The Nerve Theorem in Topological Data Analysis

Applications in Binary Classification Problems

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Quiero agradecerle a Cristian por ser mi mentor y la motivación para perseguir una carrera académica en las matemáticas puras.
A mi mamá por siempre recordarme que tenía que haber adelantado la tesis en vacaciones, a mi papá por mantenerme los ánimos altos y a Manu por siempre ser mi modelo a seguir.
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Abstract

In this thesis, we give a brief overview of Topological Data Analysis (TDA) from its mathematical foundations to state-of-the-art applications. First, we present the necessary concepts from Topology, Algebra and Algebraic Topology that make TDA possible. Next, we introduce and prove the Nerve Theorem for convex and compact covers which underlies most of the methods used in TDA. We will also show the relevance of the Nerve Theorem in TDA from the perspective of Category Theory. Then, we explain how persistent homology is defined and used in TDA. Lastly, we present an application published in [1] of the Nerve Theorem and persistent homology that proves a lower bound for the sample size of data points that faithfully recovers the homology of the decision boundary manifold in binary classification problems.

Keywords: Topological Data Analysis, Persistent Homology, Nerve Theorem, Binary Classification, Algebraic Topology.

Contents

1 Introduction

One of the central problems in data analysis is the characterization of data sets. Traditional statistics gives us a series of methods which approximate the behavior of data to linear or polynomial models by doing *regression*. These methods assume the *topology* of the data and then seek to find the best fitting instance of such a topology near the data points. We can imagine how fitting a linear regression to a point cloud forces the data to conform in the best way possible to such a model, even though the data may contain more complex topological properties. On the other hand, *clustering* algorithms can detect clusters in data but aren't suited for the study of data that isn't meaningfully representable in $\mathbb{R}^n$.

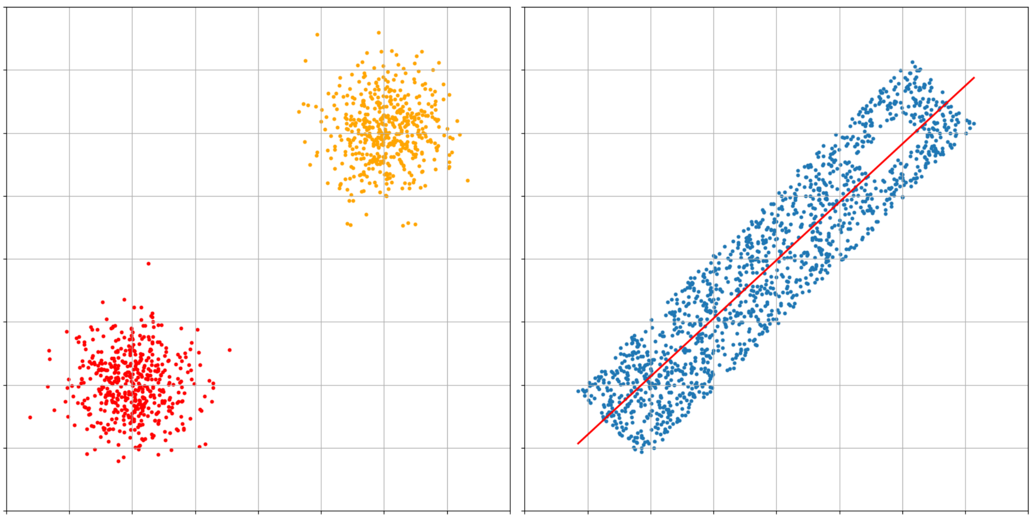

Figure 1: Test Data. A clasiffication problem on the left and a regression problem on the right. Created by the authors.

It is clear that the data points on the right do exhibit a linear behavior but the linear model doesn't capture the topological properties of the datasets, namely the number of *connected components* or the number of *holes*. Traditional *clustering* algorithms can identify the number of clusters in the data but can't filter out noise, which may introduce spurious results to the analysis.

These considerations motivate the development of **Topological Data Analysis** (TDA). This is a relatively recent research area which began with the work of Edelsbrunner in persistent homology [2] at the beginning of the 2000s. The methods that have been developed ever since seek to explore the topological properties of the latent space from which data comes from.

The objective of this thesis is to explore the mathematical foundations of TDA as well as to present some novel applications of these concepts in Machine Learning. In Section 2, we will present the necessary mathematical background in Algebra, Topology and Algebraic Topology for an undergraduate student to understand the results presented here. In Section 3, we state and prove the Nerve Theorem for convex and compact covers and show its relevance in TDA through Category Theory. Finally, in Section 4 we introduce homology, persistence and an application of these concepts developed in [1] for binary classification problems.

2 Background

The purpose of this chapter is to introduce the reader to some fundamental mathematical concepts in Topology, Algebra and Algebraic Topology which are used in TDA. The knowledgeable reader may skip this chapter but it is strongly advised to review the subsection on Algebraic Topology as TDA is mostly based on its concepts.

2.1 Algebra

In TDA, topological properties are studied by using algebraic objects. There exists a series of structures (*groups, rings, fields, modules*) which will encode topological properties that will give us relevant information about our data. We begin with the most basic definition.

Definition 2.1. A ***group*** is a set G together with a binary operation $\cdot : G \times G \longrightarrow G$ such that:

1. For all $a, b, c \in G$ we have $(a \cdot b) \cdot c = a \cdot (b \cdot c)$.
2. There exists an element $e \in G$ such that for all $x \in G$, $e \cdot x = x \cdot e = x$.
3. For all $g \in G$ there exists an element g^{-1} such that $g \cdot g^{-1} = g^{-1} \cdot g = e$.

Example 2.2. Let A be a set. A *permutation* of the set A is a function $\phi : A \longrightarrow A$ that is bijective. The set of all permutations of the set A under function composition is a group called the *symmetric group* of A denoted by S_A. When $A = \{1, \ldots, n\}$, we denote S_A simply by S_n.

As we will see later, groups form a category under a special kind of structure preserving functions called **homomorphisms**.

Definition 2.3. A ***homomorphism*** is a function between two groups $\varphi : G \longrightarrow H$ such that for all $g, h \in G$ we have $\varphi(g \cdot_G h) = \varphi(g) \cdot_H \varphi(h)$. We add a subscript as to highlight where each operation comes from.

Remark 2.4. We will omit the subscript notation for group operations where it is clear which operation we are using.

We can demand further structure from group homomorphisms in the form of group **isomorphisms**.

Definition 2.5. A bijective group homomorphism is called an ***isomorphism***. We denote two isomorphic groups as $G \cong H$.

We can progressively define further properties that the group operation must satisfy in order to better suit the context we are working in. For instance, in homology we will use a special type of groups called **abelian groups**.

Definition 2.6. We say that a group G is ***abelian*** if its operation is commutative (i.e $a \cdot b = b \cdot a$). In what follows, we denote the operation $a \cdot b$ as just ab.

Example 2.7. The classic example of an abelian group is the *cyclic group of order* n, denoted by $\mathbb{Z}_n$, which is the set of residue classes of integers modulo n with addition. Furthermore, we can define the group $\mathbb{Z}^r$ as the direct sum of r copies of $\mathbb{Z}$ (i.e $\bigoplus_{i=1}^r \mathbb{Z}$) where the operation is component by component addition. In particular, $\mathbb{Z}$ by itself is abelian under addition.

Isomorphisms induce equivalence classes for groups. This allows us to classify groups by the properties preserved under isomorphism. As expected, being abelian is one of those properties.

Example 2.8. Let G, H be two groups and $\varphi : G \longrightarrow H$ an isomorphism. Then G is abelian if and only if H is abelian.

Proof of Example 2.8. Suppose G is abelian. As φ is bijective, let $h, j \in H$ such that, $\varphi(a) = h$ and $\varphi(b) = j$ with $a, b \in G$.

$$h \cdot j = \varphi(ba) = \varphi(ab) = j \cdot h$$

So H is abelian. The other direction is analogous with the inverse function φ^{-1}. □

Definition 2.9. Let G be a group. A subset $H \subseteq G$ is a ***subgroup*** of G provided that it is itself a group under the same operation defined on G. We denote this relation by $H \leq G$.

Remark 2.10. **Cayley's Theorem** states that every group is isomorphic to a subgroup of symmetric group.

The most important and relevant examples of subgroups that will be used throughout this thesis are the **image** and the **kernel** of a homomorphism.

Example 2.11. Let G and H be groups together with a group homomorphism $\varphi : G \longrightarrow H$. The following two sets are subgroups of their respective groups.

$$\mathrm{Im}(\varphi) = \{h \in H \mid h = \varphi(g) \text{ for some } g \in G\} \leq H,$$

called the *image* of φ.

$$\mathrm{Ker}(\varphi) = \{g \in G \mid \varphi(g) = e\} \leq G,$$

called the *kernel* of φ.

In fact, the kernel of a homomorphism is a special kind of subgroup called a **normal** subgroup.

Definition 2.12. Let G be a group and $H \leq G$. We say that H is a ***normal*** subgroup of G, denoted by $H \trianglelefteq G$, if for any $x \in H$ and $g \in G$ we have $g^{-1}xg \in H$. If this is the case, we say that H is closed under *conjugation*.

Remark 2.13. Any subgroup of an abelian group G is normal.

Normal subgroups play a central role in the study of *quotient groups*.

Definition 2.14. Let G be a group and $N \trianglelefteq G$. We denote by G/N the set of left cosets of N in G. This is

$$G/N = \{g \cdot N \mid g \in G\}$$

where,

$$gN = \{g \cdot n \mid n \in N\}.$$

We call gN the quotient class of g where g is called a *representative*. The operation on the cosets is defined as follows:

$$(g_1N) \cdot (g_2N) = (g_1 \cdot g_2)N.$$

Normality of N shows that this is well defined. In this case, we refer to G/N as the quotient group.

Remark 2.15. We can think of the quotient as *factoring* the elements of N from the group G as they effectively become the identity element on G/N.

A fundamental result that relates quotient groups, the kernel and the image of a group homomorphism is the **first isomorphism theorem** which states that for a group homomorphism $\varphi : G \longrightarrow H$, we have:

$$G/\mathrm{Ker}(\varphi) \cong \mathrm{Im}(\varphi).$$

2.2 Topology

A central problem of Topology is the classification of topological spaces up to a certain notion of equivalence. There are many notions of equivalence for topological spaces from which we will discuss only two in this section, homeomorphism and homotopy, as they are the most relevant for TDA. Moreover, the proof of the Nerve Theorem is topological in nature and will require the concepts introduced in this section.

Definition 2.16. A **topology** on a set X is a collection $\mathcal{T} \subseteq \mathcal{P}(X)$ having the following properties:

1. $\varnothing \in \mathcal{T}$ and $X \in \mathcal{T}$.
2. X is closed under arbitrary unions.
3. X is closed under finite intersections.

The pair $(X, \mathcal{T})$ where X is a set and $\mathcal{T}$ is a topology defined over X is called a **topological space**. We say that a set $U \subseteq X$ is *open* if $U \in \mathcal{T}$. In this case, if $x \in U$, we say that U is an *open neighborhood* of x. The information given by a topology is fundamental to define concepts such as continuity, distance and compactness which are essential to various results that will be used throughout this thesis. In what follows, we will say that X is a topological space without specifying its topology $\mathcal{T}$ unless it is strictly necessary.

Example 2.17. We can induce a topology, called the **subspace topology**, for any subset S of a topological space X. Let $\mathcal{T}$ be the topology of X. The collection

$$\mathcal{T}_S = \{S \cap U \mid U \in \mathcal{T}\}$$

defines a topology on S. In what follows, we will assume that any subset of a topological space inherits the subspace topology.

