

A DESIGNER KNOWS THAT HE HAS ACHIEVED PERFECTION NOT WHEN THERE
IS NOTHING LEFT TO ADD, BUT WHEN THERE IS NOTHING LEFT TO TAKE
AWAY.

ANTOINE DE SAINT-EXUPÉRY

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A BASIC AND CONCISE
INTRODUCTION
TO TOPOLOGICAL
DATA ANALYSIS

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Introduction

In these lecture notes, we will illustrate some basic concepts in topological data analysis. To do so, we must first introduce the notions of abstract and geometric simplicial complexes and their main properties, and describe how simplicial complexes can be associated with point clouds in Euclidean space, in order to geometrically structure the information represented by such clouds. We will then introduce simplicial homology with coefficients in $\mathbb{Z}_2$ and use it to study the qualitative properties of the previously defined simplicial complexes. This will allow us to introduce some elementary concepts in Topological Data Analysis, based on the material presented in the first part of these notes. Specifically, we will present the concept of persistence diagrams and their applications to shape description. At the conclusion of the course, we will show how the invariance of persistence diagrams can be refined using Group Equivariant Non-Expansive Operators (GENEOs). The use of GENEOs in Machine Learning will also be briefly illustrated. The course will prioritize practical applications over theoretical aspects, often citing results without formal proofs. The main reference is the book [Herbert Edelsbrunner and John Harer (2010)]¹. For the sake of completeness, these notes contain much more material than will actually be used in the course. The course requires knowledge of basic concepts in algebra and linear algebra.

¹ Herbert Edelsbrunner and John Harer. *Computational Topology - an Introduction*. American Mathematical Society, 2010. ISBN 978-0-8218-4925-5. URL <http://www.ams.org/bookstore-getitem/item=MBK-69>

Finite Simplicial Complexes

Finite Geometric Simplicial Complexes

Definition 1. Let $u_0, \dots, u_k \in \mathbb{R}^d$ and $\lambda_0, \dots, \lambda_k \in \mathbb{R}$, with $\sum_{i=0}^k \lambda_i = 1$. The point $p = \sum_{i=0}^k \lambda_i u_i$ is called an **affine combination** of $u_0, \dots, u_k$ with coefficients $\lambda_0, \dots, \lambda_k \in \mathbb{R}$.

Definition 2. The set of all affine combinations of the points $u_0, \dots, u_k \in \mathbb{R}^d$ is called the **affine hull** of $u_0, \dots, u_k$.

Definition 3. The points $u_0, \dots, u_k \in \mathbb{R}^d$ are called **affinely independent** if this implication holds for $(\lambda_0, \dots, \lambda_k), (\mu_0, \dots, \mu_k) \in \mathbb{R}^{k+1}$: $\sum_{i=0}^k \lambda_i = \sum_{i=0}^k \mu_i = 1 \wedge \sum_{i=0}^k \lambda_i u_i = \sum_{i=0}^k \mu_i u_i \implies \lambda_i = \mu_i$ for every index i . If the points $u_0, \dots, u_k \in \mathbb{R}^d$ are not affinely independent, then they are called **affinely dependent**.

Remark 1. It is trivial to check that the definition of affinely independent points does not depend on the ordering of the points.

Proposition 1. The points $u_0, \dots, u_k \in \mathbb{R}^d$ are affinely independent if and only if the vectors $u_1 - u_0, \dots, u_k - u_0$ are linearly independent.

Proof. $\implies$) From the equality $\sum_{i=1}^k \lambda_i (u_i - u_0) = \mathbf{0}$ it follows that $u_0 + \sum_{i=1}^k \lambda_i (u_i - u_0) = u_0$. Hence $(1 - \sum_{i=1}^k \lambda_i) u_0 + \lambda_1 u_1 + \dots + \lambda_k u_k = 1 u_0 + 0 u_1 + \dots + 0 u_k$. Since $u_0, \dots, u_k$ are affinely independent, $\lambda_1 = \dots = \lambda_k = 0$. Therefore, the vectors $u_1 - u_0, \dots, u_k - u_0$ are linearly independent.

$\Leftarrow$) Let us assume $\sum_{i=0}^k \lambda_i u_i = \sum_{i=0}^k \mu_i u_i$ with $\sum_{i=0}^k \lambda_i = \sum_{i=0}^k \mu_i = 1$. Then, $(\sum_{i=0}^k \lambda_i u_i) - u_0 = (\sum_{i=0}^k \mu_i u_i) - u_0$. Since $\sum_{i=0}^k \lambda_i = \sum_{i=0}^k \mu_i = 1$, it follows that $\sum_{i=0}^k \lambda_i u_i - \sum_{i=0}^k \lambda_i u_0 = \sum_{i=0}^k \mu_i u_i - \sum_{i=0}^k \mu_i u_0$, so that $\sum_{i=1}^k \lambda_i (u_i - u_0) = \sum_{i=1}^k \mu_i (u_i - u_0)$. Since the vectors $u_1 - u_0, \dots, u_k - u_0$ are linearly independent, we have that $\lambda_1 = \mu_1, \dots, \lambda_k = \mu_k$. From the equality $\sum_{i=0}^k \lambda_i = \sum_{i=0}^k \mu_i = 1$, it follows that $\lambda_0 = \mu_0$. Therefore, the points $u_0, \dots, u_k$ are affinely independent.

□

Before proceeding, we recall these two definitions:

- A **convex** subset of a vector space X is a subset S of X such that

$$x_1, x_2 \in S, t \in [0, 1] \implies (1 - t)x_1 + tx_2 \in S.$$

- A **compact** subset of $\mathbb{R}^n$ (or a space Y homeomorphic to $\mathbb{R}^n$) is a closed and bounded subset of $\mathbb{R}^n$ (or Y). We recall that each compact set $C \subseteq Y$ has this property: if $\{U_i\}_{i \in I}$ is an infinite family of open subsets of Y such that $C \subseteq \bigcup_{i \in I} U_i$, then a finite subfamily $\{U_{i_1}, \dots, U_{i_n}\}$ exists, such that $C \subseteq \bigcup_{r=1}^n U_{i_r}$.

Corollary 1. *The points $u_0, \dots, u_k \in \mathbb{R}^d$ are affinely dependent if and only if there exists an affine space of dimension $k - 1$ that contains them.*

Proof. It immediately follows from Proposition 1, by observing that the smallest affine space containing $u_0, \dots, u_k$ has the dimension of the vector space generated by the vectors $u_1 - u_0, \dots, u_k - u_0$, since any point in such a space can be represented as $u_0 + \sum_{i=1}^k \lambda_i (u_i - u_0)$ for suitable values of $\lambda_1, \dots, \lambda_k$. $\square$

Definition 4. Each affine combination $p = \sum_{i=0}^k \lambda_i u_i$ with nonnegative coefficients is called a **convex combination** of $u_0, \dots, u_k$.

Definition 5. If $U \subseteq \mathbb{R}^d$, the set $\text{conv } U$ of all convex combinations of points of U is called the **convex hull** of U . If $U = \{u_0, \dots, u_k\}$, we will often write $\langle u_0, \dots, u_k \rangle$ in place of $\text{conv } U$.

Exercise 1. Prove that $\langle u_0, \dots, u_k \rangle$ is the smallest convex set containing $u_0, \dots, u_k$.

Definition 6. The convex hull σ of $k + 1$ affinely independent points is called a **geometric k -simplex**. The number k is called the **dimension of the geometric simplex σ** .

We say that the empty set is the unique -1 -simplex. In this text, with abuse of notation, we will often denote the 0 -simplex $\{u\}$ by u .

Exercise 2. Prove that each simplex is compact and convex.

Definition 7. If $\sigma = \langle u_0, \dots, u_k \rangle$ is a simplex, the convex hull of any subset of $\{u_0, \dots, u_k\}$ is called a **face** of σ . If τ is a face of σ we write $\tau \leq \sigma$ (or $\sigma \geq \tau$). If $\tau \leq \sigma$ and $\tau \neq \sigma$, we say that τ is a **proper face** of σ and write $\tau < \sigma$ (or $\sigma > \tau$). If τ is a (proper) face of σ , we say that σ is a (proper) **coface** of τ .

NB: The empty set is a face of any simplex.

Definition 8. The (set) boundary $\text{bd } \sigma$ of a simplex σ is the union of all proper faces of σ . The interior $\text{int } \sigma$ of σ is the set $\sigma \setminus \text{bd } \sigma$.

Definition 9. A (finite) **geometric simplicial complex** is a finite set $K \neq \{\emptyset\}$ of simplexes such that

1. if $\sigma \in K$ and $\tau \leq \sigma$, then $\tau \in K$;
2. if $\sigma_1, \sigma_2 \in K$, then $\sigma_1 \cap \sigma_2 \leq \sigma_1$ and $\sigma_1 \cap \sigma_2 \leq \sigma_2$.

The **dimension of a geometric simplicial complex** is the maximum dimension of any of its simplexes.

Definition 10. The **body** $|K|$ of a geometric simplicial complex K is the union of all simplexes in K , endowed with the topology induced by the Euclidean topology in $\mathbb{R}^d$.

Exercise 3. Prove that the body of each geometric simplicial complex is compact.

Definition 11. Let K be a geometric simplicial complex. Every geometric simplicial complex L such that $L \subseteq K$ is called a **subcomplex** of K .

Definition 12. Let K be a geometric simplicial complex. Its subcomplex $K^{(j)} := \{\sigma \in K : \dim \sigma \leq j\}$ is called the **j -skeleton** of K . $K^{(0)}$ is called the **vertex set** of K and denoted by the symbol $\text{Vert } K$.

Finite Abstract Simplicial Complexes

Definition 13. A (finite) **abstract simplicial complex** is a finite family $A \neq \{\emptyset\}$ of sets such that if $\alpha \in A$ and $\beta \subseteq \alpha$ then $\beta \in A$. Each element of an abstract simplicial complex is called an **abstract simplex**. The **dimension of an abstract simplex** $\alpha \in A$ is $\text{card } \alpha - 1$. The **dimension of an abstract simplicial complex** A is the value $\max\{\dim \alpha : \alpha \in A\}$. Any (proper) subset of $\alpha \in A$ is called a (proper) **face** of α . The union of the abstract simplexes of A is called the **vertex set** of A , and denoted by the symbol $\text{Vert } A$.

Exercise 4. Prove that each abstract simplex is a finite set.

Definition 14. Let A be an abstract simplicial complex. Every abstract simplicial complex B such that $B \subseteq A$ is called a **subcomplex** of A .

Definition 15. Two abstract simplicial complexes A, B are **isomorphic** if there exists a bijection $\varphi : \text{Vert } A \rightarrow \text{Vert } B$ such that $\alpha \in A$ implies that $\varphi(\alpha) := \{\varphi(a) : a \in \alpha\} \in B$ and $\beta \in B$ implies that $\varphi^{-1}(\beta) := \{\varphi^{-1}(b) : b \in \beta\} \in A$. The map $\bar{\varphi} : A \rightarrow B$ induced by the map φ is called an **isomorphism** between the abstract simplicial complexes A, B .

Proposition 2. Let K be a geometric simplicial complex. Let $\text{Ab}(K)$ be the set whose elements are the subsets $\{u_0, \dots, u_k\}$ of $\text{Vert } K$ such that $\langle u_0, \dots, u_k \rangle \in K$. Then $\text{Ab}(K)$ is an abstract simplicial complex, and is called the **vertex scheme** of K .

Proof. Trivial. □

Geometric realizations of Abstract Simplicial Complexes

Definition 16. Let K be a geometric simplicial complex. If an abstract simplicial complex B is isomorphic to $\text{Ab}(K)$, then K is called a **geometric realization** of B .

Geometric Realization Theorem

Theorem 1 (Geometric Realization Theorem). Every abstract simplicial complex A of dimension d has a geometric realization in $\mathbb{R}^{2d+1}$.

Proof. First of all, let us prove that for every set $\{a_0, \dots, a_{k-1}\}$ a map $f : \{a_0, \dots, a_{k-1}\} \rightarrow \mathbb{R}^{2d+1}$ exists, such that the following property holds: (*) if $S \subseteq \{a_0, \dots, a_{k-1}\}$ and $\text{card } S \leq 2d + 2$, then the points in $f(S)$ are affinely independent. If (*) holds, we say that f is a **good embedding map** for $\{a_0, \dots, a_{k-1}\}$. We observe that f is injective.

Let us prove (*) by induction on the cardinality k . The statement is trivial for $k \leq 2d + 2$, since we can consider the map $f : \{a_0, \dots, a_{k-1}\} \rightarrow \mathbb{R}^{2d+1}$ taking a_0 to $\mathbf{0}$ and each other point a_i to e_i , where $e_1, \dots, e_{2d+1}$ is the canonical basis of $\mathbb{R}^{2d+1}$. Let us now assume that the statement is true for $k = n \geq 2d + 2$, and prove that it is also true for $k = n + 1$. Therefore, assume that $k = n + 1$, and consider the set $\{a_0, \dots, a_{k-1}\} = \{a_0, \dots, a_n\}$. Let us now build a good embedding map f' for $\{a_0, \dots, a_{n-1}\}$ and denote by C the set given by the union of the affine $2d$ -dimensional subspaces of $\mathbb{R}^{2d+1}$ that contain at least (but in fact exactly) $2d + 1$ points of $f'(\{a_0, \dots, a_{n-1}\})$. We observe that set of these subspaces is finite. Therefore, C is a proper subset of $\mathbb{R}^{2d+1}$, and hence there exists a $w \in \mathbb{R}^{2d+1} \setminus C$. Let us take the map $f : \{a_0, \dots, a_n\} \rightarrow \mathbb{R}^{2d+1}$ that extends f' and is defined by setting $f(a_n) = w$. We claim that f is a good embedding map for $\{a_0, \dots, a_n\}$. If this were not true, a subset S of $\{a_0, \dots, a_n\}$ would exist, such that $\text{card } S \leq 2d + 2$ and $f(S)$ is an affinely dependent set. Up to a possible extension of S , we can assume that $S = \{a_{i_0}, \dots, a_{i_{2d+1}}\}$. Then, because of Corollary 1, there exists a $2d$ -dimensional affine subspace containing the points $f(a_{i_0}) = f'(a_{i_0}), \dots, f(a_{i_{2d}}) = f'(a_{i_{2d}})$ and the point $f(a_{i_{2d+1}}) = w$, against the assumption $w \in \mathbb{R}^{2d+1} \setminus C$.

Therefore, (*) holds for $k = n + 1$. This concludes the proof of (*) by induction.

Let us now consider a good embedding map f for A , and the set K of all the convex hulls of the sets $f(\alpha)$ for $\alpha \in A$. We have to prove that 1) K is a geometric simplicial complex and 2) $\text{Ab}(K)$ is isomorphic to A . Let us now prove these two statements.

- 1) Let $\sigma_1, \sigma_2 \in K$. The definition of K implies that $\alpha_1, \alpha_2 \in A$ exist, such that σ_1 is the convex hull of $f(\alpha_1)$ and σ_2 is the convex hull of

$f(\alpha_2)$. If $x \in \sigma_1 \cap \sigma_2$, we can write

$$x = \sum_{a_i \in \alpha_1 \cap \alpha_2} \lambda_i f(a_i) + \sum_{a_j \in \alpha_1 \setminus \alpha_2} \lambda_j f(a_j)$$

and

$$x = \sum_{a_i \in \alpha_1 \cap \alpha_2} \mu_i f(a_i) + \sum_{a_h \in \alpha_2 \setminus \alpha_1} \mu_h f(a_h)$$

where all coefficients are nonnegative and

$$\sum_{a_i \in \alpha_1 \cap \alpha_2} \lambda_i + \sum_{a_j \in \alpha_1 \setminus \alpha_2} \lambda_j = \sum_{a_i \in \alpha_1 \cap \alpha_2} \mu_i + \sum_{a_h \in \alpha_2 \setminus \alpha_1} \mu_h = 1.$$

It follows that

$$\begin{aligned} & \sum_{a_i \in \alpha_1 \cap \alpha_2} \lambda_i f(a_i) + \sum_{a_j \in \alpha_1 \setminus \alpha_2} \lambda_j f(a_j) + \sum_{a_h \in \alpha_2 \setminus \alpha_1} 0 f(a_h) \\ = & \sum_{a_i \in \alpha_1 \cap \alpha_2} \mu_i f(a_i) + \sum_{a_j \in \alpha_1 \setminus \alpha_2} 0 f(a_j) + \sum_{a_h \in \alpha_2 \setminus \alpha_1} \mu_h f(a_h). \end{aligned}$$

Since $\text{card } \alpha_1 \cup \alpha_2 \leq 2d + 2$ (we recall that $\dim \alpha_1, \dim \alpha_2 \leq \dim A \leq d$, and hence $\text{card } \alpha_1, \text{card } \alpha_2 \leq d + 1$), the points of $f(\alpha_1 \cup \alpha_2)$ are affinely independent, and hence the coefficients in the first sum are correspondingly equal to the coefficients in the second sum. In particular, $\lambda_j = 0$ for $a_j \in \alpha_1 \setminus \alpha_2$. Therefore, $x = \sum_{a_i \in \alpha_1 \cap \alpha_2} \lambda_i f(a_i)$, with $\lambda_i \geq 0$ for every $a_i \in \alpha_1 \cap \alpha_2$ and $\sum_{a_i \in \alpha_1 \cap \alpha_2} \lambda_i = 1$. Since this equality holds for every $x \in \sigma_1 \cap \sigma_2$, then $\sigma_1 \cap \sigma_2 \subseteq \text{conv } f(\alpha_1 \cap \alpha_2)$.

Since $\text{conv } f(\alpha_1 \cap \alpha_2) \subseteq \text{conv } f(\alpha_1) = \sigma_1$ and $\text{conv } f(\alpha_1 \cap \alpha_2) \subseteq \text{conv } f(\alpha_2) = \sigma_2$, the other inclusion $\text{conv } f(\alpha_1 \cap \alpha_2) \subseteq \sigma_1 \cap \sigma_2$ is trivial. Hence, $\sigma_1 \cap \sigma_2 = \text{conv } f(\alpha_1 \cap \alpha_2)$. Therefore, $\sigma_1 \cap \sigma_2$ is a simplex of K and a common face of σ_1 and σ_2 .

If $\sigma \in K$, then we can find $\alpha \subseteq \text{Vert } A$ such that $\sigma = \text{conv } f(\alpha)$. If $\tau \leq \sigma$, then there exists $Y \subseteq f(\alpha)$ such that $\tau = \text{conv } Y$. If we set $\beta := f^{-1}(Y)$, we have that $\tau = \text{conv } f(\beta)$ with $\beta \subseteq \alpha$. This proves that τ is a simplex of K .

In conclusion, K is a geometric simplicial complex.

- 2) It is easy to check that the map that takes each $\{a_{i_0}, \dots, a_{i_k}\} \in A$ to $\{f(a_{i_0}), \dots, f(a_{i_k})\} \in \text{Ab}(K)$ is an isomorphism between A and $\text{Ab}(K)$.

□

Simple Graphs

Definition 17. A (simple) **graph** G is an abstract or geometric simplicial complex of dimension $d \leq 1$. The 0-simplexes and the 1-simplexes of a graph are respectively called **vertexes** and **edges** of the graph. The vertexes of a 1-simplex in G are called **adjacent** in G . If any pair of distinct vertexes of the graph G are adjacent in G , we say that G is **complete**. Any sequence $(\langle P_1, P_2 \rangle, \langle P_2, P_3 \rangle, \dots, \langle P_{n-1}, P_n \rangle, \langle P_n, P_{n+1} \rangle)$ of edges in G with card $\{P_1, \dots, P_n\} = n$ and $P_{n+1} = P_1$ is called a **(regular) cycle**. Any vertex that is a face of exactly one edge is called a **leaf**.

In this section, we will need the following Definition 18 and Proposition 3.

Definition 18. Let Γ be a graph in $\mathbb{R}^2$. Any (bounded or unbounded) connected component of the set $\mathbb{R}^2 \setminus |\Gamma|$ is called a **region for Γ** (see Figure 1).

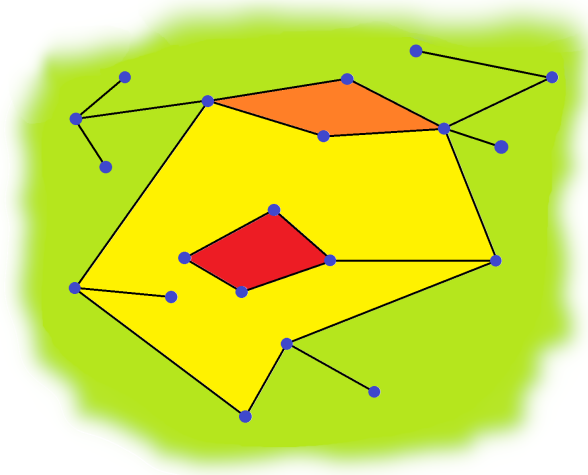


Figure 1: A graph in $\mathbb{R}^2$, its bounded regions (in yellow, orange and red), and its unbounded region (in green).

In the following, if Γ is graph in $\mathbb{R}^2$, we will set $c_\Gamma, v_\Gamma, e_\Gamma, r_\Gamma$ equal to the number of connected components of $|\Gamma|$, vertexes of Γ , edges of Γ , and regions for Γ , respectively. Sometimes, when Γ is clear from the context, we will omit the index Γ in the symbols $c_\Gamma, v_\Gamma, e_\Gamma, r_\Gamma$.

Proposition 3. Let Γ be a graph in $\mathbb{R}^2$. Then $v_\Gamma - e_\Gamma + r_\Gamma = c_\Gamma + 1$.

Proof. If the statement of Proposition 3 is false, we can find a counterexample Γ (i.e., $v_\Gamma - e_\Gamma + r_\Gamma \neq c_\Gamma + 1$) such that the value $v_\Gamma + e_\Gamma$ is minimal.

Firstly, we observe that there exists no vertex P of Γ , such that P is a face of exactly one edge a (i.e., Γ does not contain any leaf). Otherwise we could remove both a and P , and obtain a new geometric

simplicial complex $\hat{\Gamma}$ with $c_{\hat{\Gamma}} = c_{\Gamma}$, $v_{\hat{\Gamma}} = v_{\Gamma} - 1$, $e_{\hat{\Gamma}} = e_{\Gamma} - 1$, $r_{\hat{\Gamma}} = r_{\Gamma}$, respectively (see Figure 2). It would follow that $v_{\hat{\Gamma}} - e_{\hat{\Gamma}} + r_{\hat{\Gamma}} = v_{\Gamma} - e_{\Gamma} + r_{\Gamma} \neq c_{\Gamma} + 1 = c_{\hat{\Gamma}} + 1$, and hence $\hat{\Gamma}$ would be another counterexample to the statement of Proposition 3. This would be a contradiction, since $v_{\hat{\Gamma}} + e_{\hat{\Gamma}} < v_{\Gamma} + e_{\Gamma}$, while we assumed that $v_{\Gamma} + e_{\Gamma}$ had the minimum value.

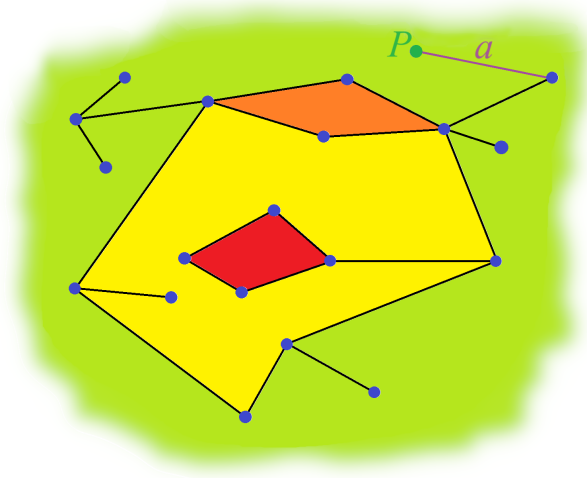


Figure 2: The graphs Γ and $\hat{\Gamma}$ in the proof of Proposition 3. The graph $\hat{\Gamma}$ is obtained from Γ by removing the vertex P and the edge a .

Secondly, no bounded region for Γ exists (i.e., Γ does not contain any cycle). Otherwise we could find a bounded region R for Γ whose closure touches the closure of the unbounded region U for Γ along an edge b (prove it! Hint: consider a suitable polygonal chain connecting a point of the unbounded region to a point of the region R). Then, we could remove b and obtain a new geometric simplicial complex $\bar{\Gamma}$ with $c_{\bar{\Gamma}} = c_{\Gamma}$, $v_{\bar{\Gamma}} = v_{\Gamma}$, $e_{\bar{\Gamma}} = e_{\Gamma} - 1$, $r_{\bar{\Gamma}} = r_{\Gamma} - 1$, respectively. Therefore $v_{\bar{\Gamma}} - e_{\bar{\Gamma}} + r_{\bar{\Gamma}} = v_{\Gamma} - e_{\Gamma} + r_{\Gamma} \neq c_{\Gamma} + 1 = c_{\bar{\Gamma}} + 1$, and hence $\bar{\Gamma}$ would be another counterexample to the statement of Proposition 3 (see Figure 3). This would be a contradiction, since $v_{\bar{\Gamma}} + e_{\bar{\Gamma}} < v_{\Gamma} + e_{\Gamma}$, while we assumed that $v_{\Gamma} + e_{\Gamma}$ had the minimum value.

In conclusion, Γ is a complex of dimension 0, i.e., $e_{\Gamma} = 0$. It follows that $c_{\Gamma} = v_{\Gamma}$ and $r_{\Gamma} = 1$. Hence $v_{\Gamma} - e_{\Gamma} + r_{\Gamma} = c_{\Gamma} + 1$, contradicting the statement that Γ is a counterexample. $\square$

Definition 19. K_n is the complete graph with n vertexes (up to isomorphisms).

Proposition 4. The graph K_5 has no geometric realization in $\mathbb{R}^2$.

Proof. By contradiction, assume that such a geometric realization Γ of K_5 exists. Proposition 3 implies that $v - e + r = 2$ (where the symbols

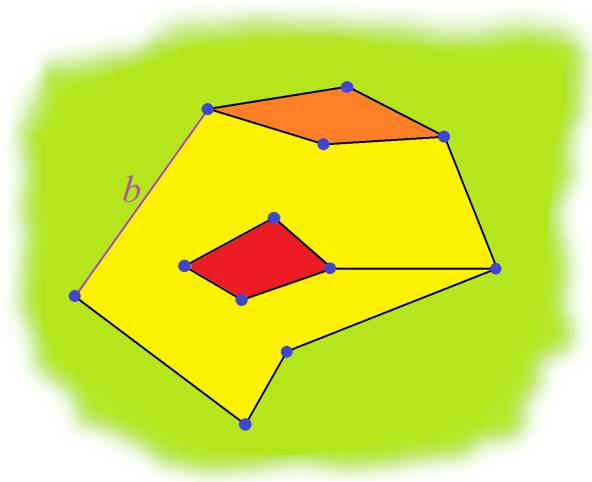
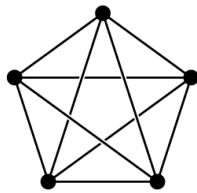


Figure 3: The graphs Γ and $\bar{\Gamma}$ in the proof of Proposition 3. The graph $\bar{\Gamma}$ is obtained from Γ by removing the edge b .

