let $(X, \mathcal{T})$ be a topological space, and let $A \subseteq X$ be a non-empty subset of X.

1. The *interior of* A is the union of all open sets of X contained in A, and it is denoted by $\mathrm{Int}(A)$.

2. The *closure of* A is the intersection of all closed sets of X containing A, and it is denoted by $\mathrm{Cl}(A)$.

3. The *boundary of* A is the set difference $\mathrm{Bd}(A) = \mathrm{Cl}(A) \setminus \mathrm{Int}(A)$.

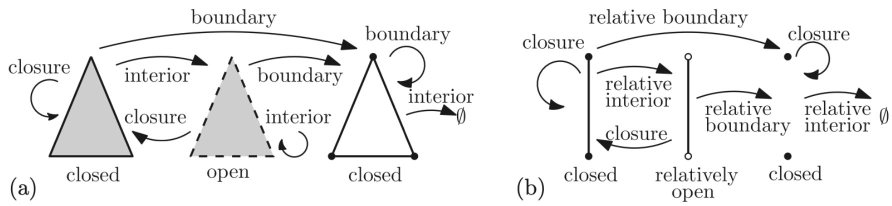


Figure 1: Visual representation of closure, interior, and boundary [6].

Definition 2.7. A space is called *Hausdorff* if every two disjoint sets have disjoint open sets containing them.

Example: Consider the set $X = \{1, 2, 3\}$. Define $\mathcal{T}_1$ as follows:

$$\mathcal{T}_1 = \{\emptyset, X, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}\}.$$

Thus, this topological space would be a Hausdorff space since every two disjoint point sets have disjoint open sets that contain them.
However, if we now consider another topology, $\mathcal{T}_2 = \{\emptyset, X, \{1, 3\}, \{2\}\}$, this satisfies the properties of a topological space, however **does not** satisfying the properties of a Hausdorff space. For instance, if we take the disjoint sets $\{1, 3\}$ and $\{2\}$, there is no disjoint open set containing them.

Definition 2.8. A topological space $(X, \mathcal{T})$ is *disconnected* if there are two disjoint non-empty open sets $U, V \in \mathcal{T}$ so that $X = U \cap V$. A topological space is therefore *connected* if it is **not** disconnected.

Examples:

1. $\mathbb{R}$ with the usual topology is connected.

2. $(0, 1) \cup (2, 3) \subseteq \mathbb{R}$ with the subspace topology is disconnected.

3. $\mathbb{N}$ with the discrete topology is disconnected.

Remark. There is a relationship between connectedness and the number of sets that are open/closed.
X is *connected* if and only if the only subjects of X that are closed and open are X and $\emptyset$.

Definition 2.9. Let $(X, \mathcal{T})$ be a topological space. An *open/closed cover* of X is a collection $\mathcal{C}$ of open/closed subsets of X s.t. $X = \bigcup_{A \in \mathcal{C}} A$.

Definition 2.10. Let $(X, \mathcal{T})$ be a topological space. We say X is *compact* if for every open cover $\mathcal{C}$ of X there exists a finite subcover $\mathcal{C}'$ of X.

Symbolically: $\forall\, \mathcal{C}, X = \bigcup_{A \in \mathcal{C}} A,\ \exists\, \mathcal{C}' \subseteq \mathcal{C}, \mathcal{C}'$ is finite and $X = \bigcup_{A \in \mathcal{C}'} A$

Example: Consider $\mathbb{R}$ with the usual topology. $\mathcal{C} = \{(-\infty, n) : n \in \mathbb{N}\}$ is an open cover of $\mathbb{R}$. $\mathbb{R}$ with the usual topology is **not** compact because $\mathcal{C} = \{(-n, n) : n \in \mathbb{N}\}$ is an open cover of $\mathbb{R}$ that cannot be reduced to a finite cover.

Intuition

Compactness can be thought of as a property having to do with the finiteness of a space. For example, spaces like $\mathbb{R}$ or $[0, \infty)$ with the usual topology are "infinitely large" and are not compact. However, compactness is defined in terms of open sets, so intervals like (a, b) and $[a, b)$ are noncompact, while closed intervals $[a, b]$ are compact.

Definition 2.11. Given a topological space $(X, \mathcal{T})$ and an equivalence relation $\sim$ defined on the set X, a *quotient space*$(S, \mathcal{S})$ induced by $\sim$ is defined by the set $S = X \backslash \sim$ and the *quotient topology* $\mathcal{S}$ where $S := \{U \subseteq S | \{x : [x] \in U\} \in \mathcal{T}\}$.

Examples:

1. Take the square $[0, 1] \times [0, 1]$ with the equivalence relation given by $(0, t) \sim (1, 1 - t)$ $\forall\, t \in [0, 1]$. The space obtained as a quotient space is called the *Möbius band*:

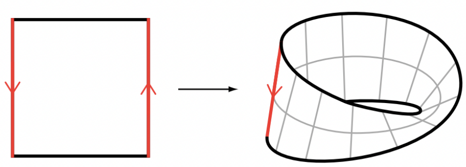


Figure 2: The visual representation for the Möbius band is given above [1].

2. Take the square $[0, 1] \times [0, 1]$ with the equivalence relation given by $(0, t) \sim (1, t)$ $\forall\, t \in [0, 1]$ and $(s, 0) \sim (s, 1)$ $\forall\, s \in [0, 1]$. The space obtained as a quotient space is called the *torus*:

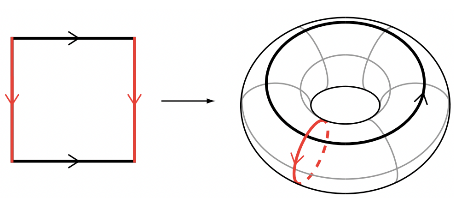


Figure 3: The visual representation for the torus is given above [1].

3. Take the square $[0,1] \times [0,1]$ with the equivalence relation given by $(0,t) \sim (1,t)$ $\forall$ $t \in [0,1]$ and $(s,0) \sim (1-s,1)$ $\forall$ $s \in [0,1]$. The space obtained as a quotient space is called the *Klein bottle*:

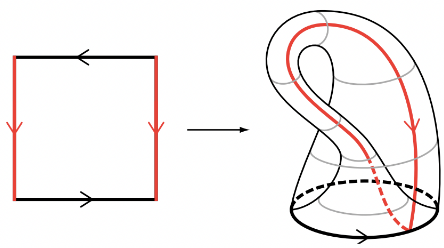


Figure 4: The visual representation for the Klein bottle is given above [1].

2.2 Metric Spaces

Definition 2.12. A *metric space* is an ordered pair (X,d) where X is a set and $d : X \times X \to \mathbb{R}^+ \cup \{0\}$ is a metric on X. In other words, d is a function such that for any x, y, and z in X the following properties hold:

- Identity: $d(x,y) = 0$ if and only if $x = y$;
- Symmetry: $d(x,y) = d(y,x)$;
- Triangle inequality: $d(x,z) \leq d(x,y) + d(y,z)$.

The function d is typically called a *distance function*.

Definition 2.13. Let (X,d) be a metric space. Fix a point $c \in X$, and let $r > 0$. We define the following sets:

- An *open ball centered at c of radius r* is the set $B_0(c,r) := \{x \in X \ : \ d(x,c) < r\}$.
- An *closed ball centered at c of radius r* is the set $B(c,r) := \{x \in X \ : \ d(x,c) \leq r\}$.

Given a metric space (X,d), the distance function induces a topology on X where the collection $\{B_0(c,r) | c \in X, 0 < r\}$ and their union are the open sets of X. In this case we use the notation $(X, \mathcal{T}_d)$ to indicate that X is considered a topological space with the topology induced by the metric d.

Examples:

1. The *Euclidean metric on* $\mathbb{R}$ is defined as follows

$$\begin{aligned} d : \mathbb{R} \times \mathbb{R} &\to \mathbb{R}^+ \cup \{0\} \\ (x,y) &\mapsto |x-y|. \end{aligned}$$

Open balls are $B_0(c,r) = \{x \in \mathbb{R} \ : \ |x-c| < r\} = (c-r, c+r)$.

The topology induced by the Euclidian metric on $\mathbb{R}$ is the usual topology on $\mathbb{R}$.

2. The *Euclidean metric on* $\mathbb{R}^n$ is defined as follows

$$\begin{aligned} d : \mathbb{R}^n \times \mathbb{R}^n &\to \mathbb{R}^+ \cup \{0\} \\ (\mathbf{x}, \mathbf{y}) &\mapsto \sqrt{(x_1 - y_1)^2 + \cdots + (x_n - y_n)^2}, \end{aligned}$$

for all $\mathbf{x} = (x_1 \ \cdots \ x_n)^T$ and $\mathbf{y} = (y_1 \ \cdots \ y_n)^T$. Open balls $B_0(c, r)$ are disks centered at $c = \begin{pmatrix} c_1 & \cdots & c_n \end{pmatrix}^T$ of radius r without boundary.

$(\mathbb{R}^n, \mathcal{T}_d)$ is known as $\mathbb{R}^n$ with the usual topology.

In this case, we denote open balls and closed balls centered at $\mathbf{c} = \mathbf{0} = (0 \ \ldots \ 0)^T$ and of radius $r = 1$ by B_0^n and B^n, respectively.

We also define the $(n-1)$*-sphere centered at* $\mathbf{c}$ *of radius* r as the set

$$S(c, r) \coloneqq \{\mathbf{x} \in \mathbb{R}^n \ : \ (x_1 - c_1)^2 + \cdots + (x_n - c_n)^2 = r^2\},$$

for all $\mathbf{x} = (x_1 \ \cdots \ x_n)^T$ and $\mathbf{c} = (c_1 \ \cdots \ c_n)^T$. When $\mathbf{x} = \mathbf{0}$ and $r = 1$, we simply write S^{n-1} and call it the $(n-1)$*-unit sphere.*

3. Let X be a nonempty set. The *discrete metric on* X is defined as follows

$$\begin{aligned} d : X \times X &\to \mathbb{R}^+ \cup \{0\} \\ (x, y) &\mapsto \begin{cases} 0, & \text{if } x = y \\ 1, & \text{if } x \neq y. \end{cases} \end{aligned}$$

Open balls $B_0(c, r) = \{x \in X \ : \ d(c, x) < r\}$ are

$$B_0(c, r) = \begin{cases} \{c\}, & \text{if } 0 < r \leq 1 \\ X, & \text{if } r > 1. \end{cases}$$

4. The *infinity metric on* $\mathbb{R}^2$ is defined as follows

$$\begin{aligned} d_\infty : \mathbb{R}^2 \times \mathbb{R}^2 &\to \mathbb{R}^+ \cup \{0\} \\ (\mathbf{x}, \mathbf{y}) &\mapsto \max\{|x_1 - y_1|, |x_2 - y_2|\}, \end{aligned}$$

for all $\mathbf{x} = (x_1 \ x_2)^T$ and $\mathbf{y} = (y_1 \ y_2)^T$.

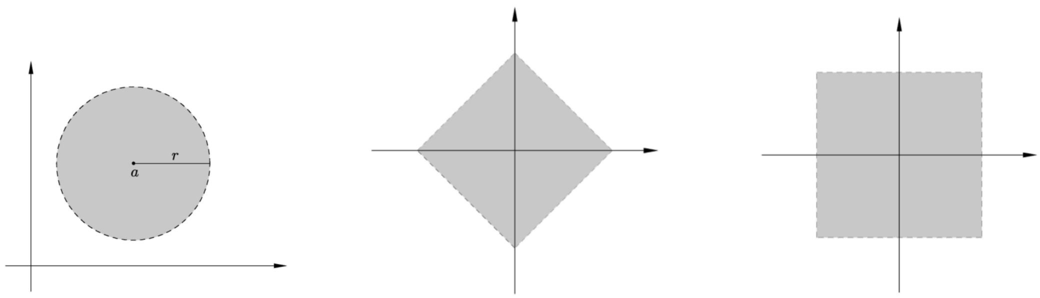
Open balls $B_0(c, r) = \{x \in \mathbb{R}^2 \ : \ \max\{|x_1 - c_1|, |x_2 - c_2|\} < r\}$ are squares centered at $c = (c_1 \ c_2)^T$ of side length $2r$ without boundary.

5. The *taxicab or Manhattan metric on* $\mathbb{R}^2$ is defined as follows

$$\begin{aligned} d_\infty : \mathbb{R}^2 \times \mathbb{R}^2 &\to \mathbb{R}^+ \cup \{0\} \\ (\mathbf{x}, \mathbf{y}) &\mapsto |x_1 - y_1| + |x_2 - y_2|, \end{aligned}$$

for all $\mathbf{x} = (x_1 \ x_2)^T$ and $\mathbf{y} = (y_1 \ y_2)^T$.

Open balls $B_0(c, r) = \{x \in \mathbb{R}^2 \ : \ |x_1 - c_1| + |x_2 - c_2| < r\}$



(a) Open ball $B_0(a, r)$ with the Euclidean metric on $\mathbb{R}^2$ (b) Open ball $B_0(\mathbf{0}, 1)$ with the taxicab metric on $\mathbb{R}^2$ (c) Open ball $B_0(\mathbf{0}, 1)$ with the infinity metric on $\mathbb{R}^2$

Figure 5: Here are examples of open balls under different metrics [15].

Definition 2.14. Suppose we have some metric space (X, d). Let $Q \subseteq X$ be a point set. A point $p \in X$ is a *limit point* of Q, if for every real number $\epsilon > 0$, Q contains a point $q \neq p$ such that $d(p, q) < \epsilon$.

In other words, there is an infinite sequence of points in Q that gets progressively closer to p, without actually being p, and gets arbitrarily close. In terms of topological spaces, a point $p \in X$ is a limit point of a set $Q \subseteq X$ if every open set containing p intersects Q.

Definition 2.15. Let $Q \subseteq X$ be a point set. Q is called *disconnected* if Q can be partitioned into two disjoint non-empty sets U and V so that there is no point in U that is a limit point of V, and no point in V that is a limit point of U. If no such partition exists, then Q is *connected*.

Definition 2.16. Cl Q is the set containing every point in Q and every limit point of Q. A point set Q is *closed* if $Q = \text{Cl } Q$, where Q contains all the limit points. Q is *open* if its complement is closed, that is, $X \backslash Q = \text{Cl } (X \backslash Q)$.

Definition 2.17. The *boundary* of a point set Q in a metric space X, denoted $\operatorname{Bd} Q$, is the intersection of the closures of Q and its complement, i.e., $\operatorname{Bd} Q = \operatorname{Cl} Q \cap \operatorname{Cl}(X \backslash Q)$. The *interior* of Q, or $\operatorname{Int} Q$, is $Q \backslash \operatorname{Bd} Q = Q \backslash \operatorname{Cl}(X \backslash Q)$.