Topological spaces are characterized by their *basis*.

Definition 2.18. Let X be a set. A ***basis*** for a topology on X is a collection $\mathcal{B} \subseteq \mathcal{P}(X)$ such that:

1. For each $x \in X$ there exists a set $B \in \mathcal{B}$ such that $x \in B$ (i.e $X = \bigcup_{B \in \mathcal{B}} B$).
2. Let $B_1, B_2 \in \mathcal{B}$. If $x \in B_1 \cap B_2$, then there exists a set $B_3 \in \mathcal{B}$ such that $x \in B_3 \subseteq B_1 \cap B_2$.

A collection $\mathcal{B}$ satisfying these conditions is said to generate the topology $\mathcal{T}$ if $U \subseteq X$ is said to be open if and only if, for each $x \in U$, there is a basis element B such that $x \in B \subseteq U$. In other words, the topology generated by $\mathcal{B}$ is the collection of all unions of elements in $\mathcal{B}$.[1]

Example 2.19. Consider the set of real numbers $\mathbb{R}$. There are various topologies that can be defined over $\mathbb{R}$ which induce different topological properties on the set. The standard Euclidean topology is defined as the topology generated by the basis of open intervals.

Another topology that can be defined over $\mathbb{R}$ is called the finite complement topology or co-finite topology, given by

$$\mathcal{T}_c \coloneqq \{U \subseteq \mathbb{R} \mid \mathbb{R} - U \text{ is finite or, } \mathbb{R} - U = \mathbb{R}\}$$

We say that a topological space X is **Hausdorff** if for each pair $x_1, x_2 \in X$ with $x_1 \neq x_2$, there exist open sets U_1 and U_2 such that $x_1 \in U_1, x_2 \in U_2$ and $U_1 \cap U_2 = \varnothing$. Lets see that $\mathbb{R}$ is Hausdorff with the topology $\mathcal{T}_E$ but not with T_c.

Proof that $\mathcal{T}_E$ is Hausdorff but not T_c . First consider $\mathbb{R}$ with the topology of the finite complement. Assume, by contradiction, that it is Hausdorff. Take $x, y \in \mathbb{R}$ and U, V their corresponding open neighborhoods such that $U \cap V = \varnothing$. Observe that, $V \subseteq \mathbb{R} - U$. Then V is finite or $\mathbb{R}$. V can't be the whole set as $U \cap V \neq \varnothing$ so V has to be finite. If V is finite then $\mathbb{R} - V$ is not finite so V isn't an open set in $\mathcal{T}_c$. Then $(\mathbb{R}, \mathcal{T}_c)$ is not Hausdorff.

Now consider $\mathbb{R}$ with the usual topology. Take $x, y \in \mathbb{R}$ with $x \neq y$. Without loss of generality, assume that $x > y$ so $\varepsilon = \frac{x-y}{2} > 0$. Then $(x-\varepsilon, x+\varepsilon)$ and $(y-\varepsilon, y+\varepsilon)$ are open sets. Clearly x and y are in their respective sets. Furthermore, $(x-\varepsilon, x+\varepsilon) \cap (y-\varepsilon, y+\varepsilon) = \varnothing$. Then $(\mathbb{R}, \mathcal{T}_E)$ is Hausdorff. □

It is clear how a topology changes the properties that a set satisfies. However, to fully grasp the importance of a topology, we will go over the definition of a continuous function; the elemental relation between topological spaces.

Definition 2.20. Let X and Y be topological spaces. A function $f : X \longrightarrow Y$ is said to be ***continuous*** if for each open set $V \subseteq Y$, $f^{-1}(V)$ is open in X.

[1]This is Lemma 13.1 in Munkres' *Topology.*

Continuous functions are central in the study of topological spaces but they are too weak distinguish them. However, it is possible to demand additional structure from a continuous function by means of a *homeomorphism*.

Definition 2.21. Let X and Y be topological spaces and $f : X \longrightarrow Y$ a bijection. If f and f^{-1} are continuous functions then f is called a ***homeomorphism***.

By demanding that a continuous function be bicontinuous we can have a 1-1 correspondence, not only at the level of points, but between open sets which, much like linear isomorphisms between vector spaces or group isomorphisms between groups, imply a structural equivalence between topological spaces. Furthermore, we look for properties that when satisfied by X, they are immediately satisfied by any space homeomorphic to X. Properties that meet this condition for any arbitrary topological space are called **topological properties**.

Example 2.22. Let X be a topological space. A separation of X is a pair U, V of disjoint nonempty open subsets of X whose union is X. A space X is said to be **connected** if X does not have a separation. Let us verify that connectedness is a topological property.

Proof of Example 2.22. Let X, Y be topological spaces and assume that X is a connected space. Let $f : X \longrightarrow Y$ be a homeomorphism. Suppose Y is not a connected space. Then there exists U, V disjoint and nonempty open sets such that $Y = U \cup V$. Note that, $f^{-1}(U)$ and $f^{-1}(V)$ are open in X. Furthermore, $f^{-1}(Y) = X$. As U and V are disjoint and nonempty and f is bijective, then $f^{-1}(U) \cup f^{-1}(V) = X$ is a separation of X. Then, Y has to be connected and so, connectedness is a topological property. □

Most of the spaces where empirical data comes from are **metric spaces**. These class of spaces carry a topology called the **metric topology** induced by a **metric**.

Definition 2.23. A ***metric*** on a set X is a function

$$d : X \times X \longrightarrow \mathbb{R}$$

having the following properties:

1. $d(x, y) \geq 0$ for all $x, y \in X$. Equality holds if and only if $x = y$.
2. $d(x, y) = d(y, x)$ for all $x, y \in X$
3. d satisfies the triangle inequality: $d(x, y) + d(y, z) \geq d(x, z)$
   for all $x, y, z \in X$

A metric defined on a space X allows us to define a notion of *distance* in the space, namely $d(x, y)$. Moreover, we can define a special kind of set called an ***open ball***. Given $\varepsilon > 0$, the set

$$B(x, \varepsilon) = \{y \in X \mid d(x, y) < \varepsilon\}$$

is called an ***open ball of radius*** $\boldsymbol{\varepsilon}$ ***centered at*** $\boldsymbol{x}$ or just an $\boldsymbol{\varepsilon}$***-ball centered at*** $\boldsymbol{x}$. These sets form a basis for a topology on the set X, which is called the **metric topology**.

Remark 2.24. Let S be a subset of a metric space X. We can define the **open neighborhood of radius** ε **of a set** S as:

$$B(S, \varepsilon) = \bigcup_{x \in S} B(x, \varepsilon).$$

Example 2.25. Data in the real world can be represented as points in $\mathbb{R}^n$ where n is the number of characteristics that are being considered in the sample. In TDA we wish to infer what shape does the data have as a subspace of $\mathbb{R}^n$. Fortunately $\mathbb{R}^n$ has very useful topological properties that make it a suitable space to work with. We can define the **standard Euclidean metric in** $\mathbb{R}^n$ as follows:

$$\begin{aligned} d : \mathbb{R}^n \times \mathbb{R}^n &\longrightarrow \mathbb{R} \\ (\mathbf{x}, \mathbf{y}) &\longmapsto \left(\sum_{i=1}^{n} (x_i - y_i)^2 \right)^{\frac{1}{2}} \end{aligned}$$

It can be shown that the function d is a metric and thus, it induces a metric topology on $\mathbb{R}^n$.

Metric spaces are central in the study of **sequences** and their **convergence**.

Definition 2.26. Let X be a topological space. A ***sequence*** is a set of points $x_i \in X$ indexed by the natural numbers denoted by (x_n). If we consider the sequence $(n_i) \subseteq \mathbb{N}$, the resulting sequence (x_{n_i}) is called a ***subsequence*** of (x_n).

Definition 2.27. Let X be a metric space with metric d and (x_n) be a sequence in X. We say that (x_n) ***converges*** if there exists a point $x \in X$ such that, for every $\varepsilon > 0$, there exists an integer N such that, if $n \geq N$ then $d(x_n, x) < \varepsilon$.

Remark 2.28. If (x_n) is a sequence of points in a metric space X that converges to x, we say that x is a limit point. The limit point of a sequence in a metric space is unique.

Most of the spaces we will encounter in TDA are called **compact** spaces. Compactness is an important topological property that is stated in terms of **open coverings**. Nevertheless, since our ambient space will be $\mathbb{R}^n$ in most applications, we can characterize compact subsets using the **Heine-Borel Theorem**.

Definition 2.29. A collection $\mathcal{U} = \{U_i\}_{i\in\Gamma}$ of subsets of a space X is said to ***cover*** X, or to be a covering of X, if the union of the elements of $\mathcal{U}$ is equal to X. It is called an ***open covering*** of X if its elements are open subsets of X. More generally, an open covering of a ***subset*** $S \subseteq X$ is a collection $\mathcal{U} = \{U_j\}_{j\in\Gamma}$ of subsets of X such that $S \subseteq \bigcup_{j\in\Gamma} U_j$. We say that a subset $V \subseteq \mathcal{U}$ is a ***subcover*** of $\mathcal{U}$ if it is itself a cover of X.

Definition 2.30. A space X is said to be ***compact*** if every open covering of X contains a finite subcover.

Theorem 2.31 (Heine-Borel)**.** *Let $S \subseteq \mathbb{R}^n$. S is compact, with the subspace topology if and only if, S is closed and bounded.*

Sequences defined on compact spaces exhibit desirable convergence properties. We say that a metric space X is called **sequentially compact** if every sequence of points has a convergent subsequence converging to a point in X.

Theorem 2.32 (Bolzano-Weirstrass)**.** *A subset of $\mathbb{R}^n$ is sequentially compact if and only if it is bounded and closed in $\mathbb{R}^n$.*

Remark 2.33. By the Heine-Borel Theorem this implies that, compact subsets and sequentially compact subsets of $\mathbb{R}^n$ are equivalent.

Recall that in Example 2.19 we introduced the notion of a *Hausdorff space.* This property is part of a family of properties which are called the **separation axioms**. For the proof of the Nerve Theorem in the next section we will need a separation axiom stronger than being Hausdorff called **normality**.

Definition 2.34. We say that a topological space X is ***normal*** if, for every two disjoint closed subsets E and F, there exist open neighborhoods U of E and V of F such that $U \cap V = \varnothing$.

Remark 2.35. All metric spaces are normal spaces. The most relevant for TDA being $\mathbb{R}^n$.

Normal spaces satisfy what is known as **Urysohn's Lemma**. The details of the proof are [3, Theorem 33.1].

Theorem 2.36 (Urysohn)**.** *Let X be a normal space, A and B be disjoint closed subsets of X, and $[a, b]$ be a closed interval in the real line. Then, there exists a continuous function $f : X \longrightarrow [a, b]$ such that $f(x) = a$ for every $x \in A$ and $f(x) = b$ for every $x \in B$.*

A function that satisfies this property is called a *Urysohn function.* These functions allow us to separate disjoint closed subsets.

2.3 Algebraic Topology

The concepts herein defined provide the mathematical basis for TDA. Most importantly, homotopy provides a notion of equivalence that is flexible enough to be used to study data but it still preserves the information captured by homology.

2.3.1 Homotopy

We will introduce the last notion of equivalence that will be relevant for our study of TDA and the Nerve Theorem, namely **homotopy equivalence**.