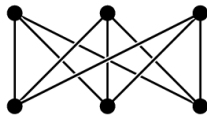
v, e, r have the usual meaning). Since Γ is a geometric realization of K_5 , each vertex of Γ is a face of exactly 4 edges, and hence $4v = 2e$ (because every edge has exactly two vertexes in its boundary). Furthermore, each region for Γ has at least 3 edges in its boundary, and each edge touches exactly two regions. Hence $3r \leq 2e$. It follows that

$$2 = v - e + r \leq v - e + \frac{2}{3}e = v - 2v + \frac{2}{3} \cdot 2v = \frac{1}{3}v.$$

Therefore, $v \geq 6$, against the equality $v = 5$. $\square$



K_5



$K_{3,3}$

Definition 20. $K_{n,n}$ is the graph with distinct vertexes $A_1, \dots, A_n, B_1, \dots, B_n$, whose edges are all the sets $\{A_i, B_j\}$ with $1 \leq i, j \leq n$ (up to isomorphisms).

Proposition 5. The graph $K_{3,3}$ has no geometric realization in $\mathbb{R}^2$.

Proof. By contradiction, assume that such a geometric realization Γ of $K_{3,3}$ exists. Proposition 3 implies that $v - e + r = 2$ (where the symbols v, e, r have the usual meaning). Since Γ is a geometric realization of $K_{3,3}$, each vertex of Γ is a face of exactly 3 edges, and

hence $3v = 2e$ (because every edge has exactly two vertexes in its boundary). Furthermore, each region for Γ has at least 4 edges in its boundary (because of the definition of $K_{3,3}$), and each edge touches exactly two regions. Hence $4r \leq 2e$. It follows that

$$2 = v - e + r \leq v - e + \frac{1}{2}e = v - \frac{3}{2}v + \frac{1}{2} \cdot \frac{3}{2}v = \frac{1}{4}v.$$

Therefore, $v \geq 8$, against the equality $v = 6$. $\square$

Definition 21. Let G be an (abstract) graph containing a vertex B that is adjacent to exactly two vertexes A, C of G . Let G' be the graph obtained from G by deleting the vertex B and the edges $\{A, B\}, \{B, C\}$, and adding the edge $\{A, C\}$. We say that G' has been obtained from G by an **elementary contraction**. If a graph G_1 is isomorphic to a graph G_2 that has been obtained from a graph G_3 by applying a finite sequence of edge contractions and inverses of edge contractions, we say that G_1 and G_3 are **isomorphic up to edge contractions**.

Propositions 4 and 5 show that the statement of the Geometric Realization Theorem is sharp. They are strengthened by the following theorem, whose proof is omitted.

Theorem 2 (Kuratowski Theorem). *A graph admits a geometric realization in $\mathbb{R}^2$ if and only if it does not contain subcomplexes isomorphic to K_5 or to $K_{3,3}$, up to edge contractions.*

Barycentric Coordinates

In this subsection we will assume that a geometric simplicial complex K is given.

Proposition 6. *For every $x \in |K|$ a unique simplex $\sigma \in K$ exists, such that $x \in \text{int } \sigma$.*

Proof. Existence. Since $x \in |K| = \bigcup_{\tau \in K} \tau$, x belongs to at least one simplex of K . Let us take a simplex σ that contains x and has minimal dimension. If $x \in \partial\sigma$, then x belongs to a face of σ , against the minimality of the dimension of σ . Therefore, $x \in \text{int } \sigma$.

Uniqueness. If $x \in \text{int } \sigma_1 \cap \text{int } \sigma_2$, then $x \in \sigma_1 \cap \sigma_2$. The simplex $\tau = \sigma_1 \cap \sigma_2$ is a face of both σ_1 and σ_2 . If τ were a proper face of σ_1 , x would belong to $\partial\sigma_1$, against the condition $x \in \text{int } \sigma_1$. Hence $\tau = \sigma_1$. Analogously, we can show that $\tau = \sigma_2$. Therefore, $\sigma_1 = \sigma_2$. $\square$

Definition 22. Let $x \in |K|$. Assume that $\sigma \in K$ and $x \in \text{int } \sigma$. Also, assume that $u_0, \dots, u_k$ are the vertexes of σ and $x = \sum_{i=0}^k \lambda_i u_i$, with $\sum_{i=0}^k \lambda_i = 1$ and $\lambda_i > 0$ for $i = 0, \dots, k$. Each value λ_i is called

the **barycentric coordinate** of x with respect to u_i , while we say that the **barycentric coordinate** of x with respect to any $u \in \text{Vert } K \setminus \{u_0, \dots, u_k\}$ is 0.

Proposition 6 implies that the **barycentric coordinate** of x with respect to u is uniquely defined for every $x \in |K|$ and every $u \in \text{Vert } K$.

Simplicial Maps

Definition 23. Let K, L be two geometric simplicial complexes. A **vertex map** is a map $\varphi : \text{Vert } K \rightarrow \text{Vert } L$ such that if $u_{i_0}, \dots, u_{i_k}$ are vertexes of a simplex of K , then $\varphi(u_{i_0}), \dots, \varphi(u_{i_k})$ are vertexes of a simplex of L .

NB: φ is not required to be injective (see Figure 4).

Definition 24. Let K, L be two geometric simplicial complexes. If $\varphi : \text{Vert } K \rightarrow \text{Vert } L$ is a vertex map, the map $f : K \rightarrow L$ defined by setting $f(\alpha) := \text{conv } \varphi(\alpha)$ is called a **simplicial map**.

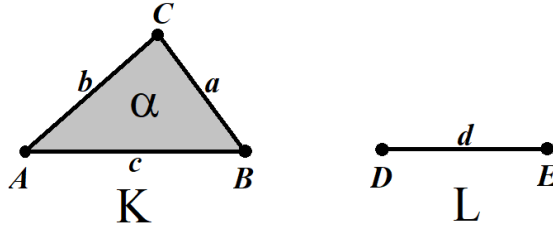


Figure 4: The map φ taking A to D , and B and C to E is a vertex map. The map taking A to D , B and C to E , a to E , and b, c and α to d is the simplicial map induced by φ .

Definition 25. Let K, L be two geometric simplicial complexes. If $f : K \rightarrow L$ is the simplicial map induced by the vertex map $\varphi : \text{Vert } K \rightarrow \text{Vert } L$, we can consider the map $|f| : |K| \rightarrow |L|$ defined by setting $|f|(x) := \sum_{u_i \in \text{Vert } K} \lambda_i \varphi(u_i)$ where λ_i is the barycentric coordinate of x with respect to u_i . The map $|f|$ is called the **PL map (piecewise linear map)** induced by φ (and f).

Proposition 7. If $\varphi : \text{Vert } K \rightarrow \text{Vert } L$ is bijective and both φ and φ^{-1} are vertex maps, then the induced PL map $|f|$ is a homeomorphism between $|K|$ and $|L|$.

Proof. Let $\sigma \in K$. It is easy to check that $|f|$ is a homeomorphism from σ to $f(\sigma)$. The statement of the proposition follows from the Gluing Lemma, since each simplex is a compact set. $\square$

Categories and Functors

A **category** $\mathbf{C}$ consists of a class $\text{ob}(\mathbf{C})$ (whose elements are called **objects** of $\mathbf{C}$) and, for every ordered pair (X, Y) of objects in $\mathbf{C}$, of a

class $\text{Hom}_{\mathbf{C}}(X, Y)$ (whose elements are called *morphisms* from X to Y). If f belongs to $\text{Hom}_{\mathbf{C}}(X, Y)$ we write $f : X \rightarrow Y$, but we do not require that f is a function (see our next examples). We require that the following properties hold:

1. There exists an associative morphism composition from $\text{Hom}_{\mathbf{C}}(X, Y) \times \text{Hom}_{\mathbf{C}}(Y, Z)$ to $\text{Hom}_{\mathbf{C}}(X, Z)$;
2. Every class $\text{Hom}_{\mathbf{C}}(X, X)$ contains a special element 1_X that acts as a unit for the composition (when it is defined).

NB: Pay attention to the fact the classes may be not sets (see Russell's Paradox). Some examples of categories:

- Groups and homomorphisms of groups;
- Abelian Groups and homomorphisms of Abelian groups;
- Vector spaces and linear transformations;
- Topological spaces and continuous maps;
- Geometric simplicial complexes and simplicial maps;
- Polyhedra and PL maps.

Two examples of categories where the morphisms are not functions:

- The category $\mathbf{C}$ where the objects are the elements of a partially ordered set $(X, \leq)$ and, for every ordered pair of objects (x_1, x_2) , $\text{Hom}_{\mathbf{C}}(x_1, x_2)$ contains just the pair (x_1, x_2) if $x_1 \leq x_2$, and is empty otherwise. The composition of (x_1, x_2) with (x_2, x_3) is simply the ordered pair (x_1, x_3) .
- The category $\mathbf{C}$ whose objects are the points P_1, P_2, P_3 , and whose morphisms from P_i to P_j are the oriented arcs from P_i to P_j represented in Figure 5. The composition of arcs is the most natural one: the composition of the arc from P_i to P_j with the arc from P_j to P_k is the arc from P_i to P_k .

Definition 26. Let $\mathbf{X}, \mathbf{Y}$ be two categories. A *covariant functor* $\mathbf{F}$ from $\mathbf{X}$ to $\mathbf{Y}$ ($\mathbf{F} : \mathbf{X} \rightarrow \mathbf{Y}$) is a map that takes each object x of $\mathbf{X}$ to an object $\mathbf{F}(x)$ of $\mathbf{Y}$ and every morphism $f : x_1 \rightarrow x_2$ to a morphism $\mathbf{F}(f) : \mathbf{F}(x_1) \rightarrow \mathbf{F}(x_2)$, and verifies these two properties with respect to the composition $\circ$ of morphisms:

1. $\mathbf{F}(g \circ f) = \mathbf{F}(g) \circ \mathbf{F}(f)$ for every ordered pair (f, g) of composable morphisms;

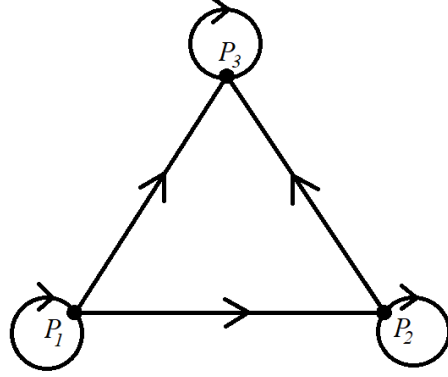


Figure 5: An example of category whose morphisms are not functions.

2. $F(1_x) = 1_{F(x)}$ for every object x in X .

Example 1. Let X be the category whose objects are the geometric simplicial complexes and whose morphisms are the simplicial maps. Let Y be the category whose objects are the polyhedra and whose morphisms are the PL maps. The map taking each geometric simplicial complex K to its body $|K|$ and each simplicial map f to the PL map $|f|$ is a covariant functor. We observe that the restriction of this functor to $\text{Hom}_X(K, L)$ is not injective, i.e., there are distinct simplicial maps that induce the same PL map (we say that it is not **faithful**).

Definition 27. Let X, Y be two categories. A **contravariant functor** F from X to Y ($F : X \rightarrow Y$) is a map that takes each object x of X to an object $F(x)$ of Y and every morphism $f : x_1 \rightarrow x_2$ to a morphism $F(f) : F(x_2) \rightarrow F(x_1)$, and verifies these two properties with respect to the composition $\circ$ of morphisms:

1. $F(g \circ f) = F(f) \circ F(g)$ for every ordered pair (f, g) of composable morphisms;
2. $F(1_x) = 1_{F(x)}$ for every object x in X .

Example 2. Let X be the category whose objects are the vector spaces and whose morphisms are the linear transformations between vector spaces. The map taking each vector space V to its dual V^* and each linear transformation $f : V \rightarrow W$ to its dual $f^* : W^* \rightarrow V^*$ is a contravariant functor.

Nerve of a finite collection of sets

Definition 28. The **nerve** $\text{Nrv } F$ of a finite collection F of subsets of a nonempty set Y is the abstract simplicial complex whose simplexes are all the subsets F' of F , such that $\bigcap_{X \in F'} X \neq \emptyset$.

Remark 2. Observe that, for $F' = \emptyset$, the statement

$$\exists y \in Y \text{ s.t. } \forall X \in F' \ y \in X$$

is true. Therefore, $\text{Nrv } F$ always contains at least the empty set.

Exercise 5. Prove that $\text{Nrv } F$ is an abstract simplicial complex.

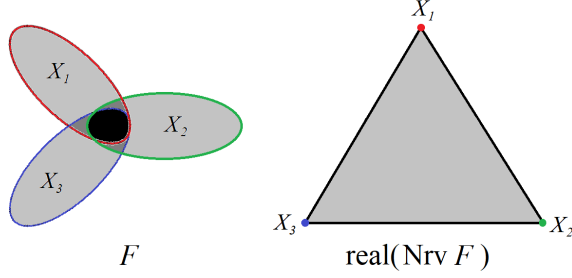


Figure 6: A family F of sets and a geometric realization of its nerve in $\mathbb{R}^2$.

Čech complexes and Vietoris-Rips complexes

Definition 29. Let F and S be a finite collection of closed balls of radius $r \geq 0$ in $\mathbb{R}^d$ and the set of their centers, respectively. The abstract simplicial complex $\text{Nrv } F$ is called the **Čech complex** of S with radius r .

We will denote the Čech complex of S with radius r by the symbol $\check{\text{Cech}}(S, r)$ (or simply by $\check{\text{Cech}}(r)$, when the set S is understood). When a Čech complex $\check{\text{Cech}}(S, r)$ is given, for each $\sigma \in \check{\text{Cech}}(S, r)$ we can consider the set $\hat{\sigma}$ of all centers of the balls belonging to σ . We denote the abstract simplicial complex $\{\hat{\sigma} : \sigma \in \check{\text{Cech}}(S, r)\}$ by the symbol $\widehat{\check{\text{Cech}}}(S, r)$. Of course, $\widehat{\check{\text{Cech}}}(S, r)$ and $\check{\text{Cech}}(S, r)$ are isomorphic.

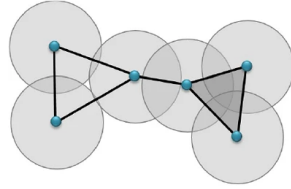


Figure 7: A set of balls of radius 1 in $\mathbb{R}^2$ and a geometric realization of the corresponding Čech complex.

Proposition 8. For each non-empty compact set $K \subset \mathbb{R}^d$ there exists a unique closed ball containing K and having minimum radius.

Proof. Existence. Let us consider a sequence of closed balls $\bar{B}_i$ of center p_i and radius r_i , such that $K \subseteq \bar{B}_i$ and $\lim_{i \rightarrow \infty} r_i$ equals the infimum $\bar{r}$ of the radii of the closed balls containing K . Let us fix a point $\bar{q} \in K$. Since $K \subseteq \bar{B}_i$, for any large enough index i the inequalities $\|\bar{q} - p_i\| \leq r_i \leq \bar{r} + 1$ hold, and hence the point p_i belongs to the closed ball of center $\bar{q}$ and radius $\bar{r} + 1$. Therefore, it

is not restrictive to assume that (p_i) converges to a point $\bar{p} \in \mathbb{R}^d$. Since $K \subseteq \bar{B}_i$, $\|q - p_i\| \leq r_i$ for every $q \in K$. Passing to the limit, we get $\|q - \bar{p}\| \leq \bar{r}$. Therefore, the closed ball $\bar{B}$ of center $\bar{p}$ and radius $\bar{r}$ must contain K . The definition of $\bar{r}$ implies that no closed ball of radius strictly smaller than $\bar{r}$ can contain K . It follows that $\bar{B}$ is a closed ball containing K and having minimum radius.

Uniqueness. We will prove our statement by contradiction. Let us assume that two distinct closed balls $\bar{B}'$, $\bar{B}''$ of radius $\bar{r}$ exist, such that $K \subseteq \bar{B}'$, $\bar{B}''$ and $\bar{r}$ is the infimum of the radii of the closed balls containing K . Let M be the middle point of the segment connecting the centers p' , p'' of $\bar{B}'$ and $\bar{B}''$, respectively. The points of the set $\partial\bar{B}' \cap \partial\bar{B}''$ have a constant distance $\hat{r} = \sqrt{\bar{r}^2 - \|M - p'\|^2}$ from M , and $\hat{r}$ is strictly smaller than $\bar{r}$. We can easily check that $\max\{\|p - M\| : p \in \bar{B}' \cap \bar{B}''\} = \hat{r}$ (it is sufficient to prove that $\max\{\|p - M\| : p \in \bar{B}' \cap \bar{B}'' \cap \alpha\} = \hat{r}$ for any plane α containing p' and p''). Therefore, the closed ball $\hat{B}$ of center M and radius $\hat{r}$ contains $\bar{B}' \cap \bar{B}''$. Since $K \subseteq \bar{B}' \cap \bar{B}''$, the closed ball $\hat{B}$ contains K , while it has a radius strictly smaller than $\bar{r}$. This contradicts the definition of $\bar{r}$.

□

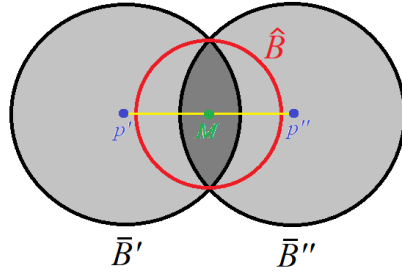


Figure 8: The construction used in the proof of uniqueness of the miniball.

Proposition 8 allows us to give the following definition.

Definition 30. For each non-empty compact set $K \subset \mathbb{R}^d$, the unique closed ball containing K and having minimum radius is called **miniball** of K .

The next proposition makes available three equivalent methods to define simplexes in Čech complexes.

Proposition 9. Let $\{p_1, \dots, p_n\} \subset \mathbb{R}^d$. If $F = \{\bar{B}_1, \dots, \bar{B}_n\}$ is the set of all closed balls $\bar{B}_i$ of center p_i and radius $r \geq 0$, for $1 \leq i \leq n$, then these three properties are equivalent:

1. $\bigcap_{i=1}^n \bar{B}_i \neq \emptyset$;

2. There exists a point $\bar{p} \in \mathbb{R}^d$, such that the closed ball of center $\bar{p}$ and radius r contains $\{p_1, \dots, p_n\}$;
3. The miniball of $\{p_1, \dots, p_n\}$ has radius less than or equal to r .

Proof. 1) $\implies$ 2) Just take a point $\bar{p} \in \bigcap_{i=1}^n \bar{B}_i$.

2) $\implies$ 3) It trivially follows from the minimality of the radius of the miniball containing $\{p_1, \dots, p_n\}$.

3) $\implies$ 1) It is sufficient to observe that the center of the miniball containing $\{p_1, \dots, p_n\}$ belongs to $\bigcap_{i=1}^n \bar{B}_i$.

□

Definition 31. Let $S = \{p_1, \dots, p_n\}$ be a finite subset of $\mathbb{R}^d$. The abstract simplicial complex whose simplexes are all the subsets of S having diameter at most $2r$ is called the **Vietoris-Rips complex** of S with radius r .

We will denote the Vietoris-Rips complex of S with radius r by the symbol $\text{VR}(S, r)$ (or simply by $\text{VR}(r)$, when the set S is understood).

Exercise 6. Prove that $\text{VR}(S, r)$ is indeed an abstract simplicial complex.

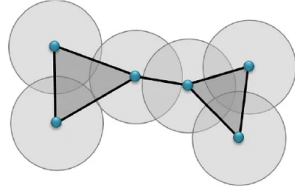


Figure 9: A set of balls of radius 1 in $\mathbb{R}^2$ and a geometric realization of $\text{VR}(S, 1)$, where S is the set of centers of the balls. Compare this figure with Figure 7.

Remark 3. Our definitions immediately imply that if $0 \leq r_1 \leq r_2$, then $\widehat{\text{Cech}}(S, r_1) \subseteq \widehat{\text{Cech}}(S, r_2) \subseteq \text{VR}(S, r_2)$.

Vietoris-Rips Lemma

Theorem 3 (Vietoris-Rips Lemma). Let $S = \{p_1, \dots, p_n\}$ be a finite subset of $\mathbb{R}^d$. For every $r \geq 0$, $\widehat{\text{Cech}}(S, r) \subseteq \text{VR}(S, r) \subseteq \widehat{\text{Cech}}(S, \sqrt{2}r)$.

Proof. The first inclusion is trivial (see Remark 3). Let $M(\sigma)$ be the miniball of a k -simplex $\sigma = \{p_{i_0}, \dots, p_{i_k}\} \in \text{VR}(r)$. Call $\bar{p}$ the center of $M(\sigma)$ and ρ its radius. We start by proving that $\sqrt{2}\rho \leq \text{diam } \sigma \leq 2\rho$. Since this statement trivially holds for $k = 0$, let us assume that $k \geq 1$ (and hence $\rho > 0$).

The inequality $\text{diam } \sigma \leq 2\rho$ is trivial, since $\sigma \subseteq M(\sigma)$ and $\text{diam } M(\sigma) = 2\rho$. Let us now prove that $\sqrt{2}\rho \leq \text{diam } \sigma$. By contradiction, let us assume that $\sqrt{2}\rho > \text{diam } \sigma$. Then a positive ε exists,

such that $\text{diam } \sigma < \varepsilon < \sqrt{2}\rho$. In σ there exists at least one point p_{ij} belonging to $\partial M(\sigma)$ (otherwise $M(\sigma)$ would not be the miniball of σ). Since $\text{diam } \sigma < \varepsilon$, the closed ball $\bar{B}(p_{ij}, \varepsilon)$ contains σ , and hence $\sigma \subseteq \bar{B}(p_{ij}, \varepsilon) \cap M(\sigma)$. We observe that $\partial \bar{B}(p_{ij}, \varepsilon) \cap \partial M(\sigma)$ is a $(d-2)$ -dimensional spherical surface having center at a point C belonging to the line s through p_{ij} and $\bar{p}$ (observe that $\bar{B}(p_{ij}, \varepsilon) \not\supseteq M(\sigma)$, because $0 < \varepsilon < \sqrt{2}\rho < 2\rho$). Let $\hat{\rho}$ be the radius of this spherical surface. Let us now prove that, for every plane α containing the line s , $\bar{B}(C, \hat{\rho}) \cap \alpha \supseteq \bar{B}(p_{ij}, \varepsilon) \cap M(\sigma) \cap \alpha$. In order to do that, let us choose a reference frame on α , such that $p_{ij} \equiv (0, 0)$ and $\bar{p} \equiv (0, \rho)$. Therefore, the circumferences $\partial(\bar{B}(p_{ij}, \varepsilon) \cap \alpha)$ and $M(\sigma) \cap \alpha$ in the plane α have respective equations $x^2 + y^2 = \varepsilon^2$ and $x^2 + (y - \rho)^2 = \rho^2$. These circumferences meet each other at the points $A \equiv \left(\sqrt{\varepsilon^2 - \frac{\varepsilon^4}{4\rho^2}}, \frac{\varepsilon^2}{2\rho}\right)$ and $B \equiv \left(-\sqrt{\varepsilon^2 - \frac{\varepsilon^4}{4\rho^2}}, \frac{\varepsilon^2}{2\rho}\right)$ (check it!). Since $\varepsilon < \sqrt{2}\rho$, it follows that $y_A = y_B = y_C = \frac{\varepsilon^2}{2\rho} < \rho$. This implies that C belongs to the interior of the segment connecting p_{ij} and $\bar{p}$. **As a consequence, it is easy to check by elementary trigonometry that A and B are the points of the set $\bar{B}(p_{ij}, \varepsilon) \cap M(\sigma) \cap \alpha$ that maximize the distance from C (just apply the law of cosines to the triangle of vertexes $C, \bar{p}, p$, with $p \in \bar{B}(p_{ij}, \varepsilon) \cap M(\sigma) \cap \alpha$).** Moreover, their distance from C is $\hat{\rho} = \sqrt{\rho^2 - \|\bar{p} - C\|^2} < \rho$. It follows that $\bar{B}(C, \hat{\rho}) \cap \alpha \supseteq \bar{B}(p_{ij}, \varepsilon) \cap M(\sigma) \cap \alpha$. Since this inclusion holds for every plane α containing the line s , we have that $\bar{B}(C, \hat{\rho}) \supseteq \bar{B}(p_{ij}, \varepsilon) \cap M(\sigma) \supseteq \sigma$. Therefore, $\bar{B}(C, \hat{\rho})$ is a closed ball that contains σ and has a radius $\hat{\rho}$ strictly less than ρ . Such a statement contradicts the assumption that $\bar{B}(\bar{p}, \rho)$ is the miniball of σ . This concludes the proof that $\sqrt{2}\rho \leq \text{diam } \sigma \leq 2\rho$.

Since $\sigma \in \text{VR}(r)$, we know that $\text{diam } \sigma \leq 2r$. It follows that $\sqrt{2}\rho \leq 2r$, and hence $\rho \leq \sqrt{2}r$. Therefore, the definition of Čech complex and Proposition 9 imply that the collection σ' of balls of radius $\sqrt{2}r$, whose centers belong to σ , is a simplex in $\check{\text{Cech}}(\sqrt{2}r)$. It follows that $\text{VR}(S, r) \subseteq \widehat{\check{\text{Cech}}(S, \sqrt{2}r)}$. $\square$

Remark 4. In the proof of the Vietoris-Rips Lemma we use the inequality $\varepsilon < \sqrt{2}\rho$. If this inequality does not hold, then our construction fails, since it is no more true that $\bar{B}(C, \hat{\rho}) \cap \alpha \supseteq \bar{B}(p_{ij}, \varepsilon) \cap M(\sigma) \cap \alpha \supseteq \sigma$ (see Figure 11).