Definition 2.18. The diameter of a point set Q is $\sup_{p,q \in Q} d(p, q)$. The set Q is *bounded* if its diameter is finite, and unbounded if its diameter is infinite. A point set Q in a metric space is *compact* if it is closed and bounded.

Intuition

The intuition of compactness in a metric space, like compactness of a topological space, can be thought of similarly to the intuition of finiteness.

2.3 Homeomorphisms and Homotopies

Definition 2.19. Let $(X, \mathcal{T}_X)$ and $(Y, \mathcal{T}_Y)$ be topological spaces. A function $f : X \to Y$ is said to be *continuous* if for all $U \in \mathcal{T}_Y$, $f^{-1}(U) \in \mathcal{T}_X$.

Example: Consider $f : \mathbb{R} \to \mathbb{R}$ given by $f(x) = x$, for all $x \in \mathbb{R}$. Then for any open set U in $\mathbb{R}$, $f^{-1}(U) = U$ and so is open. Thus, f is continuous.

Definition 2.20. A continuous map $i : X \to Y$ is an *embedding* if i is injective.
X lives inside Y and $\dim(X) \leq \dim(Y)$.
Notation: $X \hookrightarrow Y$

Definition 2.21. A continuous map $f : X \to Y$ is a *homeomorphism* if the following conditions are satisfied:

1. f is bijective
2. f^{-1} is continuous

Remark. Homeomorphisms preserve properties that depend on the topology of spaces. Thus, connectedness, compactness, Hausdorff, dimension, # of holes, and orientability are preserved by homeomorphisms.

Intuition

We can think of two spaces as being homeomorphic when they are related by a continuous deformation, meaning they are related by stretching and bending without any tearing anything apart or gluing parts together.

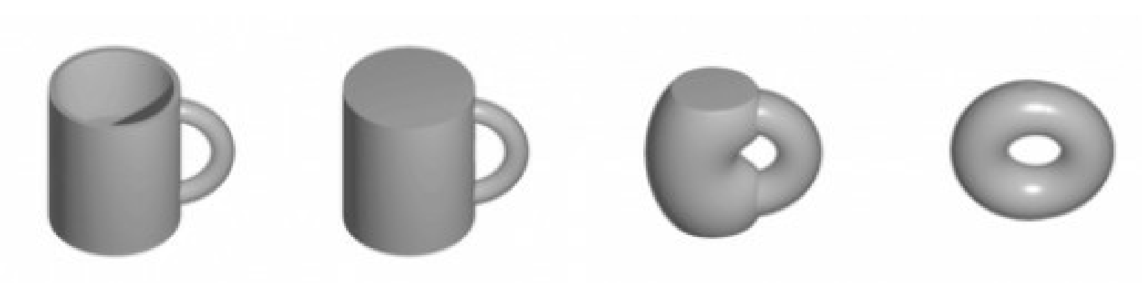


Figure 6: One common example of a homeomorphism is the deformation of a mug into a torus (or a coffee cup into a donut), via stretching and bending as per the intuition stated above. [9]

Examples:

1. Consider $\mathbb{R}^n$ with the Euclidean topology and B_0^n. Then
$$\begin{aligned} f : & B_0^n \to \mathbb{R}^n \\ X & \mapsto \frac{X}{1-||x||} \end{aligned}$$
is a homeomorphism. (To verify this, need to show that f is continuous and bijective and that f^{-1} is continuous.)

   $f^{-1}(X) = \frac{X}{1+||X||}$

2. The xy-plane is homeomorphic to a punctured two-dimensional sphere.

   $T : S^3 \backslash \{(0,0,1)\} \to \mathbb{R}^2$

   $(x,y,z) \mapsto \left(\frac{x}{1-z}, \frac{y}{1-z}\right)$

   $T^{-1} : \mathbb{R}^2 \to S^3 \backslash \{(0,0,1)\}$

   $(x,y) \mapsto \left(\frac{2x}{x^2+y^2+1}, \frac{2y}{x^2+y^2+1}, , \frac{x^2+y^2-1}{x^2+y^2+1}\right)$

   T is called the *stereographic projection of* $S^3 \backslash \{(0,0,1)\}$ *onto the plane* $z = 0$.

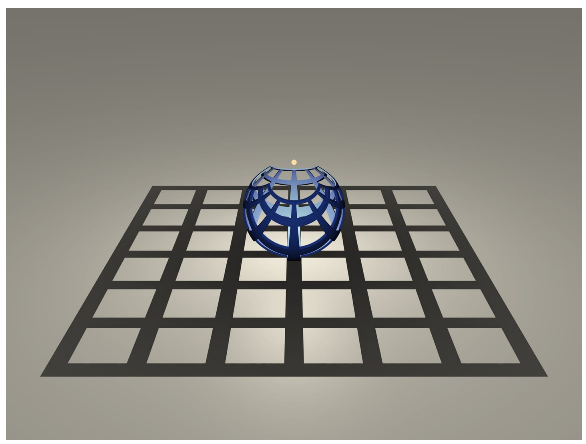


Figure 7: Here is a visual representation of the stereographic projection, mapping a sphere (with a pole punctured) onto a plane. This homeomorphism is also demonstrated well in this video. [23]

3. $\mathbb{R}^m$ and $\mathbb{R}^n$ are not homeomorphic if $m \neq n$.

   $(0,1) \ncong [0,1]$ because $(0,1)$ is not compact and $[0,1]$ is compact.

   $(\{0,1\}, discrete) \ncong (\{1,2,3\}, discrete)$ because they have different cordinality

4. A bijective map $f : X \to Y$ can be continuous without being a homeomorphism (i.e. 2nd condition in the definition is necessary)

   $f : [0, 2\pi) \to S^1$ defined by $f(0) = (\cos\theta, \sin\theta)$ is continuous and bijective, but its inverse is **not** continuous.

   Note also that $[0, 2\pi)$ (not compact) cannot be homeomorphic to S^1 (compact).

Definition 2.22. Let $f, g : X \to Y$ be continous maps. A *homotopy* between f and g is a continous map $H : X \times [0,1] \to Y$ such that

1. $H(x, 0) = f(x)\ \forall x \in X$
2. $H(x, 1) = g(x)\ \forall x \in X$

Notation/Terminology: f is *homotopic* to g, $f \simeq g$

Example: A point is homotopic to a disk. Consider the maps:

$$f : B^2 \to \{0\} \text{ and } g : \{0\} \to B^2.$$

Observe that $f \circ g = \mathrm{id}_{\{0\}}$. Let us define a homotopy between $g \circ f$ and id_{B^2}.
$H : B^2 \times [0,1] \to B^2$
$H(x, 0) = 0 = (g \circ f)(x)$
$H(x, 1) = x$

Definition 2.23. Let X and Y be topological spaces. Let $f, g : X \hookrightarrow Y$ be embeddings. An *isotopy* between f and g is a continous map $I : X \times [0,1] \to Y$ such that

1. $I(x, 0) = f(x)\ \forall x \in X$
2. $I(x, 1) = g(x)\ \forall x \in X$
3. $i_t : X \to Y$ is an embedding $\forall t \in [0,1]$, where $i_t(x) = I(x, t)$

Notation/Terminology: f is *isotopic* to g

Definition 2.24. X and Y are *homotopic* if there exist maps $f : X \to Y$ and $g : X \to Y$ such that $g \circ f \simeq id_X$ and $f \circ g \simeq id_Y$.
Notation/Terminology: X is *homotopy equivalent* to Y: $X \simeq Y$

Definition 2.25. Let $A \subseteq X$. A *retraction of X to A* is a map $r|_A = id_A$. A *deformation retraction of X onto A* is a map $R : X \times [0,1] \to X$ such that

1. $R(x, 0) = x\ \forall x \in X$
2. $R(x, 1) \in A\ \forall x \in X$
3. $R(a, t) = a\ \forall a \in A\ \forall t \in [0,1]$

Terminology: A is a *deformation retract* of X

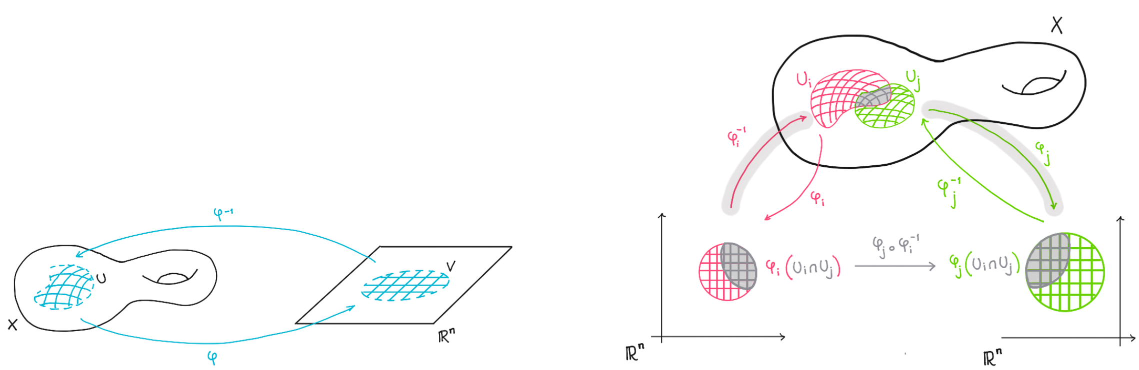
2.4 Manifolds

Definition 2.26. Let X be a topological space. Given an open set $U \subseteq X$, a *chart* is a homeomorphism $\phi : U \to V$, where $V \subseteq \mathbb{R}^n$ is an open set.

Notation/Terminology: We write (U, ϕ) for a chart, where the inverse ϕ^{-1} gives U a coordinate system.

Definition 2.27. An *atlas* for X is a collection of charts $\{U_i\}_{i \in I}$ such that the collection is an open cover of X.

Definition 2.28. If (U_i, ϕ_i) and (U_j, ϕ_j) are charts so that $U_i \cap U_j \neq \emptyset$, the map $\phi_j \circ \phi_i^{-1} : (U_i \cap U_j) \to \phi_j(U_i \cap U_j)$ is called a *transition map from ϕ_i to ϕ_j*. (See Figure 14b)



(a) A chart (b) A transition map

Figure 8: Here are examples of a chart and a transition map.

Intuition

A chart can be thought of as a patch on X that looks exactly like $\mathbb{R}^n$. Transition maps describe how coordinates change as we move from chart to chart.

Definition 2.29. Let M be a topological space. M is an *n-dimensional topological manifold* if:

1. M is a Hausdorff space (i.e., M has enough open sets)
2. M is a second-countable space (i.e., there is a countable number of basic open sets)
3. M is locally Euclidean of dimension n, i.e. $\forall m \in M \, \exists \, U$ open such that $m \in U$ and (U, ϕ) is a chart. In other words, there is an atlas for M.

Definition 2.30. Let M be an n-dimensional topological manifold. M is an *n-dimensional smooth manifold* if the transition maps are continuous and infinitely differentiable.

Examples:

1. $\mathbb{R}^n$ is an n-dim smooth manifold, covered by a single chart $(\mathbb{R}^n, \mathrm{id})$
2. S^1 is a 1-dim smooth manifold, covered by two charts. Let $\epsilon > 0$.

$$\mathcal{U}_+ := \{(x, y) \in S^1 : y > \epsilon - 1/2\} \text{ and } \mathcal{U}_- := \{(x, y) \in S^1 : y > \epsilon + 1/2\}$$

3. The n-sphere $S^n \subseteq \mathbb{R}^{n+1}$ is an n-dim smooth manifold for $n \geq 1$, covered by two charts.
4. The torus $T := ([0,1] \times [0,1])\backslash \sim, (x, 0) \sim (x, 1)$ and $(0, y) \sim (1, y)$ is a 2-dim smooth manifold.
5. The Möbius band $M := ([0,1] \times [0,1])\backslash \sim, (x, 0) \sim (1 - x, 1)$ is a 2-dim smooth manifold.

Definition 2.31. Let M be a smooth topological m-manifold. A function $f : M \to \mathbb{R}^n$ is *smooth* if $\forall p \in M \exists$ a chart (U, ϕ) for M such that $p \in U$ and $f \circ \phi^{-1} : \phi(U) \subseteq \mathbb{R}^m \to \mathbb{R}^n$ is smooth.

Definition 2.32. Let M be a smooth topological m-manifold. A smooth function $h : M \to \mathbb{R}$ is a *Morse function* if and only if:

1. None of f's critical points are degenerate
2. The critical points have distinct function values

Remark. The critical points of h are places where the inverse images of $f^{-1}(I)$ for $I \subseteq \mathbb{R}$, an open interval, behave in irregular ways, such as holes and points of discontinuity. Thus, M can be characterized by the critical points of suitable continuous functions $M \to \mathbb{R}$.

Definition 2.33. Level Sets

1. The *interval levelset of h with respect to I* is the inverse image of I under h: $M_I := h^{-1}(I) := \{x \in M : h(x) \in I\}$
2. The *sublevel set $M_{\leq a}$ of I* is if $I = (-\infty, a]$, where $M_{\leq a} := h^{-1}(I)$
3. The *superlevel set $M_{\geq a}$ of I* is if $I = [a, \infty)$, where $M_{\geq a} := h^{-1}(I)$
4. The *levelset of h at $a \in \mathbb{R}$* is if $I = \{a\}$, called $h^{-1}(a)$.

Example:

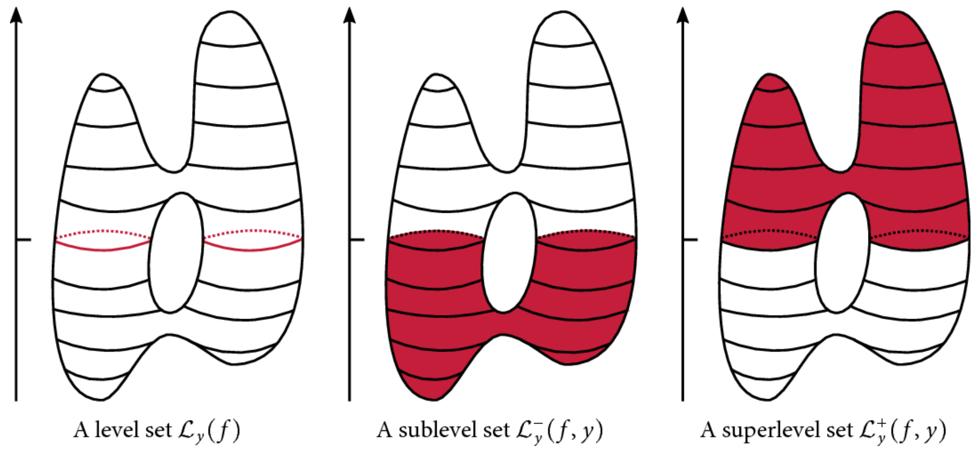


Figure 9: Here is a visual representation of level sets, sublevel sets, and superlevel sets. In this example, the level set contains two different contours, while the sublevel set and the superlevel set only have one single connected component each [21].