Definition 2.37. Let X, Y be topological spaces and $f,\ g : X \longrightarrow Y$ two continuous functions. A ***homotopy*** is a family of functions $f_t : X \longrightarrow Y$, $t \in [0,1]$ such that the associated map $F : X \times [0,1] \longrightarrow Y$ given by $F(x,t) = f_t(x)$ is continuous and $F(x,0) = f(x)$ and $F(x,1) = g(x)$.

Two maps f, g are said to be **homotopic**, denoted $f \simeq g$, if there exists a homotopy between them. If two maps are homotopic we can imagine taking the image set of one of the functions and continuously deforming it to the other in such a way that it is never broken up into pieces.

Example 2.38. It is important to note that homotopy is able to capture a notion of *equivalence* between functions but it is not precisely that they act equally on the space.

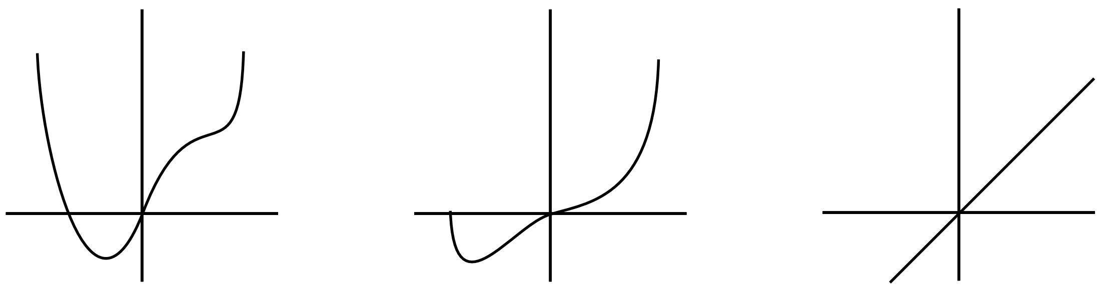

Figure 2: Some steps of a homotopy between a polynomial and the identinty in $\mathbb{R}^2$.

Homotopy is not only convenient to study the relationship between functions but it can also be used to study topological spaces as a whole.

Definition 2.39. Let X, Y be topological spaces. A map $f : X \longrightarrow Y$ is called a ***homotopy equivalence*** if there exists a map $g : Y \longrightarrow X$ such that $f \circ g \simeq \mathbb{1}$ and $g \circ f \simeq \mathbb{1}$ where $\mathbb{1}$ denotes the identity map on each space.

Remark 2.40. If the above map exists, X and Y are said to be **homotopy equivalent** or to have the same **homotopy type**, denoted $X \simeq Y$.

Example 2.41. The 1 point space, denoted by $\{\mathrm{pt}\}$, has a unique set of properties that are desirable for some spaces to have. A space X is said to be **contractible** if it has the homotopy type of the 1 point space. In other words, we say that X is contractible if the identity map id_X is homotopic to a constant map. This means that we can pick any point in our space $x \in X$ and define a homotopy from any other point to x, hence X has the same homotopy type as $\{\mathrm{pt}\}$.

For our purposes in this thesis, we shall consider a general class of contractible sets in $\mathbb{R}^n$ called **star-shaped** sets.

Definition 2.42. Let $S \subseteq \mathbb{R}^n$. We say S is a ***star-shaped*** set if there exists a point $s_0 \in S$ such that for all $s \in S$, the line segment connecting s_0 and s is contained in S.

Clearly, any star-shaped set S can be contracted to the point s_0 by a straight line homotopy.

Remark 2.43. Convex sets are particular examples of star-shaped sets and thus, they are contractible.

Homotopy equivalence is a much weaker notion than homeomorphism. In fact, a homeomorphism is a special case of a homotopy equivalence; precisely when $f \circ g = g \circ f = \mathbb{1}$.

An important question that arises in the study of homotopies is how do we *extend* homotopies that are defined on a subspace A of a larger space X. In general, this depends on the topological relationship that A has with X.

Definition 2.44. Let X and Y be topological spaces with $A \subseteq X$. Suppose that we have a continous map $f_0 : X \longrightarrow Y$ and a homotopy $f_t : A \longrightarrow Y$ of the map $f_0|_A$, which we want to extend to a homotopy $f_t : X \longrightarrow Y$ for f_0. We say that the pair (X, A) has the ***homotopy extension property*** if this extension always exists.

Remark 2.45. Let $I = [0, 1]$ denote the unit interval. Equivalently, we can say that the pair (X, A) has the homotopy extension property if any map $F : ((X \times \{0\}) \cup (A \times I)) \longrightarrow Y$ can be extended to a map $F' : X \times I \longrightarrow Y$.

2.3.2 Simplices

To work out the details of the proof of the Nerve Theorem in the following section, we need to define various properties of simplices and simplicial complexes that will be essential in understanding the arguments that will follow.

Definition 2.46. A ***geometric k-simplex*** σ in $\mathbb{R}^n$ is the convex hull of a collection of $(k+1)$ points $\{x_0, \ldots, x_k\}$, where the set $\{x_1 - x_0, \ldots, x_k - x_0\}$ is linearly independent[2]. This is independent of how we choose the point x_0. Each of the x_i is called a *vertex* of the n-simplex.

Any point inside a geometric simplex can be represented uniquely by its **barycentric coordinates**. If $\{x_0, \ldots, x_k\}$ is the set of vertices of a geometric simplex σ, then a point x is in σ if and only if,

$$x = \sum_{i=0}^{k} t_i x_i \text{ for some } t_0, \ldots, t_k \in \mathbb{R}, \text{ where} \sum_{i=0}^{k} t_i = 1.$$

The coefficients t_i are called the **barycentric coordinates** of the point x.

Remark 2.47. The function $b_{x_i}(x) = t_i$, which extracts the barycentric coordinates of x with respect to the vertex x_i is a continuous function.

Although the definition of a geometric simplex may seem abstract, it corresponds to subspaces that we are already familiar with. Figure 3 shows examples of low dimensional simplices.

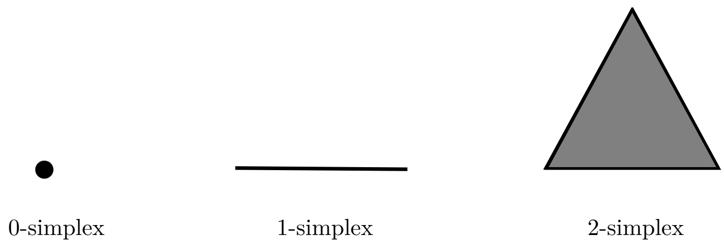

Figure 3: Low dimensional geometric simplices

The number k in the definition of a k-simplex σ is called the **dimension** of σ. Any simplex spanned by a subset $F \subseteq \{x_0, \ldots, x_k\}$ is called a **face** of σ. The most important property of simplices is precisely that each of the faces of a simplex is a simplex in itself. This property makes simplices a very convenient type of space for inductive arguments.

Definition 2.48. A ***simplicial complex*** K in $\mathbb{R}^n$ is a collection of geometric simplices in $\mathbb{R}^n$ such that:

1. Every face of a simplex of K is in K.

[2]This definition is equivalent to affine independece.

2. The intersection of any two simplices of K is a face of each of them.

Definition 2.49. If L is a subcollection of a simplicial complex K that contains all faces of its elements, then L is a simplicial complex itself, called a ***subcomplex*** of K.

Remark 2.50. The subcomplex of a simplicial complex K, which consists of all the simplices of K with dimension at most p, is called the ***p*-skeleton** of K. We denote this subcomplex by $\mathrm{sk}_p K$. The 0-skeleton of K, which consists of the collection of vertices of K, is denoted by Vert K.

So far we have worked with *geometric* simplicial complexes but there exists a class of objects which are closely related to geometric simplicial complexes called *abstract simplicial complexes*. These objects provide a combinatorial description of geometric simplices as we will specify later.

Definition 2.51. Let V be a finite nonempty set. An ***abstract simplicial complex*** on V is a collection K of nonempty subsets of V which satisfy the following conditions.

- For each $v \in V$, $\{v\} \in K$. The singletons in K are called the *vertices* of the complex.
- If $\tau \in K$ and $\sigma \subset \tau$, then $\sigma \in K$. This is equivalent to saying that K is closed under the face relation.

If $\{v_0, \ldots, v_k\}$ is the set of vertices of an abstract simplicial complex σ, we denote it by $\sigma = [v_0, \ldots, v_k]$. The face of the simplex σ spanned by all the vertices but the vertex v_i is denoted by $[v_0, \ldots, \hat{v}_i, \ldots, v_k]$.

An abstract simplicial complex captures the properties that we discussed earlier about geometric simplicial complexes. This will allow us to define a simplicial structure on other types of objects. For now, let us define formally how to relate an abstract simplicial complex to a geometric simplicial complex. We will follow the Lecture Notes given by Vidit Nanda in [4].

Definition 2.52. Let K be an abstract simplicial complex and $\phi : \mathrm{sk}_0 K \longrightarrow \mathbb{R}^n$ an injective function that sends the vertices of K to points in $\mathbb{R}^n$ such that $\phi(\mathrm{sk}_0 K)$ is affinely independent. The ***geometric realization*** of K is the union

$$|K| = \bigcup_{\sigma \in K} |\sigma|$$

where for each $\sigma = [v_0, \ldots, v_k]$, the set $|\sigma| \subseteq \mathbb{R}^n$ is the geometric k-simplex spanned by the points $\{\phi(v_0), \ldots, \phi(v_k)\}$.

As such, it is clear that the geometric realization of an abstract simplicial complex corresponds to the intuition we have built of what a geometric simplex looks like as in Figure 3. From now on, we will use the term *simplex* to refer to a geometric simplex or its associated abstract simplicial complex interchangeably. Now we will introduce the **barycentric subdivision**, a central construction for the proof of the Nerve Theorem.

Definition 2.53. Let K be a simplicial complex. The *barycentric subdivision* Sd K is a simplicial complex defined as follows. For each dimension $i \geq 0$, the i-simplices of Sd K are given by all sequences

$$\sigma_0 \subset \sigma_1 \subset \cdots \subset \sigma_{i-1} \subset \sigma_i$$

of distinct simplices in K ordered by the face relation. Each σ_j represents a vertex of Sd K and its called the *barycenter of* σ_j.

Consider the following example to ilustrate the barycentric subdivision of a simplicial complex.

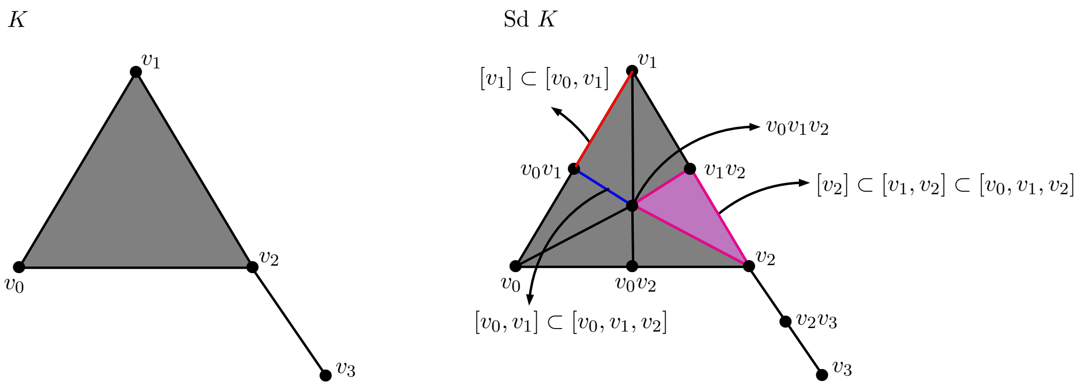

Figure 4: An example of the barycentric subdivision of a simplicial complex K with corresponding labels for some simplices.