Theorem 4 (Optimality of the Vietoris-Rips Lemma). *The statement of the Vietoris-Rips Lemma is sharp, in the sense that $\sqrt{2}$ equals the minimum of the set A of all real values α such that for any $r \geq 0$, any positive integer d and any finite subset S of $\mathbb{R}^d$ the inclusion $\text{VR}(S, r) \subseteq \widehat{\check{\text{Cech}}(S, \alpha r)}$ holds.*

Proof. Let us consider the set $\bar{S} = \{u_0, \dots, u_d\}$ of all vertexes of a regular d -simplex $\sigma \subseteq \mathbb{R}^d$, with $B(\sigma) = \mathbf{0}$, such that $\|u_i\| = 1$ for any

$i \in \{0, \dots, d\}$. Since σ is regular, for every pair $(i, j) \in \{0, \dots, d\}^2$ with $i \neq j$ we have that $\|u_i - u_j\| = \|u_1 - u_0\|$, and hence $u_i \cdot u_j = u_1 \cdot u_0$. Let us set $c := u_1 \cdot u_0$. Since $\frac{1}{d+1} \sum_{i=0}^d u_i = B(\sigma) = \mathbf{0}$, it follows that $\sum_{i=0}^d u_i = \mathbf{0}$. This implies that $0 = \left(\sum_{i=0}^d u_i\right) \cdot u_0 = \sum_{i=0}^d u_i \cdot u_0 = 1 + dc$, and hence $c = -\frac{1}{d}$. As a consequence, $\text{diam} \{u_0, \dots, u_d\} = \|u_1 - u_0\| = \sqrt{\|u_1\|^2 + \|u_0\|^2 - 2u_1 \cdot u_0} = \sqrt{2 - 2c} = \sqrt{2 + \frac{2}{d}}$. It follows that $\{u_0, \dots, u_d\} \in \text{VR} \left(\bar{S}, \frac{\sqrt{2 + \frac{2}{d}}}{2} \right)$. Then, for any $\alpha \in A$, the inclusion $\text{VR} \left(\bar{S}, \frac{\sqrt{2 + \frac{2}{d}}}{2} \right) \subseteq \widehat{\check{\text{Cech}} \left(\bar{S}, \alpha \frac{\sqrt{2 + \frac{2}{d}}}{2} \right)}$ implies that $\{u_0, \dots, u_d\} \in \widehat{\check{\text{Cech}} \left(\bar{S}, \alpha \frac{\sqrt{2 + \frac{2}{d}}}{2} \right)}$, i.e., the radius ρ of the miniball of $\{u_0, \dots, u_d\}$ verifies the inequality $\rho \leq \alpha \frac{\sqrt{2 + \frac{2}{d}}}{2}$. We now observe that $\rho = 1$, since the miniball of the set $\{u_0, \dots, u_d\}$ is the closed ball centered at $\mathbf{0}$, with radius 1. Therefore, for any $\alpha \in A$, $1 \leq \alpha \frac{\sqrt{2 + \frac{2}{d}}}{2}$, and hence $\alpha \geq \frac{2}{\sqrt{2 + \frac{2}{d}}} = \sqrt{2} \sqrt{\frac{d}{d+1}}$. Passing to the limit for $d \rightarrow \infty$, we get the inequality $\alpha \geq \sqrt{2}$, for any $\alpha \in A$. This implies that $\inf A \geq \sqrt{2}$. The Vietoris-Rips Lemma states that $\sqrt{2} \in A$, and hence $\sqrt{2} = \min A$. $\square$

Remark 5. The statement of the Vietoris-Rips Lemma is no longer optimal if we fix d . For example, if $d = 1$ then $\text{VR}(S, r) = \widehat{\check{\text{Cech}}(S, r)}$. Further information about this topic can be found in the paper [Vin de Silva and Robert Ghrist (2007)]², Theorem 2.5.

Exercise 7. Prove that if $d = 1$ then $\text{VR}(S, r) = \widehat{\check{\text{Cech}}(S, r)}$.

Delaunay complexes

The use of Čech complexes and Vietoris-Rips complexes of a set $S = \{p_1, \dots, p_n\} \subseteq \mathbb{R}^d$ has two computational drawbacks: when the parameter r is large enough, these complexes contain a large number of simplexes (2^n) and have a large dimension ($n - 1$), independently from the value of d . As a first step to solve these problems, we will introduce the concept of Delaunay simplex. Before doing that, we have to present the concept of Voronoi diagram.

Definition 32. Let $S = \{p_1, \dots, p_n\}$ be a finite subset of $\mathbb{R}^d$. The **Voronoi cell** V_u of a point $u \in S$ is the set $\{p \in \mathbb{R}^d : \forall v \in S, \|p - u\| \leq \|p - v\|\}$. The set $\{V_u : u \in S\}$ is called the **Voronoi diagram** of S . For each Voronoi cell V_u , we say that u is its center.

² Vin de Silva and Robert Ghrist. Coverage in sensor networks via persistent homology. *Algebr. Geom. Topol.*, 7:339–358, 2007. ISSN 1472-2747. DOI: 10.2140/agt.2007.7.339. URL <https://doi-org.ezproxy.unibo.it/10.2140/agt.2007.7.339>

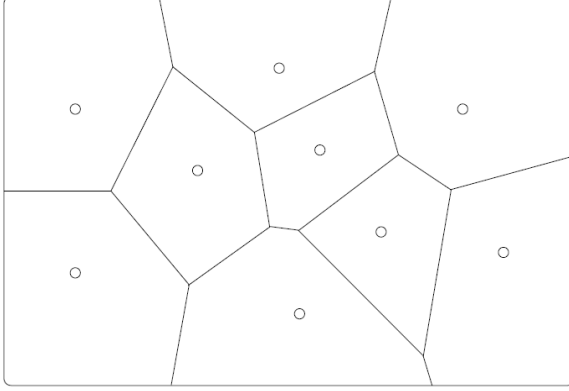


Figure 12: The Voronoi diagram of a set of nine points in $\mathbb{R}^2$.

NB: Since each Voronoi cell is an intersection of closed half-spaces, it is both closed and convex.

Definition 33. Let $S = \{p_1, \dots, p_n\}$ be a finite subset of $\mathbb{R}^d$. The **Delaunay complex** $\text{Del}(S)$ of S is the nerve of the Voronoi diagram of S .

When a Delaunay complex $\text{Del}(S)$ is given, for each $\sigma \in \text{Del}(S)$ we can consider the set $\hat{\sigma}$ of all centers of the Voronoi cells belonging to σ . We denote the abstract simplicial complex $\{\hat{\sigma} : \sigma \in \text{Del}(S)\}$ by the symbol $\widehat{\text{Del}}(S)$. Of course, $\widehat{\text{Del}}(S)$ and $\text{Del}(S)$ are isomorphic.

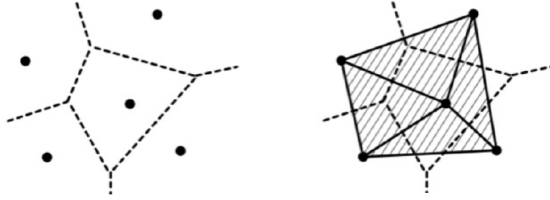


Figure 13: A Voronoi diagram and a geometric realization of the corresponding Delaunay complex.

Definition 34. We say that the points of the set $S = \{p_1, \dots, p_n\} \subseteq \mathbb{R}^d$ are in **general position** if for each subset $S' = \{p_{i_1}, \dots, p_{i_{d+2}}\}$ of cardinality $d + 2$ of S there is no spherical surface of dimension $d - 1$ that contains S' .

Exercise 8. Prove that for every set $S = \{p_1, \dots, p_n\} \subseteq \mathbb{R}^d$ and every $\varepsilon > 0$ there exists another set $\hat{S} = \{\hat{p}_1, \dots, \hat{p}_n\} \subseteq \mathbb{R}^d$ such that the points of $\hat{S}$ are in general position and $\max_{1 \leq i \leq n} \|p_i - \hat{p}_i\| \leq \varepsilon$.

The following result shows the advantage of using Delaunay complexes.

Proposition 10. If the points of the set $S = \{p_1, \dots, p_n\} \subseteq \mathbb{R}^d$ are in general position, then $\dim \text{Del}(S) \leq d$.

Proof. Let $\sigma = \{V_{p_{i_0}}, \dots, V_{p_{i_k}}\} \in \text{Del}(S)$. The definition of Delaunay complex implies that $\bigcap_{j=0}^k V_{p_{i_j}} \neq \emptyset$. Let $\tilde{p} \in \bigcap_{j=0}^k V_{p_{i_j}}$. The definition of Voronoi cell guarantees that $\|\tilde{p} - p_{i_0}\| = \dots = \|\tilde{p} - p_{i_k}\|$, and hence the spherical surface of dimension $d - 1$ and center $\tilde{p}$ contains the points $p_{i_0}, \dots, p_{i_k}$. Since the points of the set S are in general position, $k + 1 \leq d + 1$. Therefore, $\dim \sigma = k \leq d$. $\square$

Remark 6. The example represented in Figure 14 shows that the assumption of general position is indeed necessary in the statement of Proposition 10.

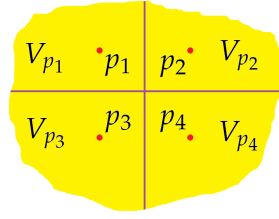


Figure 14: The statement of Proposition 10 does not hold if the points of S are not in general position. In this figure, a 3-simplex $\sigma = \{V_{p_1}, V_{p_2}, V_{p_3}, V_{p_4}\} \in \text{Del}(S)$ is represented, for $S = \{p_1, p_2, p_3, p_4\} \subseteq \mathbb{R}^2$. We observe that $\dim \text{Del}(S) = 3$.

Exercise 9. Prove that if the points of the set $S = \{p_1, \dots, p_n\} \subseteq \mathbb{R}^2$ are in general position, then $\text{card Del}(S) \leq 6n - 4$.

Before proceeding, we invite the reader to do the following exercise.

Exercise 10 (Extension of Exercise 8). Prove that for every set $S = \{p_1, \dots, p_n\} \subseteq \mathbb{R}^d$ and every $\varepsilon > 0$ there exists another set $\hat{S} = \{\hat{p}_1, \dots, \hat{p}_n\} \subseteq \mathbb{R}^d$ such that $\max_{1 \leq i \leq n} \|p_i - \hat{p}_i\| \leq \varepsilon$ and the following properties hold:

1. For each subset $S' = \{p_{i_0}, \dots, p_{i_{d+1}}\}$ of cardinality $d + 2$ of $\hat{S}$ there is no $(d - 1)$ -dimensional spherical surface that contains S' (i.e., the points of $\hat{S}$ are in general position according to Definition 34);
2. For each subset $S'' = \{p_{i_0}, \dots, p_{i_d}\}$ of cardinality $d + 1$ of $\hat{S}$ there is no $(d - 1)$ -dimensional affine space that contains S'' (i.e., the points of any subset of $\hat{S}$ of cardinality $d + 1$ are affinely independent).

Hint: use the fact that no finite union of hyperplanes and $(d - 1)$ -dimensional spherical surfaces in $\mathbb{R}^d$ can be equal to $\mathbb{R}^d$.

Lemma 1. If $S = \{p_1, \dots, p_n\}$ is a finite subset of $\mathbb{R}^d$, and $S' = \{p_{i_0}, \dots, p_{i_k}\} \in \widehat{\text{Del}}(S)$, then the following properties hold:

1. $\bigcap_{j=0}^k V_{p_{i_j}} \neq \emptyset$;
2. If $p \in \bigcap_{j=0}^k V_{p_{i_j}}$, then $\|p - p_{i_0}\| = \dots = \|p - p_{i_k}\|$, and the open ball B of center p and radius $\|p - p_{i_0}\|$ does not contain any point of S ;

3. A unique point $\bar{c}(S') \in \bigcap_{j=0}^k V_{p_{i_j}}$ exists, minimizing the continuous function $r(p) : \|p - p_{i_0}\| = \dots = \|p - p_{i_k}\|$ over $\bigcap_{j=0}^k V_{p_{i_j}}$. The point $\bar{c}(S')$ will be called the **center of the abstract simplex $S' \in \widehat{\text{Del}}(S)$** .

Proof. 1. By definition of $\widehat{\text{Del}}(S)$.

2. By definition of Voronoi cell, all points in S' take the minimum distance from p in S .
3. The existence and uniqueness of $\bar{c}(S')$ follows from the fact that the set $\bigcap_{j=0}^k V_{p_{i_j}}$ is closed and convex, and the function $r^2(p)$ is strictly convex on its domain.

□

Remark 7. We observe that if S' is a singleton $\{p_{i_0}\}$, then $\bar{c}(S') = p_{i_0}$.

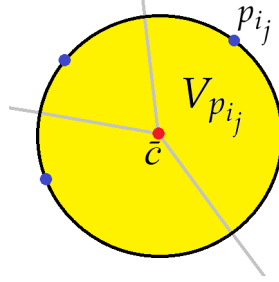


Figure 15: An example of center $\bar{c}$ (in red) of an abstract simplex $S' = \{p_{i_0}, \dots, p_{i_k}\} \in \widehat{\text{Del}}(S)$ (in blue). S' is a subset of $S = \{p_1, \dots, p_n\}$. No point in the yellow region can belong to S .

Theorem 5 (Realization Theorem for Delaunay complexes). *Let us assume that $S = \{p_1, \dots, p_n\}$ is a finite set of points of $\mathbb{R}^d$ with $n > d$, verifying the following properties:*

1. *For each subset $S' = \{p_{i_0}, \dots, p_{i_{d+1}}\}$ of cardinality $d + 2$ of S there is no $(d - 1)$ -dimensional spherical surface that contains S' ;*
2. *For each subset $S'' = \{p_{i_0}, \dots, p_{i_d}\}$ of cardinality $d + 1$ of S there is no $(d - 1)$ -dimensional affine space that contains S'' .*

Then the set $K := \{\text{conv } \tilde{S} : \emptyset \neq \tilde{S} \subseteq S, \bigcap_{p \in \tilde{S}} V_p \neq \emptyset\} \cup \{\emptyset\}$ is a geometric simplicial complex that realizes $\text{Del}(S)$.

Proof. The case $d = 1$ is trivial, and hence we can assume $d \geq 2$. By definition, if $\emptyset \neq \tilde{S} = \{p_{i_0}, \dots, p_{i_k}\} \subseteq S$ and $\bigcap_{j=0}^k V_{p_{i_j}} \neq \emptyset$ (so implying $\text{conv } \tilde{S} \in K$), then statement 2 in Lemma 1 guarantees that the points $p_{i_0}, \dots, p_{i_k}$ belong to at least one $(d - 1)$ -dimensional spherical surface centered at a point of $\bigcap_{j=0}^k V_{p_{i_j}}$. Assumption 1) implies that $k + 1 \leq d + 1$. Then, from assumption 2) it follows that the points $p_{i_0}, \dots, p_{i_k}$ are affinely independent (since $n > d$,

we can indeed complete $\{p_{i_0}, \dots, p_{i_k}\}$ to an affinely independent set $\{p_{i_0}, \dots, p_{i_d}\} \subseteq S$, and hence $\sigma := \text{conv} \{p_{i_0}, \dots, p_{i_k}\}$ is a geometric simplex, which can be written as $\langle p_{i_0}, \dots, p_{i_k} \rangle$.

Furthermore, if $\tau \leq \sigma$, the definition of K immediately implies that $\tau \in K$. Therefore, the only nontrivial property we have to prove in order to show that K is indeed a geometric simplicial complex is that if $\sigma_1 = \langle p_{i_0}, \dots, p_{i_r} \rangle$ and $\sigma_2 = \langle p_{j_0}, \dots, p_{j_s} \rangle$ belong to K (i.e., $\bigcap_{a=0}^r V_{p_{i_a}} \neq \emptyset$ and $\bigcap_{b=0}^s V_{p_{j_b}} \neq \emptyset$), then $\sigma_1 \cap \sigma_2$ is a common face of σ_1 and σ_2 . In order to do that, let us consider the sets $S_1 = \{p_{i_0}, \dots, p_{i_r}\}$ and $S_2 = \{p_{j_0}, \dots, p_{j_s}\}$, the centers $q_1 = \bar{c}(S_1)$ of S_1 and $q_2 = \bar{c}(S_2)$ of S_2 (see Lemma 1), and the closed balls $\bar{B}_1 := \bar{B}(\bar{c}(S_1), \|p_{i_0} - \bar{c}(S_1)\|)$ and $\bar{B}_2 := \bar{B}(\bar{c}(S_2), \|p_{j_0} - \bar{c}(S_2)\|)$.

First of all, let us examine the trivial case in which at least one of the two closed balls reduces to a singleton $\{p_i\}$ (remember Remark 7!). In this case, assuming $\sigma_1 = \{p_i\}$, either $\sigma_1 \cap \sigma_2 = \emptyset$, and hence $\sigma_1 \cap \sigma_2$ is a trivial common face of σ_1 and σ_2 in K , or $\sigma_1 \cap \sigma_2 = \{p_i\}$. In this last case, since $p_i \notin \text{int } \bar{B}_2$ (because of statement 2 in Lemma 1) and the vertexes of σ_2 are the only points of σ_2 that do not belong to $\text{int } \bar{B}_2$, the point p_i is a vertex of σ_2 , and hence $\sigma_1 \cap \sigma_2 \in K$.

Therefore, we can assume that both $\bar{B}_1$ and $\bar{B}_2$ are different from singletons, i.e., $\text{card } S_1 \geq 2$ and $\text{card } S_2 \geq 2$. Since S_1 is included in the $(d-1)$ -dimensional spherical surface $\partial \bar{B}_1$, we observe that assumption 1) implies the inequality $\text{card } S_1 \leq d+1$. Then assumption 2) guarantees that the points of S_1 are affinely independent. Similarly, the points of S_2 are affinely independent.

If $\bar{B}_1 \cap \bar{B}_2 = \emptyset$, then $\sigma_1 \cap \sigma_2 = \emptyset \in K$, since $\sigma_1 \subseteq \bar{B}_1$ and $\sigma_2 \subseteq \bar{B}_2$.

If $\bar{B}_1 = \bar{B}_2$, then $q_1 = q_2$ and hence $S_1 \cup S_2 \in \text{Del}(S)$, because $q_1 = q_2 \in (\bigcap_{a=0}^r V_{p_{i_a}}) \cap (\bigcap_{b=0}^s V_{p_{j_b}})$. Since $S_1 \cup S_2$ is included in the $(d-1)$ -dimensional spherical surface $\partial \bar{B}_1 = \partial \bar{B}_2$, assumption 1) implies that $\text{card } S_1 \cup S_2 \leq d+1$. Then assumption 2) guarantees that the points of $S_1 \cup S_2$ are affinely independent. It follows that $\sigma_1 \cap \sigma_2 = \text{conv } S_1 \cap \text{conv } S_2 = \text{conv } (S_1 \cap S_2) \in K$.

If $\bar{B}_1 \neq \bar{B}_2$ and $\bar{B}_1 \cap \bar{B}_2 \neq \emptyset$, we can observe that $\bar{B}_1$ cannot be a proper subset of $\bar{B}_2$, and $\bar{B}_2$ cannot be a proper subset of $\bar{B}_1$, because of statement 2 in Lemma 1. As a consequence, if $\bar{B}_1$ and $\bar{B}_2$ are tangent to each other, then their interiors cannot meet, and hence either $\sigma_1 \cap \sigma_2 = \emptyset$, or $\sigma_1 \cap \sigma_2$ is a singleton containing a vertex of both σ_1 and σ_2 (because $\partial \bar{B}_1$ cannot meet $\text{int } \sigma_1$ and $\partial \bar{B}_2$ cannot meet $\text{int } \sigma_2$). In both cases, $\sigma_1 \cap \sigma_2$ is a common face of σ_1 and σ_2 in K . **In summary, we can assume that $\bar{B}_1 \neq \bar{B}_2$, $\bar{B}_1 \cap \bar{B}_2 \neq \emptyset$, $\bar{B}_1$ and $\bar{B}_2$ are not tangent to each other, and are not singletons.** Then $\partial \bar{B}_1 \cap \partial \bar{B}_2$ is a $(d-2)$ -dimensional spherical surface, and we can consider the hyperplane α containing such a surface. Let us now

define the (possibly empty) sets $S_1^\alpha := S_1 \cap \alpha$, $S_2^\alpha := S_2 \cap \alpha$.

Since the sets S_1, S_2 are affinely independent, their respective subsets S_1^α, S_2^α are affinely independent too. As a consequence, we can define the geometric simplexes $\sigma_1^\alpha := \text{conv } S_1^\alpha$ and $\sigma_2^\alpha := \text{conv } S_2^\alpha$. Since $S_1 \subseteq \bar{B}_1 \setminus \text{int } \bar{B}_2$ (because of statement 2 in Lemma 1), there exists a closed half-space π_1 such that $\alpha = \partial\pi_1$ and $S_1 \subseteq \pi_1$. Moreover, since $S_2 \subseteq \bar{B}_2 \setminus \text{int } \bar{B}_1$, there exists a closed half-space $\pi_2 \neq \pi_1$ such that $\alpha = \partial\pi_2$ and $S_2 \subseteq \pi_2$. Of course, this implies that $\sigma_1 \subseteq \pi_1$ and $\sigma_2 \subseteq \pi_2$ (see Figure 16). Since $\pi_1 \cap \pi_2 = \alpha$, it follows that if $p \in \sigma_1 \cap \sigma_2$, then $p \in \alpha$. In other words, the simplexes σ_1, σ_2 are respectively contained in two opposed half-spaces, and can meet each other only at points of α . If we represent $p \in \sigma_1 \cap \sigma_2$ as $\sum_{a=0}^r \lambda_a p_{i_a} \in \sigma_1$ and as $\sum_{b=0}^s \mu_b p_{j_b} \in \sigma_2$, it follows that $\lambda_a = 0$ for $p_{i_a} \in S_1 \setminus S_1^\alpha$, and $\mu_b = 0$ for $p_{j_b} \in S_2 \setminus S_2^\alpha$. This implies that $p \in \sigma_1^\alpha \cap \sigma_2^\alpha$, and hence $\sigma_1 \cap \sigma_2 = \sigma_1^\alpha \cap \sigma_2^\alpha$. Since $S_1^\alpha \cup S_2^\alpha$ is included in the $(d-2)$ -dimensional spherical surface $\partial\bar{B}_1 \cap \partial\bar{B}_2$, we have that $S_1^\alpha \cup S_2^\alpha \subseteq \partial\bar{B}_1$. Assumption 1) implies that $\text{card } S_1^\alpha \cup S_2^\alpha \leq d+1$. Then assumption 2) guarantees that the points of $S_1^\alpha \cup S_2^\alpha$ are affinely independent, and hence $\text{conv } (S_1^\alpha \cup S_2^\alpha)$ is a geometric simplex. Since $\sigma_1^\alpha \cap \sigma_2^\alpha$ is a face of $\text{conv } (S_1^\alpha \cup S_2^\alpha)$, then $\sigma_1^\alpha \cap \sigma_2^\alpha$ is a geometric simplex too. This concludes the proof that K is a geometric simplicial complex. Finally, we observe that the geometric simplicial complex K realizes $\text{Del}(S)$ by construction. $\square$

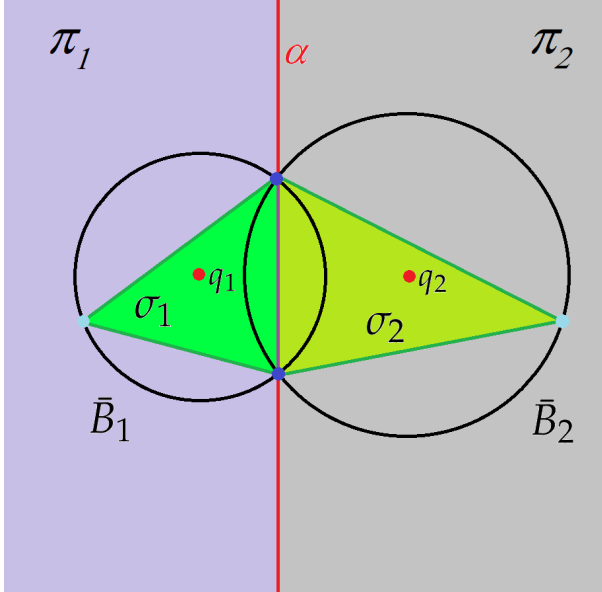


Figure 16: A (rough) description of the key step in the proof of Theorem 5.

Alpha complexes

The concepts of Čech complex and Delaunay complex can be combined. This leads to the definition of Alpha complex.

Definition 35. Let us choose a finite subset $S = \{p_1, \dots, p_n\}$ of $\mathbb{R}^d$ and a nonnegative value r . For each $p_i \in S$ let us consider the Voronoi cell V_{p_i} , the closed ball $\bar{B}(p_i, r)$, and the set $R(p_i, r) := V_{p_i} \cap \bar{B}(p_i, r)$. The nerve of the collection of sets $\{R(p_i, r) : p_i \in S\}$ is called the **Alpha complex** of S with radius r .

We will denote the Alpha complex of S with radius r by the symbol $\text{Alpha}(S, r)$ (or simply by $\text{Alpha}(r)$, when the set S is understood). When an Alpha complex $\text{Alpha}(S, r)$ is given, for each $\sigma \in \text{Alpha}(S, r)$ we can consider the set $\hat{\sigma}$ of all centers of the balls belonging to σ . We denote the abstract simplicial complex $\{\hat{\sigma} : \sigma \in \text{Alpha}(S, r)\}$ by the symbol $\widehat{\text{Alpha}}(S, r)$. Of course, $\widehat{\text{Alpha}}(S, r)$ and $\text{Alpha}(S, r)$ are isomorphic.

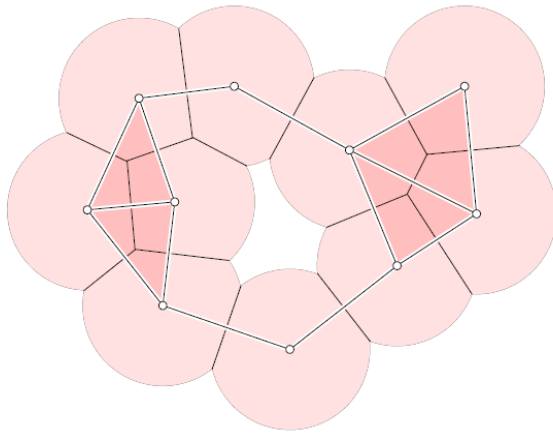


Figure 17: A geometric realization of the Alpha complex $\text{Alpha}(S, r)$ of a set S of ten points in $\mathbb{R}^2$.

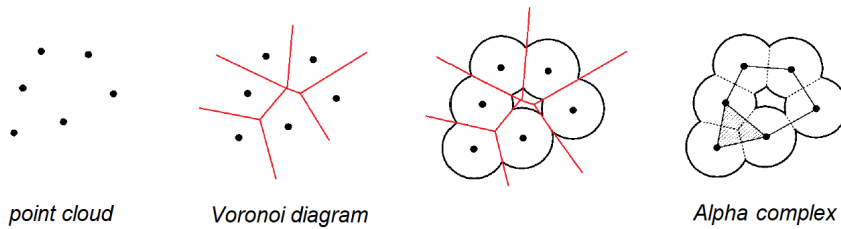


Figure 18: An example of Alpha complex obtained from a point cloud.