Theorem 2.34. Let $h : M \to \mathbb{R}$ be a smooth function on a manifold M. Let $a, b \in \mathbb{R}$ where $a < b$. Suppose $M_{[a,b]}$ is compact and contains no critical points of h. Then:

1. $M_{\leq a}$ is diffeomorphic to $M_{\leq b}$
2. $M_{\leq a}$ is a deformation retract of $M_{\leq b}$
3. The inclusion $i : M_{\leq a} \hookrightarrow M_{\leq b}$ is a homotopy equivalence.

Example: Consider the height function $h : M \to \mathbb{R}$ defined as a vertical torus. There are four critical points of h: u (minimum), v, w (saddles), and z (maximum). Here, $M_{\leq a}$ is empty for $a < h(u)$, homeomorphic to a 2-disk for $h(u) < a < f(v)$, homeomorphic to a cylinder for $h(v) < a < h(w)$, homeomorphic to a compact genus-one surface with a circle as a boundary for $h(w) < a < h(z)$, and a full torus for $a > h(z)$.

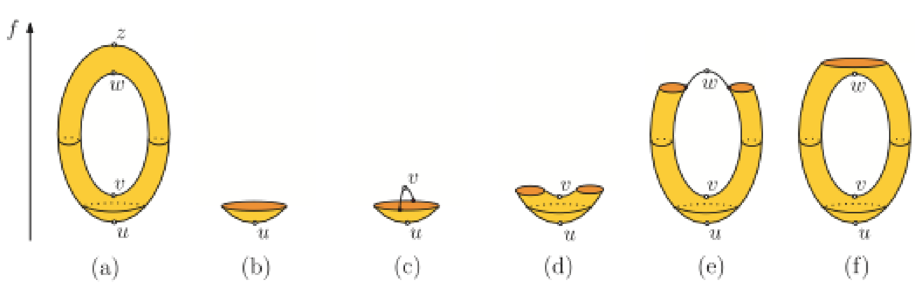


Figure 10: A visual representation of height function h. In (a), h is defined as a torus with four critical points. In (b)-(f), note that passing through each index-k critical point is the same attaching a k-cell from the homotopy point of view [6].

2.5 Basics of Topology Exercises

1. A topological space $\mathbb{T}$ is called *path connected* if any two points $x, y \in \mathbb{T}$ can be joined by a path, that is, there exists a continuous map $f : [0,1] \to \mathbb{T}$ of the secment $[0,1] \subset \mathbb{R}$ onto $\mathbb{T}$ so that $f(0) = x$ and $f(1) = y$. Prove that a path connected space is also connected but the converse may not be true; however, if $\mathbb{T}$ is finite, then the two notions are equivalent.

   Proof. Suppose X is not connected. Then, there exist $U, V \in \mathcal{T}_x$ such that $U \cap V = \emptyset$ and $U \cup V = X$ by definition. Let $x \in U, y \in V$. Since X is path connected, $\exists \alpha : [0,1] \to X$ that is a continuous map, where $\alpha(0) = x$ and $\alpha(1) = y$. By hypothesis, $\alpha^{-1}(U) \cap \alpha^{-1}(V) = \emptyset$ and $\alpha^{-1}(U) \cup \alpha^{-1}(V) = [0,1]$. Also, $\alpha^{-1}(U), \alpha^{-1}(V)$ are open in $[0,1]$ by the continuity of α, and $0 \in \alpha^{-1}(U)$ and $1 \in \alpha^{-1}(V)$. Thus, $[0,1]$ is disconnected, which is a contradiction, since α is continuous. Thus, by contradiction, a path connected space is also connected, as required.

   In order to prove the converse may not be true, take the counterexample of the topologist's sine curve. This space is the graph of the function $f(x) = sin(1/x)$ for x in the interval $(0,1]$ with the point $(0,0)$. The space is connected because it is a continuous curve that cannot be disconnected, but it is not path connected because if we try to get from a point on the graph of $f(x)$ to the point $(0,0)$, there is an infinitely long path to approach $(0,0)$. Thus, the converse is not necessarily true.

   Now, suppose X is a finite connected space. For $x \in X$, let $U_x := \bigcap\{U \subseteq X : U$ open, $x \in U\}$ denote the smallest open set containing x. Let $A \subseteq X$ denote the set of points $y \in X$ for which there exists a sequence $x_0 = x, x_1, ..., x_n = y$ such that for each i, either $x_i \in U_{x_{i+1}}$ or $x_{i+1} \in U_{x_i}$. We have that $x \in A$, and for any $y \in A, U_y \subseteq A$, hence A is open. If $z \notin A$, then $U_z \subseteq X\ A$, hence A is closed. Since X is connected, $A = X$. Now, define $\beta : [0,1] \to X$ by $\beta(t) = x$ for $t < 1$ and $\beta(1) = y$ and let $x \in U_y$. Let $U \subseteq X$ open, thus if $y \notin U$, then $\beta^{-1}[U] \in \{\emptyset, [0,1\}\}$, hence $\beta^{-1}[U]$ is open. If $y \in U$, then $U_y \subseteq U$, hence $x \in U$, thus $\beta^{-1}[U] = [0,1]$. Thus, β is continuous. Now, if we take the aforementioned sequence, x_i and x_{i+1} are connectable by a path β_i. As this is true for all i, x_0 and x_n are connected by a path, and so X is path connected, as required. □

2. Prove that for every subset X of a metric space Cl Cl X = Cl X. In other words, augmenting a set with its limit points does not give it more limit points.

   Proof. Take a topological space (X, $\mathcal{T}_x$) and $A \subseteq X$. Recall by definition that Cl(A) $:= \bigcap\{C \subseteq X : C$ is closed and $A \subseteq C\}$. Let B := Cl(A). Then, we want to show that Cl(B) = B, i.e. B is closed. Recall that by definition of closure, B $\subseteq$ Cl(B). In addition, let p be a limit point of Cl(B). We want to show that p is also a limit point of B. Let $\epsilon > 0$. Then, there is a point $q \neq p \in$ Cl(B), $d(p,q) =: s < \epsilon$ by definition. Thus, either $q \in$ B, or q is a limit point of B. In the latter case, the ball $B_{r-s}(q)$ of radius $r-s$ is contained in $B_r(p)$ and intersects B, so $B_r(p)$ intersects B for any $\epsilon > 0$. Thus, p is also a limit point of B. Thus, Cl(B) $\subseteq$ B. As a result, Cl(B) = B, i.e. B is closed, as required. □

3. Show that any metric on a finite set induces the discrete topology.

Proof. Let (X,d) be finite and non-empty. We want to show that $\{x\}$, a finite set, is open $\forall x \in X$. If X=$\{x\}$, then it is trivial that any metric on the finite set induces the discrete topology. Now, let $\#(X) > 1$. Let $x \in X$ and $S := \{d(x,y) : \forall y \in X\ \{x\}$, where r := min(S). Then, $B_0(x,r) = \{x\}$. Thus, $\forall x \in X$, $\{x\}$ is open, as required. □

4. Give an example of a bijective function that is continuous, but its inverse is not.

Proof. Let X be a set and $\mathcal{T}_1, \mathcal{T}_2$ be two topologies on X with $\mathcal{T}_2 \not\subseteq \mathcal{T}_1$. Then, the identity function from the topological space $(X, \mathcal{T}_1)$ to $(X, \mathcal{T}_2)$ is a continuous bijection, but the inverse function, the identity function from $(X, \mathcal{T}_2)$ to $(X, \mathcal{T}_1)$ is not continuous, as required. □

5. Let $f : \mathbb{T} \to \mathbb{U}$ be a continuous function of a compact space $\mathbb{T}$ into another space $\mathbb{U}$. Prove that the image $f(\mathbb{T})$ is compact.

Proof. Let $f : X \to Y$ be a continuous function of a compact space X into another space Y. Let $\{V_i\}_{i \in I}$ be an open cover of $f(X)$. Since f is continuous, then $\{f^{-1}(V_i)\}$ is a collection of open sets in X. Also, $\bigcup_{i \in I} f^{-1}(V_i) = X$ because $\forall x \in X, f(x) \in Y$, and so $\exists i$ s.t. $f(x) \in V_i$, where $x \in f^{-1}(V_i)$. Since X is compact, there exists a finite subcover, $\{f^{-1}(V_i)\}_{i \in I'}$. If $y \in f(X), \exists x \in X$ such that $f(x) = y$ and $\exists i \in I'$ such that $x \in f^{-1}(V_i)$. Thus, $f(x) \in V_i$ for some $i \in I'$. Hence, $\{V_i\}_{i \in I'}$ is a finite subcover of $f(X)$, which means that the image $f(X)$ is compact, as required. □

6. Deduce that homeomorphism is an equivalence relation. Show that the relation of homotopy among maps is an equivalence relation.

Proof. In order to show that homotopy is an equivalence relation, consider the continuous maps $f, g : X \to Y$, where X, Y are topological spaces. We must verify that $\sim$ is reflexive, symmetric, and transitive.

(a) Reflexivity: Consider the continuous map $F : X \times [0,1] \to X$. Then, $F(x,t) = f(x)$ is a homotopy from f to f, and $f \cong f$.

(b) Symmetry: Consider the continuous map $F : X \times [0,1] \to X$ and suppose it is a homotopy from f to g. Then, the map $G : X \times [0,1] \to X$, $G(x,t) = F(x, 1-t)$ is a homotopy from g to f. Thus, $f \cong g \Rightarrow g \cong f$.

(c) Transitivity: Consider the same continuous map F and another continuous map $G : X \times [0,1] \to X$, which is a homotopy from g to h. Then, the map $H : X \times [0,1] \to X$, defined by:

$$H(x,t) = \begin{cases} F(x,2t) & \text{if } 0 \leq t \leq 1/2 \\ G(x,2t-1) & \text{if } 1/2 \leq t \leq 1 \end{cases}$$

is a homotopy from f to h since in topology two continuous functions can be pasted together to form another continuous function. Thus, $f \cong g$ & $g \cong h \Rightarrow f \cong h$.

Since the properties of an equivalence relation have been satisfied, the relation of homotopy among maps is an equivalence relation, as required. Moreover, homeomorphism can also be proven to be an equivalence relation by considering the same properties. For any topological space X, the continuous identity map is a homeomorphism from X to X, satisfying the reflexive property. In addition, if we let $f : X \to Y$ be a homeomorphism, then f^{-1} is a continuous bijection. Also, $(f^{-1})^{-1} = f$, so f^{-1} has a continuous inverse. Thus, $f^{-1} : Y \to X$ is a homeomorphism, satisfying the symmetric property. Finally, if we let $f : X \to Y$ and $g : Y \to Z$ be homeomorphisms, $f \circ g : X \to Z$ is also a homeomorphism, since $(f^{-1} \circ g^{-1}) \circ (g \circ f) = id_X$ and $(g \circ f) \circ (f^{-1} \circ g^{-1}) = id_Z$, and so $f \circ g$ is a bijection, and since this is a composition of continuous functions, it is also continuous , and since $f^{-1} \circ g^{-1}$ is a composition of continuous functions, it is also continuous; thus, satisfying the transitive property. Thus, we can deduce that homeomorphism is an equivalence relation, as required. □

3 Complexes

Simplicial complexes are spaces constructed from building blocks called simplices, which are points, line segments, filled-in triangles, and solid tetrahedra that provide a useful way to construct topological spaces from sets of points. There are different types of complexes that algorithmically allow us to construct topological spaces and view their geometric realizations, and each are useful in their own ways, especially when the original topological space is unknown.

3.1 Simplicial Complexes

Definition 3.1. Suppose $\{x_0, x_1, ..., x_k\} \subseteq \mathbb{R}^n$ satisfy the condition that the set of vectors $\{x_1 - x_0, x_2 - x_0, ..., x_k - x_0\}$ in $\mathbb{R}^n$ are linearly independent. The *k-simplex* spanned by $\{x_0, x_1, ..., x_k\}$ is the set of all points

$$z = \sum_{i=0}^{k} a_i x_i \text{ such that } a_1, a_2, ..., a_k \in \mathbb{R}^+ \text{ and } \sum_{i=0}^{k} a_i = 1.$$

For a given point z, we refer to a_i as the *i-th barycentric coordinate.*

Example: We can geometrically describe simplices as follows:

1. A 0-simplex is a point where $\{x_0\} \subseteq \mathbb{R}^n$.

2. A 1-simplex is a line segment with endpoints x_0 and x_1.

3. A 2-simplex is a filled-in triangle with vertices x_0, x_1 and x_2.

4. A 3-simplex is a solid tetrahedron with vertices x_0, x_1, x_2 and x_3.

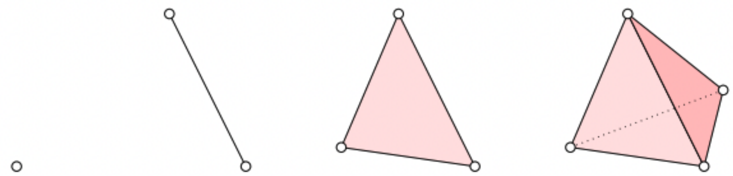


Figure 11: From left to right: 0-simplex, 1-simplex, 2-simplex, 3-simplex [8].

Definition 3.2. Let S be a k-simplex spanned by $\{x_0, x_1, ..., x_k\} \subseteq \mathbb{R}^n$.

1. A *face of* S is any simplex spanned by a subset of $\{x_0, x_1, ..., x_k\}$. Any k-simplex has $k+1$ faces of dimension $(k-1)$.

2. The *interior of* S is the subset of S where $a_i > 0$ for all barycentric coordinates a_i, we denote it by $Int(S)$.

3. The *boundary of* S is $Bd(S) := S \setminus Int(S)$.

Definition 3.3. A *simplicial complex* X in $\mathbb{R}^n$ is a set of simplices in $\mathbb{R}^n$ such that

1. every face of a simplex in X is also a simplex in K, and

2. for any two simplices $\sigma, \tau \in X$, their intersection $\sigma \cap \tau$ is either empty or a face of both σ and τ.