Note that the label in the blue simplex corresponds to a truncated sequence of the simplex $[v_1] \subset [v_0, v_1] \subset [v_0, v_1, v_2]$. Although this isn't defined explicitly in the barycentric subdivision, it will be a useful way of labeling simplices for Lemma 3.6.

In general, for a simplicial complex K, an algorithm to draw Sd K has the following structure.

1. Label the barycenter of the j-simplex $[v_{i_0}, \dots, v_{i_j}]$ by $v_{i_0} \dots v_{i_j}$.

2. Add the j-simplex according to the sequences of simplices of j elements as in Definition 2.53. This simplex is spanned by the barycenters that appear in the sequence.

We begin this process with the 1-simplices and continue inductively until we are done with all the simplices in K.

Observe that in Figure 4 reveals how similar the underlying topological space of the barycentric subdivision and its original complex are. This fact is encapsulated in the following proposition.

Proposition 2.54. *Let K be a simplicial complex. There exists a homeomorphism α_K between $|K|$ and $|\mathrm{Sd}\ K|$.*

We can imagine α_K as a retraction of the new simplices created in Sd K to each of the vertices of the old simplices.

3 The Nerve Theorem

For the main result of this thesis we will follow [5]. Their proof of the Nerve Theorem requires a collection of closed convex subsets of $\mathbb{R}^n$, $\mathcal{C} = \{C_i\}_{i\in[n]}$, which covers the data points appropriately. Upon closer inspection of the paper [5] and an active discussion with its authors, we discovered a mistake in their construction for an associated open cover. As such, we will require for our cover to be convex and *compact*. This extra requirement does not affect any applications of the theorem as its practical uses are on finite sets of data points in $\mathbb{R}^n$ which are easily covered in such a way.

First, we will define the **nerve** of a cover $\mathcal{U} = \{U_i\}_{i\in J}$ and work towards seeing how it is related to the original topological space we started with. The Nerve Theorem provides us with a homotopy equivalence between a topological space and a simplicial complex, called the nerve, associated to such covering. Roughly speaking, the nerve may be seen as a discrete approximation of a topological space. As any sort of approximation, it preserves certain information of the original object. This intuition will be made precise in the following Section on Homology.

Definition 3.1. The ***nerve***[3] of the cover $\mathcal{U} = \{U_i\}_{i\in J}$ is the abstract simplicial complex $\mathrm{Nrv}(\mathcal{U})$ with simplices given by the finite subsets $W \subseteq J$ such that

$$\bigcap_{i\in W} U_i \neq \varnothing.$$

[3]The nerve is also referred in the literature as the Čech Complex of the cover $\mathcal{U}$.

From now on, let X denote the union of the elements of the cover $\mathcal{C}$. The main idea behind the proof of the Nerve Theorem is to define a continuous function $\Gamma : |\text{Sd Nrv}(\mathcal{C})| \longrightarrow X$ which takes a vertex on the barycentric subdivision of the nerve and maps a point on its corresponding intersection of cover elements. We can see the map Γ illustrated in Figure 5. Formally, consider a point $x_{k\ldots\ell} \in C_k \cap \cdots \cap C_\ell$ and let $|v_k \ldots v_\ell|$ be the barycenter corresponding to that intersection in $|\text{Sd Nrv}(\mathcal{C})|$. Let $\Gamma(|v_k \ldots v_\ell|) = x_{k\ldots\ell}$. As each point of a simplex $|\sigma| \in |\text{Sd Nrv}(\mathcal{C})|$ is defined by its barycentric coordinates with respect to the vertices of $|\sigma|$ then, $x = \sum_i \alpha_i |v_i|$ where $\sum_i \alpha_i = 1$. As each intersection of the cover elements is convex we have that $\Gamma(x) = \sum_i \alpha_i \Gamma(|v_i|)$ is also in that intersection. This map is well defined as convexity of the cover elements allows us to uniquely extend our choice of the points associated to each simplex in the nerve to an embedding of $|\text{Sd Nrv}(\mathcal{C})|$ in X that is *affine linear*[4].

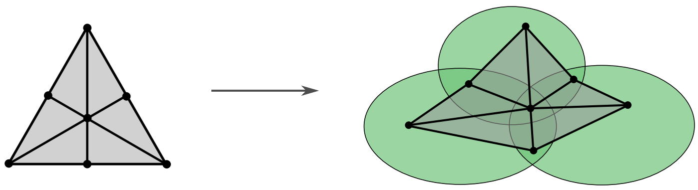

Figure 5: Illustration of the map Γ. Taken from [5, Figure 6].

We will prove that Γ is a homotopy equivalence by constructing a homotopy inverse Ψ to Γ. We will detail its explicit construction in Section 3.1. The main Theorem that we are going to prove is:

Theorem 3.2 (The Nerve Theorem)**.** *The map Γ is a homotopy equivalence. In particular, $|\text{Nrv}(\mathcal{C})|$ is homotopy equivalent to X.*

Remark 3.3. In this thesis we will work with the *barycentric subdivision of the nerve* and prove the homotopy equivalence to this space. Given that homotopy type is preserved under homeomorphism, this will not affect the main result as the nerve and its barycentric subdivision are homeomorphic.

3.1 Some results about Geometric Simplicial Complexes

To prove the Nerve Theorem we will need various lemmas about geometric simplicial complexes. The following construction will aid in our study of the map Γ.

[4]A map is said to be ***affine linear*** if its a linear transformation that does not preserve the origin. These sort of transformations need not preserve euclidean distances, only lines and parallelisms.

Definition 3.4. For every vertex v of a simplicial complex K we define the ***closed barycentric star*** as the subspace

$$\text{bst } v = |\text{Cl St}_{\text{Sd } K}\, v| \subseteq |\text{Sd } K|,$$

where $\text{Cl St}_{\text{Sd } K}\, v = \{\sigma \in \text{Sd } K \mid \sigma \cup \{v\} \in \text{Sd } K\}$ is the closure of the star of v in the barycentric subdivision of K.

Remark 3.5. The closed barycentric star is just the union of all simplices of the barycentric subdivision that have v as a vertex.

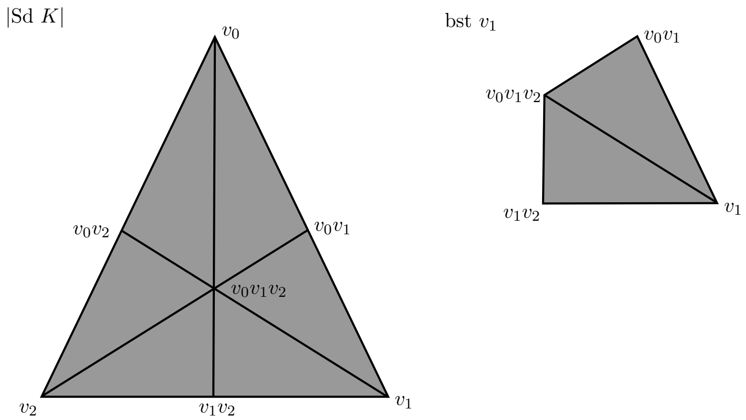

Figure 6: An example of the closed barycentric star bst v_1.

Lemma 3.6. *Let K be a simplicial complex and σ a simplex spanned by the vertices $\{v_0, \dots, v_k\} \in K$ and consider the subcomplex $L = \{\tau_0 \subset \cdots \subset \tau_m \mid \sigma \subseteq \tau_0\} \subseteq \text{Sd } K$. Then $\bigcap_{i=0}^k$ bst $v_i = |L|$.*

Proof. Let $\phi = (\tau_0 \subset \cdots \subset \tau_m) \in L$ be a simplex. By definition, this simplex is in bst v_i as it is a face of the simplex $(v_i \subset \tau_0 \subset \cdots \subset \tau_m) \in$ bst v_i. Furthermore, this is true for every vertex in σ so $\phi \in \cap_{i=0}^k$ bst v_i and then $L \subseteq \cap_{i=0}^k$ bst v_i.

For the reverse inclusion, lets take $\phi \in \cap_{i=0}^k$ bst v_i. By definition, $\phi = |\tau_0 \subset \cdots \subset \tau_m|$ where for each i, $v_i \in \tau_0$. Then, it is clear that $\sigma \subseteq \tau_0$. So $\phi \in L$ and $\cap_{i=0}^k$ bst $v_i \subseteq L$. □

Remark 3.7. The point in Sd K labeled $v_1 v_2 \dots v_k$ is the barycenter of the simplex σ. According to the preceding lemma, it is clear that the subcomplex L is just the closed barycentric star of this vertex in Sd K.

With this in mind, the following lemma is an immediate result.

Lemma 3.8. *Let K be a simplicial complex and let $\sigma \in K$ be a simplex. Then the intersection $\cap_{v\in\sigma}$ bst v is contractible. In particular, the collection of closed barycentric stars forms a good cover of $|K|$.*

Remark 3.9. By good cover we mean a cover $\mathcal{U}$ of a topological space X such that all sets and all non-empty intersections of finitely many sets are contractible.

Proof. For a vertex v, the closed barycentric star bst v is a simplicial complex. We can contract each simplex through a straight line homotopy to v because each simplex is a convex set. As, $\bigcap_{v\in\sigma}$ bst v is the closed barycentric star for the barycenter of σ, it is also contractible. This implies that each closed barycentric star is contractible and non-empty intersections are contractible. Finally, the collection of closed barycentric stars cover the simplex $|K|$ as $\bigcup_{v\in \text{Vert } K}$ bst $v = |\text{Sd } K|$ and $|\text{Sd } K| \cong K$. □

Finally, we have the last lemma which characterizes the points in closed barycentric stars in terms of their barycentric coordinates.[5]

Lemma 3.10. *Let K be a simplicial complex and let v be a vertex of K. The closed barycentric star* bst v *consists of all points $x \in |K|$ that satisfy*

$$b_v(x) \geq b_w(x) \text{ for all } w \in \text{Vert } K,$$

where the function $b_v(x)$ is defined in Remark 2.47.

3.2 Constructing a homotopy inverse for Γ

To construct Ψ we use the concept of a partition of unity to define a family of functions that will allow us to detect in which cover element a point lies and associate its corresponding element in the nerve. We use the definition of partition of unity given in [6].

Definition 3.11. Let $\mathfrak{U} = \{U_\alpha\}_{\alpha\in A}$ be a finite open covering of a topological space X. A ***partition of unity subordinate to the open covering*** $\mathfrak{U}$ is a family of real valued functions $\{\varphi_\alpha\}_{\alpha\in A}$ with the following properties.

- $0 \leq \varphi_\alpha(x) \leq 1$ for all $\alpha \in A$ and $x \in X$.
- $\sum_{\alpha\in A} \varphi_\alpha(x) = 1$ for all $x \in X$.

[5] The proof for this lemma requires various calculations that are out of the scope of this thesis. All the details may be found in [5, Appendix A].

- $\overline{\text{Supp } \varphi_\alpha} = \overline{\{x \in X \mid \varphi_\alpha(x) \neq 0\}} \subseteq U_\alpha, \forall\, \alpha \in A$

As such, we first need to build an open cover $\mathcal{U}$ which respects the nerve of our convex and compact cover $\mathcal{C}$. We will first prove a more general statement about compact neighborhoods in metric spaces.