Proposition 11. Let S be a finite nonempty subset of $\mathbb{R}^d$. For every non-negative value r , $\widehat{\text{Alpha}}(S, r) \subseteq \widehat{\text{Čech}}(S, r)$ and $\widehat{\text{Alpha}}(S, r) \subseteq \widehat{\text{Del}}(S)$.

Proof. If $S = \{p_1, \dots, p_n\}$, it is sufficient to observe that $\bigcap_{i=1}^n R(p_i, r) \neq \emptyset$ implies that $\bigcap_{i=1}^n \bar{B}(p_i, r) \neq \emptyset$ and $\bigcap_{i=1}^n V_{p_i} \neq \emptyset$. $\square$

Proposition 12. If the points of the finite nonempty set $S \subseteq \mathbb{R}^d$ are in general position, then $\dim \text{Alpha}(S, r) \leq d$ for every nonnegative value r .

Proof. It follows from Proposition 10 and Proposition 11. $\square$

Collapsibility

Definition 36. Let K be a geometric simplicial complex, and assume that the simplex τ has only one coface σ in K (we say that τ is a **free face**). Then we say that the geometric simplicial complex $K' := K \setminus \{\tau, \sigma\}$ has been obtained from K by an **elementary collapse**. We also say that K has been obtained from K' by the **inverse of an elementary collapse**.

NB: Since τ has only one coface σ in K , $\dim \sigma = \dim \tau + 1$.

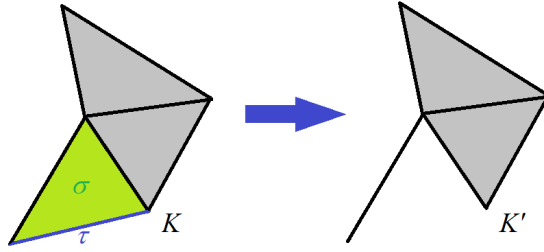


Figure 19: An example of elementary collapse.

Definition 37. If we can reduce a geometric simplicial complex K to a geometric simplicial complex K' having only one vertex by a sequence of elementary collapses, we say that K is **collapsible**.

Simplicial homology over $\mathbb{Z}_2$

Homology groups of a chain complex

Definition 38. A **chain complex** $\mathcal{C}$ is a sequence of vector spaces V_p over a field $\mathbb{K}$ and homomorphisms $v_p : V_p \rightarrow V_{p-1}$ indexed by the integer numbers, such that $v_{p-1} \circ v_p$ is the null homomorphism, for every $p \in \mathbb{Z}$. Each homomorphism v_p is called a **p -boundary map**. The elements of V_p , $\ker v_p$, $\text{Im } v_{p+1}$ are respectively called **p -chains**, **p -cycles** and **p -boundaries**.

NB: The assumption $v_p \circ v_{p+1} \equiv 0$ immediately implies that $\text{Im } v_{p+1} \subseteq \ker v_p$, and hence the quotient vector space $\frac{\ker v_p}{\text{Im } v_{p+1}}$ is well defined. Sometimes, we will use the symbols $Z_p(\mathcal{C})$ and $B_p(\mathcal{C})$ to denote the vector spaces $\ker v_p$ and $\text{Im } v_{p+1}$, respectively.

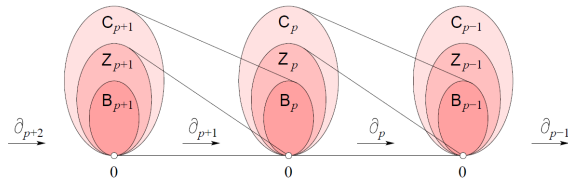


Figure 20: Representation of a chain complex.

Definition 39. If a chain complex $\mathcal{C} = (V_p, v_p)_{p \in \mathbb{Z}}$ is given, we say that the vector space $\frac{\ker v_p}{\text{Im } v_{p+1}}$ is the **p -th homology group** (or homology group in degree p) of $\mathcal{C}$. We use the symbol $H_p(\mathcal{C})$ to denote such a vector space.

As we will see in the following, for any geometric simplicial complex K a chain complex $\mathcal{C}(K)$ can be easily defined.

Definition 40. If X is a set, a **formal linear combination** of elements of X with coefficients in a field $\mathbb{K}$ is a finitely supported function $f : X \rightarrow \mathbb{K}$. The set of all such functions is a vector space with respect to the usual sum of functions and the usual multiplication by elements of the field $\mathbb{K}$.

Each formal linear combination f of elements of X with coefficients in a field $\mathbb{K}$ is usually represented in the form $\sum_{i=1}^k a_i x_i$, where

each x_i belongs to X and each coefficient a_i equals $f(x_i)$. The null function (i.e., the trivial formal linear combination) is often represented by the symbol $\mathbf{0}$.

Definition 41. Let K be a geometric simplicial complex. For every integer p with $0 \leq p \leq \dim K$, we can consider the vector space $C_p(K)$ of all formal linear combinations $\sum_{i=1}^k a_i \sigma_i$ of p -simplexes of K with coefficients in $\mathbb{Z}_2$ (for any positive integer k). If $p < 0$ or $p > \dim K$, we set $C_p(K) := \mathbf{0}$ (i.e., the trivial vector space over $\mathbb{Z}_2$).

In the following, if a p -simplex $\langle u_0, \dots, u_p \rangle$ is given for $p > 0$, we will set $\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle := \text{conv}(\{u_0, \dots, u_p\} \setminus \{u_i\})$.

Proposition 13. Let K be a geometric simplicial complex. For each $p \in \mathbb{Z}$ with $0 < p \leq \dim K$, let us consider the homomorphism $\partial_p : C_p(K) \rightarrow C_{p-1}(K)$ that takes each p -simplex $\langle u_0, \dots, u_p \rangle$ to the vector $\sum_{i=0}^p \langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle$. If $p \leq 0$ or $p > \dim K$, we set $\partial_p : C_p(K) \rightarrow C_{p-1}(K)$ equal to the null homomorphism. The sequence $\mathcal{C}(K) := (C_p(K), \partial_p)_{p \in \mathbb{Z}}$ is a chain complex.

Proof. The statement $\partial_{p-1} \circ \partial_p \equiv \mathbf{0}$ is trivial for $p \leq 0$ and for $p > \dim K$. Therefore, we can assume that $0 < p \leq \dim K$. We have just to prove that $\partial_{p-1} \circ \partial_p(\sigma)$ is the null chain, for every $p \in \mathbb{Z}$ and every p -simplex $\sigma = \langle u_0, \dots, u_p \rangle$ of K . Let us define the symbol σ_{ij} by setting

$$\sigma_{ij} := \begin{cases} \langle u_0, \dots, \hat{u}_i, \dots, \hat{u}_j, \dots, u_p \rangle, & \text{if } i < j \\ \text{null chain in } C_{p-2}(K), & \text{if } i \geq j. \end{cases}$$

We have that

$$\begin{aligned} \partial_{p-1} \circ \partial_p(\sigma) &= \partial_{p-1} \left(\sum_{i=0}^p \langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle \right) \\ &= \sum_{i=0}^p \partial_{p-1} (\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle) \\ &= \sum_{i=0}^p \left(\sum_{j=0}^{i-1} \langle u_0, \dots, \hat{u}_j, \dots, \hat{u}_i, \dots, u_p \rangle + \sum_{j=i+1}^p \langle u_0, \dots, \hat{u}_i, \dots, \hat{u}_j, \dots, u_p \rangle \right) \\ &= \sum_{i=0}^p \left(\sum_{j=0}^{i-1} \sigma_{ji} + \sum_{j=i+1}^p \sigma_{ij} \right) \\ &= \sum_{i=0}^p \left(\sum_{j=0}^p \sigma_{ji} + \sum_{j=0}^p \sigma_{ij} \right) \\ &= \sum_{i=0}^p \sum_{j=0}^p \sigma_{ji} + \sum_{i=0}^p \sum_{j=0}^p \sigma_{ij} \\ &= \sum_{i=0}^p \sum_{j=0}^p \sigma_{ij} + \sum_{i=0}^p \sum_{j=0}^p \sigma_{ij} \\ &= \mathbf{0} \end{aligned}$$

where the last equality follows from the fact that $\mathbb{K} = \mathbb{Z}_2$. $\square$

In the following, for any given geometric simplicial complex K and every $p \in \mathbb{Z}$ we will use the symbols $Z_p(K)$, $B_p(K)$ and $H_p(K)$ to denote $Z_p(\mathcal{C}(K)) = \ker \partial_p$, $B_p(\mathcal{C}(K)) = \text{Im } \partial_{p+1}$ and the p -th homology group $H_p(\mathcal{C}(K)) = \frac{\ker \partial_p}{\text{Im } \partial_{p+1}}$, respectively. The vector space $H_p(K)$ is called the *p -th homology group of K with coefficients in $\mathbb{Z}_2$* . Moreover, we will set

- $n_p(K) := \dim C_p(K)$ (= number of p -simplexes in K , for $p \neq -1$, and 0 for $p = -1$);
- $z_p(K) := \dim Z_p(K)$;
- $b_p(K) := \dim B_p(K)$;
- $\beta_p(K) := \dim H_p(K)$.

The number $\beta_p(K)$ will be called the p -th *Betti number* of K . We observe that $\text{card } C_p(K) = 2^{n_p(K)}$, and $H_p(K)$ is isomorphic to $\sum_{i=1}^{\beta_p(K)} \mathbb{Z}_2$ (where the empty sum is set equal to $\mathbf{0}$).

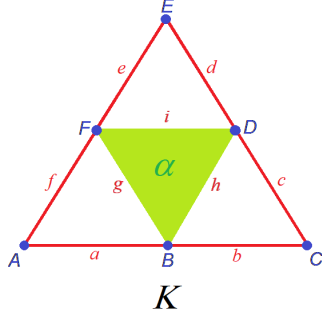
Proposition 14. *If K is a geometric simplicial complex, then $\beta_p(K) = n_p(K) - b_p(K) - b_{p-1}(K)$ for any $p \in \mathbb{Z}$.*

Proof. Let us consider the dimensional equations for the linear maps $\partial_p : C_p(K) \rightarrow C_{p-1}(K)$ and $\pi_p : Z_p(K) \rightarrow H_p(K) = \frac{Z_p(K)}{B_p(K)}$, where π_p is the quotient projection map. They respectively state that $n_p(K) = z_p(K) + b_{p-1}(K)$ and $z_p(K) = b_p(K) + \beta_p(K)$. Our thesis immediately follows from these two equalities. $\square$

Since $H_p(K)$ is isomorphic to $\sum_{i=1}^{\beta_p(K)} \mathbb{Z}_2$, the computation of homology groups over the field $\mathbb{Z}_2$ reduces to compute Betti numbers. The equality $\beta_p(K) = n_p(K) - b_p(K) - b_{p-1}(K)$ shows that the computation of Betti numbers reduces to compute the values b_p , i.e., $\dim \text{Im } \partial_{p+1}$. For $0 \leq p \leq \dim K - 1$, the value b_p equals the rank of the matrix associated with the linear map ∂_{p+1} with respect to any bases of $C_{p+1}(K)$ and $C_p(K)$. We observe that the natural bases for these vector spaces are respectively given by the sets of all $(p+1)$ -simplexes and all p -simplexes in K .

Remark 8. *Since $B_p(K) \subseteq C_p(K)$ for any index p , and $C_p(K)$ is the null space for every $p < 0$ and every $p > \dim K$, it follows that $b_p(K) = 0$ for every $p < 0$ and every $p > \dim K$. Moreover, since $C_{\dim K+1}(K)$ is the null space, $b_{\dim K}(K) := \dim \partial_{\dim K+1}(C_{\dim K+1}(K)) = 0$. Therefore, $b_p(K) = 0$ for every $p < 0$ and every $p \geq \dim K$.*

Example 3. Let us compute the homology groups of the geometric simplicial complex represented in Figure 21. We will call $A_{p+1}(K)$ the matrix associated with the linear map ∂_{p+1} with respect to the natural bases of $C_{p+1}(K)$ and $C_p(K)$. The natural ordered bases of $C_0(K)$, $C_1(K)$ and $C_2(K)$ are respectively (A, B, C, D, E, F) , $(a, b, c, d, e, f, g, h, i)$ and (α) .

Figure 21: The complex K in Example 3.

We have that $n_0(K) = 6$, $n_1(K) = 9$, $n_2(K) = 1$, and $n_p(K) = 0$ for every $p < 0$ and every $p > 2$. Let us now compute the matrixes $A_1(K)$ and $A_2(K)$:

$$A_1(K) = \begin{pmatrix} a & b & c & d & e & f & g & h & i \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \end{pmatrix} \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix}$$

$$A_2(K) = \begin{pmatrix} \alpha \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{matrix}$$

We can easily check that $\text{rank } A_1(K) = 5$ and $\text{rank } A_2(K) = 1$. Therefore, $b_0(K) = 5$ and $b_1(K) = 1$. Moreover, $b_p(K) = 0$ for every $p < 0$ and every $p \geq 2$ because of Remark 8. Hence

- $\beta_0(K) = n_0(K) - b_0(K) - b_{-1}(K) = 6 - 5 - 0 = 1$;
- $\beta_1(K) = n_1(K) - b_1(K) - b_0(K) = 9 - 1 - 5 = 3$;

- $\beta_2(K) = n_2(K) - b_2(K) - b_1(K) = 1 - 0 - 1 = 0$;
- $\beta_p(K) = n_p(K) - b_p(K) - b_{p-1}(K) = 0 - 0 - 0 = 0$ for $b \neq 0, 1, 2$.

It follows that $H_0(K) \cong \mathbb{Z}_2$, $H_1(K) \cong \mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2$ and $H_p(K) \cong \mathbf{0}$ for $p \neq 0, 1$.

Computation of bases for $Z_p(K)$, $B_p(K)$ and $H_p(K)$

Let K be a geometric simplicial complex. A method to compute bases for the vector spaces $Z_p(K)$, $B_p(K)$ and $H_p(K)$ consists in the following steps:

1. For every index p with $1 \leq p \leq \dim K$, compute the matrix A_p associated with the homomorphism ∂_p , with respect to the standard bases of the vector spaces $C_p(K)$ and $C_{p-1}(K)$. Label each column of A_p with the corresponding vector in the basis of $C_p(K)$.
2. For every index p with $1 \leq p \leq \dim K$, by means of a finite sequence of elementary column operations, transform A_p into its reduced column echelon form R_p . Each time you apply an elementary column operation, apply the same operation also to the labels of the columns. Now, the labels of the null columns represent a basis $\mathcal{B}_{Z_p(K)}$ of $Z_p(K)$. The $(p-1)$ -chains in $C_{p-1}(K)$ whose coordinates are given by the non-null columns of R_p are a basis $\mathcal{B}_{B_p(K)}$ for $B_p(K)$.
3. For every index p with $0 \leq p \leq \dim K$, build a matrix M_p whose first $b_p(K)$ columns are the columns of the coordinates of the vectors in $\mathcal{B}_{B_p(K)}$, while the remaining $z_p(K)$ columns are the columns of the coordinates of the vectors in $\mathcal{B}_{Z_p(K)}$. Call $\hat{M}_p$ the submatrix of M_p containing the first $b_p(K)$ columns of M_p .
4. Add some of the columns of $\hat{M}_p$ to some of the last $z_p(K)$ columns of M_p until the new matrix M'_p does not contain units in the cells belonging to the rows of the pivot elements in $\hat{M}_p$. Observe that now the last $z_p(K)$ columns of M'_p may be linearly dependent. However, if two columns in this set are different from each other, then they represent different elements of $H_p(K)$, since the difference between them cannot contain units at the positions corresponding to pivots in $\hat{M}_p$, and hence it cannot be a boundary. Furthermore, the equivalence classes represented by these columns are a system of generators for $H_p(K)$.
5. By means of a finite sequence of elementary column operations involving only the last $z_p(K)$ columns of M'_p , transform M'_p into a new matrix M''_p where the last $z_p(K)$ columns are in column

echelon form. The equivalence classes of the $(p - 1)$ -chains in $C_{p-1}(K)$ whose coordinates are given by the non-null columns among the last $z_p(K)$ columns in M_p'' are a basis $\mathcal{B}_{H_p(K)}$ for $H_p(K)$.

Example 4. Let us apply the algorithm previously described to the geometric simplicial complex considered in Example 3.

1. Computation of A_p :

$$A_1(K) = \begin{pmatrix} a & b & c & d & e & f & g & h & i \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \end{pmatrix} \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix}$$

$$A_2(K) = \begin{pmatrix} \alpha \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{matrix}$$

2. Reduction of $A_1(K)$ and $A_2(K)$ to their respective column echelon forms $R_1(K)$ and $R_2(K)$:

$$R_1(K) = \begin{pmatrix} a & b & c & d & e & a+b+c+d+e+f & b+c+d+e+g & b+c+h & d+e+i \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix}$$

Therefore, $\mathcal{B}_{Z_1(K)} = \{a + b + c + d + e + f, b + c + d + e + g, b + c + h, d + e + i\}$ and $\mathcal{B}_{B_0(K)} = \{A + B, B + C, C + D, D + E, E + F\}$.

$$R_2(K) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{matrix}$$

Therefore, $\mathcal{B}_{Z_2(K)} = \emptyset$ and $\mathcal{B}_{B_1(K)} = \{g + h + i\}$.

3. Computation of M_p (remember that $Z_0(K) = C_0(K)$):

$$M_0(K) = \begin{pmatrix} \textcircled{1} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix}$$

The first $b_0(K)$ columns are colored in red. These are the columns of $\hat{M}_0$.
The pivots in $\hat{M}_0$ are circled.

$$M_1(K) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ \textcircled{1} & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{matrix}$$

The first $b_1(K)$ columns are colored in red. These are the columns of $\hat{M}_1$.
The pivot in $\hat{M}_1$ is circled.

4. Computation of M'_p :

$$M'_0(K) = \begin{pmatrix} \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix}$$

$$M'_1(K) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ \textcircled{1} & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{pmatrix} \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{matrix}$$

5. Computation of M''_p :

$$M''_0(K) = \begin{pmatrix} \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \textcircled{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} A \\ B \\ C \\ D \\ E \\ F \end{matrix}$$

Therefore, $\mathcal{B}_{H_0(K)} = \{[F]\}$.

$$M''_1(K) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \textcircled{1} & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \end{pmatrix} \begin{matrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{matrix}$$

Therefore, $\mathcal{B}_{H_1(K)} = \{[a + f + h + i], [b + c + h], [d + e + i]\}$.

Exercise 11. Choose a geometric simplicial complex and compute its homology groups.

Exercise 12. Choose a geometric simplicial complex and compute the bases of its homology groups.

Chain maps

Definition 42. Let $\mathcal{U} = (U_p, u_p)_{p \in \mathbb{Z}}$ and $\mathcal{V} = (V_p, v_p)_{p \in \mathbb{Z}}$ be two chain complexes. An indexed family of homomorphisms $\varphi = (\varphi_p : U_p \rightarrow V_p)_{p \in \mathbb{Z}}$ is called a **chain map** from $\mathcal{U}$ to $\mathcal{V}$ if $v_p \circ \varphi_p = \varphi_{p-1} \circ u_p$ for every index p . If each homomorphism φ_p is an isomorphism, we say that φ is an **isomorphism between chain complexes**.

$$\begin{array}{ccc}
U_p & \xrightarrow{u_p} & U_{p-1} \\
\downarrow \varphi_p & \square & \downarrow \varphi_{p-1} \\
V_p & \xrightarrow{v_p} & V_{p-1}
\end{array}$$

Figure 22: According to the definition of chain map, this diagram must commute. We express this by inserting a square in the diagram.

The importance of the concept of chain map is given by the next proposition.

Proposition 15. Let $\varphi = (\varphi_p : U_p \rightarrow V_p)_{p \in \mathbb{Z}}$ be a chain map from $\mathcal{U} = (U_p, u_p)_{p \in \mathbb{Z}}$ to $\mathcal{V} = (V_p, v_p)_{p \in \mathbb{Z}}$. Then each map $\varphi_{p*} : H_p(\mathcal{U}) \rightarrow H_p(\mathcal{V})$ defined by setting $\varphi_{p*}([z]) := [\varphi_p(z)]$ is a well defined homomorphism for every $p \in \mathbb{Z}$. If φ is an isomorphism between chain complexes, then each map $\varphi_{p*} : H_p(\mathcal{U}) \rightarrow H_p(\mathcal{V})$ is an isomorphism.

Proof. Each element of $H_p(\mathcal{U})$ can be represented as $[z]$, where z is a p -cycle, i.e., $u_p(z) = \mathbf{0}$. First of all, $v_p(\varphi_p(z)) = \varphi_{p-1}(u_p(z)) = \varphi_{p-1}(\mathbf{0}) = \mathbf{0}$, and hence $\varphi_p(z) \in Z_p(\mathcal{V})$. Therefore, $\varphi_p(z)$ identifies an element $[\varphi_p(z)]$ of $H_p(\mathcal{V})$. Furthermore, if $[z'] = [z]$ we have that $z' - z$ is a p -boundary, i.e., a $(p+1)$ -chain $c \in U_{p+1}$ exists, such that $z' - z = u_{p+1}(c)$. It follows that $\varphi_p(z') - \varphi_p(z) = \varphi_p(z' - z) = \varphi_p(u_{p+1}(c)) = v_{p+1}(\varphi_{p+1}(c))$, and hence $\varphi_p(z') - \varphi_p(z)$ is a p -boundary. This implies that $[\varphi_p(z')] = [\varphi_p(z)]$ in $H_p(\mathcal{V})$. Therefore, the map φ_{p*} is well defined. The linearity of φ_{p*} immediately follows from the linearity of φ_p . If φ is an isomorphism from $\mathcal{U}$ to $\mathcal{V}$ and $[z] \in H_p(\mathcal{U})$, then we can easily check that $\varphi^{-1} = (\varphi_p^{-1} : V_p \rightarrow U_p)_{p \in \mathbb{Z}}$ is a chain map from $\mathcal{V}$ to $\mathcal{U}$. Furthermore, $(\varphi_p^{-1})_* \circ \varphi_{p*}([z]) = [\varphi_p^{-1} \circ \varphi_p(z)] = [z]$, and hence φ_{p*} is an isomorphism, for every index $p \in \mathbb{Z}$. $\square$

Definition 43. Let $\varphi = (\varphi_p : U_p \rightarrow V_p)_{p \in \mathbb{Z}}$ be a chain map from $\mathcal{U}$ to $\mathcal{V}$. The indexed family of homomorphisms $\varphi_* = (\varphi_{p*} : H_p(\mathcal{U}) \rightarrow H_p(\mathcal{V}))_{p \in \mathbb{Z}}$ defined in Proposition 15 is called an **induced map** from $H(\mathcal{U}) := (H_p(\mathcal{U}))_{p \in \mathbb{Z}}$ to $H(\mathcal{V}) := (H_p(\mathcal{V}))_{p \in \mathbb{Z}}$.

Proposition 16. Let $f : K \rightarrow L$ be a simplicial map. For every index $p \in \mathbb{Z}$ with $0 \leq p \leq \dim K$, let us consider the linear map $f_{p\#} : C_p(K) \rightarrow C_p(L)$ defined by setting, for every p -simplex $\sigma \in K$,

$$f_{p\#}(\sigma) := \begin{cases} f(\sigma), & \text{if } \dim f(\sigma) = \dim \sigma \\ \text{null chain in } C_p(L), & \text{if } \dim f(\sigma) < \dim \sigma. \end{cases}$$

For $p < 0$ and for $p > \dim K$ we set $f_{p\#} : C_p(K) \rightarrow C_p(L)$ equal to the null map. The collection of maps $f_{\#} = (f_{p\#} : C_p(K) \rightarrow C_p(L))_{p \in \mathbb{Z}}$ is a chain map from $\mathcal{C}(K)$ to $\mathcal{C}(L)$.

Proof. We have just to prove that $f_{(p-1)\#}(\partial_p(\sigma)) = \partial_p(f_{p\#}(\sigma))$ for every index p with $1 \leq p \leq \dim K$ and every p -simplex $\sigma = \langle u_0, \dots, u_p \rangle$ in K . We can indeed observe that such an equality is trivial for $p \leq 0$ and for $p > \dim K$. Before proceeding, we recall that the points $f(u_0), \dots, f(u_p)$ are (possibly coinciding) vertexes of a simplex τ in L , because of the definition of a simplicial map. The following cases are possible:

$\text{card } \{f(u_0), \dots, f(u_p)\} = p + 1$. In this case the points $f(u_0), \dots, f(u_p)$ are distinct vertexes of a simplex in L and $\dim f(\sigma) = \dim \sigma$. Moreover,

$$\begin{aligned} f_{(p-1)\#}(\partial_p(\sigma)) &= f_{(p-1)\#} \left(\sum_{i=0}^p \langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle \right) \\ &= \sum_{i=0}^p f_{(p-1)\#} (\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle) \\ &= \sum_{i=0}^p \langle f(u_0), \dots, \widehat{f(u_i)}, \dots, f(u_p) \rangle \\ &= \partial_p (\langle f(u_0), \dots, f(u_p) \rangle) \\ &= \partial_p \circ f_{p\#}(\sigma). \end{aligned}$$

$\text{card } \{f(u_0), \dots, f(u_p)\} = p$ In this case exactly two of the points $f(u_0), \dots, f(u_p)$ coincide (say $f(u_r)$ and $f(u_s)$), and $\dim f(\sigma) = \dim \sigma - 1$. Therefore, $f_{(p-1)\#}(\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle) = \mathbf{0}$ for $i \notin \{r, s\}$, since in this case two of the points $f(u_0), \dots, \widehat{f(u_i)}, \dots, f(u_p)$ coincide. For the same reason, $f_{p\#}(\langle u_0, \dots, u_p \rangle) = \mathbf{0}$. We also observe that $\langle f(u_0), \dots, \widehat{f(u_r)}, \dots, f(u_p) \rangle = \langle f(u_0), \dots, \widehat{f(u_s)}, \dots, f(u_p) \rangle$. It follows that

$$\begin{aligned} f_{(p-1)\#}(\partial_p(\sigma)) &= f_{(p-1)\#} \left(\sum_{i=0}^p \langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle \right) \\ &= \sum_{i=0}^p f_{(p-1)\#} (\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle) \\ &= \langle f(u_0), \dots, \widehat{f(u_r)}, \dots, f(u_p) \rangle + \langle f(u_0), \dots, \widehat{f(u_s)}, \dots, f(u_p) \rangle \\ &= \mathbf{0} \\ &= \partial_p(\mathbf{0}) \\ &= \partial_p(f_{p\#}(\langle u_0, \dots, u_p \rangle)) \\ &= \partial_p(f_{p\#}(\sigma)). \end{aligned}$$

$\text{card } \{f(u_0), \dots, f(u_p)\} < p$ In this case $\dim f(\sigma) < \dim \sigma - 1$

and for any choice of i at least two of the points $f(u_0), \dots, \widehat{f(u_i)}, \dots, f(u_p)$ coincide. Hence, $f_{p\#}(\langle u_0, \dots, u_p \rangle) = \mathbf{0}$, and $f_{(p-1)\#}(\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle) = \mathbf{0}$ for any index i . It follows that

$$\begin{aligned} f_{(p-1)\#}(\partial_p(\sigma)) &= f_{(p-1)\#} \left(\sum_{i=0}^p \langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle \right) \\ &= \sum_{i=0}^p f_{(p-1)\#}(\langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle) \\ &= \mathbf{0} \\ &= \partial_p(\mathbf{0}) \\ &= \partial_p(f_{p\#}(\langle u_0, \dots, u_p \rangle)) \\ &= \partial_p(f_{p\#}(\sigma)). \end{aligned}$$

Therefore, the equality $f_{(p-1)\#}(\partial_p(\sigma)) = \partial_p(f_{p\#}(\sigma))$ holds in any case. $\square$

The following theorem states one of the most important properties of homology.