Terminology:

1. We say X has *dimension* k if k is the maximum dimension among all simplices in X.

2. We say X is *finite* if X has finitely many simplices.

3. The collection of simplices of dimension at most L is referred to as the l-*skeleton* of the simplicial complex; we denote it by X_l.

4. The *geometric realization* $|X|$ of a finite simplicial complex X is the topological space given by the union of simplices in X, given the subspace topology.

Definition 3.4. Let X be a simplicial complex. Any subset $X' \subseteq X$ that is itself a simplcial complex is called a *subcomplex* of X.

Example: Consider the l-skeleton consisting of all simplices of dimension l or less, such that $X' = \{\sigma \in X | \dim \sigma \leq l\}$. X' is a subcomplex of X since the union of simplices of dimension l or less forms a simplicial complex.

Definition 3.5. Let X and Y be simplicial complexes. A *simplicial map* $f : X \to Y$ is specified by a map $f_0 : X_0 \to Y_0$ such that whenever $\{x_0, ..., x_k\} \subseteq X_0$ span a simplex of X, $\{f(x_0), ..., f(x_k)\} \subseteq Y_0$ span a simplex of Y.

The map $f : X \to Y$ is an *isomorphism of simplicial complexes* if:

1. f_0 is a bijection, and
2. $\forall\, k > 1$ $\{x_0, ..., x_k\}$ is a simplex of X if and only if $\{f(x_0), ..., f(x_k)\}$ is a simplex of Y.

Example: Consider the simplicial map $f : [0, 1]^2 \to \mathbb{T}^2$ below:

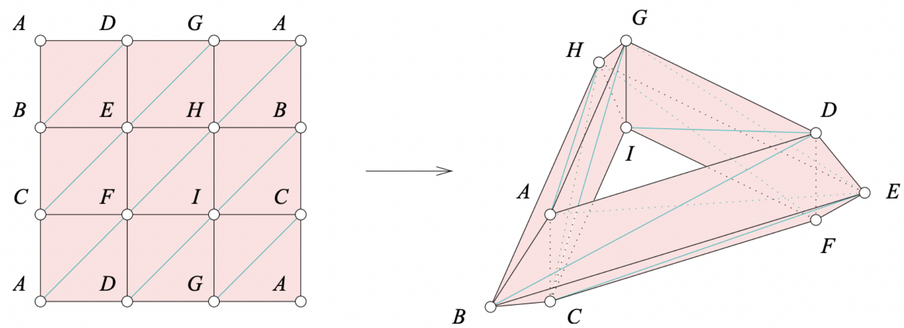


Figure 12: The simplicial map from the square to the torus [8].

This simplicial map glues the simplices of the triangulation of the square to obtain a triangulation of the torus. If we then take the vertex map f_0 : Vert$([0, 1]^2)$ $\to$Vert$(\mathbb{T}^2)$, we observe that f_0 is bijective since every vertex that spans the triangulation of the square also spans the triangulation of the torus. In addition, if we take the inverse map of f_0, it is also a vertex map, and thus induces a simplicial isomorphism between the square and the torus.

Definition 3.6. An *abstract simplicial complex* is a collection $\mathcal{K}$ of nonempty finite sets such that if $\sigma \in \mathcal{K}$, then every nonempty subset of σ is in $\mathcal{K}$.

1. Elements of $\mathcal{K}$ are called *simplices*.
2. The *dimension* of $\sigma \in \mathcal{K}$ is $dim\sigma := \#(\sigma) - 1$ where $\#(\sigma)$ is the number of elements of the set σ.
3. Any non-empty subset of a simplex σ is called a *face of* σ.
4. The *vertices* of $\mathcal{K}$ are the one-point sets in $\mathcal{K}$.
5. The *n-skeleton* of $\mathcal{K}$ is the subset of $\mathcal{K}$ consisting of set of cardinality $\leq n + 1$, we write $\mathcal{K}_l$.

6. The map $f : \mathcal{K} \to \mathcal{L}$ is a *map of abstract simplicial complexes* if there is a map $f_0 : \mathcal{K}_0 \to \mathcal{L}_0$ such that whenever $\{k_0, ..., k_k\} \subseteq \mathcal{K}_0$ span a simplex of $\mathcal{K}$, $\{f(k_0), ..., f(k_k)\} \subseteq \mathcal{L}_0$ span a simplex of $\mathcal{Y}$.

7. The map $f : \mathcal{K} \to \mathcal{L}$ is an *isomorphism of abstract simplicial complexes* if: f_0 is a bijection, and $\forall\ k > 1$ $\{k_0, ..., k_k\}$ is a simplex of $\mathcal{K}$ if and only if $\{f(k_0), ..., f(k_k)\}$ is a simplex of $\mathcal{L}$.

3.2 Nerves & Čech, Vietoris-Rips, and Delaunay Complexes

Definition 3.7. A *nerve* is the simplicial complex $N(U)$ such that if we take the finite collection of sets $U = \{U_i\}_{i=0}^n$, then:

1. $N(U)_0 = \{x_0, ..., x_n\}$, and
2. $\forall \{i_0, ..., i_k\} \subseteq \{0, 1, ..., n\}, \{x_{i_0}, ..., x_{i_k}\} \subseteq N(U)_0$ spans a k-simplex in $N(U)$, which occurs if and only if $U_{i_0} \cap U_{i_1} \cap ... \cap U_{i_k} \neq \emptyset$.
3. If U is a cover of a topological space, we call $N(U)$ the *nerve of a cover.*

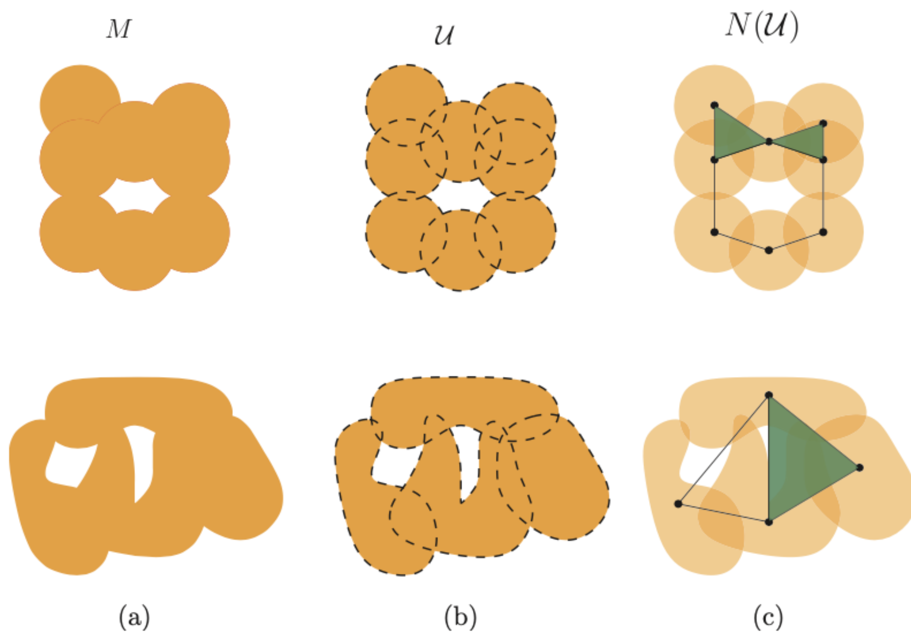


Figure 13: Here is an example of two spaces (a), open covers of them (b), and their nerves (c). [6].

Intuition

From Figure 13, we can see that practically, every cover gives a vertex, a double intersection of covers gives an edge, a triple intersection of covers gives a triangle with its interior, and a quadruple intersection of covers gives a tetrahedron with its interior.

Theorem 3.8. Let U be a finite cover of a metric space X. If every non-empty intersection $\bigcap_{i=0}^{k} U_{\alpha_i}$ of elements of U is contractible, then $X \simeq |N(U)|$.

Definition 3.9. Let (X, d) be a finite metric space, and $r > 0$ be a real number. Then, we can form topological spaces from distances in a set of points using the following two methods:

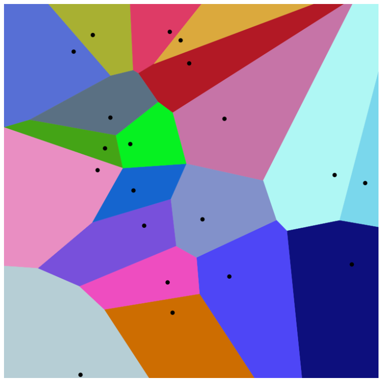
1. The *Čech complex* $C^r(X)$ is the abstract simplicial complex with:
   - vertices the points of X, and
   - a k-simplex when a set of points $\{x_0, x_1, ..., x_k\} \subseteq X$ satisfy $\bigcap_{i=0}^{k} B(x_i, r) \neq \emptyset$.
2. The *Vietoris-Rips complex* $VR^r(X)$ is the abstract simplicial complex with:
   - vertices the points of X, and
   - a k-simplex when a set of points $\{x_0, x_1, ..., x_k\}$ when $d(x_i, x_j) \leq 2r \; \forall \; 0 \leq i, j \leq k$.

Proposition 3.10. Let (X, d) be a finite metric space. For all $r > 0$, $C^r(X) \subseteq VR^r(X) \subseteq C^{2r}(X)$.

Proof. If there is a point $x' \in \bigcap_{i=0}^{k} B(x_i, r)$, then for every pair $(i, j), d(x_i, x_j) \leq 2r \; \forall \; 0 \leq i, j \leq k$. Thus, every simplex $\{x_0, x_1, ..., x_k\} \in C^r(X) \subseteq VR^r(X)$. In addition, let us consider another simplex $\{x_0, x_1, ..., x_k\} \in VR^r(X)$. Since by definition of Vietoris-Rips complex $d(x_i, x_0) \leq 2r \; \forall \; 0 \leq i \leq k$, we have that $\bigcap_{i=0}^{k} B(x_i, 2r) \supset x_0 \neq \emptyset$. Thus, by definition, $\{x_0, x_1, ..., x_k\}$ is also a simplex in $C^{2r}(X)$, as required. ☐

Definition 3.11. Let $X \subseteq \mathbb{R}^n$ be a finite set with given points $\{x_0, x_1, ..., x_k\}$. Assume that these points satisfy the condition that the set of vectors $\{x_1 - x_0, x_2 - x_0, ..., x_k - x_0\}$ in $\mathbb{R}^n$ are linearly independent, where for $\alpha_1, \alpha_2, ..., \alpha_k \in \mathbb{R}$: if $\alpha_1(x_1 - x_0) + \alpha_2(x_2 - x_0) + ... + \alpha_k(x_k - x_0) = \mathbf{0}$, then $\alpha_1 = \alpha_2 = ... = \alpha_k = 0$. Also, let d be a metric on X.

1. The *Voronoi diagram* Vor(X) of X is the tessellation of $\mathbb{R}^n$ into convex cells V_x for $x \in X$ called *Voronoi cells* where all the points in $\mathbb{R}^n$ are closer to x than to any other $x' \in X$, such that: $V_x := \{z \in \mathbb{R}^n : d(x, z) \leq d(x', z) \forall x' \in X\}$.
2. The *Delaunay complex* Del(X) is the simplicial complex obtained as the nerve of the cover of $\mathbb{R}^n$ by Voronoi cells, where Del(X) $= N(\{V_x\}_{x \in X})$.



(a) Euclidean distance

(b) Taxicab distance

Figure 14: Voronoi diagrams of 20 points in $\mathbb{R}^2$ using two different metrics [24].

3. The *Alpha complex* D_x^α is a subcomplex of the Delaunay complex containing all simplices in Del(X) that have a circumscribing ball of radius at most α, where for each $x \in X$, we let $B(x, \alpha)$ be denoted as a closed ball of radius α centering x, such that: $D_x^\alpha := \{p \in B(x, \alpha) : d(p, x) \leq d(p, x')\forall x' \in X\}$.

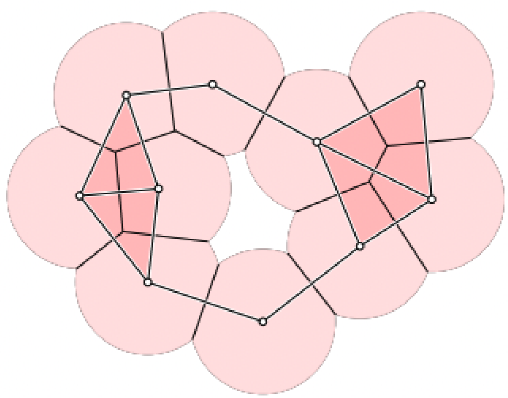


Figure 15: Here is an example of the union of balls decomposed into convex cells V_x by the Voronoi cells, with the corresponding alpha complex superimposed. Weighed alpha complexes, where we permit balls of different sizes, are also useful in modeling biomolecules, where each radius reflects the intermolecular forces of specific atom types [7].

4. The *Witness complex* $\mathcal{W}(W, L)$ is a simplicial complex intended to behave like a Delaunay triangulation but with two point sets, W called witnesses and L called landmarks, built with vertices in the landmarks and the remaining points determining which simplices occur in the complex. Thus, $\mathcal{W}(W, L)$ is defined as the collection of all simplices whose faces are all weakly witnessed by a point in $W \setminus L$.

If we let W be a point set with a real-valued function on pairs $d : W \times W \to \mathbb{R}$ and $L \subseteq W$ be a finite subset, a simplex $\sigma = \{l_1, ..., l_k\}$ with $l_i \in L$ is weakly witnessed by $x \in W \setminus L$ if $d(l, x) \leq d(w, x)$ for every $l \in \{l_1, ..., l_k\}$ and $w \in L \setminus \{l_1, ..., l_k\}$.

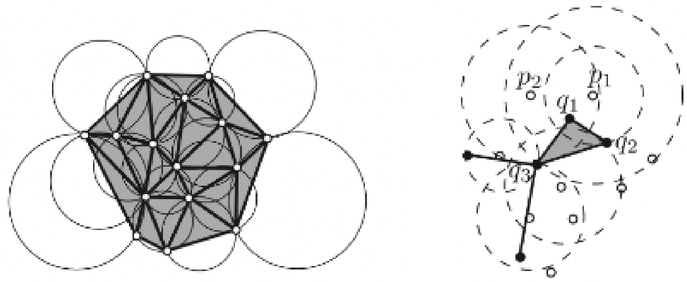


Figure 16: A Delaunay complex is shown to the left and a witness complex is shown to the right, constructed out of the points from the left figure, where landmarks are the black dots and the witness points are the hollow dots. The witnesses for five edges and the triangle are the centers of the six circles. For example, the triangle $q_1q_2q_3$ and the edge q_1q_3 are weakly witnessed by the points p_1 and p_2, respectively [6].