Lemma 3.12. *Let $U_1, \dots, U_n$ be compact neighborhoods of a metric space X such that $U_1 \cap \cdots \cap U_\ell = \varnothing$. Then, there exists an $\varepsilon > 0$ such that, $B(U_1, \varepsilon) \cap \cdots \cap B(U_\ell, \varepsilon) = \varnothing$.*[6]

Proof [7]. Suppose that this Lemma is not true. Then, for all $n \in \mathbb{Z}^+$ there exists $x_n \in B(U_1, \frac{1}{n}) \cap \cdots \cap B(U_\ell, \frac{1}{n})$. This implies that there exists a $y_{i,n} \in U_i$ such that

$$d(x_n, y_{i,n}) < \frac{1}{n}, \text{ for all } i = 1, \dots, \ell.$$

Then $(y_{i,n})_{n=1}^{\infty}$ is a sequence of points in U_i. As U_i is compact, there exists a subsequence (y_{i,n_k}) which converges to y_i. Without loss of generality, we can assume that we have the same n_k for each i. By applying the triangle inequality we have,

$$d(y_i, y_j) \leq d(y_i, y_{i,n_k}) + d(y_{i,n_k}, x_{n_k}) + d(x_{n_k}, y_j).$$

The first two terms of the right hand side tend to 0 as k tends to infinity, by definition. The third term also tend to 0 because of our remark regarding the indices of each convergent subsequence. This implies that $y_1 = y_2 = \cdots = y_\ell$. As U_i is closed, $y_i \in U_i$ for all $i = 1, \dots, \ell$. Thus, $U_1 \cap \cdots \cap U_\ell \neq \varnothing$, which contradicts our hypothesis. □

The original lemma in the paper, modified for convex and compact covers, is an immediate conclusion of Lemma 3.12.

Lemma 3.13. *Let $\mathcal{C} = \{C_i\}_{i \in [n]}$ be a collection of convex and compact subsets of $\mathbb{R}^n$. Then, there exists a collection of open sets $\mathcal{U} = \{U_i \supseteq C_i\}_{i \in [n]}$ satisfying $\mathrm{Nrv}(\mathcal{C}) = \mathrm{Nrv}(\mathcal{U})$.*

Proof. For each C_i, consider the set of $\varepsilon_{i,\ell}$ radii given by the preceding lemma for each empty intersection with ℓ number of cover elements. This set is finite and we can take the minimum ε_i which satisfies the property for all possible empty intersections. Define the cover elements as

$$\mathcal{U} = \{U_i = B(C_i, \varepsilon_i)\}_{i \in [n]}.$$

Clearly, $\mathrm{Nrv}(\mathcal{C}) \subseteq \mathrm{Nrv}(\mathcal{U})$ by definition. The previous lemma ensures no new intersections are created, thus $\mathrm{Nrv}(\mathcal{C}) \supseteq \mathrm{Nrv}(\mathcal{U})$. □

[6] We thank Professor Mario Velásquez for suggesting this approach towards proving the original Lemma.

Using Lemma 3.13 we construct an open cover $\mathcal{U}$ of X. Define the function φ_i which separates the set C_i from the other C_k where $\varphi_i(C_i) = 1$ and $\varphi_i(\mathbb{R}^n - U_i) = 0$.

$$\begin{aligned} \varphi_i : \mathbb{R}^n &\longrightarrow [0,1] \\ x &\longmapsto \frac{d(x, \mathbb{R}^n \setminus U_i)}{d(x, C_i) + d(x, \mathbb{R}^n \setminus U_i)}. \end{aligned}$$

Normalizing each of the functions φ_i leads to a partition of unity on X subordinate to the cover $\{(U_i \cap X)\}_{i \in [n]}$ with the following family of functions $\{\psi_i\}_{i \in [n]}$ defined as

$$\begin{aligned} \psi_i : X &\longrightarrow [0,1] \\ x &\longmapsto \frac{\varphi_i(x)}{\sum_{j=0}^{n} \varphi_j(x)}. \end{aligned}$$

We can now define the map $\Phi : X \longrightarrow |\mathrm{Nrv}(\mathcal{C})|$ in barycentric coordinates for $|\mathrm{Nrv}(\mathcal{C})|$ as

$$\begin{aligned} \Phi : X &\longrightarrow |\mathrm{Nrv}(\mathcal{C})| \\ x &\longmapsto \sum_{i=0}^{n} \psi_i(x) \cdot |v_i|. \end{aligned}$$

This map associates to each point of X its corresponding simplex in the nerve. This simplex encodes which sets cover the point x. The vertex v_i represents the cover element C_i in the nerve and $|v_i|$ is its geometric realization.

The map $\Psi = \alpha_{\mathrm{Nrv}(\mathcal{C})} \circ \Phi : X \longrightarrow |\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|$ is given by the composition with the standard homeomorphism of the nerve to its barycentric subdivision. To understand the compatibility of the map Γ and Ψ we need to introduce the concept of morphism of **covered spaces**, which will fit in the categorical approach that will be described in the following subsection.

Definition 3.14. Let $(U_i)_{i \in I}$ and $(V_\ell)_{\ell \in L}$ be indexed covers of the topological spaces X and Y, respectively. A ***morphism of covered spaces*** is a pair of functions $(f, \varphi) : (X, (U_i)_{i \in I}) \longrightarrow (Y, (V_\ell)_{\ell \in L})$ where $f : X \longrightarrow Y$ is a continous map and $\varphi : I \longrightarrow L$ is a map between the indexing sets such that for all i we have $f(U_i) \subseteq V_{\varphi(i)}$. In this case, we say that the map f is *carried* by φ.

Remark 3.15. There is a well defined notion of *composition* between morphisms of covered spaces. If f is carried by φ and g is carried by ψ, then $g \circ f$ is carried by $\psi \circ \varphi$ if the compositions are defined.

Proposition 3.16. *The pair of maps* $(\Psi, \mathrm{id}_{[n]})$ *is a morphism of covered spaces*

$$(X, \mathcal{C} = (C_i)_{i\in[n]}) \longrightarrow (|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|, (\mathrm{bst}\ v_i)_{[n]}).$$

Proof. Recall that $\Psi = \alpha_{\mathrm{Nrv}(\mathcal{C})} \circ \Phi$, where the barycentric coordinates are given by each of the ψ_i. Note that, if $x \in C_i$ then $\varphi_i(x) = 1$. Hence, we have that $\psi_i(x)$ is maximal along the $\psi_j(x)$. By Lemma 3.10 we know that $\Psi(x) \in \mathrm{bst}\ v_i$ and then, $\Psi(C_i) \subseteq \mathrm{bst}\ v_i$. □

Proposition 3.17. *The pair of maps* $(\Gamma, \mathrm{id}_{[n]})$ *is a morphism of covered spaces*

$$(|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|, (\mathrm{bst}\ v_i)_{[n]}) \longrightarrow (X, \mathcal{C} = (C_i)_{i\in[n]})$$

Proof. By definition, the map Γ sends the vertices of a geometric simplex σ in bst v_i to C_i. As the cover element C_i is convex and Γ is affine linear on σ, it follows that $\Gamma(\sigma) \subseteq C_i$. This shows that $\Gamma(\mathrm{bst}\ v_i) \subseteq C_i$. □

Knowing that these maps are compatible with their covers, we can now state the proof of the Nerve Theorem for convex and compact covers relying on one final result on morphisms of covered spaces whose proof will be deferred to Appendix A.

Proposition 3.18. *Let K be a finite simplicial complex and let Y be a topological space. Assume we have two morphisms of covered spaces*

$$(f, \varphi), (g, \varphi) : (|K|, (|L_i|)_{i\in[n]}) \longrightarrow (Y, (V_j)_{j\in J}),$$

with the same map of index sets $\varphi : [n] \longrightarrow J$, where $(|L_i|)_{i\in[n]}$ is a cover by subcomplexes and $(V_j)_{j\in J}$ is a good cover. Then f is homotopic to g.

Proof of Theorem 3.2. From Proposition 3.16 and Proposition 3.17 we have that the pair of maps $(\Gamma \circ \Psi, \mathrm{id}_{[n]})$ constitutes a morphism of covered spaces carried by the identity on $\mathcal{C}$. Then, for every $x \in C_i$, we have $(\Gamma \circ \Psi)(x) \in C_i$. As each of the C_i are convex, we have that the line segment joining x and $(\Gamma \circ \Psi)(x)$ lies on C_i thus making $\Gamma \circ \Psi$ homotopic to id_X by straight line homotopy. Conversely, the pair of maps $(\Psi \circ \Gamma, \mathrm{id}_{[n]})$ also constitutes a morphism of covered spaces. Consider the following pair of morphisms of covered spaces

$$(\Psi \circ \Gamma, \mathrm{id}_{[n]}), (\mathrm{id}_{|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|}, \mathrm{id}_{[n]}) : (|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|, (\mathrm{bst}\ v_i)_{[n]}) \longrightarrow (|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|, (\mathrm{bst}\ v_i)_{[n]}).$$

Observe that we can regard the covered space $(|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|, (\mathrm{bst}\ v_i)_{[n]})$ as a finite simplicial complex covered by subcomplexes but also as topological space with a good cover because of Lemma 3.8. Finally, by Proposition 3.18 we have that $\Psi \circ \Gamma \simeq \mathrm{id}_{|\mathrm{Sd}\ \mathrm{Nrv}(\mathcal{C})|}$, proving the claim. $\square$

3.3 A categorical point of view of the Nerve Theorem

Category theory offers a very interesting perspective to the study of mathematics as it lends itself to the study of general structures shared among different areas of mathematics. In particular, the richness of the Nerve Theorem in TDA can be seen clearly with the tools and concepts defined in the field. We begin with these basic concepts.

Definition 3.19. A ***category*** $\mathbf{C}$[7] consists of the following data:

1. A collection $\mathrm{ob}(\mathbf{C})$ of **objects**.
2. For $A, B \in \mathrm{ob}(\mathbf{C})$ a set $\mathrm{Hom}(A, B)$ of maps, called **morphisms**, from A to B.
3. For each $A \in \mathrm{ob}(\mathbf{C})$ a morphism $id_A : A \longrightarrow A$ called the **A-identity**.
4. For $A, B, C \in \mathrm{ob}(\mathbf{C})$, a **composition law**

$$\begin{aligned} \circ : \mathrm{Hom}(B, C) \times \mathrm{Hom}(A, B) &\longrightarrow \mathrm{Hom}(A, C) \\ (g, f) &\longmapsto (g \circ f) \end{aligned}$$

   Satisfying the following properties

   (a) Associativity: Let $A, B, C, D \in \mathcal{O}$ where $f \in \mathrm{Hom}(A, B)$, $g \in \mathrm{Hom}(B, C)$, $g \in \mathrm{Hom}(C, D)$ such that $(h \circ g) \circ f = h \circ (g \circ f)$

   (b) Object identities act as composition identities: if $f \in \mathrm{Hom}(A, B)$, $f \circ id_A = f = id_B \circ f$

Categories allow a level of generality where most results are applicable to a very diverse class of objects. The expressivity of categories forces mathematicians to shift their focus from particular objects to the structure of their relationships at a very high level.

Example 3.20. Some examples of categories that we have worked with throughout this thesis:

- **Top**: the category of topological spaces with continuous functions and compositions thereof.

[7] This is really the definition of a **localy small category**. This is the only type of categories we will work with in this thesis.

- **Grp**: the category of groups with group homomorphisms and compositions thereof.
- **Set**: the category of sets under set functions and compositions thereof.

A natural question that arises in the study of categories is how to define relationships between them that preserve their structure. A **functor** is precisely the type of "function" that formalizes this intuition.