Theorem 6. *The map F_p taking each geometric simplicial complex K to $H_p(K)$ and each simplicial map $f : K \rightarrow L$ to the map $f_{p\#} : H_p(K) \rightarrow H_p(L)$ (induced by the chain map $f_{p\#}$ defined in Proposition 16) is a co-variant functor for every $p \in \mathbb{Z}$.*

Proof. First of all, let us prove that if $f : K \rightarrow L$ and $g : L \rightarrow M$ are simplicial maps, and $p \in \mathbb{Z}$, then $(g \circ f)_{p\#} = g_{p\#} \circ f_{p\#}$. This equality is trivial for $p < 0$ and for $p > \dim K$, hence we can assume that $0 \leq p \leq \dim K$. It will be sufficient to prove that for each p -simplex $\sigma = \langle u_0, \dots, u_p \rangle$ in K , the equality $(g \circ f)_{p\#}(\sigma) = g_{p\#}(f_{p\#}(\sigma))$ holds. Since $\dim \sigma \geq \dim f(\sigma) \geq \dim g(f(\sigma))$, there are four possibilities:

1. $\dim \sigma = \dim f(\sigma) = \dim g(f(\sigma))$. In this case $(g \circ f)_{p\#}(\sigma) = (g \circ f)(\sigma) = g(f(\sigma)) = g_{p\#}(f_{p\#}(\sigma)) = g_{p\#} \circ f_{p\#}(\sigma)$.
2. $\dim \sigma > \dim f(\sigma) = \dim g(f(\sigma))$. In this case $f_{p\#}(\sigma) = \mathbf{0}$ and $(g \circ f)_{p\#}(\sigma) = \mathbf{0}$. Hence $(g \circ f)_{p\#}(\sigma) = \mathbf{0} = g_{p\#}(\mathbf{0}) = g_{p\#}(f_{p\#}(\sigma)) = g_{p\#} \circ f_{p\#}(\sigma)$.
3. $\dim \sigma = \dim f(\sigma) > \dim g(f(\sigma))$. In this case $g_{p\#}(f(\sigma)) = \mathbf{0}$ and $(g \circ f)_{p\#}(\sigma) = \mathbf{0}$. Hence $(g \circ f)_{p\#}(\sigma) = \mathbf{0} = g_{p\#}(f(\sigma)) = g_{p\#}(f_{p\#}(\sigma)) = g_{p\#} \circ f_{p\#}(\sigma)$.
4. $\dim \sigma > \dim f(\sigma) > \dim g(f(\sigma))$. In this case $f_{p\#}(\sigma) = \mathbf{0}$ and $(g \circ f)_{p\#}(\sigma) = \mathbf{0}$. Hence $(g \circ f)_{p\#}(\sigma) = \mathbf{0} = g_{p\#}(\mathbf{0}) = g_{p\#}(f_{p\#}(\sigma)) = g_{p\#} \circ f_{p\#}(\sigma)$.

Therefore, $(g \circ f)_{p\#} = g_{p\#} \circ f_{p\#}$ in any case. Because of this equality, if $[z] \in H_p(K)$, then

$$\begin{aligned}
 F_p(g \circ f)([z]) &= (g \circ f)_{p\#*}([z]) \\
 &= [(g \circ f)_{p\#}(z)] \\
 &= [g_{p\#} \circ f_{p\#}(z)] \\
 &= [g_{p\#}(f_{p\#}(z))] \\
 &= F_p(g)([f_{p\#}(z)]) \\
 &= F_p(g)(F_p(f)([z])) \\
 &= F_p(g) \circ F_p(f)([z]).
 \end{aligned}$$

Therefore, $F_p(g \circ f) = F_p(g) \circ F_p(f)$. Finally, if $\text{id} : K \rightarrow K$ is the identity, then $\text{id}_{p\#} : C_p(K) \rightarrow C_p(K)$ is the identity. It follows that $F_p(\text{id})([z]) = [\text{id}_{p\#}(z)] = [z]$ for every $[z] \in H_p(K)$, and hence $F_p(\text{id}) : H_p(K) \rightarrow H_p(K)$ is the identity. $\square$

The following result simplifies the computation of homology groups.

Theorem 7. *If a geometric simplicial complex L can be obtained from a geometric simplicial complex K by applying a sequence of elementary collapses and inverses of elementary collapses, then $H_p(L)$ is isomorphic to $H_p(K)$ for every $p \in \mathbb{Z}$.*

Proof. It is sufficient to prove that $H_p(L)$ is isomorphic to $H_p(K)$ in the case that L can be obtained from K by applying an elementary collapse involving the pair (τ, σ) , where $\tau = \langle v_1, \dots, v_k \rangle$ is a $(k-1)$ -simplex whose only coface is $\sigma = \langle v_0, \dots, v_k \rangle$.

Let us consider the inclusion $\psi : \text{Vert } L \rightarrow \text{Vert } K$. If $k > 1$, then ψ is a bijection. In any case, ψ is a **vertex map**. (We observe that, even if ψ^{-1} exists, it may not be a vertex map.) Let $g : L \rightarrow K$ be the simplicial map induced by ψ , i.e, the inclusion of L into K . We will show that the homomorphism $g_{p\#*} = F_p(g) : H_p(L) \rightarrow H_p(K)$ is bijective, and hence an isomorphism. In the following, if z is a p -cycle in L (K), we will denote by $[z]_L$ ($[z]_K$) the equivalence class of z in $H_p(L)$ ($H_p(K)$).

$g_{p\#*}$ is surjective Let $[z]_K \in H_p(K)$. Of course, z is a p -cycle in K .

If $p \notin \{k-1, k\}$, then z is also a p -cycle in L . Since $g_{p\#}(z) = z$, then $g_{p\#*}([z]_L) = [g_{p\#}(z)]_K = [z]_K$.

If $p = k-1$, then $z = \sum_{j=1}^m \lambda_j \tau_j + a\tau \in C_p(K)$, for suitable values $\lambda_1, \dots, \lambda_m, a \in \mathbb{Z}_2$ and $(k-1)$ -simplexes $\tau_1, \dots, \tau_m \in L$. Let us consider the p -chain $\tilde{z} = \sum_{j=1}^m \lambda_j \tau_j + a \sum_{r=1}^k \langle v_0, \dots, \hat{v}_r, \dots, v_k \rangle \in C_p(L)$. Since $\tau = \langle v_0, v_1, \dots, v_k \rangle$, then $\tilde{z} - z = a\partial\sigma$ (remember that the coefficients we are considering belong to $\mathbb{Z}_2$). Therefore,

$\partial\tilde{z} = \partial z + a\partial\partial\sigma = \mathbf{0}$ (i.e., $\tilde{z}$ is a cycle), and $[\tilde{z}]_K = [z]_K$. Moreover, $g_{p\#}(\tilde{z}) = \tilde{z}$, and hence $g_{p\#*}([\tilde{z}]_L) = [g_{p\#}(\tilde{z})]_K = [\tilde{z}]_K = [z]_K$.

If $p = k$, then the chain z cannot contain σ as a summand, because otherwise ∂z should contain τ as a summand, and hence z could not be a cycle. It follows that z is a cycle in L . Since $g_{p\#}(z) = z$, then $g_{p\#*}([z]_L) = [g_{p\#}(z)]_K = [z]_K$.

Therefore, in any case $[z]_K$ is the image by $g_{p\#*}$ of an element of $H_p(L)$.

$g_{p\#*}$ is injective Let $[z]_L \in H_p(L)$, with $g_{p\#*}([z]_L) = \mathbf{0} \in H_p(K)$.

Of course, z is a p -cycle in L and $g_{p\#}(z) = z$ is a p -boundary in K . Therefore, we can write $z = \partial\gamma$ for a suitable $\gamma \in C_{p+1}(K)$.

If $p+1 \notin \{k-1, k\}$, then $C_{p+1}(K) = C_{p+1}(L)$, and hence z is a p -boundary in L too. Therefore, $[z]_L = \mathbf{0} \in H_p(L)$.

If $p+1 = k-1$, then $\gamma = \sum_{j=1}^m \mu_j \tau_j + b\tau \in C_{p+1}(K)$, for suitable values $\mu_1, \dots, \mu_m, b \in \mathbb{Z}_2$ and $(k-1)$ -simplexes $\tau_1, \dots, \tau_m \in L$. Let us consider the $(p+1)$ -chain $\tilde{\gamma} = \sum_{j=1}^m \mu_j \tau_j + b \sum_{r=1}^k \langle v_0, \dots, \hat{v}_r, \dots, v_k \rangle \in C_{p+1}(L)$. Since $\tau = \langle \hat{v}_0, v_1, \dots, v_k \rangle$, then $\tilde{\gamma} - \gamma = b\partial\sigma$. Therefore, $\partial\tilde{\gamma} = \partial\gamma + b\partial\partial\sigma = \partial\gamma$. Hence, $\partial\tilde{\gamma} = \partial\gamma = z$. It follows that z is a p -boundary not only in K , but also in L , and hence $[z]_L = \mathbf{0} \in H_p(L)$.

If $p+1 = k$, then the chain γ cannot contain σ as a summand, because otherwise $z = \partial\gamma$ should contain τ as a summand, against the assumption $z \in C_p(L)$. Therefore, $\gamma \in C_{p+1}(L)$. Since $z = \partial\gamma$, then $[z]_L = \mathbf{0} \in H_p(L)$.

It follows that, in any case, $g_{p\#*}([z]_L) = \mathbf{0} \in H_p(K)$ implies that $[z]_L = \mathbf{0} \in H_p(L)$.

□

Reduced homology

The reader can observe that the chain complex we have used to define the homology groups of a geometric simplicial complex K is a little weird: while we assume that K contains the (-1) -dimensional simplex $\emptyset$, we have set $C_{-1}(K)$ equal to the trivial vector space, and the 0-boundary map equal to the null map. This choice has some important consequences. For example, we get that if K is trivial (in the sense that it contains only one vertex), then $H_0(K)$ is not trivial, while any other homology group is trivial. Moreover, while $\dim H_p(K)$ counts the “number of p -dimensional holes in K ” for $p \neq 0$, $\dim H_0(K)$ counts the “number of connected components in K ” (this number differs by one unit from the “number of

0-dimensional holes in K ", i.e., "gaps between connected components"). These asymmetries can be removed if we consider a new chain complex and the corresponding "reduced homology".

Definition 44. Let K be a geometric simplicial complex. For every integer p with $-1 \leq p \leq \dim K$, we can consider the vector space $\tilde{C}_p(K)$ of all formal linear combinations $\sum_{i=1}^k a_i \sigma_i$ of p -simplexes of K with coefficients in $\mathbb{Z}_2$ (for any positive integer k). If $p < -1$ or $p > \dim K$, we set $\tilde{C}_p(K) := \mathbf{0}$ (i.e., the trivial vector space over $\mathbb{Z}_2$).

NB: For $p \neq -1$, $\tilde{C}_p(K) = C_p(K)$, while $\tilde{C}_{-1}(K) \cong \mathbb{Z}_2 \neq \mathbf{0} = C_{-1}(K)$.

Proposition 17. Let K be a geometric simplicial complex. For each $p \in \mathbb{Z}$ with $1 \leq p \leq \dim K$, let us consider the homomorphism $\tilde{\partial}_p : \tilde{C}_p(K) \rightarrow \tilde{C}_{p-1}(K)$ that takes each p -simplex $\langle u_0, \dots, u_p \rangle$ to the vector $\sum_{i=0}^p \langle u_0, \dots, \hat{u}_i, \dots, u_p \rangle$. We set $\tilde{\partial}_0 : \tilde{C}_0(K) \rightarrow \tilde{C}_{-1}(K)$ equal to the homomorphism that takes each 0-simplex of K to the (-1) -simplex $\emptyset \in \tilde{C}_{-1}(K)$ (seen as a (-1) -chain). If $p < 0$ or $p > \dim K$, we set $\tilde{\partial}_p : \tilde{C}_p(K) \rightarrow \tilde{C}_{p-1}(K)$ equal to the null homomorphism. The sequence $\tilde{C}(K) := (\tilde{C}_p(K), \tilde{\partial}_p)_{p \in \mathbb{Z}}$ is a chain complex.

Proof. Since $\tilde{\partial}_p \equiv \partial_p$ for $p \neq 0, -1$, because of Proposition 13 we can limit ourselves to prove that both $\tilde{\partial}_{-1} \circ \tilde{\partial}_0$ and $\tilde{\partial}_0 \circ \tilde{\partial}_1$ are null homomorphisms. On the one hand, the map $\tilde{\partial}_{-1} \circ \tilde{\partial}_0$ is null because $\tilde{\partial}_{-1}$ is null. On the other hand, if $\sigma = \langle v_0, v_1 \rangle$ is a 1-simplex in K , then $\tilde{\partial}_0 \circ \tilde{\partial}_1(\sigma) = \tilde{\partial}_0(v_0 + v_1) = \tilde{\partial}_0(v_0) + \tilde{\partial}_0(v_1) = \emptyset + \emptyset = \mathbf{0}$. It follows that $\tilde{\partial}_0 \circ \tilde{\partial}_1$ is the null map. $\square$

NB: The homomorphism $\tilde{\partial}_0$ is called *augmentation map* and often denoted by the symbol ϵ . For $p \neq 0, -1$, we have that $\tilde{\partial}_p \equiv \partial_p$. We will use the symbols $\tilde{Z}_p(K)$ and $\tilde{B}_p(K)$ to denote the vector spaces $Z_p(\tilde{C}(K)) = \ker \tilde{\partial}_p$ and $B_p(\tilde{C}(K)) = \text{Im } \tilde{\partial}_{p+1}$, respectively. We observe that $\tilde{Z}_p(K) = Z_p(K)$ for $p \neq 0, -1$, and $\tilde{B}_p(K) = B_p(K)$ for $p \neq -1$.

In the following, for any given geometric simplicial complex K and every $p \in \mathbb{Z}$ we will use the symbol $\tilde{H}_p(K)$ to denote the vector space $H_p(\tilde{C}(K)) = \frac{\ker \tilde{\partial}_p}{\text{Im } \tilde{\partial}_{p+1}}$. We will call $\tilde{H}_p(K)$ the p -th *reduced homology group* of K with coefficients in $\mathbb{Z}_2$. Moreover, we will set

- $\tilde{n}_p(K) := \dim \tilde{C}_p(K)$ = number of p -simplexes in K (for any integer p);
- $\tilde{z}_p(K) := \dim \tilde{Z}_p(K)$;
- $\tilde{b}_p(K) := \dim \tilde{B}_p(K)$;
- $\tilde{\beta}_p(K) := \dim \tilde{H}_p(K)$.

The number $\tilde{\beta}_p(K)$ will be called the p -th *reduced Betti number* of K . We observe that $\text{card } \tilde{C}_p(K) = 2^{\tilde{n}_p(K)}$, and $\tilde{H}_p(K)$ is isomorphic to $\sum_{i=1}^{\tilde{\beta}_p(K)} \mathbb{Z}_2$ (where the empty sum is set equal to $\mathbf{0}$). We stress that $\dim \tilde{B}_{-1}(K) = 1$ and $\dim B_{-1}(K) = 0$, since $\tilde{B}_{-1}(K)$ is generated by the (-1) -simplex $\emptyset$, while $B_{-1}(K) = \mathbf{0}$.

Proposition 18. *If K is a geometric simplicial complex, then $\tilde{\beta}_p(K) = \tilde{n}_p(K) - \tilde{b}_p(K) - \tilde{b}_{p-1}(K)$ for any $p \in \mathbb{Z}$.*

Proof. Completely analogous to the one of Proposition 14. $\square$

Proposition 19. *If K is a geometric simplicial complex, then $\tilde{\beta}_p(K) = \beta_p(K)$ for every $p \neq 0$, and $\tilde{\beta}_0(K) = \beta_0(K) - 1$.*

Proof. For $p \neq 0, -1$, the equality $\tilde{\beta}_p(K) = \beta_p(K)$ follows from Propositions 14 and 18, by recalling that $\tilde{n}_p(K) = n_p(K)$ and $\tilde{b}_p = b_p$ for $p \neq -1$. Moreover, since $b_0(K) = \tilde{b}_0(K)$, $b_{-1}(K) = 0$ and $\tilde{b}_{-1}(K) = 1$, we have that $\tilde{\beta}_0(K) = \tilde{n}_0(K) - \tilde{b}_0(K) - \tilde{b}_{-1}(K) = n_0(K) - b_0(K) - b_{-1}(K) - 1 = \beta_0(K) - 1$. $\square$

The reader could wonder why we defined non-reduced homology groups, given that reduced homology groups have better properties. The reason is that non-reduced homology groups are of use for Poincaré Duality (a topic not illustrated in these lecture notes).

Exercise 13. *Choose a geometric simplicial complex and compute its reduced homology groups.*

Exercise 14. *Prove or disprove this statement: For every ordered $(n+1)$ -tuple $(a_0, \dots, a_n)$ of natural numbers, there exists a geometric simplicial complex K of dimension n , such that $\tilde{\beta}_p(K) = a_p$ for $p \in \{0, \dots, n\}$ and $\tilde{\beta}_p(K) = 0$ for $p \notin \{0, \dots, n\}$.*

Euler-Poincaré Theorem

Theorem 8. *If K is a geometric simplicial complex, then $\chi(K) = \sum_{p=0}^{\dim K} (-1)^p \beta_p(K)$.*

Proof. Proposition 14 states that $\beta_p(K) = n_p(K) - b_p(K) - b_{p-1}(K)$. From this equality and the equalities $b_{\dim K}(K) = b_{-1}(K) = 0$, it follows that

$$\begin{aligned} & \sum_{p=0}^{\dim K} (-1)^p \beta_p(K) \\ &= \sum_{p=0}^{\dim K} (-1)^p n_p(K) - \sum_{p=0}^{\dim K} (-1)^p b_p(K) - \sum_{p=0}^{\dim K} (-1)^p b_{p-1}(K) \\ &= \sum_{p=0}^{\dim K} (-1)^p n_p(K) - \sum_{p=0}^{\dim K} (-1)^p b_p(K) - \sum_{q=-1}^{\dim K-1} (-1)^{q+1} b_q(K) \end{aligned}$$

$$\begin{aligned}
&= \sum_{p=0}^{\dim K} (-1)^p n_p(K) - \sum_{p=0}^{\dim K} (-1)^p b_p(K) + \sum_{q=-1}^{\dim K-1} (-1)^q b_q(K) \\
&= \sum_{p=0}^{\dim K} (-1)^p n_p(K) - (-1)^{\dim K} b_{\dim K}(K) - b_{-1}(K) \\
&= \sum_{p=0}^{\dim K} (-1)^p n_p(K) \\
&= \chi(K).
\end{aligned}$$

□

The natural pseudo-distance

In this chapter, we introduce the concept of the natural pseudo-distance (restricted to the case of simplicial complexes) and illustrate its fundamental properties.

Perception pairs and topological groups

Let us consider a geometric simplicial complex K and a set Φ of bounded functions from $V = \text{Vert } K$ to $\mathbb{R}$. Φ is a metric space with respect to the distance D_Φ defined by setting $D_\Phi(\varphi, \psi) = \|\varphi - \psi\|_\infty := \max_{v \in V} |\varphi(v) - \psi(v)|$. The functions in Φ will be called *admissible functions* or *admissible measurements* or *admissible signals*, and represent the data that can be produced by the measuring tools or the observers we are interested in. The set V is endowed with the (extended) pseudo-metric D_V which distinguishes points only if they are seen as different by some measurement:

$$D_V(v_1, v_2) = \sup_{\varphi \in \Phi} |\varphi(v_1) - \varphi(v_2)| \quad (1)$$

for every $v_1, v_2 \in V$. We recall that a *pseudo-metric* is just a distance d without the property that $d(a, b) = 0$ implies $a = b$. We say that a pseudo-metric is *extended* if it can take an infinite value. We observe that every function $\varphi \in \Phi$ is nonexpansive with respect to D_V .

In the following, we will denote by $\text{Iso}_\Phi(K)$ the set of all bijections $g : V \rightarrow V$ such that:

1. If $v_0, \dots, v_k$ are vertexes of a k -simplex of K , then $g(v_0), \dots, g(v_k)$ and $g^{-1}(v_0), \dots, g^{-1}(v_k)$ are also vertexes of k -simplexes of K .
2. $\varphi \circ g, \varphi \circ g^{-1} \in \Phi$ for every $\varphi \in \Phi$.

The set $\text{Iso}_\Phi(K)$ is a group with respect to the composition of maps, called the group of *Φ -preserving isomorphisms* of K .

Definition 45. If G is a subgroup of $\text{Iso}_\Phi(K)$, we say that (Φ, G) is a *perception pair*.

In some sense, considering a perception pair (Φ, G) means that G represents a set of data transformations that are relevant for our analysis. If V is a bounded pseudo-metric space with respect to D_V , then the group G is a pseudo-metric space with respect to the pseudo-metric D_G defined by setting

$$D_G(g_1, g_2) := \sup_{\varphi \in \Phi} D_\Phi(\varphi \circ g_1, \varphi \circ g_2) \quad (2)$$

for every $g_1, g_2 \in G$.

We observe that

$$\begin{aligned} D_G(g_1, g_2) &= \sup_{\varphi \in \Phi} D_\Phi(\varphi \circ g_1, \varphi \circ g_2) \\ &= \sup_{\varphi \in \Phi} \max_{v \in V} |\varphi(g_1(v)) - \varphi(g_2(v))| \\ &= \max_{v \in V} \sup_{\varphi \in \Phi} |\varphi(g_1(v)) - \varphi(g_2(v))| \\ &= \max_{v \in V} D_V(g_1(v), g_2(v)). \end{aligned}$$

Exercise 15. Prove that D_V and D_G are indeed pseudo-metrics.

We leave the simple proof of the following proposition to the reader.

Proposition 20. The following statements hold:

1. $D_\Phi(\varphi_1 \circ g, \varphi_2 \circ g) = D_\Phi(\varphi_1, \varphi_2)$ for every $\varphi_1, \varphi_2 \in \Phi$ and $g \in G$;
2. $D_V(g(v_1), g(v_2)) = D_V(v_1, v_2)$ for every $v_1, v_2 \in V$ and $g \in G$;
3. $D_G(g_1 \circ g, g_2 \circ g) = D_G(g_1, g_2)$ for every $g_1, g_2, g \in G$.

Exercise 16. Prove Proposition 20.

We recall that a *right action* of a group $(\hat{G}, \star)$ on a set $\hat{\Phi}$ is a map $\alpha : \hat{\Phi} \times \hat{G} \rightarrow \hat{\Phi}$ such that the following two properties hold:

1. $\alpha(\varphi, e) = \varphi$ for any $\varphi \in \hat{\Phi}$ (where e is the unit of $\hat{G}$);
2. $\alpha(\alpha(\varphi, g_1), g_2) = \alpha(\varphi, g_1 \star g_2)$ for any $\varphi \in \hat{\Phi}$ and any $g_1, g_2 \in \hat{G}$.

In our setting G acts on Φ by right composition: $\alpha(\varphi, g) := \varphi \circ g$ for every $\varphi \in \Phi$ and every $g \in G$.

Natural pseudo-distance with respect to a group G

Let us assume that (Φ, G) is a perception pair and call V the domain of the functions in Φ .

Definition 46. The function $d_G : \Phi \times \Phi \rightarrow \mathbb{R}$ defined by setting $d_G(\varphi_1, \varphi_2) := \min_{g \in G} \|\varphi_1 - \varphi_2 \circ g\|_\infty$ is called the **natural pseudo-distance** associated with the perception pair (Φ, G) (or simply with the group G , in the case the set Φ is understood).

Proposition 21. The function d_G is a pseudo-metric.

Proof. 1. $0 \leq d_G(\varphi, \varphi) := \min_{g \in G} \|\varphi - \varphi \circ g\|_\infty \leq \|\varphi - \varphi \circ \text{id}_{\text{Vert } K}\|_\infty = \|\varphi - \varphi\|_\infty = 0$, and hence $d_G(\varphi, \varphi) = 0$ for every $\varphi \in \Phi$.

2. From Proposition 20 it follows that $d_G(\varphi_1, \varphi_2) := \min_{g \in G} \|\varphi_1 - \varphi_2 \circ g\|_\infty = \min_{g \in G} \|\varphi_1 \circ g^{-1} - \varphi_2\|_\infty = \min_{g \in G} \|\varphi_2 - \varphi_1 \circ g^{-1}\|_\infty = \min_{g^{-1} \in G} \|\varphi_2 - \varphi_1 \circ g^{-1}\|_\infty = \min_{g \in G} \|\varphi_2 - \varphi_1 \circ g\|_\infty = d_G(\varphi_2, \varphi_1)$ for every $\varphi_1, \varphi_2 \in \Phi$.