5. The *graph induced complex* (GIC) retains the simplicity of the Vietoris-Rips complex, the sparsity of the witness complex, and the similarity of the Delaunay triangulation. Given a graph G on (X, d) and subset $Y \subseteq X$, a simplex is in the complex if and only if its vertex set $V \subseteq Y$ has the property that a set of points in X, each being closest to exactly one vertex in V, forms a clique in G, which is an all-to-all connected set of vertices such that every two distinct vertices in the clique are adjacent.

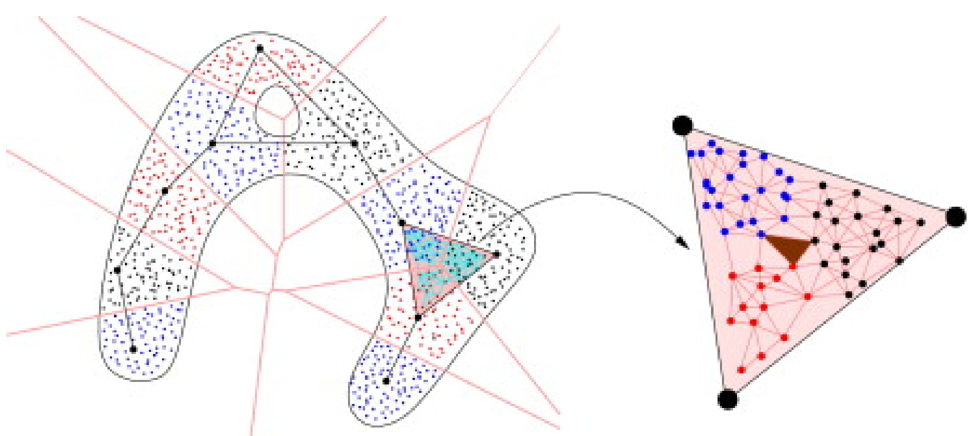


Figure 17: A graph induced complex is shown to the left and the input graph is shown to the right. Subsets of points are the darker vertices, and input points are grouped according to the proximity to the darker vertices, indicated by the superimposed Voronoi cells. The enlarged triangle to the right is in the GIC since there is a 3-clique in the graph whose 3 vertices have 3 different closest points in the subset [6].

3.3 Comparison of Complexes

Much of our interest in understanding topology and its application to data analysis is taking a finite set of points X and organizing these points in a topological space X. By choosing a metric on the set X, we attempt to create these various spaces using various algorithmic complexes with given metrics. Each of these complexes have various benefits in terms of our objective: if we attempt to build a simplicial complex K from a sample of points from given space X, it is desirable to construct if it satisfies the following conditions:

I. The homology of the simplicial complex approximates the homology of the space (meaning that the simplicial complex resembles in structure the topological space X, see section 3 for further detail on homology)

II. The simplicial complex does not have many simplices, especially in high dimensions

See below for a more detailed comparison of the primary complexes mathematicians use to compute simplicial complexes of higher dimensional data:

Complex K	Satisfies (I)?	Satisfies (II)?	Worst-case computational time of K
Čech	Equal by Nerve Theorem	No	$2^{O(N)}, N = \|K_0\|$
Vietoris-Rips	Approximates Čech	Yes, in dim ≤ 3	$2^{O(N)}, N = \|K_0\|$
Alpha	Equal by Nerve Theorem	Yes, in dim 2	$N^{O(\lceil d/2 \rceil)}$, N points $\in \mathbb{R}^d$
Witness	For curves and surfaces in Euclidean space	Yes, in dim ≤ 2	$2^{O(\|L\|)}$, L set of landmark points
GIC	Approximates Vietoris-Rips	Yes	$2^{O(\|Q\|)}$, Q subsample set

Note: The Delaunay complex is used to satisfy condition (II) in order to avoid computational problems for the Čech and Vietoris-Rips complexes. [17]

3.4 Algorithms of Complexes

In order to compute the aforementioned complexes, we must further develop and utilize computer algorithms. The below references provide initial frameworks for computations:

1. Čech algorithm [4]

2. Vietoris-Rips algorithm [25]

3. Delaunay algorithm [14]

4. Alpha algorithm [22]

5. Witness algorithm [2]

6. Graph Induced Complex (GIC) algorithm [5]

4 Homology Groups

The study of homology is the practice of associating a sequence of algebraic objects, such as groups and modules, with other mathematical objects, primarily topological spaces. Homology groups are algebraic tools used to quantify topological features in a space. By considering the homology of simplicial complexes, such as their path-connected components, loops, voids, and holes, we can better translate the shapes formed by simplicial complexes into a rigorous study of algebra, studying particular numerical structures and symmetries amongst topological spaces, without ever having a clear geometric representation of the topological space itself.

4.1 Chains, Cycles and Boundaries

Definition 4.1. Let G be an abelian group. G is *free* if $\exists A \subseteq G$ such that every element of G can be written uniquely as a linear combination $\sum_{i=1}^{r} n_i a_i$ for some $r \in \mathbb{N}, n_i \in \mathbb{Z}, a_i \in A$. We call A a *basis of G*, and its cardinality is called the *rank of G*, written as $G = \mathbb{Z}[A]$ or G $= < A >$. When uniqueness is not a condition, we say A *generates* G.

Definition 4.2. Let R be a commutative ring with identity, and let M be an abelian group. We say M is an *R-module* if there is an operation $\cdot : R \times M \to M$ such that $\forall r, s \in R \, \forall m, n \in M$

1. $r \cdot (m + n) = r \cdot m + r \cdot n$
2. $(r + s) \cdot m = r \cdot m + s \cdot m$
3. $(rs) \cdot m = r \cdot (s \cdot m)$
4. $1_R \cdot m = m$

Terminology: When R is a field, we say M is an *R-vector space.*

Definition 4.3. Let M and N be R-modules. A function $\varphi : M \to N$ is an *R-homomosphism* if $\forall r \in R$ and $\forall m, n \in M$

1. $\varphi(m + n) = \varphi(m) + \varphi(n)$
2. $\varphi(r \cdot m) = r \cdot \varphi(m)$

Examples:

1. Let M be a smooth manifold. The set $C^\infty(M) := \{f : M \to \mathbb{R} \mid f \text{ is a smooth map}\}$ is a ring under additiona and multiplication of function. Then, $C^\infty(M)$ is an $\mathbb{R}$-vector space.

   Proof. Since $C^\infty(M)$ is a ring, then in particular it is an abelian group. $\forall r \in \mathbb{R}\, \forall f \in C^\infty(M)$, define $r \cdot f \in C^\infty(M)$ as:

   $$r \cdot f : M \to \mathbb{R}, \text{ where } (r \cdot f)(m) = rf(m), \text{ which is multiplication in } \mathbb{R}.$$

   Now that we have defined an operation, we must check the axioms from the definition of an R-module, as follows:

   (a) We must confirm that $r \cdot (f + g) = (r \cdot f) + (r \cdot g)$, where $f, g \in C^\infty(M)$. Observe that $\forall m \in M$:
   $(r \cdot (f+g))(m) = r((f+g)(m)) = r(f(m)+g(m)) = rf(m)+rg(m) = (r \cdot f)(m) + (r \cdot g)(m)$, as required.

   (b) We must confirm that $(r + s) \cdot f = (r \cdot f) + (s \cdot f)$, where $r, s \in \mathbb{R}$. Observe that $\forall m \in M$:
   $((r+s) \cdot f)(m) = (r+s)f(m) = rf(m)+sf(m) = r \cdot f(m) + s \cdot f(m)$, as required.

   (c) We must confirm that $(rs) \cdot f = r \cdot (s \cdot f)$, where $r, s \in \mathbb{R}$. Observe that $\forall m \in M$:
   $((rs) \cdot f)(m) = (rs)f(m) = rs \cdot f(m) = r \cdot s \cdot f(m) = r \cdot (s \cdot f(m))$, as required.

   (d) We must confirm that $1_R \cdot f = f$. Observe that $\forall m \in M$:
   $1_R \cdot f(m) = (1_R f(m)) = f(m) = f$, as required.

   Thus, since $\mathbb{R}$ is a field, and $C^\infty(M)$ satisfies the axioms to be considered a $\mathbb{R}$-module, then $C^\infty(M)$ is an $\mathbb{R}$-vector space. □

2. Building off of the previous example, now suppose we have

   $$V := \{X : C^\infty(M) \to C^\infty(M) | X \text{ is a linear transformation over } \mathbb{R}, \text{ and } X(fg) = fX(g) + X(f)g \;\forall r \in \mathbb{R}, f, g \in C^\infty(M)\}.$$

   Then, V is a $C^\infty(M)$-module.

   Proof. By hypothesis, we know that X is a linear transformation over $\mathbb{R}$. By definition, this means that $X(f + g) = X(f) + X(g)$ and $X(r \cdot f) = r \cdot X(f)$.
   Now, we must first prove that V is an abelian group, as follows:
   Define: $X + Y : C^\infty(M) \to C^\infty(M)$, where $(X + Y)(f) = X(f) + Y(f)$. Since $X + Y$ is a linear transformation by definition and also a derivation, $X + Y \in V$.
   Now, let us define scalar multiplication. Take $\alpha \in C^\infty(M), X \in V$.
   Define $\alpha \cdot X : C^\infty(M) \to C^\infty(M)$, where $(\alpha \cdot X)(f) = \alpha X(f)$, such that $(\alpha X(f))(m) = \alpha(m) \cdot X(f)(m) \forall m \in C^\infty(M)$, which is multiplication in $\mathbb{R}$. Now that we have defined an operation, we must check the axioms from the definition of an R-module, as follows:

(a) We must confirm that $\alpha \cdot (X+Y) = \alpha \cdot X + \alpha \cdot Y$, where $X, Y \in V$:
$\alpha \cdot (X+Y) = \alpha(X+Y)(f) = \alpha(X(f)+Y(f)) = \alpha \cdot X(f) + \alpha \cdot Y(f) = \alpha \cdot X + \alpha \cdot Y$, as required.

(b) We must confirm that $(\alpha+\beta) \cdot X = \alpha \cdot X + \beta \cdot X$, where $X \in V, \alpha, \beta \in C^\infty(M)$:
$(\alpha+\beta) \cdot X = (\alpha+\beta) \cdot X(f) = \alpha \cdot X(f) + \beta \cdot X(f) = \alpha \cdot X + \beta \cdot X$, as required.

(c) We must confirm that $(\alpha\beta) \cdot X = \alpha \cdot (\beta \cdot X)$, where $X \in V, \alpha, \beta \in C^\infty(M)$:
$(\alpha\beta) \cdot X = (\alpha\beta) \cdot X(f) = X(\alpha\beta \cdot f) = \alpha \cdot X(\beta \cdot f) = \alpha \cdot (\beta \cdot X(f)) = \alpha \cdot (\beta \cdot X)$, as required.

(d) We must confirm that $1_R \cdot X = X$. Observe that $\forall X \in V$:
$1_R \cdot X = 1_R \cdot X(f) = X(1_R \cdot f) = X(f) = X$, as required.

Thus, since the axioms are satisfied, by definition, V is a $C^\infty(M)$-module. $\square$

Definition 4.4. Let R be a commutative ring with identity. Let K be a k-simplicial complex, and $0 \leq p < k$.

1. Let $S_p \subseteq K$ be the set of p-simplices of K, and $m_p := \#(S_p)$
2. An element of $C_p(K,R) := \left\{\sum_{i=1}^{m_p} r_i\sigma_i : r_i \in R, \sigma_i \in S_p\right\}$ is called a *p-chain* in K. We call r_i *coefficients* for all $1 \leq i \leq m_p$.

Convention: When writing a chain, we omit simplices with coefficient 0_R.

Example: Consider the 3-simplicial complex K shown below:

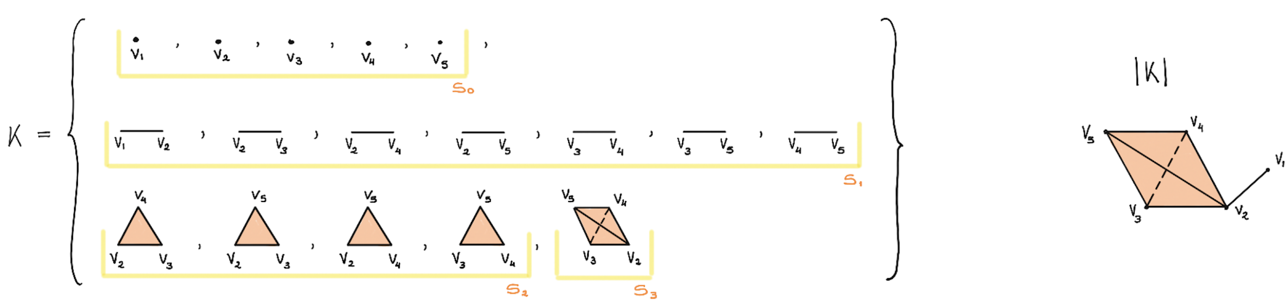


Figure 18: Visual representation of a 3-simplicial complex K with associated set of p-simplices.

From the above complex K, we can observe the following:

vertices	edges	faces	tetrahedra
$m_0 = 5$	$m_1 = 7$	$m_2 = 4$	$m_3 = 1$
$S_0 = \{v_1, ..., v_5\}$	$S_1 = \{e_1, ..., e_7\}$	$S_2 = \{f_1, ..., f_4\}$	$S_3 = \{\sigma\}$

Let $R = \mathbb{Z}$, then the following are examples of p-chains in K:

0-chains: $C_0(K;\mathbb{Z})$	$20v_5, -3v_1 - 6v_4$
1-chains: $C_1(K;\mathbb{Z})$	$6e_2 + 5e_4, \sum_{i=1}^{7} e_i$
2-chains: $C_2(K;\mathbb{Z})$	$f_2 - 3f_4$
3-chains: $C_3(K;\mathbb{Z})$	$11\sigma, -63\sigma$

Let $R = \mathbb{F}_2$, then the p-chains have coefficients 0 or 1:

In $C_0(K;\mathbb{F}_2)$ $\quad (v_1 + v_2) + (v_2 + v_3) = v_1 + 2v_2 (= 0v_2) + v_3 = v_1 + v_3$

Proposition 4.5. For all $0 \leq p \leq k$, $C_p(K;R)$ is an R-module where $r \cdot \Sigma_{i=1}^{m_p} r_i\sigma_i := \Sigma_{i=1}^{m_p}(rr_i)\sigma_i$ for all $r, r_i \in R$ and $\sigma_i \in S_p$.