Definition 3.21. A ***functor*** F between categories $\mathbf{A}, \mathbf{B}$ is a pair of maps where, one of them associates to each object of $\mathbf{A}$ an object of $\mathbf{B}$ and the other associates to each morphism in $\mathbf{A}$ a morphism between the corresponding object images, $\mathrm{Hom}(A, B) \xrightarrow{F} \mathrm{Hom}(F(A), F(B))$, such that:

1. F preserves composition whenever its defined.
2. F preserves identity morphisms.

Example 3.22. The main idea behind functors is to see how certain information is *translated* from one category to another. This does NOT imply that information should be preserved, rather the most interesting insights are those that characterize precisely how information morphs and ends up being represented in the other category. For example, we can define what is called the **forgetful functor** between **Top** and **Set** as a function that assigns to each topological space the underlying set structure of their topology. Then, any continuous function looses its topological information and just becomes a set function.

In the context of the Nerve Theorem, the category in which we are working with is called the **category of covered spaces Cov**. Recall Definition 3.14, in which we introduced the notion of a *covered space* as a pair $(X, \{U_i\}_{i\in I})$ and a *morphism of covered spaces* as a pair of functions $(f, \varphi) : (X, \{U_i\}_{i\in I}) \longrightarrow (Y, \{V_\ell\}_{\ell\in L})$ where f is *carried* by φ. These elements will be the *objects* and *morphisms* of our category **Cov**. Furthermore, Remark 3.15 gives us a well defined *composition law*; the final condition to have a category according to our definition.

The other relevant category for this thesis is the **category of abstract simplicial complexes Simp**. In Definition 2.51 we defined the notion of an *abstract simplicial complex*. These will be the objects of **Simp**. The morphisms of our category are called **simplicial maps**.

Definition 3.23. Let L and K be two abstract simplicial complexes. We say that a map $f : \mathrm{Vert}\ L \longrightarrow \mathrm{Vert}\ K$ is a ***simplicial map*** if for every simplex $\sigma \in L$, $f(\sigma) \in K$.

As we have seen, taking the nerve of a covered space associates an abstract simplicial complex to it. To prove the functoriality of the nerve, we have to check that morphisms of covered spaces induce simplicial maps between the corresponding nerves.

Proof of the functoriality of the nerve. Let $(X, \mathcal{U} = \{U_i\}_{i \in I}), (Y, \mathcal{V} = \{V_j\}_{j \in J})$ be two covered spaces and (f, φ) a morphism of covered spaces. Let, $\varphi(i) = j$. By definition, we have $f(U_i) \subseteq V_j$. Each of the cover elements corresponds to one of the vertices of the nerve, so this gives us a correspondence between vertices given by φ. Thus, the induced map on the nerves is

$$\begin{aligned} \varphi_* : \mathrm{Nrv}(\mathcal{U}) &\longrightarrow \mathrm{Nrv}(\mathcal{V}) \\ v_i &\longmapsto v_j. \end{aligned}$$

Consider the simplex $\sigma \in \mathrm{Nrv}(\mathcal{U})$. Take $U_{i_1}, \ldots, U_{i_k}$ the corresponding cover elements which generate σ on $\mathrm{Nrv}(\mathcal{U})$ and take $V_{j_1}, \ldots, V_{j_w}$ their corresponding cover elements when carried by φ. We have that, $f(U_{i_1} \cap \cdots \cap U_{i_k}) \subseteq V_{j_1} \cap \cdots \cap V_{j_w}$ is non empty, which implies that the simplex $\varphi_*(\sigma) = \sigma'$ exists on $\mathrm{Nrv}(\mathcal{V})$. Then, φ_* is a simplicial map. □

In Definition 2.52, we defined how to associate a topological space to a simplicial complex K called the **geometric realization** of K. We can prove that it is a functor between **Simp** and **Top** by following [8, Lemma 2.7]. This Lemma provides a way to linearly extend a simplicial map to all the points inside the geometric realization of a simplex continuously. Then, each simplicial map induces a continuous function between geometric realizations of simplices. We can now define the functor which enables the homological techniques used in TDA that will be introduced in the next section.

$$\begin{tikzcd} \mathbf{Cov} \arrow[r, "\mathrm{Nrv}"] \arrow[rr, bend right, "|\mathrm{Nrv}|"'] & \mathbf{Simp} \arrow[r, "|\cdot|"] & \mathbf{Top} \end{tikzcd}$$

Figure 7: The geometric realization of the nerve Functor.

The geometric realization of the nerve functor associates to each covered space a geometric simplicial complex which corresponds to the nerve of its cover. By functoriality, any homological calculations carried out on the geometric realization of the nerve preserve the topological information of the original covered space.

4 Homology and Applications

4.1 Homology

Homology is the algebraic tool at the center of TDA. It is a way to associate to a topological space a group in such a way that it captures some of its topological properties. There are many ways to define homology but, for the purposes of this thesis, we will define and work with **simplicial homology** as it is the most well suited type of homology for computational applications. We use [9] and [8] as our main references to introduce these concepts.

Consider a simplicial complex K. Let K_p be the set of all p-simplices in K. We can define an *orientation* on the vertices of a p-simplex $\sigma = [v_0, \ldots, v_p]$ by following the order of the vertices inside the brackets.

To define a group related to our simplicial complex K we will define a the concept of a **free abelian group generated by a basis** S.

Definition 4.1. A ***free abelian group generated by a basis*** S is an abelian group where each element g may be uniquely written as a linear combination of basis elements

$$g = \sum_{s_\alpha \in S} \eta_\alpha s_\alpha$$

where each $\eta_\alpha \in \mathbb{Z}$.[8]

Remark 4.2. We regard the representation of the element g as a *formal sum* where the operation defined on the group is addition over the coefficients of each basis element, just as in vector spaces.

We take the set K_p and define the *group of p-chains* $\mathcal{C}_p(K)$ as the free abelian group generated by all p-simplices in K. In this setting, we consider each simplex as having an orientation as defined earlier. As such, if we have the simplex $\sigma = [v_0, \ldots, v_p]$ then the p-chain represented by $-\sigma = [v_p, \ldots, v_0]$ has the opposite orientation.

As we have seen in previous figures, there exists a relationship between higher dimensional simplices and its lower dimensional counterparts, namely that a subset of the vertices of a p-simplex σ spans a *face* of σ. In particular, a simplex spanned by $p - 1$ vertices of σ is called a *boundary* of σ. We can capture this property algebraically with the **boundary operator**.

[8]For the purposes of this thesis we will use $\mathbb{Z}$ as our coefficient group. Nevertheless, there are theories of homology that use other algebraic structures as coefficients.

Definition 4.3. The ***boundary operator*** $\partial_p : \mathcal{C}_p(K) \longrightarrow \mathcal{C}_{p-1}(K)$ is a group homomorphism where, for each basis element $\sigma_\alpha \in K_p$,

$$\partial_p(\sigma_\alpha) = \sum_{i=0}^{p} (-1)^i \, \sigma_\alpha|_{[v_0,\ldots,\hat{v}_i,\ldots v_p]}$$

This operator captures how the orientation defined on a p-simplex changes when traversing its boundary. The boundary operator satisfies the equation $\partial_p \circ \partial_{p+1} = 0$[9]. This equation implies that Im $\partial_{p+1} \subset$ Ker ∂_p. The algebraic situation we have now is a sequence of homomorphisms of abelian groups called a **chain complex**.

$$\ldots \longrightarrow \mathcal{C}_{p+1}(K) \xrightarrow{\partial_{p+1}} \mathcal{C}_p(K) \xrightarrow{\partial_p} \mathcal{C}_{p-1}(K) \longrightarrow \ldots \longrightarrow \mathcal{C}_1(K) \xrightarrow{\partial_1} \mathcal{C}_0(K) \xrightarrow{\partial_0} 0$$

The elements of Ker ∂_p are called ***p*-cycles**. The set of all ***p*-cycles** of the simplex K is denoted by Z_p. Similarly, an element of Im ∂_{p+1} is called a ***p*-boundary**. The collection of all ***p*-boundaries** is denoted by B_p. By Remark 2.13, Z_p and B_p are normal subgroups of $\mathcal{C}_p(K)$ and thus, the following quotient is well defined.

Definition 4.4. The ***p-th simplicial homology group*** $H_p(K)$ is defined as the quotient

$$H_p(K) = \text{Ker } \partial_p / \text{Im } \partial_{p+1} \;=\; Z_p/B_p$$

In general, applications in TDA use *finite* simplicial complexes. As such, the p-th homology groups for $p \gg 0$ will be the trivial group as there are no simplices which match said dimension that generate a non trivial group. In practice, TDA uses **Betti numbers** which store the homological information of the space in a computationally-friendly manner.

Definition 4.5. The ***p-th Betti number*** is defined as the *rank* of $H_p(K)$, i.e the cardinality of the smallest generating set of the free part of the group $H_p(K)$.

$$\beta_p = \text{rank } H_p(K) = \text{rank } Z_p - \text{rank } B_p$$

As we stated earlier, homology groups capture certain topological properties of the spaces for which they are computed. The following proposition tells us one of the properties that can be identified by homology groups.

Proposition 4.6. *If K is a simplicial complex such that its geometric realization $|K|$ is non-empty and path-connected, then $H_0(K) \cong \mathbb{Z}$, i.e., $\beta_0 = 1$. In general, β_0 counts the number*

[9] A proof of this statement is in [10, Lemma 2.1]

of path connected components of $|K|$[10].

The generators of a homology group $H_p(K)$ correspond to p-cycles that are not boundaries of a $(p+1)$-simplex. These generators must be thought as topological holes of dimension p. Thus, each homology group has a topological interpretation but its significance in TDA is dependent on the context of each application.

The most relevant property of homology, in light of the Nerve Theorem, is the **homotopy invariance of homology groups**. The proof of this property may be found in [10, Corollary 2.11]. This means that spaces that are homotopy equivalent, such as the space X which is the union of the cover elements defined in the preceding subsection and its nerve, have **isomorphic homology groups**[11]. In general, continuous functions between topological spaces induce *homomorphisms* between corresponding homology groups. This implies that homology $H_*(\,\cdot\,) : \mathbf{Top} \longrightarrow \mathbf{Grp}$ is a functor. In the context of TDA, this allows computational methods to work with the nerve of a space, which is usually far simpler than the original topological space, and not lose any homological information in the process.

4.2 Persistent Homology

In 2002, Herbert Edelsbrunner, David Letscher, and Afra Zomorodian introduced in [2] the foundational concept of *persistence*. This paper would later come to define TDA as a research area as their algorithms were efficient enough for applications in a broad range of subjects. Furthemore, the philosophy of persistence became the basis for developing new algorithms in TDA, which are still being researched to this day.

Let $S = \{v_0, v_1, \ldots, v_k\} \subseteq \mathbb{R}^n$ be a finite set of points[12]. The following two objects will let us define a suitable simplicial complex for the points in S. The work of Edelsbrunner in [11] and [12] details the relationship between the following constructions along with other families of objects parametrized by α.

Definition 4.7. A ***Voronoi cell*** of a point p with respect to a point set $S \subseteq \mathbb{R}^n$ is the set

$$V_p = \{x \in \mathbb{R}^n \mid d(x,p) \leq d(x,p_i) \text{ for all } p_i \in S\}.$$

Remark 4.8. The Voronoi cell of a point p is a convex set according to [13]. The collection of all Voronoi cells for the points in a set S is called the **Voronoi diagram** of S.