3. Proposition 20 implies that for $\varphi_1, \varphi_2 \in \Phi$ and every fixed $f \in G$

$$\begin{aligned} d_G(\varphi_1, \varphi_2) &:= \min_{g \in G} \|\varphi_1 - \varphi_2 \circ g\|_\infty \\ &= \min_{g \in G} \|\varphi_1 - \varphi_2 \circ g \circ f\|_\infty \\ &\leq \min_{g \in G} (\|\varphi_1 - \varphi_3 \circ f\|_\infty + \|\varphi_3 \circ f - \varphi_2 \circ g \circ f\|_\infty) \\ &= \min_{g \in G} (\|\varphi_1 - \varphi_3 \circ f\|_\infty + \|\varphi_3 - \varphi_2 \circ g\|_\infty) \\ &= \|\varphi_1 - \varphi_3 \circ f\|_\infty + \min_{g \in G} \|\varphi_3 - \varphi_2 \circ g\|_\infty \\ &= \|\varphi_1 - \varphi_3 \circ f\|_\infty + d_G(\varphi_3, \varphi_2). \end{aligned}$$

It follows that for every $\varphi_1, \varphi_2, \varphi_3 \in \Phi$

$$\begin{aligned} d_G(\varphi_1, \varphi_2) &= \min_{f \in G} d_G(\varphi_1, \varphi_2) \\ &\leq \min_{f \in G} (\|\varphi_1 - \varphi_3 \circ f\|_\infty + d_G(\varphi_3, \varphi_2)) \\ &= \min_{f \in G} \|\varphi_1 - \varphi_3 \circ f\|_\infty + d_G(\varphi_3, \varphi_2) \\ &= d_G(\varphi_1, \varphi_3) + d_G(\varphi_3, \varphi_2). \end{aligned}$$

□

If G is the trivial group Id_V , then $d_G = D_\Phi$. Moreover, if G_1 and G_2 are subgroups of $\text{Iso}_\Phi(K)$ and $G_1 \subseteq G_2$, then

$$d_{\text{Iso}_\Phi(K)}(\varphi_1, \varphi_2) \leq d_{G_2}(\varphi_1, \varphi_2) \leq d_{G_1}(\varphi_1, \varphi_2) \leq D_\Phi(\varphi_1, \varphi_2)$$

for every $\varphi_1, \varphi_2 \in \Phi$.

The direct computation of d_G is usually difficult, due to the size of G . In the section “*Non-expansive equivariant operators*” we will see that this difficulty can be worked around by means of persistent homology and the concept of group equivariant non-expansive operator.

The role of d_G in Topological Data Analysis

The key property of the natural pseudo-distance d_G is that it is strongly invariant under the action of the group G . More explicitly, $d_G(\varphi_1 \circ f, \varphi_2 \circ g) = d_G(\varphi_1, \varphi_2)$ for every $\varphi_1, \varphi_2 \in \Phi$ and every $f, g \in G$. This property is of great use when we wish to compare data “up to transformations in G ”.

Exercise 17. *Prove that the natural pseudo-distance d_G is strongly invariant under the action of the group G .*

Persistent homology

Let K be a simplicial complex. If a function $\varphi : \text{Vert } K \rightarrow \mathbb{R}$ is given, a filtration $K_t^\varphi := \{\sigma \in K : \varphi(v) \leq t \text{ for any vertex } v \text{ of } \sigma\}$ is defined, for $t \in \mathbb{R}$. We will think of t as a time. Note that K_t^φ is still a simplicial complex. After fixing a degree $p \in \mathbb{Z}$, for every ordered pair $(s, t) \in \mathbb{R}^2$ with $s \leq t$ we can consider the linear map $i_{s,t}^{\varphi*} : H_p(K_s^\varphi) \rightarrow H_p(K_t^\varphi)$ induced by the inclusion $i_{s,t}^\varphi : K_s^\varphi \rightarrow K_t^\varphi$ (in practice, $i_{s,t}^{\varphi*}$ takes the homology class of a cycle in K_s^φ to the homology class of the same cycle in K_t^φ).

Definition 47. A **persistence module** is a set $\{V_t\}_{t \in \mathbb{R}}$ of vector spaces on $\mathbb{Z}_2$, such that for every ordered pair $(s, t) \in \mathbb{R}^2$ with $s \leq t$ there exists a linear map $v_{s,t} : V_s \rightarrow V_t$ for which $v_{t,t} = \text{id}_{V_t} : V_t \rightarrow V_t$ and $v_{s,t} \circ v_{r,s} = v_{r,t}$ for $r \leq s \leq t$.

In the following, the symbol $i_{s,\infty}^{\varphi*}$ will represent the map induced by the inclusion of K_s^φ into $K = K_{\max \varphi}^\varphi = K_\infty^\varphi$. The functoriality of homology (Theorem 6) implies that $i_{v,w}^{\varphi*} \circ i_{u,v}^{\varphi*} = i_{u,w}^{\varphi*}$ for $u \leq v \leq w$. Therefore, the maps $i_{s,t}^{\varphi*}$ define a persistence module.

1-dimensional PBNFs

Definition 48 (Persistent homology group). For $u \in \mathbb{R}$, $v \in \mathbb{R} \cup \{\infty\}$ with $u < v$, the group $\text{Im } i_{u,v}^{\varphi*} \subseteq H_p(K_v^\varphi)$ is denoted by the symbol $H_p^\varphi(u, v)$ and called the **pth persistent homology group** at (u, v) . The dimension $\beta_p^\varphi(u, v)$ of $H_p^\varphi(u, v)$ is called the **pth persistent Betti numbers function** (PBNF) (or **rank invariant**) of φ , computed at the point (u, v) ³.

Remark 9. We observe that $K_v^\varphi = K_{\max \varphi}^\varphi = K_\infty^\varphi$, and hence $\beta_p^\varphi(\cdot, v) \equiv \beta_p^\varphi(\cdot, \max \varphi) \equiv \beta_p^\varphi(\cdot, \infty)$, for every $v \geq \max \varphi$.

Remark 10. We observe that $\beta_p^\varphi(u, v) \leq \dim H_p(K_v^\varphi) \leq \text{card } \left(K_v^\varphi\right)^{(p)} \leq \text{card } K < \infty$.

Proposition 22. The function $\beta_p^\varphi(u, v)$ is right-continuous in both its variables.

³ Herbert Edelsbrunner, David Letscher, and Afra Zomorodian. Topological persistence and simplification. *Discrete Comput. Geom.*, 28(4):511–533, 2002

Proof. For each $v \in \mathbb{R}$ an $\varepsilon > 0$ exists such that if $v \leq v' \leq v + \varepsilon$ then $K_{v'}^\varphi = K_v^\varphi$. This implies that $i_{v,v'}^\varphi$ is the identity. Therefore, $\beta_p^\varphi(u, v') = \text{Im } i_{u,v'}^{\varphi*} = \text{Im } i_{v,v'}^{\varphi*} \circ i_{u,v}^{\varphi*} = \text{Im } i_{u,v}^{\varphi*} = \beta_p^\varphi(u, v)$. This proves that $\beta_p^\varphi(u, v)$ is right-continuous in the variable v .

Analogously, For each $u \in \mathbb{R}$ an $\varepsilon > 0$ exists such that if $u \leq u' \leq u + \varepsilon$ then $K_{u'}^\varphi = K_u^\varphi$. This implies that $i_{u,u'}^\varphi$ is the identity. Therefore, $\beta_p^\varphi(u, v) = \text{Im } i_{u,v}^{\varphi*} = \text{Im } i_{u',v}^{\varphi*} \circ i_{u,u'}^{\varphi*} = \text{Im } i_{u',v}^{\varphi*} = \beta_p^\varphi(u', v)$. This proves that $\beta_p^\varphi(u, v)$ is right-continuous in the variable u . $\square$

The following statement holds.

Lemma 2. *Let U, V, W be finite dimensional vector spaces over the field $\mathbb{K}$. If $f : U \rightarrow V$ and $g : V \rightarrow W$ are linear maps, then the following equality holds: $\dim \text{Im } g \circ f = \dim \text{Im } f - \dim \ker g|_{\text{Im } f}$.*

Proof. The rank–nullity theorem applied to the linear map $g|_{\text{Im } f} : \text{Im } f \rightarrow W$ states that $\dim \text{Im } f = \dim \text{Im } g \circ f + \dim \ker g|_{\text{Im } f}$. $\square$

Proposition 23. *The function $\beta_p^\varphi(u, v)$ is nondecreasing in the variable u and nonincreasing in the variable v .*

Proof. If $u \leq u'$, then $i_{u,v}^{\varphi*} = i_{u',v}^{\varphi*} \circ i_{u,u'}^{\varphi*}$. This implies that $\text{Im } i_{u,v}^{\varphi*} \subseteq \text{Im } i_{u',v}^{\varphi*}$, i.e., $H_p^\varphi(u, v) \subseteq H_p^\varphi(u', v)$. Hence $\dim H_p^\varphi(u, v) \leq \dim H_p^\varphi(u', v)$. Moreover, by applying Lemma 2 for $f = i_{u,v}^{\varphi*}$ and $g = i_{v,v'}^{\varphi*}$ with $v' \geq v$ we get that $\dim \text{Im } i_{u,v'}^{\varphi*} \leq \dim \text{Im } i_{u,v}^{\varphi*}$, i.e., $\dim H_p^\varphi(u, v') \leq \dim H_p^\varphi(u, v)$. $\square$

Hereafter, the symbol Δ denotes the diagonal $\{(u, v) \in \mathbb{R}^2 : u = v\}$, the symbol Δ^+ denotes the half-plane $\{(u, v) \in \mathbb{R}^2 : u < v\}$, while Δ^* is the set $\Delta^+ \cup \{(u, \infty) : u \in \mathbb{R}\}$. The finiteness of K implies that the vector spaces $H_p(K_t^\varphi)$ are finitely generated for every time t . This fact guarantees that $\beta_p^\varphi(u, v) < \infty$ for every $(u, v) \in \Delta^*$. Hereafter, we will assume that a degree $p \in \mathbb{Z}$ has been chosen, and that the symbols $\varepsilon, \eta, \varepsilon', \eta'$ refer to finite values.

The following result illustrates an interesting invariance property of the persistent Betti numbers functions, in the case that $g : K \rightarrow L$ is an isomorphism between two simplicial complexes (i.e. a bijective map such that both it and its inverse take vertexes of simplexes to vertexes of simplexes). We consider the filtrations K_t^φ and $L_t^{\varphi \circ g^{-1}}$.

Proposition 24. $\beta_p^\varphi \equiv \beta_p^{\varphi \circ g^{-1}}$ for every isomorphism $g : K \rightarrow L$.

Proof. It is sufficient to consider the chain map $g_{p\#} : C_p(K) \rightarrow C_p(L)$ induced by g (Proposition 16) and check that it is an isomorphism between chain complexes. From Proposition 15 it follows that the linear map $g_{p\#*} : H_p(K) \rightarrow H_p(L)$ taking each homology class $\left[\sum_{i=1}^k \sigma_i \right]$ to the homology class $\left[\sum_{i=1}^k g \circ \sigma_i \right]$ is an isomorphism.

Since $i_{x,y}^{\varphi \circ g^{-1}*} \circ g_{p\#*} = g_{p\#*} \circ i_{x,y}^{\varphi*}$, the map $\rho : H_p^\varphi(u, v) \rightarrow H_p^{\varphi \circ g^{-1}}(u, v)$ taking $i_{x,y}^{\varphi*}([z])$ to $i_{x,y}^{\varphi \circ g^{-1}*}(g_{p\#*}([z]))$ is an isomorphism, for every pair $(u, v) \in \Delta^+$. $\square$

Definition 49. Let $\varepsilon \geq 0, \eta \geq 0$, and $u < v < \infty$. If $u + \varepsilon < v - \eta$, we define $\mu_{\varepsilon, \eta}^\varphi(u, v) := \beta_p^\varphi(u + \varepsilon, v - \eta) - \beta_p^\varphi(u - \varepsilon, v - \eta) - \beta_p^\varphi(u + \varepsilon, v + \eta) + \beta_p^\varphi(u - \varepsilon, v + \eta)$. If $u + \varepsilon \geq v - \eta$, we define $\mu_{\varepsilon, \eta}^\varphi(u, v) := \infty$. The value $\mu_{\varepsilon, \eta}^\varphi(u, v)$ will be called the **total multiplicity of the (ε, η) -box centered at (u, v)** .

The next proposition shows that the value $\mu_{\varepsilon, \eta}^\varphi(u, v)$ is always nonnegative.

Proposition 25. If $\varepsilon \geq 0, \eta \geq 0$, and $u + \varepsilon < v - \eta < \infty$, $\mu_{\varepsilon, \eta}^\varphi(u, v) = \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*}} - \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*}} \geq 0$.

Proof. By applying Lemma 2 for $f = i_{u+\varepsilon, v-\eta}^{\varphi*}$ and $g = i_{v-\eta, v+\eta}^{\varphi*}$ we get

$$\dim \text{Im } i_{u+\varepsilon, v+\eta}^{\varphi*} = \dim \text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*} - \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*}}.$$

By applying Lemma 2 for $f = i_{u-\varepsilon, v-\eta}^{\varphi*}$ and $g = i_{v-\eta, v+\eta}^{\varphi*}$ we get

$$\dim \text{Im } i_{u-\varepsilon, v+\eta}^{\varphi*} = \dim \text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*} - \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*}}.$$

It follows that

$$\begin{aligned} \mu_{\varepsilon, \eta}^\varphi(u, v) &= \beta_p^\varphi(u + \varepsilon, v - \eta) - \beta_p^\varphi(u - \varepsilon, v - \eta) \\ &\quad - \beta_p^\varphi(u + \varepsilon, v + \eta) + \beta_p^\varphi(u - \varepsilon, v + \eta) \\ &= \dim \text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*} - \dim \text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*} \\ &\quad - \dim \text{Im } i_{u+\varepsilon, v+\eta}^{\varphi*} + \dim \text{Im } i_{u-\varepsilon, v+\eta}^{\varphi*} \\ &= \dim \text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*} - \dim \text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*} \\ &\quad - \dim \text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*} + \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*}} \\ &\quad + \dim \text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*} - \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*}} \\ &= \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*}} - \dim \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*}} \geq 0 \end{aligned}$$

where the last inequality follows from the inclusion

$$\text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*} = \text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*} \circ i_{u-\varepsilon, u+\varepsilon}^{\varphi*} \subseteq \text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*}$$

which implies

$$\ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u-\varepsilon, v-\eta}^{\varphi*}} \subseteq \ker i_{v-\eta, v+\eta}^{\varphi*} |_{\text{Im } i_{u+\varepsilon, v-\eta}^{\varphi*}}.$$

$\square$

In the following, unless otherwise specified, we will assume that $v < \infty$. The next proposition shows that the function $\mu_{\varepsilon,\eta}^\varphi(u, v)$ is non-decreasing in the variables ε and η .

Proposition 26. *If $0 \leq \varepsilon \leq \varepsilon'$, $0 \leq \eta \leq \eta'$ and $u < v$, then $\mu_{\varepsilon,\eta}^\varphi(u, v) \leq \mu_{\varepsilon',\eta'}^\varphi(u, v)$.*

Proof. If $u + \varepsilon' \geq v - \eta'$, then $\mu_{\varepsilon',\eta'}^\varphi(u, v) = \infty$, and in this case the statement of the proposition is trivial. Therefore, we can assume that $u + \varepsilon' < v - \eta'$. By directly applying Definition 49, it is easy to check that

$$\begin{aligned} & \mu_{\varepsilon',\eta'}^\varphi(u, v) \\ &= \mu_{\frac{\varepsilon'-\varepsilon}{2}, \frac{\eta'-\eta}{2}}^\varphi\left(u - \frac{\varepsilon + \varepsilon'}{2}, v + \frac{\eta + \eta'}{2}\right) + \mu_{\varepsilon, \frac{\eta'-\eta}{2}}^\varphi\left(u, v + \frac{\eta + \eta'}{2}\right) + \mu_{\frac{\varepsilon'-\varepsilon}{2}, \frac{\eta'-\eta}{2}}^\varphi\left(u + \frac{\varepsilon + \varepsilon'}{2}, v + \frac{\eta + \eta'}{2}\right) \\ &+ \mu_{\frac{\varepsilon'-\varepsilon}{2}, \eta}^\varphi\left(u - \frac{\varepsilon + \varepsilon'}{2}, v\right) + \color{red}{\mu_{\varepsilon, \eta}^\varphi(u, v)} + \mu_{\frac{\varepsilon'-\varepsilon}{2}, \eta}^\varphi\left(u + \frac{\varepsilon + \varepsilon'}{2}, v\right) \\ &+ \mu_{\frac{\varepsilon'-\varepsilon}{2}, \frac{\eta'-\eta}{2}}^\varphi\left(u - \frac{\varepsilon + \varepsilon'}{2}, v - \frac{\eta + \eta'}{2}\right) + \mu_{\varepsilon, \frac{\eta'-\eta}{2}}^\varphi\left(u, v - \frac{\eta + \eta'}{2}\right) + \mu_{\frac{\varepsilon'-\varepsilon}{2}, \frac{\eta'-\eta}{2}}^\varphi\left(u + \frac{\varepsilon + \varepsilon'}{2}, v - \frac{\eta + \eta'}{2}\right). \end{aligned}$$

From the nonnegativity of the function $\mu_{\varepsilon,\eta}^\varphi$ (Proposition 25), it follows that $\mu_{\varepsilon,\eta}^\varphi(u, v) \leq \mu_{\varepsilon',\eta'}^\varphi(u, v)$. $\square$

Let us explain the proof of Proposition 26 in plain words. The value $\mu_{\varepsilon,\eta}^\varphi(u, v)$ is equal to the sum of the values at the red points in Figure 23, with alternate signs. The value $\mu_{\varepsilon',\eta'}^\varphi(u, v)$ is equal to the sum of the values at the green points in Figure 23, with alternate signs. This last value is equal to the sum of the total multiplicities of the nine boxes in the figure since the contributions of the non-green points cancel each other out.

Lemma 3. *Any open arcwise connected neighborhood of a discontinuity point for the function $\beta_p^\varphi(u, v)$ contains at least one discontinuity point in the variable u or v .*

Proof. Let $p \in \mathbb{R}^2$ be a discontinuity point for the function $\beta_p^\varphi(p)$. Then, in any open arcwise connected neighborhood $U \subseteq \mathbb{R}^2$ of p , a point q exists such that $\beta_p^\varphi(p) \neq \beta_p^\varphi(q)$. We can connect p and q by a path entirely contained in U and made of horizontal and vertical segments. Since β_p^φ cannot be constant along this path, our claim follows. $\square$

Proposition 27 (Propagation of discontinuities). *The following statements hold:*

1. *If $\tilde{u}$ is a discontinuity point for $\beta_p^\varphi(\cdot, \tilde{v})$ and $\tilde{u} < v < \tilde{v} < \infty$, then $\tilde{u}$ is a discontinuity point also for $\beta_p^\varphi(\cdot, v)$;*

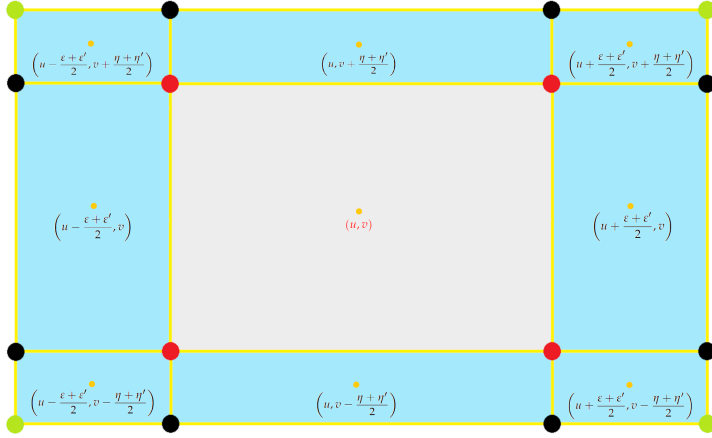


Figure 23: The grid used in the proof of Proposition 26.

2. If $\tilde{v}$ is a discontinuity point for $\beta_p^\varphi(\tilde{u}, \cdot)$ and $\tilde{u} < u < \tilde{v} < \infty$, then $\tilde{v}$ is a discontinuity point also for $\beta_p^\varphi(u, \cdot)$.

Proof. 1. Since β_p^φ is nondecreasing in its first variable, we have that $\beta_p^\varphi(\tilde{u} + \varepsilon, \tilde{v}) - \beta_p^\varphi(\tilde{u} - \varepsilon, \tilde{v}) \geq 0$ for any $\varepsilon \geq 0$ (Proposition 23). The assumption that $\tilde{u}$ is a discontinuity point for $\beta_p^\varphi(\cdot, \tilde{v})$ implies that $\beta_p^\varphi(\tilde{u} + \varepsilon, \tilde{v}) - \beta_p^\varphi(\tilde{u} - \varepsilon, \tilde{v}) > 0$ for any $\varepsilon > 0$. This last inequality and the inequality

$$\begin{aligned} & \beta_p^\varphi(\tilde{u} + \varepsilon, v) - \beta_p^\varphi(\tilde{u} - \varepsilon, v) \\ & - \beta_p^\varphi(\tilde{u} + \varepsilon, \tilde{v}) + \beta_p^\varphi(\tilde{u} - \varepsilon, \tilde{v}) \geq 0 \end{aligned}$$

(Proposition 25) imply that $\beta_p^\varphi(\tilde{u} + \varepsilon, v) - \beta_p^\varphi(\tilde{u} - \varepsilon, v) > 0$ for any $\varepsilon > 0$. It follows that $\tilde{u}$ is a discontinuity point also for $\beta_p^\varphi(\cdot, v)$;

2. Since β_p^φ is nonincreasing in its second variable, $\beta_p^\varphi(\tilde{u}, \tilde{v} + \varepsilon) - \beta_p^\varphi(\tilde{u}, \tilde{v} - \varepsilon) \leq 0$ for any $\varepsilon \geq 0$ (Proposition 23). The assumption that $\tilde{v}$ is a discontinuity point for $\beta_p^\varphi(\tilde{u}, \cdot)$ implies that $\beta_p^\varphi(\tilde{u}, \tilde{v} + \varepsilon) - \beta_p^\varphi(\tilde{u}, \tilde{v} - \varepsilon) < 0$ for any $\varepsilon > 0$. This last inequality and the inequality

$$\begin{aligned} & \beta_p^\varphi(u, \tilde{v} - \varepsilon) - \beta_p^\varphi(\tilde{u}, \tilde{v} - \varepsilon) \\ & - \beta_p^\varphi(u, \tilde{v} + \varepsilon) + \beta_p^\varphi(\tilde{u}, \tilde{v} + \varepsilon) \geq 0 \end{aligned}$$

(Proposition 25) imply that $\beta_p^\varphi(u, \tilde{v} - \varepsilon) - \beta_p^\varphi(\tilde{u}, \tilde{v} + \varepsilon) > 0$ for any $\varepsilon > 0$. It follows that $\tilde{v}$ is a discontinuity point also for $\beta_p^\varphi(u, \cdot)$. $\square$

Proposition 28. *For every point $\bar{p} = (\bar{u}, \bar{v}) \in \Delta^+$ an $\varepsilon > 0$ exists such that the open set*

$$V_\varepsilon(\bar{p}) := \{(u, v) \in \mathbb{R}^2 : |u - \bar{u}| < \varepsilon, |v - \bar{v}| < \varepsilon, u \neq \bar{u}, v \neq \bar{v}\}$$

is contained in Δ^+ and does not contain any discontinuity point for β_p^φ .

Proof. Suppose, contrary to our assertion, that for every positive integer n a discontinuity point $p_n = (u_n, v_n) \in V_{\frac{1}{n}}(\bar{p})$ exists. By applying Lemma 3, possibly by extracting a subsequence from (p_n) , we can assume that each p_n is a discontinuity point in either the u or v direction. In the following, we shall assume that each p_n is a discontinuity point in the variable u . The case in which each p_n is a discontinuity point in the variable v has a similar proof. Let us fix a natural number N that is so large that $\bar{u} + \frac{1}{N} < \bar{v} - \frac{1}{N}$, i.e., the sets $V_{\frac{1}{n}}(\bar{p})$ with $n \geq N$ lie entirely above the diagonal Δ . Let us consider the function $\beta_p^\varphi(\cdot, \bar{v} - \frac{1}{N}) :]\bar{u} - \frac{1}{N}, \bar{u} + \frac{1}{N}[\rightarrow \mathbb{N}$. From Proposition 27 we know that discontinuities in u spread downwards. Thus the function $\beta_p^\varphi(\cdot, \bar{v} - \frac{1}{N})$ should have an infinite number of integer jumps. Now, since $\beta_p^\varphi(u, v)$ is non-decreasing in the variable u (Proposition 23), this fact would imply that $\beta_p^\varphi(\bar{u} + \frac{1}{N}, \bar{v} - \frac{1}{N}) = \infty$, against the finiteness of β_p^φ (Remark 10). $\square$

Persistence diagrams and Representation Theorem

One of the main properties of the persistent Betti numbers functions is that they admit a simple and compact representation. Precisely, under our assumptions, it is possible to prove that each PBNF can be compactly described by a multiset of points, proper and at infinity, of the real plane ^{4, 5}. This multiset will be called a *persistence diagram*. Before proceeding, we need to recall the definition of a *multiset* and a *matching between multisets*.

Definition 50 (Multiset). A **multiset** is a function f from a set S to $\mathbb{N} \cup \{\infty\}$. If $s \in S$ and $f(s) > 0$, we say that s is an element of the multiset and its **multiplicity** is $f(s)$. The **realization of a multiset** f is the set $S_f := \{(s, n) \in S \times (\mathbb{N} \cup \{\infty\}) : 0 < n \leq f(s)\}$. A **finite multiset** is a multiset whose realization is a finite set.

Definition 51 (Map between multisets). Let $f_1 : S_1 \rightarrow \mathbb{N} \cup \{\infty\}$, $f_2 : S_2 \rightarrow \mathbb{N} \cup \{\infty\}$ be two multisets. Any map from S_{f_1} to S_{f_2} is called a **multiset map** from the multiset f_1 to the multiset f_2 .

Definition 52 (Matching between multisets). Let $f_1 : S_1 \rightarrow \mathbb{N} \cup \{\infty\}$, $f_2 : S_2 \rightarrow \mathbb{N} \cup \{\infty\}$ be two multisets. Any bijection from S_{f_1} to S_{f_2} is called a **matching** from the multiset f_1 to the multiset f_2 .

⁴ Andrea Cerri, Barbara Di Fabio, Massimo Ferri, Patrizio Frosini, and Claudia Landi. Betti numbers in multidimensional persistent homology are stable functions. *Math. Methods Appl. Sci.*, 36(12):1543–1557, 2013. ISSN 0170-4214. DOI: 10.1002/mma.2704. URL <http://dx.doi.org/10.1002/mma.2704>

⁵ David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Stability of persistence diagrams. *Discrete Comput. Geom.*, 37(1):103–120, 2007. ISSN 0179-5376. DOI: 10.1007/s00454-006-1276-5. URL <http://dx.doi.org/10.1007/s00454-006-1276-5>

However, for the sake of simplicity, we will often denote a finite multiset K with the standard notation $K = \{p_1, \dots, p_k\}$, assuming that each point p_j has a multiplicity m_j .