Remark. From now on, we will assume $R = \mathbb{F}_2$, and simply write $C_p(K)$. In this case:

- The inverse of every $\sigma \in C_p(K)$ is itself.
- A p-chain $\sigma_1 + \sigma_2 + \cdots + \sigma_n$ can be treated as a set $\{\sigma_1, \sigma_2, ..., \sigma_n\}$, where addition of two p-chains A and B is given by $(A \cup B) - (A \cap B)$, and the zero chain is the empty set.

Example: Consider again the example in Figure 18. From this example, we have the following:

$C_1(K)$	$\{e_1, e_2, e_3\} + \{e_4 + e_5\} = \{e_1, e_2, e_3, e_4, e_5\}$
$C_2(K)$	$\{f_2, f_3, f_4\} + \{f_1, f_3, f_4\} = \{f_1 + f_2\}$
$C_3(K)$	$\{\sigma\} + \{\sigma\} = \emptyset$

Definition 4.6. Let R be a commutative ring with identity. Let $(C_i, \partial_i)_{i=0}^{\infty}$ be a sequence of R-modules connected by R-homomophisms as follows

$$\cdots \to C_i \xrightarrow{\partial_i} C_{i-1} \to \cdots \to C_1 \xrightarrow{\partial_1} C_0 \to 0$$

We say $(C_i, \partial_i)_{i=0}^{\infty}$ is a *chain of R-modules* (or *chain complex over R*) if the composition $\partial_{i-1} \circ \partial_i$ equals zero for all $i \leq 1$.

The R-homomorphisms are called *boundary homomorphisms* (or *differentials*).

4.2 Homology

Definition 4.7. Let $\mathcal{C} := (C_i, \partial_i)_{i \geq 0}$ be a chain complex over a commutative ring with identity, R. The *i-th homology group of $\mathcal{C}$ with coefficient in R* is the quotient R-module $H_i(\mathcal{C}, R) := Z_i/B_{i+1} (= \operatorname{Ker}\partial_i / \operatorname{Im}\partial_{i+1})$.

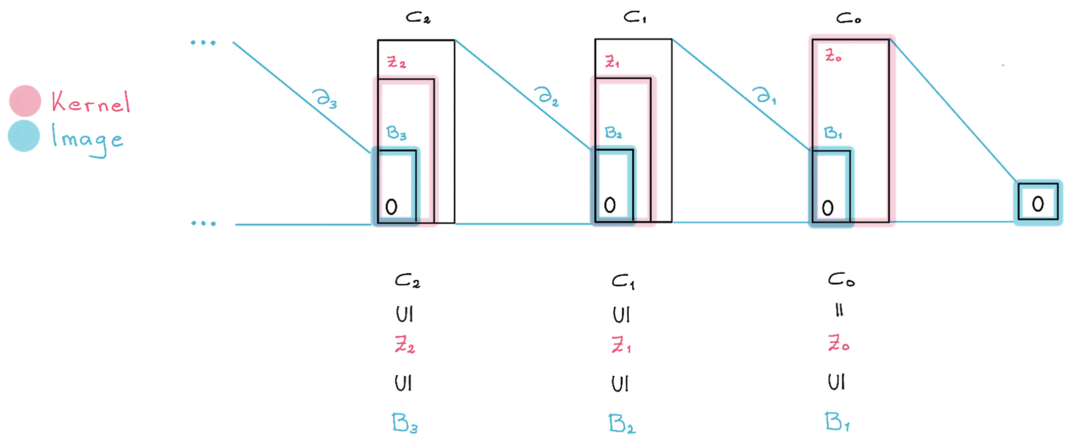


Figure 19: Visual representation of $\operatorname{Ker}\partial_{i-1}$ (which is denoted by Z_{i-1} and its elements are called (i-1)-cycles) and $\operatorname{Im}\partial_i$ (which is denoted by B_i and its elements are called i-boundaries). Note that B_i and Z_{i-1} are R-modules. This figure also allows us to visualize an important consequence of the condition $\partial_{i-1} \circ \partial_i = 0 \; \forall i \geq 1$ from Definition 4.6. Namely that $\forall i \geq 1 \operatorname{Im}\partial_i \subset \operatorname{Ker}\partial_{i-1}$

Intuition

$\operatorname{Ker}\partial_i / \operatorname{Im}\partial_{i+1}$ can be through of as "consider $\operatorname{Im}\partial_{i+1}$ and all elements of $\operatorname{Ker}\partial_i$ that are **not** images of ∂_{i+1}".
This quotient can also be thought of as a measure of the failure of $\operatorname{Im}\partial_{i+1}$ to be equal to $\operatorname{Ker}\partial_i$.

Definition 4.8. Let K be a simplicial complex. The *p-th homology group with $\mathbb{F}_2$-coefficients associated to K*, $H_p(K; \mathbb{F}_2)$, is the p-th homology group of $(C_p(K), \partial_p)_{p\geq 0}$, i.e.

$$H_p(K, \mathbb{F}_2) := Z_p/B_{p+1} (= \operatorname{Ker}\partial_p / \operatorname{Im}\partial_{p+1}).$$

Definition 4.9. The dimension of $H_p(K; \mathbb{F}_2)$ as a vector space over $\mathbb{F}_2$ receives the name of *p-th Betti number*, and it is denoted by $\beta_p := dim_{\mathbb{F}_2}(H_p(K; \mathbb{F}_2))$.

Remark. Let $p \geq 1$, a *p-dimensional hole* in the simplicial complex formed by the boundary of a $(p+1)$-simplex (without the interior).

- H_0 gives the number of path-connected components of $|K|$.
- H_1 gives the number of loops in $|K|$.
- H_2 gives the number of voids in $|K|$.
- H_p gives the number of p-dimensional holes in $|K|$.

Example: Consider the simplicial complex K with geometric realization as shown below.

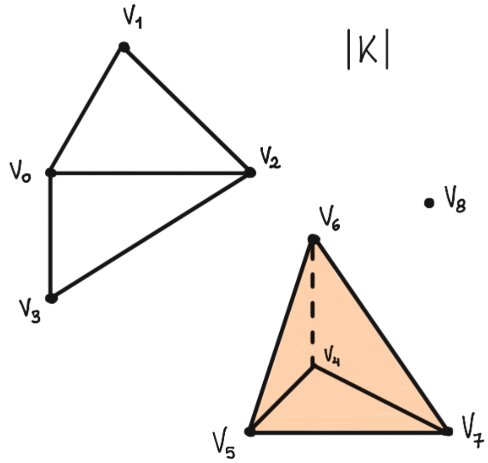


Figure 20: Simplicial complex K. Note that the tetrahedron formed by v_4, v_5, v_6, v_7 is hollow.

We claim that the homology groups and associated Betti numbers of K are as follows:

$$\begin{array}{lll} H_0(K;\mathbb{F}_2) \cong \mathbb{F}_2^3 & \text{i.e.} & \beta_0 = 3 \\ H_1(K;\mathbb{F}_2) \cong \mathbb{F}_2^2 & \text{i.e.} & \beta_1 = 2 \\ H_2(K;\mathbb{F}_2) \cong \mathbb{F}_2 & \text{i.e.} & \beta_2 = 1 \\ H_p(K;\mathbb{F}_2) \cong 0 & \text{i.e.} & \beta_p = 0, \quad \forall p \geq 0. \end{array}$$

We will calculate H_0 and H_1, and the rest will be left as an exercise.

Notation:

- $v_0, v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8$
- $e_1 = v_0v_1$ $\quad e_2 = v_0v_2$ $\quad e_3 = v_0v_3$ $\quad e_4 = v_1v_2$ $\quad e_5 = v_2v_3$ $\quad e_6 = v_4v_5$ $\quad e_7 = v_4v_6$ $\quad e_8 = v_4v_7$ $\quad e_9 = v_5v_6$ $\quad e_{10} = v_5v_7$ $\quad e_{11} = v_6v_7$
- $f_1 = v_4v_5v_6$ $\quad f_2 = v_4v_5v_7$ $\quad f_3 = v_4v_6v_7$ $\quad f_4 = v_5v_6v_7$
- $\sigma = v_4v_5v_6v_7$

Recall from Definition 4.4 that $C_p(K, R) := \left\{\sum_{i=1}^{m_p} r_i\sigma_i : r_i \in R, \sigma_i \in S_p\right\}$. Thus, using $R = \mathbb{F}_2$, observe that $C_p(K, \mathbb{F}_2)$ takes the form:

$$C_p(K) = C_p(K, \mathbb{F}_2) = \left\{\sum_{i=1}^{m_p} r_i\sigma_i : r_i \in \mathbb{F}_2, \sigma_i \in S_p\right\}$$

Therefore, we have:

$$
\begin{aligned}
C_3(K) &= \{0, \sigma\} \cong \mathbb{F}_2 \\
C_2(K) &= \left\{ \sum_{i=1}^{4} r_i f_i : r_i \in \mathbb{F}_2 \right\} \cong \mathbb{F}_2 \times \mathbb{F}_2 \times \mathbb{F}_2 \times \mathbb{F}_2 =: \mathbb{F}_2^4 \\
C_1(K) &= \left\{ \sum_{i=1}^{11} r_i e_i : r_i \in \mathbb{F}_2 \right\} \cong \mathbb{F}_2^{11} \\
C_0(K) &= \left\{ \sum_{i=0}^{8} r_i v_i : r_i \in \mathbb{F}_2 \right\} \cong \mathbb{F}_2^{9}
\end{aligned}
$$

Thus, we have the chain complex:

$$0 \to \mathbb{F}_2 \xrightarrow{\partial_3} \mathbb{F}_2^4 \xrightarrow{\partial_2} \mathbb{F}_2^{11} \xrightarrow{\partial_1} \mathbb{F}_2^9 \to 0$$

Let us now compute ∂_p for all p:

p	$\partial_p : C_p(K) \to C_{p-1}(K)$	$\partial_p : \mathbb{F}_2^{m_p} \to \mathbb{F}_2^{m_{p-1}}$
3	$\partial_3(\sigma) = f_1 + f_2 + f_3 + f_4$	$\partial_3(1) = (1,1,1,1)$
2	$\partial_2(f_1) = e_6 + e_7 + e_9$ $\partial_2(f_2) = e_6 + e_8 + e_{10}$ $\vdots$	$\partial_2(1,0,0,0) = (0,0,0,0,0,1,1,0,1,0,0)$ $\partial_2(0,1,0,0) = (0,0,0,0,0,1,0,1,0,1,0)$ $\vdots$
1	$\partial_2(e_1) = v_0 + v_1$ $\partial_2(e_2) = v_0 + v_2$ $\vdots$	$\partial_1(1,0,...,0) = (1,1,0,0,0,0,0,0,0)$ $\partial_1(0,1,...,0) = (1,0,1,0,0,0,0,0,0)$ $\vdots$

Therefore, we can represent ∂_p as an $m_{p-1} \times m_p$ matrix, which we will denote A_p. In this case,

$$A_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0&0&0&0 \\ 0&0&0&0 \\ 0&0&0&0 \\ 0&0&0&0 \\ 0&0&0&0 \\ 1&1&0&0 \\ 1&0&1&0 \\ 0&1&1&0 \\ 1&0&0&1 \\ 0&1&0&1 \\ 0&0&1&1 \end{bmatrix}, \quad \text{and,} \quad A_1 = \begin{bmatrix} 1&1&1&0&0&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0&0 \\ 0&1&0&1&1&0&0&0&0&0&0 \\ 0&0&1&0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&1&0&0&1&1&0 \\ 0&0&0&0&0&0&1&0&1&0&1 \\ 0&0&0&0&0&0&0&1&0&1&1 \\ 0&0&0&0&0&0&0&0&0&0&0 \end{bmatrix}.$$

Having our chain complex completely described, we can now compute H_0 and H_1. By definition, $H_p = \mathrm{Ker}(\partial_p)/\mathrm{Im}(\partial_{p+1}) = \mathrm{Null}(A_p)/\mathrm{Col}(A_{p+1})$. Thus, if we row reduce our above matrices and apply the rank-nullity theorem,

- $H_0(K) = \mathrm{Null}(A_0)/\mathrm{Col}(A_1) \cong \mathbb{F}_2^9/\mathbb{F}_2^6 \cong \mathbb{F}_2^3$
- $H_1(K) = \mathrm{Null}(A_1)/\mathrm{Col}(A_2) \cong \mathbb{F}_2^2$

Intuition

In the above example, we started with a combinatorial object simplicial complex, then moved to an algebraic object "vector spaces" and used linear algebra to understand the geometric realization of the simplicial complex, which is a topological object.

Proposition 4.10. *Functorial properties of* $H_*(-;\mathbb{F}_2)$

1. The induced map of the identity is the identity, i.e. $\mathrm{id}_* : H_p(K;\mathbb{F}_2) \to H_p(K;\mathbb{F}_2)$ is equal to $\mathrm{id}_{H_p(K;\mathbb{F}_2)}$ for all $p \geq 0$.
2. Let $f : K \to L$ and $g : L \to M$ be simplicial maps. Then $(g \circ f)_* = g_* \circ f_*$.

Proposition 4.11. Let $f : K \to L$ be a simplicial map s.t. $f : |K| \to |L|$ is a homeomorphism. Then $f_* : H_p(K;\mathbb{F}_2) \to H_p(L;\mathbb{F}_2)$ is an isomorphism.

Example: The 2-sphere S^2 is not homeomorphic to the torus $\mathbb{T} := S^1 \times S^1$. If $S^2 \cong \mathbb{T}$, then their homology groups are isomorphic. However,

$$H_1(S^2;\mathbb{F}_2) \cong 0 \ncong \mathbb{F}_2^2 \cong H_1(\mathbb{T};\mathbb{F}_2).$$

Proposition 4.12. Let $f, g : K \to L$ be simplicial maps. If $f, g : |K| \to |L|$ are homotopic, then $f_* = g_*$.

Proof. Omitted. See Theorem 2.10, Algebraic Topology, Hatcher. [10] □

Intuition

The above proposition implies that homotopy equivalent spaces will have the same homology (hence, equivalent Betti numbers). Therefore, we can use homology as a tool to tell some spaces apart. However, there are some spaces that have the same homology despite not being homotopy equivalent.