[10] This is [10, Proposition 2.7] restated in terms of Betti numbers.

[11] Homology groups can be defined for arbitrary topological spaces by looking at simplices mapping continously to the topological space.

[12] The original formulation of persistent homology in [2] was limited to points in $\mathbb{R}^3$. We will work with a generalized version which is entirely analogous to what is presented in the original paper.

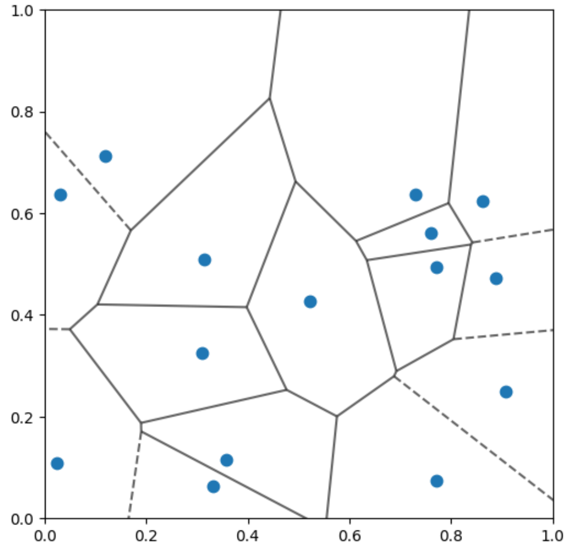

Figure 8: Voronoi diagram for a set of points.

Definition 4.9. Let $B_\alpha(p)$ be the closed ball of radius α with center at $p \in S$. The ***α-complex of** S* is the simplicial complex whose simplices are given by the finite subsets $J \subseteq S$ such that

$$\bigcap_{p \in J} (V_p \cap B_\alpha(p)) \neq \varnothing.$$

Remark 4.10. An α-complex is precisely the nerve of the cover given by $\{V_p \cap B_\alpha(p)\}_{p \in S}$.

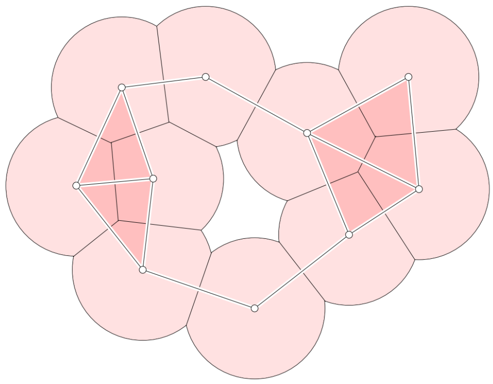

Figure 9: Example of an α-complex of a set of closed balls covering the points of S. Taken from [11, Figure III.15].

Persistent homology studies the evolution of an α-complex as the parameter α changes.

Let α_0, α_1 be some arbitrary value for the parameter α such that $\alpha_0 \leq \alpha_1$. Let K_{α_0} and K_{α_1} be their respective alpha complexes. Then, $K_{\alpha_0} \subseteq K_{\alpha_1}$. As the parameter α grows, the induced α-complexes define a **filtration**. When $\alpha = \infty$, i.e taking $B_\alpha(p) = \mathbb{R}^n$, the resulting α-complex is called the **Delaunay complex** $\mathcal{D}$. This complex is defined as the nerve of the Voronoi diagram of the set of points S. As the Delaunay complex is a finite simplicial complex, there exists a *finite* set of values $A = \{\alpha_0, \ldots, \alpha_k\}$, where their corresponding α-complexes are unique in the filtration. For $\alpha = 0$, let $K_\alpha = \varnothing$. As such, the filtration induced on the Delaunay complex by changing the parameter α is

$$\varnothing \subset K_{\alpha_0} \subset K_{\alpha_1} \subset \cdots \subset K_{\alpha_{k-1}} \subset K_{\alpha_k} = \mathcal{D}.$$

We say that a simplex σ is *born* at the time α_i if it is not in the image of the inclusion $\iota : K_{\alpha_{i-1}} \longhookrightarrow K_{\alpha_i}$[13].

Remark 4.11. If any two simplices are born at the same time, we order them according to their dimension. If they have the same dimension, they are ordered arbitrarily.

To understand how homology classes evolve as α changes in the filtration we introduce **persistent homology groups** using the notation in [2].

Definition 4.12. The ***p-persistent k-th homology group of*** $\boldsymbol{K_{\alpha_\ell}}$ is the group defined by the quotient

$$H_k^{\alpha_\ell, p} = Z_k^{\alpha_\ell} \Big/ (B_k^{\alpha_{\ell+p}} \cap Z_k^{\alpha_\ell}) \ .$$

Where, $Z_k^{\alpha_\ell}$ corresponds to the *k-cycles* of the simplicial complex K_{α_ℓ} and $B_k^{\alpha_{\ell+p}}$ corresponds to the *k-boundaries* of the simplicial complex $K_{\alpha_{\ell+p}}$.

We can define the notion of a ***p*-persistent k-th Betti number** $\beta_k^{\alpha_\ell, p}$ as the rank of the group $H_k^{\alpha_\ell, p}$. Persistent homology groups allows us to track the behavior of individual simplices across different time scales in the filtration. In general, if a k-simplex σ is born at a time α_i it means that it becomes a generator of $H_k(K_{\alpha_i})$. We say that σ dies at a time α_j if in the homomorphism induced by the inclusion on homology groups $\iota_* : H_k(K_{\alpha_i}) \longhookrightarrow H_k(K_{\alpha_j})$, $\iota_*(\sigma) = 0$. Equivalently, σ generates a homology class for the groups $H_k^{\alpha_i, \alpha_w}$ with $\alpha_i < \alpha_w < \alpha_j$. Precisely in K_{α_j}, a simplex σ' such that $\partial(\sigma') = \sigma$ must appear. The **persistence** of σ is defined as $\alpha_j - \alpha_i - 1$. Simplices which generate homology classes in $H_k(\mathcal{D})$ are said to have infinite persistence.

[13]This definition comes from [14] and is particularly interesting when we study how the inclusion in the filtration induces maps in homology groups.

Persistent homology is useful to filter out noise in data and to precisely take into account the data which generates topological information in the latent topological space where the data come from. In practice, topological features which correspond to small persistence values are discarded and only topological features with a large persistence are considered to be *true*.

4.3 Applications in Binary Classification problems

In this last section we will focus on how the Nerve Theorem, TDA and persistent homology are being used in problems derived from **supervised machine learning**. In particular, we will focus on **binary classification problems** where, given a labeled set $X = \{(z_1, c_1), \dots, (z_k, c_k)\}$ where each $z_i \in \mathbb{R}^n$ is called a *data point* and each $c_i \in \{0, 1\}$ corresponds to a label[14], we need to train a model to predict a surface which will partition the ambient space in such a way that the members of each class are separated in the most accurate way possible.

Ramamurthy, Varshney and Mody proposed in [1] a novel application of the seminal work done by Niyogi, Smale and Weinberger in [15] to estimate with high confidence the homology of the decision boundary manifold of a binary classification problem. We will briefly present the main ideas in [1]. There are a few concepts from *differential topology* that will be needed[15].

Definition 4.13. We say that a function $f : U \subset \mathbb{R}^n \longrightarrow \mathbb{R}^m$ is ***smooth*** if it has continous partial derivatives of all orders.

Definition 4.14. A smooth map $f : X \longrightarrow Y$ of subsets of two Euclidean spaces is said to be a ***diffeomorphism*** if it is a bijection whose inverse $f^{-1} : Y \longrightarrow X$ is also smooth.

Definition 4.15. A subset $X \subseteq \mathbb{R}^N$ is said to be a ***k-dimensional manifold*** if for each point $x \in X$ we have a neighborhood V of x such that V is diffeomorphic to an open set $U \subseteq \mathbb{R}^k$.

We assume that each of the classes has an associated probability density function p_X for $c_i = 1$ and p_Y for $c_i = 0$. These distributions depend on an indicator random variable that follows a Bernoulli distribution (i.e, being of class $c_i = 1$ has a probability of q and being of class $c_i = 0$ a probability of $1 - q$). If we assume that a given point z is of class c_i then, the probability of that event follows its corresponding distribution specified above. By the law of total probability, the space as a whole has an associated probability density function given by

$$p_Z(z) = p_X(z) \cdot q + p_Y(z) \cdot (1 - q).$$

[14] All the points with a label c_i are said to be the members of the *class* c_i.
[15] All of the details may be found on [16].

We define the decision boundary manifold $\mathcal{M} = \{z \in \mathbb{R}^n \mid p_X(z) = p_Y(z)\}$ as the points which have the same probability of being from either class. We also define the set $\mathcal{D} = \{z \in \mathbb{R}^n \mid p_X(z) > 0,\, p_Y(z) > 0\}$ which corresponds to the set where both distributions have some mass.

One of the contributions of [1] is the introduction of the **labeled Čech complex**.

Definition 4.16. An ***(ε, γ)-labeled Čech complex***, (ε, γ)-LČ complex, is a simplicial complex with a collection of simplices such that each simplex σ is formed on the points in the set S aided by the reference set W, when the following conditions are satisfied:

1. $\bigcap_{s_i \in \sigma} B(s_i, \varepsilon) \neq \varnothing$, where s_i are the vertices of σ.
2. For each $s_i \in \sigma$ there exists $w \in W$ such that $d(s_i, w) \leq \gamma$.

This variation of an Čech complex takes into account the labeling of the data by choosing the data points in S to be elements of one class and the elements of W to be from the other class. The first condition is simply the definition of the ε-Čech complex while the second condition forces the elements of the other class to be γ-*dense* on the simplices of the complex. Therefore, this new complex is suitable to represent a simplicial complex of the decision boundary of our original classification problem. The following Lemma guarantees that we can define a filtration on the (ε, γ)-LČ complex to calculate its persistent homology.

Lemma 4.17. *As ε varies from 0 to ∞, a filtration is induced on the (ε, γ)-LČ complex for a fixed γ.*

Proof of Lemma 4.17. Fixing γ, we choose $S_\gamma \subseteq S$, such that W is γ-dense in S_γ. Therefore, the (ε, γ)-LČ complex on S is equivalent to an ε-Čech complex on S_γ. Thus, varying ε induces a filtration on the (ε, γ)-LČ complex. □

[1, Theorem 3] provides the conditions for the (ε, γ)-LČ complex of a sample of points to be homotopic to $\mathcal{M}$. It requires the following assumptions about the distributions of both classes in $\mathbb{R}^n$. We are going to defer the explanation of some concepts from *differential topology* to Appendix B to preserve readability.

First, we assume that $\mathcal{M}$ has a condition number $1/\tau$. This means we can define a tubular neighborhood $\mathrm{Tub}_\tau(\mathcal{M})$ around $\mathcal{M}$ in such a way that any manifold in this region is homotopic to $\mathcal{M}$ via the projection map given by the normal bundle of $\mathcal{M}$. We also assume that the set of points where both distributions have mass $\mathcal{D}$ is contained in a tubular neighborhood of radius r around $\mathcal{M}$, i.e, $\mathcal{D} \subset \mathrm{Tub}_r(\mathcal{M})$. This will allow us to focus our study on the boundary manifold and not lose any relevant topological information in the process. The last condition defines a technical requirement for the measures μ_{c_i} derived from the probability distributions for each class. For every $0 < s < r$, the mass around a point p in $\mathcal{M}$ is at least $k_s^{(c_i)}$ for the class c_i. This means that, in the decision boundary, there are no isolated regions where only elements of one class can be found.