Set $\bar{\Delta}^* = \Delta^* \cup \{\Delta\}$, where Δ is the line $\{(u, v) \in \mathbb{R}^2 : u = v\}$. The nonnegativity of the function $\mu_{\varepsilon, \eta}^\varphi$ (Proposition 25) and Proposition 26 imply that the following definition is well given.

Definition 53 (Persistence diagram). *The **persistence diagram** $\text{Dgm}(\varphi)$ of the continuous function $\varphi : X \rightarrow \mathbb{R}$ is the multiset $f : \bar{\Delta}^* \rightarrow \mathbb{N} \cup \{\infty\}$ defined by setting, for every $p = (u, v) \in \bar{\Delta}^*$,*

$$f(p) := \begin{cases} \mu^\varphi(p) := \lim_{\varepsilon \rightarrow 0^+} \mu_{\varepsilon, \varepsilon}^\varphi(u, v), & \text{if } u < v < \infty \\ \nu^\varphi(p) := \lim_{\varepsilon \rightarrow 0^+} \beta_p^\varphi(u + \varepsilon, \infty) - \beta_p^\varphi(u - \varepsilon, \infty), & \text{if } u < v = \infty \\ \infty, & \text{if } p = \Delta. \end{cases}$$

Each element (u, v) of $\text{Dgm}(\varphi)$ with $u < v < \infty$ is called a **proper cornerpoint**. Each element (u, v) of $\text{Dgm}(\varphi)$ with $u < v = \infty$ is called a **cornerpoint at infinity** (or a **cornerline**, or an **essential cornerpoint**). The point Δ is called the **trivial cornerpoint**.

Proposition 29. $\text{Dgm}(\varphi) = \text{Dgm}(\varphi \circ g^{-1})$ for every isomorphism $g : K \rightarrow L$.

Proof. It immediately follows from Proposition 24 and the definition of persistence diagram. $\square$

The two following statements hold.

Proposition 30 (Position of proper cornerpoints). *If $p = (u, v) \in \text{Dgm}(\varphi)$ and $v < \infty$, then $u, v \in \varphi(V)$ (i.e., two vertexes $x, y \in V$ exist, such that $u = \varphi(x)$ and $v = \varphi(y)$). Consequently, the number of proper cornerpoints is finite.*

Proof. Since $\mu^\varphi(p) := \lim_{\varepsilon \rightarrow 0^+} \mu_{\varepsilon, \varepsilon}^\varphi(u, v) > 0$, a positive and arbitrarily small ε exists, such that $\beta_p^\varphi(u + \varepsilon, v - \varepsilon) - \beta_p^\varphi(u - \varepsilon, v - \varepsilon) - \beta_p^\varphi(u + \varepsilon, v + \varepsilon) + \beta_p^\varphi(u - \varepsilon, v + \varepsilon) > 0$. This implies that $\beta_p^\varphi(u + \varepsilon, v - \varepsilon) - \beta_p^\varphi(u + \varepsilon, v + \varepsilon) > \beta_p^\varphi(u - \varepsilon, v - \varepsilon) - \beta_p^\varphi(u - \varepsilon, v + \varepsilon) \geq 0$, and hence $\beta_p^\varphi(u + \varepsilon, v - \varepsilon) > \beta_p^\varphi(u + \varepsilon, v + \varepsilon)$. From Definition 48, it follows that $\dim \text{Im } i_{u+\varepsilon, v-\varepsilon}^{\varphi*} > \dim \text{Im } i_{u+\varepsilon, v+\varepsilon}^{\varphi*} = \dim \text{Im } (i_{v-\varepsilon, v+\varepsilon}^{\varphi*} \circ i_{u+\varepsilon, v-\varepsilon}^{\varphi*})$. As a consequence, $i_{v-\varepsilon, v+\varepsilon}^{\varphi*}$ is not an isomorphism, and hence the inclusion $i_{v-\varepsilon, v+\varepsilon}^\varphi : K_{v-\varepsilon}^\varphi \rightarrow K_{v+\varepsilon}^\varphi$ must be proper. Since ε is arbitrarily small, v must belong to $\varphi(V)$. Analogously, by observing that $\beta_p^\varphi(u + \varepsilon, v - \varepsilon) > \beta_p^\varphi(u - \varepsilon, v - \varepsilon)$ for an arbitrarily small $\varepsilon > 0$, we can show that $u \in \varphi(V)$. $\square$

Proposition 31 (Position of cornerpoints at infinity). *If $p = (u, \infty) \in \text{Dgm}(\varphi)$, then $u \in \varphi(V)$ (i.e., a vertex $x \in V$ exists, such that $u = \varphi(x)$). Consequently, the number of cornerpoints at infinity is finite.*

Proof. Since $v^\varphi(p) := \lim_{\varepsilon \rightarrow 0^+} \beta_p^\varphi(u + \varepsilon, \max \varphi) - \beta_p^\varphi(u - \varepsilon, \max \varphi) > 0$, a positive and arbitrarily small ε exists, such that $\beta_p^\varphi(u + \varepsilon, \max \varphi) > \beta_p^\varphi(u - \varepsilon, \max \varphi)$. From Definition 48, it follows that $\dim \operatorname{Im} i_{u+\varepsilon, \max \varphi}^{\varphi*} > \dim \operatorname{Im} i_{u-\varepsilon, \max \varphi}^{\varphi*} = \dim \operatorname{Im} (i_{u+\varepsilon, \max \varphi}^{\varphi*} \circ i_{u-\varepsilon, u+\varepsilon}^{\varphi*})$. As a consequence, $i_{u-\varepsilon, u+\varepsilon}^{\varphi*}$ is not an isomorphism, and hence the inclusion $i_{u-\varepsilon, u+\varepsilon}^\varphi : K_{u-\varepsilon}^\varphi \rightarrow K_{u+\varepsilon}^\varphi$ must be proper. Since ε is arbitrarily small, u must belong to $\varphi(V)$. $\square$

Proposition 32 (Propagation of discontinuities from cornerpoints). *If $\bar{p} = (\bar{u}, \bar{v}) \in \operatorname{Dgm}(\varphi)$, the following statements hold:*

1. *If $\bar{u} < v < \bar{v} < \infty$, then $\bar{u}$ is a discontinuity point for $\beta_p^\varphi(\cdot, v)$;*
2. *If $\bar{u} < u < \bar{v} < \infty$, then $\bar{v}$ is a discontinuity point for $\beta_p^\varphi(u, \cdot)$;*
3. *If $\bar{u} < v < \bar{v} = \infty$, then $\bar{u}$ is a discontinuity point for $\beta_p^\varphi(\cdot, v)$.*

Proof. 1. Because of Proposition 26, since $\bar{p} = (\bar{u}, \bar{v})$ is a proper cornerpoint in $\operatorname{Dgm}(\varphi)$, we have that

$$\begin{aligned} i) \quad & \beta_p^\varphi(\bar{u} + \eta, \bar{v} - \varepsilon) - \beta_p^\varphi(\bar{u} - \eta, \bar{v} - \varepsilon) \\ & - \beta_p^\varphi(\bar{u} + \eta, \bar{v} + \varepsilon) + \beta_p^\varphi(\bar{u} - \eta, \bar{v} + \varepsilon) > 0 \end{aligned}$$

for any small enough $\varepsilon > 0$ and any positive $\eta < \varepsilon$.

Since β_p^φ is nondecreasing in its first variable, we have that

$$ii) \quad \beta_p^\varphi(\bar{u} + \eta, \bar{v} + \varepsilon) - \beta_p^\varphi(\bar{u} - \eta, \bar{v} + \varepsilon) \geq 0$$

for any small enough $\varepsilon > 0$ and any positive $\eta < \varepsilon$ (Proposition 23).

From *i)* and *ii)* it follows that $\beta_p^\varphi(\bar{u} + \eta, \bar{v} - \varepsilon) - \beta_p^\varphi(\bar{u} - \eta, \bar{v} - \varepsilon) > 0$ for any small enough $\varepsilon > 0$ and any positive $\eta < \varepsilon$. It follows that $\bar{u}$ is a discontinuity point of $\beta_p^\varphi(\cdot, \bar{v} - \varepsilon)$ for any small enough $\varepsilon > 0$. Then Statement 1) in this proposition follows from Statement 1) in Proposition 27.

2. Because of Proposition 26, since $\bar{p} = (\bar{u}, \bar{v})$ is a proper cornerpoint in $\operatorname{Dgm}(\varphi)$, we have that

$$\begin{aligned} i) \quad & \beta_p^\varphi(\bar{u} + \varepsilon, \bar{v} - \eta) - \beta_p^\varphi(\bar{u} - \varepsilon, \bar{v} - \eta) \\ & - \beta_p^\varphi(\bar{u} + \varepsilon, \bar{v} + \eta) + \beta_p^\varphi(\bar{u} - \varepsilon, \bar{v} + \eta) > 0 \end{aligned}$$

for any small enough $\varepsilon > 0$ and any positive $\eta < \varepsilon$.

Since β_p^φ is nonincreasing in its second variable, we have that

$$ii) \quad \beta_p^\varphi(\bar{u} - \varepsilon, \bar{v} + \eta) - \beta_p^\varphi(\bar{u} - \varepsilon, \bar{v} - \eta) \leq 0$$

for any small enough $\varepsilon > 0$ and any positive $\eta < \varepsilon$ (Proposition 23).

From i) and ii) it follows that $\beta_p^\varphi(\bar{u} + \varepsilon, \bar{v} - \eta) - \beta_p^\varphi(\bar{u} + \varepsilon, \bar{v} + \eta) > 0$ for any small enough $\varepsilon > 0$ and any positive $\eta < \varepsilon$. It follows that $\bar{v}$ is a discontinuity point of $\beta_p^\varphi(\bar{u} + \varepsilon, \cdot)$ for any small enough $\varepsilon > 0$. Then Statement 2) in this proposition follows from Statement 2) in Proposition 27.

3. Since $\bar{p} = (\bar{u}, \infty)$ is an essential cornerpoint in $\text{Dgm}(\varphi)$, we have that $\beta_p^\varphi(\bar{u} + \varepsilon, \max \varphi) - \beta_p^\varphi(\bar{u} - \varepsilon, \max \varphi) > 0$ for any $\varepsilon > 0$. Because of Remark 9, if $v \geq \max \varphi$ then $\beta_p^\varphi(\bar{u} + \varepsilon, v) - \beta_p^\varphi(\bar{u} - \varepsilon, v) > 0$ for any $\varepsilon > 0$. It follows that for any $v \geq \max \varphi$, $\bar{u}$ is a discontinuity point of $\beta_p^\varphi(\cdot, v)$. Then Statement 3) in this proposition follows from Statement 1) in Proposition 27.

□

The following result completes the statement of Proposition 32, showing that each discontinuity of a PBNF “comes from a cornerpoint”.

Proposition 33 (All discontinuities come from cornerpoints). *The following statements hold:*

1. If $\bar{u} < \bar{v}$ is a discontinuity point for $\beta_p^\varphi(\cdot, \bar{v})$, then there exists at least one cornerpoint $(\bar{u}, v')$ (proper or at infinity) with $v' \geq \bar{v}$;
2. If $\bar{v} > \bar{u}$ is a discontinuity point for $\beta_p^\varphi(\bar{u}, \cdot)$, then there exists at least one proper cornerpoint $(u', \bar{v})$ with $u' \leq \bar{u}$;

Proof. 1. If $\lim_{\varepsilon \rightarrow 0^+} \beta_p^\varphi(\bar{u} + \varepsilon, \max \varphi) - \beta_p^\varphi(\bar{u} - \varepsilon, \max \varphi) > 0$, then $(\bar{u}, \infty)$ is a cornerpoint at infinity and hence property 1) holds. Therefore, we can assume that an $\bar{\varepsilon} > 0$ exists, such that $\beta_p^\varphi(\bar{u} + \varepsilon, \max \varphi) - \beta_p^\varphi(\bar{u} - \varepsilon, \max \varphi) = 0$ for any positive $\varepsilon \leq \bar{\varepsilon}$. Let us now consider the open cover $\mathcal{V} = \{V_p\}_{p \in c}$ of the closed segment c connecting the points $p_1 = (\bar{u}, \bar{v})$ and $p_2 = (\bar{u}, \max \varphi)$, where V_p is an open square centered at $p \in c$, with the sides parallel to the axes. If c does not contain cornerpoints, we can assume that $\mu_{\varepsilon(p), \varepsilon(p)}^\varphi(p) = 0$ for every $p \in c$, where $\varepsilon(p)$ is a suitable positive constant depending on p . Since c is compact, $\mathcal{V}$ admits a finite subcover $\{V_{p_1}, \dots, V_{p_n}\}$. Let us set $\varepsilon' := \min \varepsilon(p_i)$ and η' equal to half the length of c . From Proposition 25 and Proposition 26, it easily follows that $\mu_{\varepsilon', \eta'}^\varphi(\hat{p}) = \sum_{i=1}^n \mu_{\varepsilon(p_i), \varepsilon(p_i)}^\varphi(p_i) = 0$, where $\hat{p}$ is the middle point of c . This implies that

$$\begin{aligned} & \beta_p^\varphi(\bar{u} + \varepsilon', \bar{v}) - \beta_p^\varphi(\bar{u} - \varepsilon', \bar{v}) \\ &= \beta_p^\varphi(\bar{u} + \varepsilon', \max \varphi) - \beta_p^\varphi(\bar{u} - \varepsilon', \max \varphi) = 0, \end{aligned}$$

against the assumption that $\bar{u} < \bar{v}$ is a discontinuity point for $\beta_p^\varphi(\cdot, \bar{v})$.

2. We know that $\beta_p^\varphi(\min \varphi - 1, \bar{v} + \varepsilon) = \beta_p^\varphi(\min \varphi - 1, \bar{v} - \varepsilon) = 0$ for any positive ε . Let us now consider the open cover $\mathcal{V} = \{V_p\}_{p \in c}$ of the closed segment c connecting the points $p_1 = (\bar{u}, \bar{v})$ and $p_2 = (\min \varphi - 1, \bar{v})$, where V_p is an open square centered at $p \in c$, with the sides parallel to the axes. If c does not contain cornerpoints, we can assume that $\mu_{\varepsilon(p), \varepsilon(p)}^\varphi(p) = 0$ for every $p \in c$, where $\varepsilon(p)$ is a suitable positive constant depending on p . Since c is compact, $\mathcal{V}$ admits a finite subcover $\{V_{p_1}, \dots, V_{p_n}\}$. Let us set $\varepsilon' := \min \varepsilon(p_i)$ and η' equal to half the length of c . From Proposition 25 and Proposition 26, it easily follows that $\mu_{\varepsilon', \eta'}^\varphi(\hat{p}) = \sum_{i=1}^n \mu_{\varepsilon(p_i), \varepsilon(p_i)}^\varphi(p_i) = 0$, where $\hat{p}$ is the middle point of c . This implies that

$$\begin{aligned} & \beta_p^\varphi(\bar{u}, \bar{v} - \varepsilon') - \beta_p^\varphi(\min \varphi - 1, \bar{v} - \varepsilon') \\ &= \beta_p^\varphi(\bar{u}, \bar{v} + \varepsilon') - \beta_p^\varphi(\min \varphi - 1, \bar{v} + \varepsilon') = 0, \end{aligned}$$

i.e., $\beta_p^\varphi(\bar{u}, \bar{v} - \varepsilon') = \beta_p^\varphi(\bar{u}, \bar{v} + \varepsilon')$, against the assumption that $\bar{v} > \bar{u}$ is a discontinuity point for $\beta_p^\varphi(\bar{u}, \cdot)$. □

In the following we will need the next lemma, where the continuity of β_p^φ at $(\bar{u}, \infty)$ means the continuity of $\beta_p^\varphi(\cdot, \max \varphi)$ at $\bar{u}$. We recall that the sum over an empty set of indexes is defined to be equal to 0.

Lemma 4. *If $(\bar{u}, \infty) \in \Delta^*$, then $\beta_p^\varphi(\bar{u}, \infty) = \sum_{u \leq \bar{u}} \nu^\varphi(u, \infty)$.*

Proof. We can assume that $\text{Dgm}(\varphi)$ contains at least one cornerpoint at infinity with abscissa less than or equal to $\bar{u}$, otherwise our statement is trivial. Because of Propositions 30 and 31, we can find $u_0 < \dots < u_m$ such that

1. $u_0 < \min \varphi$ (and hence $K_{u_0}^\varphi = \emptyset$; moreover, because of Proposition 31, the abscissa of each cornerpoint at infinity of $\text{Dgm}(\varphi)$ is greater than u_0);
2. $u_m > \bar{u}$, and there is no essential cornerpoint (u, ∞) for β_p^φ having its abscissa in $]\bar{u}, u_m]$ (and hence, because of Proposition 33, no value in $]\bar{u}, u_m]$ is a discontinuity point of the function $\beta_p^\varphi(\cdot, \infty)$);
3. There is no essential cornerpoint for β_p^φ having its abscissa in $\{u_0, \dots, u_m\}$ (and hence, because of Proposition 33, no value u_i is a discontinuity point of the function $\beta_p^\varphi(\cdot, \infty)$);
4. Each open interval $]u_{i-1}, u_i[$ with $1 \leq i \leq m$, contains exactly one abscissa of a cornerpoint p_i at infinity (possibly endowed with a multiplicity greater than 1). If we set $\beta_i := \beta_p^\varphi(u_i, \infty)$ for any i with $0 \leq i \leq m$, we can write that $\nu^\varphi(p_i) = \beta_i - \beta_{i-1}$.

Due to assumption 1, $\beta_0 = 0$. Therefore

$$\begin{aligned}
 \sum_{u \leq \bar{u}} v^\varphi(u, \infty) &= \sum_{1 \leq i \leq m} v^\varphi(p_i) \\
 &= \sum_{1 \leq i \leq m} \beta_i - \beta_{i-1} \\
 &= \sum_{1 \leq i \leq m} \beta_i - \sum_{1 \leq i \leq m} \beta_{i-1} \\
 &= \sum_{1 \leq i \leq m} \beta_i - \sum_{0 \leq i \leq m-1} \beta_i \\
 &= \beta_m - \beta_0 \\
 &= \beta_m := \beta_p^\varphi(u_m, \infty) = \beta_p^\varphi(\bar{u}, \infty)
 \end{aligned}$$

because the function $\beta_p^\varphi(u, \infty)$ is right-continuous in the variable u (Proposition 22), and no value in $] \bar{u}, u_m]$ is a discontinuity point of the function $\beta_p^\varphi(\cdot, \infty)$. $\square$

The key role of persistence diagrams is shown in the following Representation Theorem^{6,7}, claiming that persistence diagrams uniquely determine 1-dimensional PBNFs (the converse also holds by definition of persistence diagram).

Theorem 9 (Representation Theorem). *If $(\bar{u}, \bar{v}) \in \Delta^+$, then*

$$\beta_p^\varphi(\bar{u}, \bar{v}) = \sum_{\substack{(u,v) \in \Delta^+ \\ u \leq \bar{u}, v > \bar{v}}} \mu^\varphi(u, v) + \sum_{u \leq \bar{u}} v^\varphi(u, \infty).$$

Proof. We can assume that $\text{Dgm}(\varphi)$ contains at least one proper cornerpoint (u', v') with $u' \leq \bar{u}$ and $v' > \bar{v}$, otherwise our statement is trivial because of Proposition 33 (implying $\beta_p^\varphi(\bar{u}, \bar{v}) = \beta_p^\varphi(\bar{u}, \infty)$) and Lemma 4. Propositions 30 and 31 guarantee that we can find $u_0 < \dots < u_m$ and $v_0 < \dots < v_n$ such that

1. $u_0 < \min \varphi$ (and hence $K_{u_0}^\varphi = \emptyset$; moreover, because of Proposition 31, the abscissa of each cornerpoint at infinity of $\text{Dgm}(\varphi)$ is greater than u_0);
2. $\bar{v} > u_m > \bar{u}$, and there is no (proper or essential) cornerpoint (u, v) for β_p^φ having its abscissa in $] \bar{u}, u_m]$, with $v \geq v_0$ (and hence, because of Proposition 33, no value in $] \bar{u}, u_m]$ is a discontinuity point of the function $\beta_p^\varphi(\cdot, v)$, for any $v \geq v_0$);
3. $v_0 > \bar{v}$, and there is no cornerpoint (u, v) for β_p^φ having its ordinate in $] \bar{v}, v_0]$, with $u \leq \bar{u}$ (and hence, because of Proposition 33, no value in $] \bar{v}, v_0]$ is a discontinuity point of the function $\beta_p^\varphi(u, \cdot)$, for any $u \leq \bar{u}$);
4. $v_n > \max \varphi$;

⁶ Andrea Cerri, Barbara Di Fabio, Massimo Ferri, Patrizio Frosini, and Claudia Landi. Betti numbers in multidimensional persistent homology are stable functions. *Math. Methods Appl. Sci.*, 36(12):1543–1557, 2013. ISSN 0170-4214. DOI: 10.1002/mma.2704. URL <http://dx.doi.org/10.1002/mma.2704>

⁷ David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Stability of persistence diagrams. *Discrete Comput. Geom.*, 37(1):103–120, 2007. ISSN 0179-5376. DOI: 10.1007/s00454-006-1276-5. URL <http://dx.doi.org/10.1007/s00454-006-1276-5>

5. There is no cornerpoint (and hence, because of Proposition 33, no discontinuity point) for β_p^φ having its abscissa in $\{u_0, \dots, u_m\}$;
6. There is no cornerpoint (and hence, because of Proposition 33, no discontinuity point) for β_p^φ having its ordinate in $\{v_0, \dots, v_n\}$;
7. For $1 \leq i \leq m, 1 \leq j \leq n$, each open rectangle R_i^j of vertexes $(u_i, v_{j-1}), (u_{i-1}, v_{j-1}), (u_i, v_j), (u_{i-1}, v_j)$ contains at most one cornerpoint p_i^j (possibly endowed with a multiplicity greater than 1). If we set $\beta_i^j := \beta_p^\varphi(u_i, v_j)$ for any i, j with $0 \leq i \leq m, 0 \leq j \leq n$, we can write that $\mu^\varphi(p_i^j) = \beta_i^{j-1} - \beta_{i-1}^{j-1} - \beta_i^j + \beta_{i-1}^j$. If R_i^j does not contain any cornerpoint, we set p_i^j equal to an arbitrarily chosen point in R_i^j (in this case $\mu^\varphi(p_i^j) = 0$).

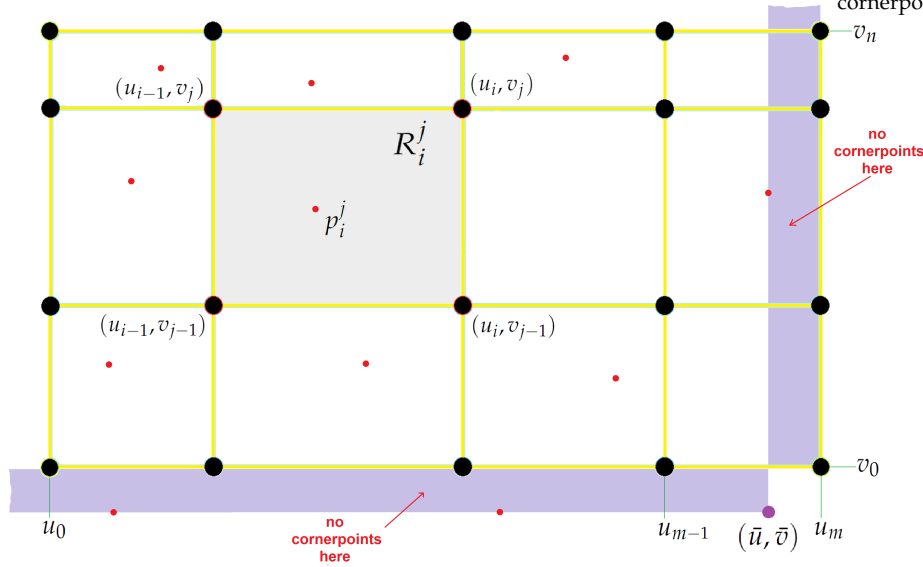


Figure 24: The grid used in the proof of Theorem 9. The red points are cornerpoints of $\text{Dgm}(\varphi)$.

Due to assumption 1, $\beta_0^j = 0$ for any index j . Moreover, by recalling that the function $\beta_p^\varphi(u, v)$ is right-continuous in the variable u and no value in $]\bar{u}, u_m]$ is a discontinuity point of the function $\beta_p^v(\cdot, v)$, for any $v \geq v_0$, Lemma 4 guarantees that $\beta_m^n = \beta_p^\varphi(u_m, v_n) = \beta_p^\varphi(\bar{u}, \infty) = \sum_{u \leq \bar{u}} \nu^\varphi(u, \infty)$. Furthermore, by recalling that (1) the function $\beta_p^\varphi(u, v)$ is right-continuous in both its variables, (2) no value in $]\bar{u}, u_m]$ is a discontinuity point of the function $\beta_p^v(\cdot, v)$, for any $v \geq v_0$, and (3) no value in $]v_0, \bar{v}]$ is a discontinuity point of the function $\beta_p^u(u, \cdot)$, for any $u \leq \bar{u}$, we obtain that $\beta_p^\varphi(u_m, v_0) = \beta_p^\varphi(\bar{u}, \bar{v})$. It

follows that

$$\begin{aligned}
\sum_{\substack{(u,v) \in \Delta^* \\ u \leq \bar{u}, v > \bar{v}}} \mu^\varphi(u,v) &= \sum_{\substack{(u,v) \in \Delta^* \\ u < u_m, v > v_0}} \mu^\varphi(u,v) \\
&= \sum_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \mu^\varphi(p_i^j) \\
&= \sum_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \beta_i^{j-1} - \sum_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \beta_{i-1}^{j-1} - \sum_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \beta_i^j + \sum_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \beta_{i-1}^j \\
&= \sum_{\substack{1 \leq i \leq m \\ 0 \leq j \leq n-1}} \beta_i^j - \sum_{\substack{0 \leq i \leq m-1 \\ 0 \leq j \leq n-1}} \beta_i^j - \sum_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \beta_i^j + \sum_{\substack{0 \leq i \leq m-1 \\ 1 \leq j \leq n}} \beta_i^j \\
&= \sum_{0 \leq j \leq n-1} \beta_m^j - \sum_{0 \leq j \leq n-1} \beta_0^j - \sum_{1 \leq j \leq n} \beta_m^j + \sum_{1 \leq j \leq n} \beta_0^j \\
&= \beta_m^0 - \beta_m^n \\
&= \beta_p^\varphi(u_m, v_0) - \beta_p^\varphi(u_m, v_n) \\
&= \beta_p^\varphi(\bar{u}, \bar{v}) - \beta_p^\varphi(\bar{u}, \infty) \\
&= \beta_p^\varphi(\bar{u}, \bar{v}) - \sum_{u \leq \bar{u}} \nu^\varphi(u, \infty).
\end{aligned}$$

□

In plain words, [Theorem 9](#) states that the value assumed by β_p^φ at a point $(\bar{u}, \bar{v}) \in \Delta^+$ equals the number of cornerpoints lying above and on the left of $(\bar{u}, \bar{v})$. The following corollary of [Theorem 9](#) gives a useful interpretation of the value $\mu_{\eta,\eta}^\varphi(\bar{p})$.