Definition 4.13. Let Δ_p denote the p-simplex spanned by the following points in $\mathbb{R}^{p+1}$ $\{(1,0,...,0),(0,1,0,...,0),...,(0,...,0,1)\}$. We call Δ_p a *standard p-simplex.*

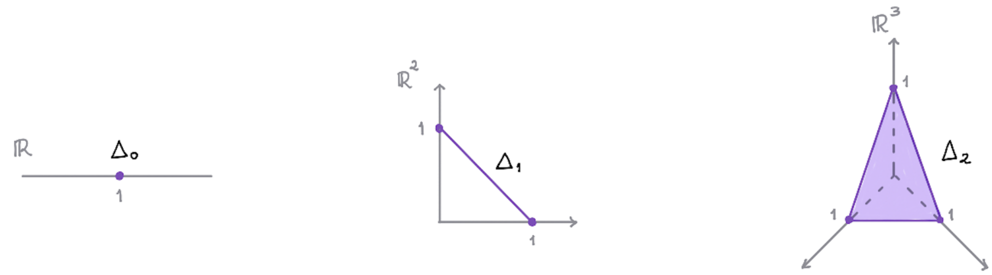


Figure 21: Illustration of the standard p-simplex in $\mathbb{R}, \mathbb{R}^2$, and $\mathbb{R}^3$.

Definition 4.14. Let X be a topological space. A *singular p-simplex* for X is a continuous map $\sigma : \Delta_p \to X$.

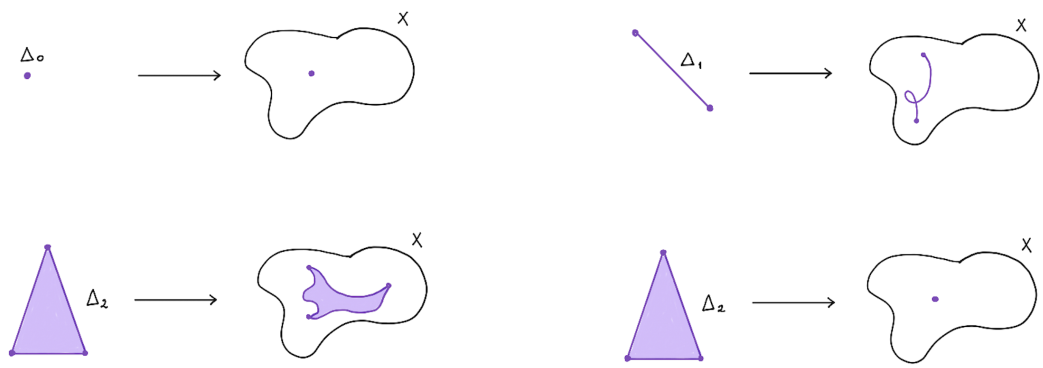


Figure 22: Visual representation of various maps $\sigma : \Delta_p \to X$. Note that σ is not necessarily injective, which is why it is called "singular".

Definition 4.15. We can define a chain complex $(S_p(X), \partial_p)_{p\geq 0}$ and $H_*(X; \mathbb{F}_2)$.

- $S_p(X) = \left\{\sum_{i=0}^{n} r_i\sigma_i : n \in \mathbb{N}, r_i \in \mathbb{F}_2 \text{ and } \sigma_i \text{ is a singular } p\text{-simplex}\right\}$
  Elements of $S_p(X)$ are called *(singular) p-chains*.
- $\partial_p : S_p(X) \to S_{p-1}(X)$ is defined as follows:
  - If $\sigma : \Delta_p \to X$ is a singular p-simplex, $\partial_p\sigma := \tau_0 + \tau_1 + ... + \tau_p$ where $\tau_i : \Delta^i_{p-1} \to X$ is the composite $\Delta^i_{p-1} \overset{d_i}{\hookrightarrow} \Delta_p \xrightarrow{\sigma} X$ where d_i is the inclusion of the ith facet of Δ_p into Δ_p.
  - $\partial_p\left(\sum_{i=0}^{n} r_i\sigma_i\right) := \sum_{i=0}^{n} r_i\partial_p\sigma_i$
- The *singular homology group of X of degree p with $\mathbb{F}_2$-coefficients* is

$$H_p(X; \mathbb{F}_2) := Z_p/B_{p+1} \; (= \operatorname{Ker}\partial_p/\operatorname{Im}\partial_{p+1}).$$

5 Persistent Homology

Persistent homology takes the principles of homology and studies the qualitative features of data that persist across multiple scales. By observing patterns in what homological features of data persist over particular, varied intervals, beginning with a simplicial complex and then applying homology to it, one can better characterize data and observe patterns that could potentially be useful for applications of topological data analysis.

Definition 5.1. Let K be a r-simplicial complex. A *filtration* $\mathcal{F}$ of K is a finite sequence of nested subcomplexes of K (not its skeleta necessarily):

$$\mathcal{F} : K_0 \subseteq K_1 \subseteq \cdots \subseteq K_n \subseteq \cdots \subseteq K_r = K$$

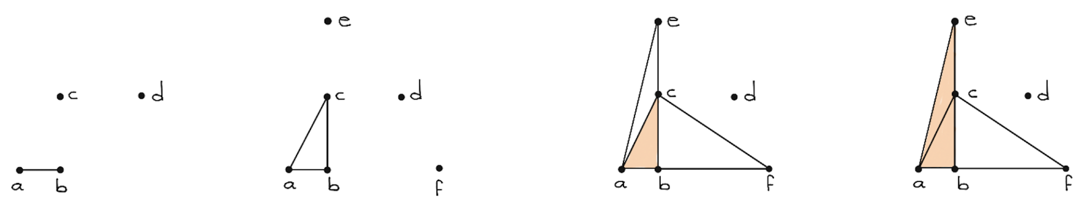


Figure 23: This is a simple example of a filtration with $\mathcal{F} : K_0 \subseteq K_1 \subseteq K_2 \subseteq K_3$.

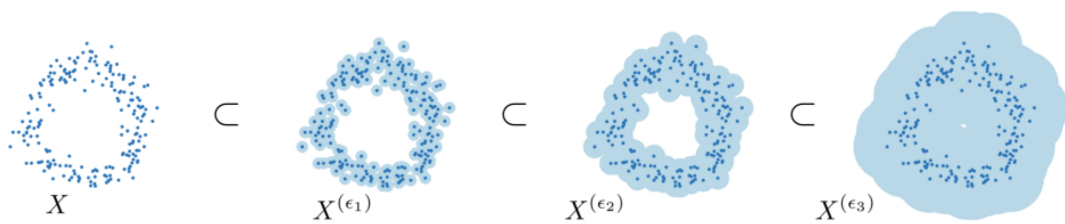


Figure 24: This is another, more complex example of a filtration using real data. [18]

Definition 5.2. Let $\mathcal{F} : K_0 \subseteq K_1 \subseteq \cdots \subseteq K_r = K$ be a filtration for K. The *p-th homology of* $\mathcal{F}$ is the pair

$$H_p(\mathcal{F}) : \left(\left\{ H_p(K_i; \mathbb{F}_2) \right\}_{i=0}^{r} ; \left\{ f_{ij} \right\}_{0 \leq i \leq j \leq r} \right),$$

where for all $0 \leq i \leq j \leq r$ the linear transformations $f_{ij} : H_p(K_i; \mathbb{F}_2) \to H_p(K_j; \mathbb{F}_2)$ are introduced by the inclusion $K_i \hookrightarrow K_j$.

$$H_p(\mathcal{F}) : H_p(K_0) \to H_p(K_1) \to \cdots \to H_p(K_i) \to \overset{f_{ij}}{\cdots} \to H_p(K_j) \to \cdots \to H_p(K)$$

Definition 5.3. Let $\mathcal{F} : K_0 \subseteq K_1 \subseteq \cdots \subseteq K_r = K$ be a filtration for K.

1. The (i, j)*-persistent p-th homology group of* K is the image of f_{ij} in the p-th homology group of $\mathcal{F}$, and it is denoted by $H_p^{i,j}$:

$$H_p^{i,j} := \mathrm{Im}\Big(f_{ij} : H_p(K_i;\mathbb{F}_2) \to H_p(K_j;\mathbb{F}_2)\Big) \text{ for } 0 \le i \le j \le r \text{ where } f_{ii} = \mathrm{id}.$$

2. The *(i,j)-persistent p-th Betti number of K* is the dimension of $H_p^{(}i,j)$ over $\mathbb{F}_2$, i.e. $\beta_p^{i,j} := \dim_{\mathbb{F}_2}(H_p^{i,j})$.

Definition 5.4. Let $\mathcal{F} : K_0 \subseteq K_1 \subseteq \cdots \subseteq K_r = K$ be a filtration for K. Let $\alpha \in H_p(K_a)$ be a non-trivial p-th homology class. We say

- *α is born at K_i* (for $i \le a$) if $\alpha \in H_p^{i,a}$ but $\alpha \notin H_p^{i-1,a}$.
- *α dies entering K_j* (for $a < j$) if $F_{a,j-1}(\alpha) \neq 0$ but $f_{a,j}(\alpha) = 0$.
- *α lives forever* if $f_{a,i}(\alpha) \neq 0$ for all $a < i \le r$.

Note, there are two ways to visualize/represent the lifetime of α: persistence diagrams and persistence barcodes (introduced in Definition 5.8 and Definition 5.9, respectively).

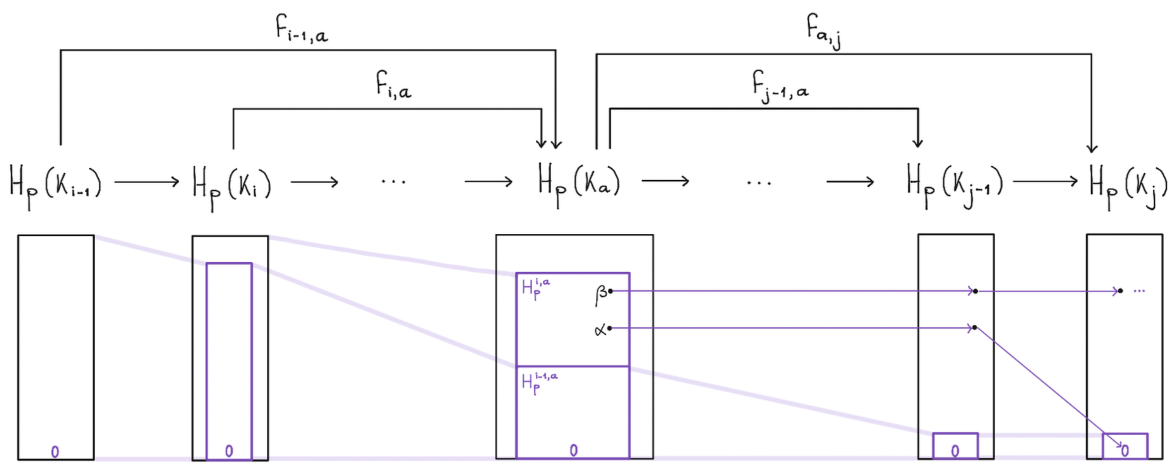
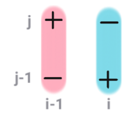


Figure 25: This figure illustrates how homology classes persist through filtration steps. We can see that class α is born at K_i since it is not in the image of $f_{i-1,i}$ and dies entering K_j since this is the first time its image becomes 0. This visual also shows that class β is born at K_i and lives forever (β persists through all of the filtration steps).

Definition 5.5. A *persistence pair* is a pair of the form (a_i, a_j) with $0 \le a_i < a_j \le r$, or of the form $(a_i, \inf)$ with $0 \le a_i \le r$ such that

1. (a_i, a_j) represents a non-trivial homology class that is born at step a_i of $\mathcal{F}$ and dies at step a_j of $\mathcal{F}$.
2. (a_i, ∞) represents a non-trivial homology class that is born at step a_i of $\mathcal{F}$ and lives forever.

$$\mu_p^{i,j} := (\beta_p^{i,j-1} - \beta_p^{i,j}) - (\beta_p^{i-1,j-1} - \beta_p^{i,j}),$$



Definition 5.6. Let $p \geq 0$. For $0 < i < j \leq r+1$, the *persistence paring function (or multiplicity)* $\mu_p^{i,j}$ of a persistence pair (a_i, a_j) is given by
where $a_{r+1} = \inf$.

- $(\beta_p^{i,j-1} - \beta_p^{i,j}\ )$ = Number of independent classes born at or before K_i, and die entering K_j
- $(\beta_p^{i-1,j-1} - \beta_p^{i-1,j}\ )$ = Number of independent classes born at or before K_{i-1}, and die entering K_j
- $\mu_p^{i,j}$ = Number of independent classes born at K_i and die entering K_j
- $j = r+1 \implies \mu_p^{i,r+1}$ = Number of independent classes born at K_i and remain alive till the end in the filtration $\mathcal{F}$.

Definition 5.7. Let α be a class with persistence pair (a_i, a_j). If $\mu_p^{i,j} \neq 0$, we define the *persistence* of α as its life span and we denote it by $\mathrm{Per}(\alpha)$.

1. If $j < r+1$, then $\mathrm{Per}(\alpha) = a_j - a_i$.
2. If $j = r+1$, then $\mathrm{Per}(\alpha) = \infty$.

Definition 5.8. The *persistence diagram* $\mathrm{Dgm}_p(\mathcal{F})$ of a filtration $\mathcal{F}$ is obtained by drawing a point (a_i, a_j) with nonzero multiplicity $\mu_p^{i,j}, i < j$, on the extended plane $\overline{\mathbb{R}}^2 := (\mathbb{R} \cup \{+\inf\})^2$ where the points on the diagonal $\Delta = \{(x, x)\}$ are added with infinite multiplicity.

Definition 5.9. The *persistence barcode* $\mathrm{bcd}(\mathcal{F})$ of a filtration $\mathcal{F}$ is obtained by where

1. (a_i, a_j) is represented by a semi-open interval $[a_i, a_j)$ called a *bar*,
2. (a_i, ∞) is represented by a ray $[a_i, \inf)$ called an *infinite bar*.

Example: Consider the filtration shown below.

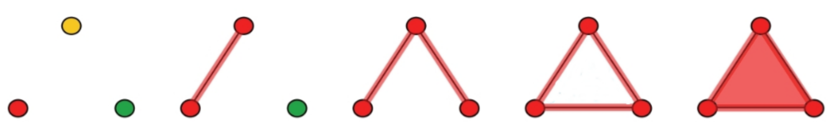


Figure 26: This is a filtration with $\mathcal{F} : K_0 \subseteq K_1 \subseteq K_2 \subseteq K_3 \subseteq K_3 = K$.

We can redraw and relabel the above filtration as shown below.

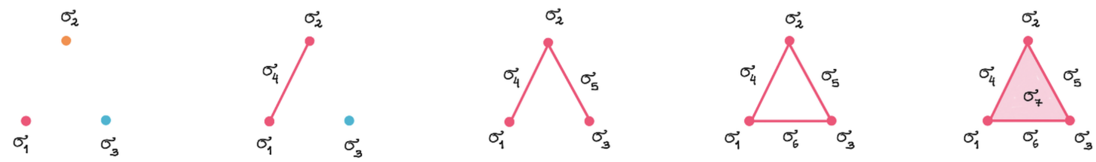


Figure 27: A redrawing of Figure 26 with classes $\alpha_1, ..., \alpha_6$ labelled.