Theorem 4.18. *[1, Theorem 3]. Let $N_{r/2}$ and $N_{s/2}$ be the $r/2$ and $s/2$ covering numbers of the submanifold $\mathcal{M}$ of $\mathbb{R}^n$. Let $\bar{z}$ be generated by identically distributed independent sampling from the probability distribution p_Z whose two component measures satisfy the constraint of minimum mass stated earlier and have mixing probabilities q and $1-q$ for $q > 0$. Let the two component samples be $\bar{x}$ and $\bar{y}$. Then if*

$$|\bar{z}| > \max\left(\frac{1}{qk_{r/2}^{(0)}}\left(\log\left(2N_{r/2}\right) + \log\left(\frac{1}{\delta}\right)\right), \frac{1}{(1-q)k_{s/2}^{(0)}}\left(\log\left(2N_{s/2}\right) + \log\left(\frac{1}{\delta}\right)\right)\right),$$

with probability greater than $1-\delta$, the $(\varepsilon, r+s)$-LČ complex will be homotopy equivalent to $\mathcal{M}$ if:

(a) $r < (\sqrt{9} - \sqrt{8})\tau$

(b) $\varepsilon \in \left(\frac{(r+\tau)-\sqrt{r^2+\tau^2-6\tau r}}{2}, \frac{(r+\tau)+\sqrt{r^2+\tau^2-6\tau r}}{2}\right)$.

This lower bound on the number of samples we have to take is a very strong result on the homotopy type of the resulting $(\varepsilon, r+s)$-LČ complex. From the Nerve Theorem we know that this complex has the same homotopy type as the union of open balls of radius ε centered at the sampled data points. It was impossible to know if the cover derived from these sampled points reconstructed the latent manifold $\mathcal{M}$ in such a way that homological information is preserved. Indeed, Theorem 4.18 ensures that this is the case, provided we have enough samples. However, the explicit computation of this lower bound incorporates topological information about the manifold $\mathcal{M}$ that, *a priori*, can't be obtained from the data. Still, this result provides a robust mathematical justification for the constructions the authors introduce to deal with labeled data in the decision boundary computationally.

5 Conclusions

Throughout this thesis it has been shown how the mathematical foundations of TDA allows these methods to revolutionize each subject in which they are used. Although TDA has an applied nature it never lacks the rigor and elegance that characterizes its birthplace in Algebraic Topology. We have seen a proof of the Nerve Theorem for convex and compact covers which serves as the backbone for the algorithms of TDA. Homology and persistent homology were introduced as the main tool which extracts topological properties from data points and quantifies them to be used in data analysis of all kinds. Finally, all of these concepts collide in a central result of the sample complexity to reconstruct the homology of the decision boundary in binary classification problems. This result aims to guarantee a precise reconstruction of the homology of the decision boundary manifold that will allow users to assess the models performance.

The full potential of the methods described in this thesis has yet to be explored at its fullest. The power of TDA lies in its capacity to describe topological features of complex objects. They are becoming more relevant to study neural networks as in [17], where the authors proved upper and lower bounds on neural network complexity to quantify their ability to approximate high complexity functions. Results like this hint at a possible explanation on the success of neural networks in a wide range of applications. Coupled with the complexity results given by [1], the study of how topological information is handled by machine learning and deep learning methods appears to be an area that deserves further research.

Appendix A: Proof of Proposition 3.18

Proof of Proposition 3.18. We will prove the proposition by induction on the dimension of the skeleton of K. Let $I = [0, 1]$ denote the unit interval. For the base case, take $m = 0$ and consider the 0-skeleton $\operatorname{sk}_0 K$. Let $p \in \operatorname{sk}_0 K$ and take $W = \{i_1, i_2, \ldots, i_k\} \subseteq [n]$ to be the indices corresponding to the cover elements $\{|L_w|\}_{w\in W}$ where $|p| \in |L_w|$. By assumption, both $f(|p|)$ and $g(|p|)$ are contained in $S := \cap_{l=0}^{k} V_{\varphi(i_l)}$ which is contractible. We define the homotopy T^0 by contracting the set S and choosing a path between these two points. We now need to verify that the homotopy T^0 is carried by the induced map φ restricted to the cover elements for the 0-skeleton. Let $(|p|, t) \in |p| \times I$ be a point. If $(|p|, t) \in |L_i| \times I$, then $i = i_\ell$ is an index frow W. Thus, by construction, $T^0((|p|, t)) \in S \subseteq V_{\varphi(i_\ell)} = V_{\varphi(i)}$.

For the induction step, suppose we have the homotopy between $f|_{|\operatorname{sk}_{m-1} K|}$ and $g|_{|\operatorname{sk}_{m-1} K|}$ $T^{m-1} : |\operatorname{sk}_{m-1} K| \times I \longrightarrow Y$ carried by the restriction of φ as described before. Let σ be an m-simplex in $\operatorname{sk}_m K$. Let $i_0, \ldots, i_w \in [n]$ be those indices i such that $\sigma \in L_i$. By the induction hypothesis, we have

$$T^{m-1}(|\partial\sigma| \times I) \subseteq S := \bigcap_{\ell=0}^{k} V_{\varphi(i_\ell)}$$

As the cover $\{V_j\}_{j\in J}$ is good, the space S is contractible. Hence, we can extend the homotopy $T^{m-1}|_{|\partial\sigma|\times I}$ to a homotopy $T^m|_{|\sigma|\times I}$, following the diagram, as the pair $(|\sigma|, |\partial\sigma|)$ is a CW pair[16].

$$\begin{tikzcd}
(|\partial\sigma| \times I) \cup (|\sigma| \times \{0\}) \arrow[r, hook] \arrow[dr, dotted, "T^m"'] & (|\sigma| \times I) \arrow[d, "T^{m-1}"] \\
 & S
\end{tikzcd}$$

Note that the simplex σ is arbitrary, we can fully extend the homotopy T^{m-1} to the homotopy $T^m : |\operatorname{sk}_m K| \times I \longrightarrow Y$. Finally, we must verify that the homotopy T^m is carried by φ. By the induction hypothesis, we already have this condition for all $x \in |\operatorname{sk}_{m-1} L_i|$. Then, we must show the claim for the points x in the *interior* of an arbitrary m-simplex $\sigma \in L_i$. As such, $i = i_\ell$ is one of the indices above and, by construction, we have

$$T^m(x, t) \in T^m(|\sigma| \times I) \subseteq S \subseteq V_{\varphi(i_\ell)} = V_{\varphi(i)}$$

proving that the extension of the homotopy is also carried by φ. $\square$

[16]Following [10, Proposition 0.16].

Appendix B: Concepts from Differential Topology

Recall Definition 4.15 where a differential structure was given to a topological space. Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ be a smooth function. We denote the derivative of f in the direction $h \in \mathbb{R}^n$ at the point x as $df_x(h)$. Let X be a k dimensional manifold in $\mathbb{R}^N$ and $\phi : \mathbb{R}^k \supseteq U \longrightarrow X$ be a parametrization of the points around $x \in X$. Letting $\phi(0) = x$, we can define the **tangent space** of X at x as the image of the map $d\phi_0 : \mathbb{R}^k \longrightarrow \mathbb{R}^N$, denoted by $T_x(X)$. A *tangent vector* to X at x is just a vector $v \in T_x(X)$. As the derivative is a linear map, we may imagine $T_x(X)$ as the space that linearly approximates the points near $x \in X$.

In general, tangent spaces at various points of X may overlap one another thus preventing us to define a useful structure on the set of all tangent spaces. Precisely the **tangent bundle** will be the object that can group the tangent spaces and allow a manifold structure to be defined over them.

Definition B.1. The ***tangent bundle*** $T(X)$ of a manifold X in $\mathbb{R}^N$ is the set

$$T(X) = \{(x, v) \in X \times \mathbb{R}^N \mid v \in T_x(X)\}.$$

$T(X)$ contains a copy X_0 of X consisting of the points $(x, 0)$. As each vector is perpendicular to the 0 vector, we have that each copy of $T_x(X)$ is perpendicular to X_0. The properties of the resulting manifold of the tangent bundle are dependent on the original manifold X as, for example, $\dim T(X) = 2 \dim X$.

A related concept is that of the **normal space**. For each $x \in X$, the normal space of X at x, denoted by $N_x(X)$ is the orthogonal complement of $T_x(X)$ in $\mathbb{R}^N$.

Definition B.2. The ***normal bundle*** $N(X)$ of a manifold X in $\mathbb{R}^N$ is the set

$$N(X) = \{(x, v) \in X \times \mathbb{R}^N \mid v \in N_x(X)\}.$$

As before, the normal bundle is also a manifold but, unlike the tangent bundle, its dimension is dependent on the *ambient space* as $\dim X = N$. Most importantly, each bundle comes equipped with its own *projection map*. Notably, the projection map

$$\begin{aligned} \pi : N(X) &\longrightarrow X \\ (x, v) &\longmapsto x \end{aligned}$$

is what is called a *submersion*, which will be defined later in this section.

Smooth functions between manifolds induce functions with specific properties between tangent spaces. Let $f : X \longrightarrow Y$ be a smooth function between two manifolds X and Y. The behavior of df_x at each $x \in X$ defines fundamental properties of the original function. If $df_x : T_x(X) \longrightarrow T_{f(x)}(Y)$ is an isomorphism, the *Inverse Function Theorem*[17] states that f is a local diffeomorphism. This assumes that both manifolds have the same dimension. If we relax those conditions and assume that dim $X \leq$ dim Y, we can only demand that df_x be injective. If so, we say that f is an **immersion**. In general, we may think of the local behavior of an immersion as just the standard inclusion map of $\mathbb{R}^k \hookrightarrow \mathbb{R}^l$ where $k \leq l$ because of the *Local Immersion Theorem*[18].

We wish that immersions respect the manifold structure of X but, in general, the image of an immersion is not a manifold in itself. We say that a function $f : X \longrightarrow Y$ is *proper* if the preimage of any compact set in Y is compact in X. If an immersion f is injective and proper we say that f is an **embedding**. Embeddings provide a convenient way to study how manifolds behave inside of an ambient space as they map diffeomorphically X onto a submanifold of Y. Finally, if dim $X \geq$ dim Y the strongest condition we can impose on df_x is surjectivity. If df_x is surjective, f is called a **submersion** at x. If f is a submersion at every point it is simply called a submersion. As it is the case with immersions, we can picture a submersion as the standard projection of $\mathbb{R}^k$ onto $\mathbb{R}^l$ where $k \geq l$ which is, locally, the canonical submersion by the *Local Submersion Theorem*[19].

There is a way to embed $N(X)$ inside an open neighborhood of the manifold X. This is done with the **Tubular Neighborhood Theorem**.

Theorem B.3 (Tubular Neighborhood Theorem)**.** *Let $X \subset M$ be a manifold. Then there exists a diffeomorphism from an open neighborhood of X in $N(X)$ onto an open neighborhood of X in M.*

We say that this is a *tubular* neighborhood as the normal vectors around the manifold are orthogonal to it and as such, may be seen as the radius of a tube going *around* the manifold. Following this idea, what the authors of [15] call the **condition number** $1/\tau$ of a manifold X is defined as the largest numbers which satisfies the following property. The open normal bundle about X of radius r is embedded in $\mathbb{R}^N$ for every $r < \tau$. Its image Tub_τ is a tubular neighborhood of X with its canonical projection map $\pi_0 : \text{Tub}_\tau \longrightarrow X$.

[17] This theorem may be found in [16, Section 1.3].
[18] Ibid.
[19] Details in [16, Section 1.4].

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