Observe the following:

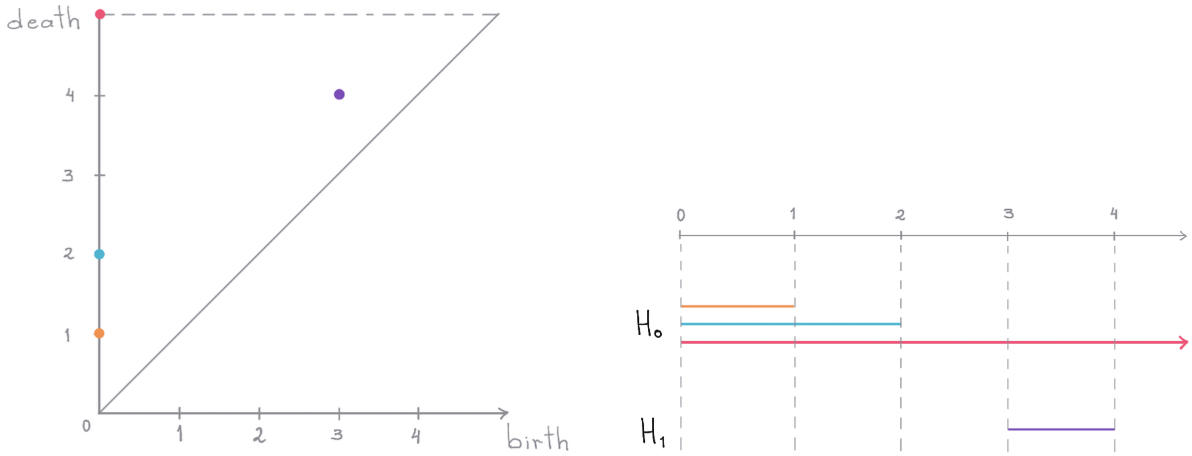
- H_0 :
  - At $t = 0$, we have 3 connected components, i.e. three classes are born.
  - At $t = 1$, two components merged, i.e. σ_2 dies whereas both σ_3 and the class "anchored" to σ_1 persist.
  - At $t = 2$, two components merged, i.e. σ_3 dies and the class "anchored" to σ_1 persists.
  - At $t = 3$ and $t = 4$, an edge and a face are added but they do not created new connected components, i.e. the class "anchored" to σ_1 persists.

Intuition

When a class dies, it can be thought of as a merger of several classes, among which the youngest one persists and determines the birth point.

- H_1 :
  - At $t = 0, t = 1$ and $t = 2$, there are no loops.
  - At $t = 3$, on loop appears, i.e. the class $\sigma_4 + \sigma_5 + \sigma_6$ is born.
  - At $t = 4$, the loop is filled up, i.e. $\sigma_4 + \sigma_5 + \sigma_6$ dies.

Therefore, the persistence diagram and barcode can be seen below.



(a) Persistence Diagram (b) Persistence Barcode

Figure 28: Persistence diagram and barcode for the filtration show in Figure 26.

Example:

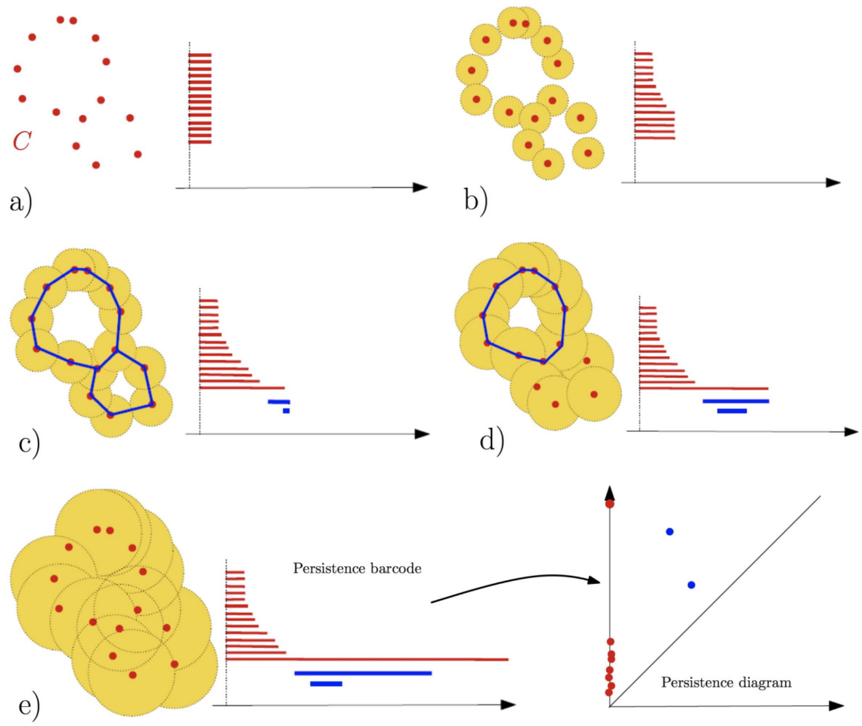


Figure 29: Here is a visual representation of persistence barcodes and a persistence diagram for a filtration using real data. The red points and bars represent 0-cycles, while the blue curves represent 1-cycles associated to the blue bars in the barcodes. [3]

6 Applications in Data Analysis

Topological data analysis provides a powerful tool in both recognizing and understanding patterns within data sets, seeking to understand the shape of data in lower-dimensions, using the aforementioned principles of persistent homology and complexes to do so.

6.1 Application in Chemistry

One application of topological data analysis is in chemistry, particularly in the study of aqueous solubility, or the ability of a molecule to be dissolved in water. In drug development, many drugs are often abandoned during the discovery process due to problems with bioactivity, in particular with the drug remaining insoluble during the oral delivery stage, leading it to be unabsorbed and with low bioavailability. Many statistical data models are inherently flawed, with experimental difficulties resulting in significant margins of error, and thus unable to generate accurate predictors of what features might explain the solubility properties of molecules. As an alternative, topological data analysis can be used to represent solubility models - using the *mapper algorithm*, a topological data analysis method that creates low-dimension representations of data, a network visualization of the solubility space for particular molecules can be formed, aiming to understand the descriptors that affect solubility prediction and the interplay between them. In addition, persistence barcodes of the chemical space are utilized from persistent homology in order to create a measure of the similarity between molecules that takes account their three-dimensional connectivity bond structure [19].

In one study, an analysis of a publicly available data set of 3663 drug-like molecules with regards to their solubility in water was used. First, they were given in Sybyl line notation (SLN), and conversion to SMILES, or molecular descriptors, was performed using computer software as one- and two-dimensional features, leaving 1521 descriptors. The SMILES strings then uniquely determined molecular graphs, with three-dimensional coordinates generated to perform classical geometry optimization. The coordinates together are then considered to be weighted, undirected graphs defined by Euclidean distances between the coordinates of the atom centers. After performing implementation of graph persistence using low-dimensional embeddings of the H_0 and H_1 distance matrices and also implementation of the mapper algorithm, the following results were found [19]:

According to the mapper algorithm:

1. nCIC, the number of cycles, or molecular rings, determined most strongly the similarity between molecules, and best accounted for the formation of cluster-like groupings within the output graphs.

2. After partitioning the data set according to the number of cycles, the feature that changed the most was the percentage of halogen atoms.

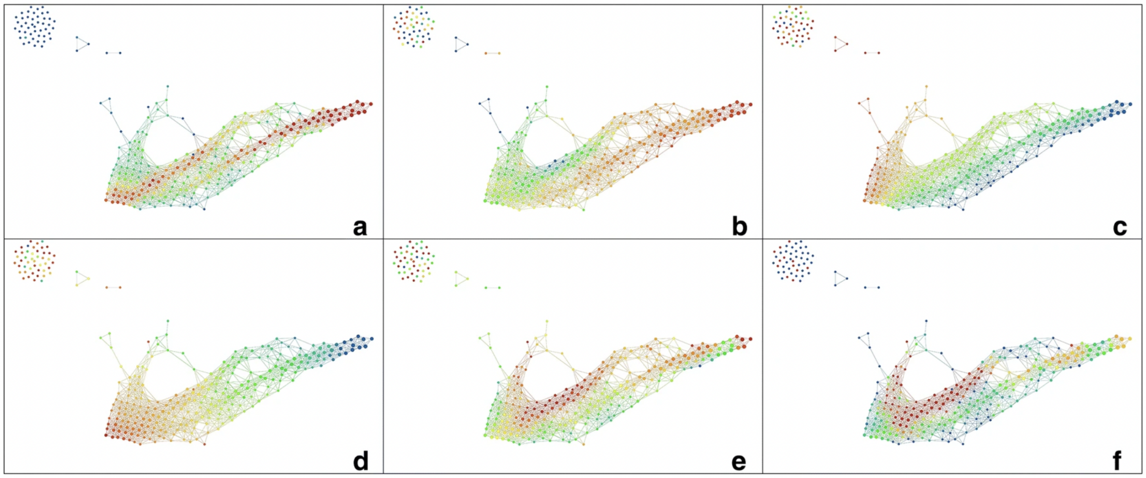


Figure 30: Here, the mapper algorithm analysis is colored by different relevant features. In (a), several distinct groupings of nodes are observed, with the red color indicating a higher number of molecules per node. In (b), the average solubility values decrease from left to right. In (c), the number of cycles in the molecular graph separate the groupings the best. In (d), the same graph is colored by molecular weight. In (e), the same graph is colored by average molecular weight. In (f), the same graph is colored by the number of chlorine atoms. According to the given research, in the red region in (d), this corresponds to the high number of chlorine atoms, which matches the blue region in (b), a lower solubility value. From (c), we can see that these are molecules with two rings [19].

According to persistent homology:

1. A radial gradient is observed with respect to the number of rings (nCIC) and an angular gradient is observed with respect to the number of atoms.
2. When colored by the number of chlorines, small, distinct subsets correspond to molecules with two rings.

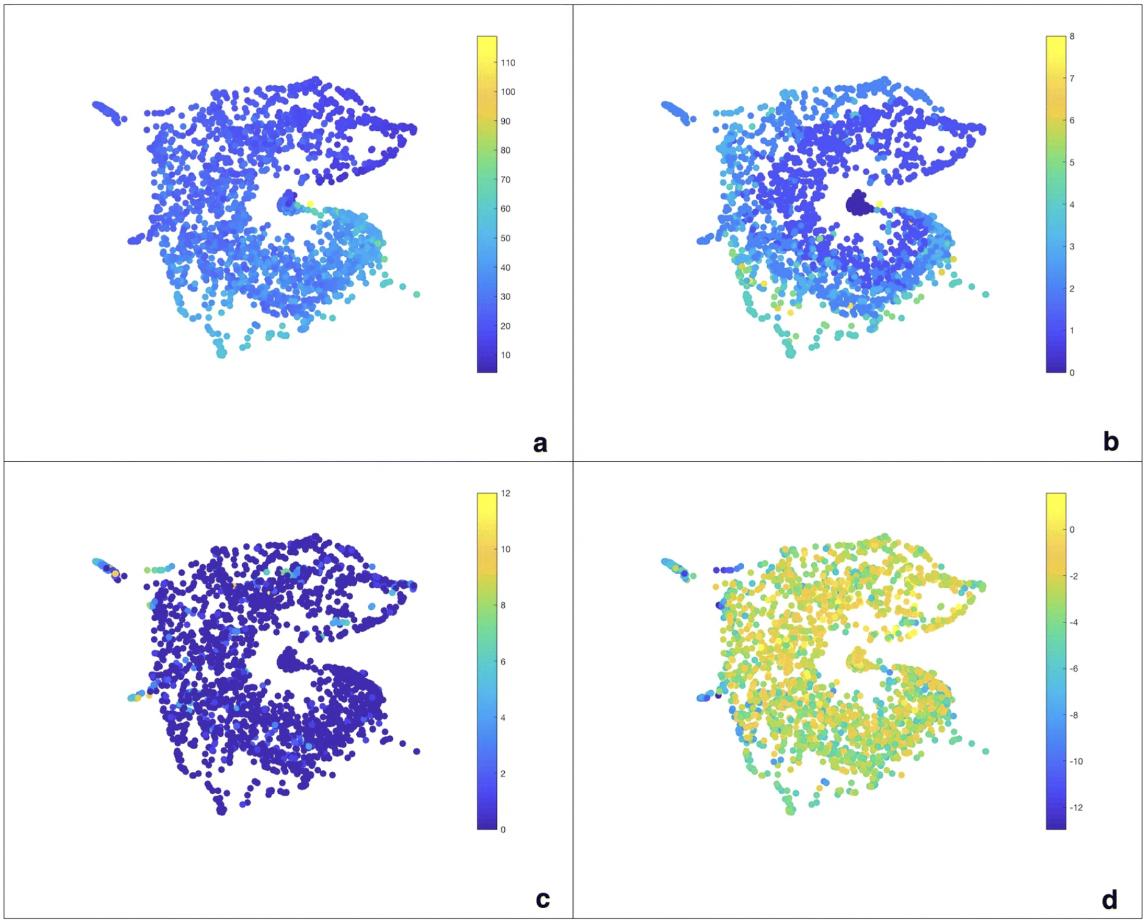


Figure 31: Here, the persistent homology analysis colored by the number of atoms (a), the number of cycles (b), the number of chlorines (c), and solubility (d). As in the mapper algorithm, the number of rings and chlorine atoms are highly representative of a lower solubility value [19].

By using topological data analysis, we can now better understand some of the correlations between ring structure of molecules and how that affects solubility. In particular, using the techniques of the mapper algorithm and persistent homology, it is observed that the effect of chlorinated groups on reducing solubility was far more powerful in larger molecules in the given data set. In addition, the molecules with chlorinated groups were particularly evenly distributed as a function of the number of rings. These graphical depictions of chemical space might be useful down the line in drug development, particularly in solubility studies, along with further exploration of chemical structures [19].

6.2 Additional Resources

Below are additional resources for further exploration of applications of TDA:

1. Torus and Klein Bottle

2. Spaces of 3×3 natural image patches
3. The Mapper Algorithm
4. The Mapper Algorithm: An Introduction
5. Persistence and Local geometry
   (a) Part A
   (b) Part B
6. Coordinate free coverage in sensor networks
7. TDA for genomics & Evolution topology in biology [20]
8. More applications of toplogy and TDA: See AATRN

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