Corollary 2. Let $\bar{p} = (\bar{u}, \bar{v}) \in \Delta^+$. Assume that $\bar{u} + \eta < \bar{v} - \eta$, with $\eta > 0$. Then $\mu_{\eta,\eta}^\varphi(\bar{p})$ equals the number of (proper) points of $\text{Dgm}(\varphi)$ (counted with their multiplicities) that belong to the semi-open square

$$\widehat{Q}_\eta := \{(u,v) \in \Delta^+ : \bar{u} - \eta < u \leq \bar{u} + \eta, \bar{v} - \eta < v \leq \bar{v} + \eta\}.$$

Proof. The statement follows from the definition of $\mu_{\eta,\eta}^\varphi(\bar{p})$ ([Definition 49](#)) and the Representation Theorem ([Theorem 9](#)), since

$$\begin{aligned}
\mu_{\eta,\eta}^\varphi(\bar{p}) &= \beta_p^\varphi(\bar{u} + \eta, \bar{v} - \eta) - \beta_p^\varphi(\bar{u} - \eta, \bar{v} - \eta) \\
&\quad - \beta_p^\varphi(\bar{u} + \eta, \bar{v} + \eta) + \beta_p^\varphi(\bar{u} - \eta, \bar{v} + \eta) \\
&= \sum_{\substack{(u,v) \in \Delta^* \\ u \leq \bar{u} + \eta \\ v > \bar{v} - \eta}} \mu^\varphi(u,v) + \sum_{u \leq \bar{u} + \eta} \nu^\varphi(u, \infty) - \sum_{\substack{(u,v) \in \Delta^* \\ u \leq \bar{u} - \eta \\ v > \bar{v} - \eta}} \mu^\varphi(u,v) - \sum_{u \leq \bar{u} - \eta} \nu^\varphi(u, \infty) \\
&\quad - \sum_{\substack{(u,v) \in \Delta^* \\ u \leq \bar{u} + \eta \\ v > \bar{v} + \eta}} \mu^\varphi(u,v) - \sum_{u \leq \bar{u} + \eta} \nu^\varphi(u, \infty) + \sum_{\substack{(u,v) \in \Delta^* \\ u \leq \bar{u} - \eta \\ v > \bar{v} + \eta}} \mu^\varphi(u,v) + \sum_{u \leq \bar{u} - \eta} \nu^\varphi(u, \infty) \\
&= \sum_{\substack{(u,v) \in \Delta^* \\ \bar{u} - \eta < u \leq \bar{u} + \eta \\ v > \bar{v} - \eta}} \mu^\varphi(u,v) - \sum_{\substack{(u,v) \in \Delta^* \\ \bar{u} - \eta < u \leq \bar{u} + \eta \\ v > \bar{v} + \eta}} \mu^\varphi(u,v)
\end{aligned}$$

$$= \sum_{\substack{(u,v) \in \Delta^* \\ \bar{u}-\eta < u \leq \bar{u}+\eta \\ \bar{v}-\eta < v \leq \bar{v}+\eta}} \mu^\varphi(u,v)$$

□

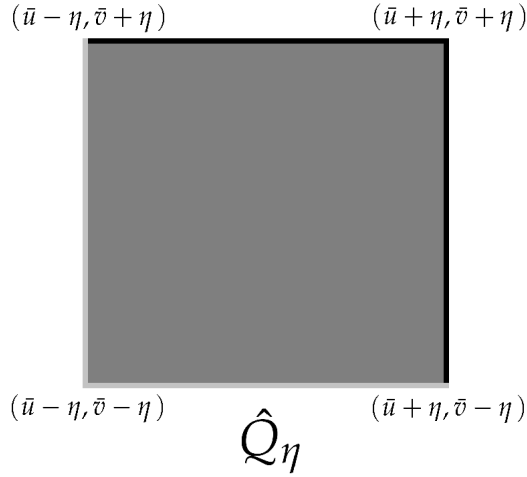


Figure 25: The set $\hat{Q}_\eta$ cited in Corollary 2. The points in black are included.

Bottleneck distance and stability of persistence diagrams

Our next goal is to introduce a metric for the space of persistence diagrams. To do that, we have to see how $\beta_p^\varphi(u, v)$ changes when φ changes. In the following, we will use the symbol $C_p^\varphi(u)$ to denote the set of p -chains in K_u^φ .

A lower bound for the natural pseudo-distance

Proposition 34. *Assume $\varphi, \psi : \text{Vert } K \rightarrow \mathbb{R}$ and $\|\varphi - \psi\|_\infty \leq \eta$. Then for every $(u, v) \in \Delta^+$ we have that $\beta_p^\varphi(u - \eta, v + \eta) \leq \beta_p^\psi(u, v)$.*

Proof. Let us choose an ordered basis $(\alpha_1, \dots, \alpha_m)$ of the vector space $H_p^\varphi(u - \eta, v + \eta) \subseteq H_p(K_{v+\eta}^\varphi)$. Let us arbitrarily choose $z_i \in \alpha_i$ with $z_i \in C_p^\varphi(u - \eta)$ for $i = 1, \dots, m$. For each index i , we can consider the homology class $\hat{\alpha}_i \in H_p^\psi(u, v)$ that contains z_i (observe that $z_i \in C_p^\psi(u)$, because $\|\varphi - \psi\|_\infty \leq \eta$). Let us now prove that the homology classes $\hat{\alpha}_i$ are linearly independent in $H_p^\psi(u, v)$. If $\lambda_1 \hat{\alpha}_1 + \dots + \lambda_m \hat{\alpha}_m = \mathbf{0} \in H_p^\psi(u, v) := \text{Im } i_{u,v}^{\psi*} \subseteq H_p(K_v^\psi)$, we can find a chain $\gamma \in C_{p+1}^\psi(v)$ such that $\partial_{p+1} \gamma = \lambda_1 z_1 + \dots + \lambda_m z_m$. Since $\|\varphi - \psi\|_\infty \leq \eta$, we have that $\gamma \in C_{p+1}^\varphi(v + \eta)$, and hence $\lambda_1 \alpha_1 + \dots + \lambda_m \alpha_m =$

$\mathbf{0} \in H_p^\varphi(u - \eta, v + \eta) := \text{Im } i_{u-v, v+\eta}^{\varphi*} \subseteq H_p(K_{v+\eta}^\varphi)$. We know that $\alpha_1, \dots, \alpha_m$ are linearly independent, and hence $\lambda_1 = \dots = \lambda_m = 0$. Therefore, $\hat{\alpha}_1, \dots, \hat{\alpha}_m$ are linearly independent too. This proves that $\dim H_p^\varphi(u - \eta, v + \eta) \leq \dim H_p^\psi(u, v)$. $\square$

Corollary 3. Assume $\varphi, \psi : \text{Vert } K \rightarrow \mathbb{R}$ and G is a group of isomorphisms from K to K . If $(u, v) \in \Delta^+$ and $\beta_p^\varphi(u - \eta, v + \eta) > \beta_p^\psi(u, v)$, then $d_G(\varphi, \psi) \geq \eta$.

Proof. Proposition 24 guarantees that $\beta_p^{\psi \circ g}(u, v) = \beta_p^\psi(u, v)$ for every $(u, v) \in \Delta^+$ and every $g \in G$. Because of Proposition 34, the inequality $\beta_p^\varphi(u - \eta, v + \eta) > \beta_p^\psi(u, v) = \beta_p^{\psi \circ g}(u, v)$ implies that $\|\varphi - \psi \circ g\|_\infty > \eta$ for every $g \in G$. It follows that $d_G(\varphi, \psi) := \min_{g \in G} \|\varphi - \psi \circ g\|_\infty \geq \eta$. $\square$

Proposition 34 has the following interesting consequence.

Proposition 35 (Local constancy of multiplicity). Assume $\varphi : \text{Vert } K \rightarrow \mathbb{R}$. If $\bar{p} = (\bar{u}, \bar{v}) \in \Delta^+$, then there is a real number $\bar{\eta} > 0$ such that if $\psi \in \Phi$ and $\|\varphi - \psi\|_\infty \leq \eta$ with $0 < \eta \leq \bar{\eta}$, then the closed square

$$\overline{Q_\eta} := \{(u, v) \in \Delta^+ : |u - \bar{u}| \leq \eta, |v - \bar{v}| \leq \eta\}$$

contains exactly $\mu^\varphi(\bar{p})$ (proper) points (counted with their multiplicities) of the persistence diagram $\text{Dgm}(\psi)$.

Proof. By Proposition 28, a sufficiently small $\varepsilon > 0$ exists such that the set $V_\varepsilon(\bar{p}) := \{(u, v) \in \mathbb{R}^2 : |u - \bar{u}| < \varepsilon, |v - \bar{v}| < \varepsilon, u \neq \bar{u}, v \neq \bar{v}\}$ is contained in Δ^+ and does not contain any discontinuity point of β_p^φ . Proposition 32 (Propagation of discontinuities from cornerpoints) implies that $\bar{p}$ is the only point of Δ^+ that could belong to both $\text{Dgm}(\varphi)$ and the open square

$$Q_\varepsilon := \{(u, v) \in \Delta^+ : |u - \bar{u}| < \varepsilon, |v - \bar{v}| < \varepsilon\}.$$

Let $\bar{\eta}$ be a real number such that $0 < \bar{\eta} < \frac{\varepsilon}{2}$. For each real number η with $0 < \eta \leq \bar{\eta}$, let us take a sufficiently small positive real number $\delta < \eta$ with $2\eta + \delta < \varepsilon$, so that $\bar{u} + 2\eta + \delta < \bar{v} - 2\eta - \delta$ (we recall that $\bar{u} + \varepsilon < \bar{v} - \varepsilon$, since $V_\varepsilon(\bar{p}) \subseteq \Delta^+$). We define $a = (\bar{u} + \eta + \delta, \bar{v} - \eta - \delta)$, $b = (\bar{u} - \eta - \delta, \bar{v} - \eta - \delta)$, $c = (\bar{u} + \eta + \delta, \bar{v} + \eta + \delta)$, $e = (\bar{u} - \eta - \delta, \bar{v} + \eta + \delta)$ as illustrated in Figure 26.

By applying Proposition 34 twice,

$$\beta_p^\varphi(\bar{u} + \delta, \bar{v} - \delta) \leq \beta_p^\psi(a) \leq \beta_p^\varphi(\bar{u} + 2\eta + \delta, \bar{v} - 2\eta - \delta).$$

Since β_p^φ is constant in each connected component of the set $V_\varepsilon(\bar{p})$,

$$\beta_p^\varphi(\bar{u} + \delta, \bar{v} - \delta) = \beta_p^\varphi(a) = \beta_p^\varphi(\bar{u} + 2\eta + \delta, \bar{v} - 2\eta - \delta).$$

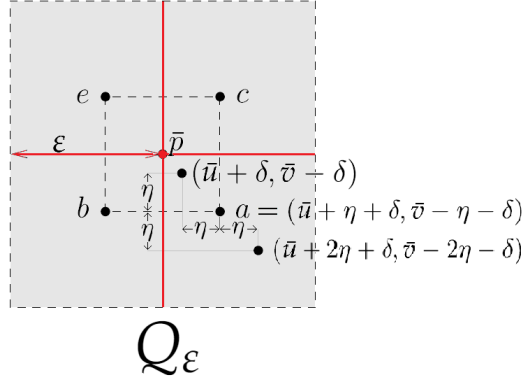


Figure 26: The set Q_ε used in the proof of Proposition 35. The set V_ε is obtained from Q_ε by removing the points displayed in red.

This implies that $\beta_p^\varphi(a) = \beta_p^\psi(a)$. Analogously, we can prove that $\beta_p^\varphi(b) = \beta_p^\psi(b)$, $\beta_p^\varphi(c) = \beta_p^\psi(c)$, and $\beta_p^\varphi(e) = \beta_p^\psi(e)$. Hence, $\mu^\varphi(\bar{p}) = \mu_{\eta+\delta, \eta+\delta}^\varphi(\bar{p}) = \mu_{\eta+\delta, \eta+\delta}^\psi(\bar{p})$. From Corollary 2 (applied to ψ), it follows that $\mu^\varphi(\bar{p})$ is equal to the number of cornerpoints in $\text{Dgm}(\psi)$ that are contained in the semi-open square $\hat{Q}_{\eta+\delta}$ with vertexes a, b, c, e , defined by setting

$$\hat{Q}_{\eta+\delta} := \{(u, v) \in \Delta^+ : \bar{u} - \eta - \delta < u \leq \bar{u} + \eta + \delta, \bar{v} - \eta - \delta < v \leq \bar{v} + \eta + \delta\}.$$

This is true for any sufficiently small $\delta > 0$. Therefore, $\mu^\varphi(\bar{p})$ is equal to the number of cornerpoints in $\text{Dgm}(\psi)$ contained in the closed square $\overline{Q}_\eta = \bigcap_{\delta>0} \hat{Q}_{\eta+\delta}$. $\square$

To proceed, we have to endow the set $\bar{\Delta}^* = \Delta^* \cup \{\Delta\}$ with the extended metric d introduced in the following definition.

Definition 54. For every $p, q \in \bar{\Delta}^*$ we set $d(p, q)$ equal to

$$\begin{cases} \min \left\{ \max \{|u - u'|, |v - v'|\}, \max \left\{ \frac{v-u}{2}, \frac{v'-u'}{2} \right\} \right\} & \text{if } p = (u, v), q = (u', v') \in \Delta^+ \\ |u - u'| & \text{if } p = (u, \infty), q = (u', \infty) \\ \frac{v-u}{2}, & \text{if } p = (u, v) \in \Delta^+, q = \Delta \\ \frac{v'-u'}{2} & \text{if } p = \Delta, q = (u', v') \in \Delta^+ \\ 0 & \text{if } p = \Delta, q = \Delta \\ \infty & \text{otherwise.} \end{cases}$$

Proposition 36. The function d given in Def. 54 is an extended metric.

Exercise 18. Prove Proposition 36.

We can now introduce a metric between persistence diagrams.

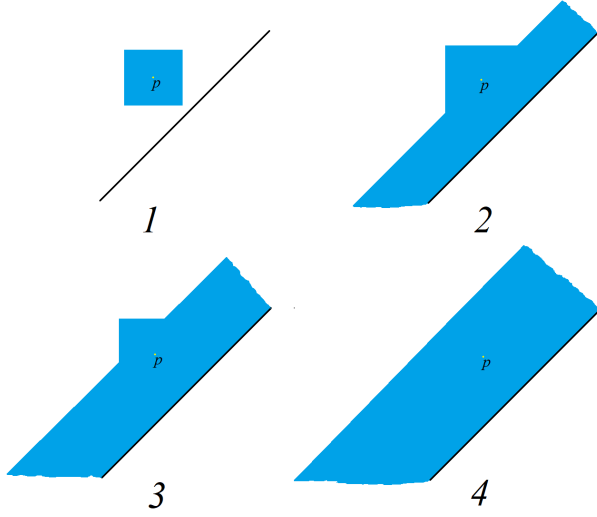


Figure 27: The open ball of center p and radius r with respect to the metric d in the cases 1) $r < d(p, \Delta)$, 2) $r = d(p, \Delta)$, 3) $d(p, \Delta) < r < 2d(p, \Delta)$, 4) $r \geq 2d(p, \Delta)$.

Definition 55. For each pair $(\text{Dgm}(\varphi), \text{Dgm}(\varphi'))$ we set

$$d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi')) := \inf_{\sigma \in S(\varphi, \varphi')} \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma(p))$$

where $S(\varphi, \varphi')$ is the set of all matchings from $\text{Dgm}(\varphi)$ to $\text{Dgm}(\varphi')$.

Proposition 37. The function d_{match} is a metric.

Proof. 1. We have that

$$\begin{aligned} d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi)) &:= \inf_{\sigma \in S(\varphi, \varphi)} \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma(p)) \\ &\leq \sup_{p \in \text{Dgm}(\varphi)} d(p, \text{id}(p)) = 0. \end{aligned}$$

2. If $d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi')) = 0$, then for every $\varepsilon > 0$ we can find a matching $\sigma_\varepsilon \in S(\varphi, \varphi')$ such that $d(p, \sigma_\varepsilon(p)) \leq \varepsilon$ for every $p \in \text{Dgm}(\varphi)$, and hence $\mu^\varphi(p) \leq \mu^{\varphi'}(p)$ for any $p \in \Delta^+$ and $\nu^\varphi(p) \leq \nu^{\varphi'}(p)$ for any $p = (u, \infty)$. Analogously, $\mu^{\varphi'}(p) \leq \mu^\varphi(p)$ for any $p \in \Delta^+$ and $\nu^{\varphi'}(p) \leq \nu^\varphi(p)$ for any $p = (u, \infty)$. Therefore, $\text{Dgm}(\varphi) = \text{Dgm}(\varphi')$;

3. We have that

$$\begin{aligned} d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi')) &:= \inf_{\sigma \in S(\varphi, \varphi')} \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma(p)) \\ &= \inf_{\sigma \in S(\varphi, \varphi')} \sup_{p \in \text{Dgm}(\varphi)} d(\sigma(p), p) \\ &= \inf_{\sigma^{-1} \in S(\varphi', \varphi)} \sup_{q \in \text{Dgm}(\varphi')} d(q, \sigma^{-1}(q)) \end{aligned}$$

$$\begin{aligned}
&= \inf_{\sigma^{-1} \in S(\varphi', \varphi)} \sup_{q \in \text{Dgm}(\varphi')} d(q, \sigma^{-1}(q)) \\
&= d_{\text{match}}(\text{Dgm}(\varphi'), \text{Dgm}(\varphi));
\end{aligned}$$

4. If $\sigma \in S(\varphi, \varphi')$ and $\sigma' \in S(\varphi', \varphi'')$, then $d(p, \sigma'(\sigma(p))) \leq d(p, \sigma(p)) + d(\sigma(p), \sigma'(\sigma(p)))$ for every $p \in \text{Dgm}(\varphi)$, and hence

$$\begin{aligned}
\sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma'(\sigma(p))) &\leq \sup_{p \in \text{Dgm}(\varphi)} (d(p, \sigma(p)) + d(\sigma(p), \sigma'(\sigma(p)))) \\
&\leq \sup_{p \in \text{Dgm}(\varphi)} (d(p, \sigma(p)) + \sup_{p \in \text{Dgm}(\varphi)} d(\sigma(p), \sigma'(\sigma(p)))) \\
&= \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma(p)) + \sup_{q \in \text{Dgm}(\psi)} d(q, \sigma'(q)).
\end{aligned}$$

It follows that for every $\sigma' \in S(\varphi, \varphi')$

$$\begin{aligned}
d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi'')) &= \inf_{\sigma'' \in S(\varphi, \varphi'')} \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma''(p)) \\
&= \inf_{\sigma' \in S(\varphi', \varphi'')} \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma'(\sigma(p))) \\
&\leq \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma(p)) + \inf_{\sigma' \in S(\varphi', \varphi'')} \sup_{q \in \text{Dgm}(\psi)} d(q, \sigma'(q)) \\
&\leq \sup_{p \in \text{Dgm}(\varphi)} d(p, \sigma(p)) + d_{\text{match}}(\text{Dgm}(\varphi'), \text{Dgm}(\varphi'')).
\end{aligned}$$

By computing the infimum for σ varying in $S(\varphi, \varphi')$, we obtain the triangle inequality

$$d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi'')) \leq d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\varphi')) + d_{\text{match}}(\text{Dgm}(\varphi'), \text{Dgm}(\varphi'')).$$

□

The metric d_{match} is called *bottleneck distance* or *matching distance*.

Proposition 38. *If $\varphi, \psi : \text{Vert } K \rightarrow \mathbb{R}$ and $\|\varphi - \psi\|_\infty \leq \varepsilon$, then for any finite multiset $X \subseteq \text{Dgm}(\varphi) \cap \Delta^+$ with $\min_{x \in X} d(x, \Delta) > \varepsilon$, there is an injective multiset map $\sigma : X \rightarrow \text{Dgm}(\psi)$ s.t. $\max_{x \in X} d(x, \sigma(x)) \leq \varepsilon$.*

Proof. Let $X = \{p_1, \dots, p_k\}$, where each $p_j = (u_j, v_j)$ has multiplicity in X equal to $m_j \leq \mu^\varphi(p_j)$, and set $m := \sum_{j=1}^k m_j$. Let us set $\varphi_t := \frac{\varepsilon-t}{\varepsilon}\varphi + \frac{t}{\varepsilon}\psi$ for every $t \in [0, \varepsilon]$. Then, for every $t, t' \in [0, \varepsilon]$, $\|\varphi_t - \varphi_{t'}\|_\infty \leq |t - t'|$. Now we will consider the set A of all values $\delta \in [0, \varepsilon]$ for which an injective multiset map $\sigma_\delta : X \rightarrow \text{Dgm}(\varphi_\delta)$ exists, such that $d(p_j, \sigma_\delta(p_j)) \leq \delta$ for every $p_j \in X$. In other words, if we think of the variation of t as the flow of time, A is the set of times δ for which the cornerpoints in X move less than δ itself, when φ is changed into φ_δ . We want to prove that $\sup A = \varepsilon$. First of all, we observe that A is non-empty, since $0 \in A$. Let us set $\bar{\delta} = \sup A$ and

show that $\bar{\delta} \in A$. Indeed, let (δ_n) be a non-decreasing sequence in A , converging to $\bar{\delta}$. Since $\delta_n \in A$, for each n there exists an injective map $\sigma_{\delta_n} : X \rightarrow \text{Dgm}(\varphi_{\delta_n})$, such that $\max_j d(p_j, \sigma_{\delta_n}(p_j)) \leq \delta_n$. Since $\delta_n \leq \varepsilon$, $\max_j d(p_j, \sigma_{\delta_n}(p_j)) \leq \varepsilon$ for any n . Thus, $\sigma_{\delta_n}(p_j) \in \overline{Q_\varepsilon}(p_j)$ for any n , where $\overline{Q_\varepsilon}(p_j) := \{(u, v) \in \Delta^+ : u_j - \varepsilon \leq u \leq u_j + \varepsilon, v_j - \varepsilon \leq v \leq v_j + \varepsilon\}$ for $1 \leq j \leq k$, because $\min_{x \in X} d(x, \Delta) > \varepsilon$ and hence the closed square $\overline{Q_\varepsilon}(p_j)$ does not meet the diagonal Δ . Possibly by extracting a subsequence, we can assume that the sequence $\sigma_{\delta_n}(p_j)$ converges for any index j . We set $\bar{p}_j := \lim_{n \rightarrow \infty} \sigma_{\delta_n}(p_j)$. We have that $d(p_j, \bar{p}_j) \leq \bar{\delta}$. Also, the following property holds:

(*) If $p_{j_1}, \dots, p_{j_r} \in X$ and $\bar{q} = \bar{p}_{j_1} = \dots = \bar{p}_{j_r}$, then the multiplicity of $\bar{q} = (\bar{u}, \bar{v})$ in $\text{Dgm}(\varphi_{\bar{\delta}})$ is not smaller than r .

In other words, if a submultiset of cardinality r of X becomes a singleton at time $\bar{\delta}$, then the point $\bar{q}$ in such a singleton has a multiplicity not smaller than r .

Let us prove (*). We know that $\delta_n \leq \varepsilon$ for any index n . Let $\eta > 0$. If n is large enough then $|\delta_n - \bar{\delta}| \leq \eta$, and hence $\|\varphi_{\delta_n} - \varphi_{\bar{\delta}}\|_\infty \leq \eta$. As a consequence, on the one hand, if η is small enough then Proposition 35 (local constancy of multiplicity) guarantees that for any large enough n the multiplicity $\bar{m}$ of $\bar{q}$ in $\text{Dgm}(\varphi_{\bar{\delta}})$ equals the number of cornerpoints of $\text{Dgm}(\varphi_{\delta_n})$ that belong to the closed square $\overline{Q_\eta}(\bar{q}) := \{(u, v) \in \Delta^+ : \bar{u} - \eta \leq u \leq \bar{u} + \eta, \bar{v} - \eta \leq v \leq \bar{v} + \eta\}$. On the other hand, $\overline{Q_\eta}(\bar{q})$ contains at least the r cornerpoints $\sigma_{\delta_n}(p_{j_1}), \dots, \sigma_{\delta_n}(p_{j_r})$ of $\text{Dgm}(\varphi_{\delta_n})$, since $\lim_{n \rightarrow \infty} \sigma_{\delta_n}(p_{j_i}) = \bar{q}$ for $1 \leq i \leq r$. Therefore, $\bar{m} \geq r$, and (*) is proved.

In particular, $\bar{q}$ is a cornerpoint in $\text{Dgm}(\varphi_{\bar{\delta}})$. In order to conclude that $\bar{\delta} \in A$, it is now sufficient to consider the multiset map $\sigma_{\bar{\delta}} : X \rightarrow \text{Dgm}(\varphi_{\bar{\delta}})$ taking p_j to $\bar{p}_j$ for every $p_j \in X$. Property (*) guarantees that $\sigma_{\bar{\delta}}$ is injective. So we have proved that $\sup A \in A$, i.e. $\sup A = \max A$. We end the proof by showing that $\max A = \varepsilon$. In fact, if $\bar{\delta} < \varepsilon$, by using Proposition 35 once again, it is not difficult to show that there exists $\eta > 0$, with $\bar{\delta} + \eta < \varepsilon$, and an injective multiset map $\sigma_{\bar{\delta}, \bar{\delta} + \eta}$ from the multiset $\{\bar{p}_1, \dots, \bar{p}_k\}$ to the multiset $\text{Dgm}(\varphi_{\bar{\delta} + \eta})$ such that $d(\bar{p}_j^i, \sigma_{\bar{\delta}, \bar{\delta} + \eta}(\bar{p}_j^i)) \leq \eta$ for $1 \leq j \leq k$, where $\bar{p}_j^i$ denotes the i -th copy of $\bar{p}_j$ in the multiset $\sigma_{\bar{\delta}}(X)$. Hence $\sigma_{\bar{\delta}, \bar{\delta} + \eta} \circ \sigma_{\bar{\delta}} : X \rightarrow \text{Dgm}(\varphi_{\bar{\delta} + \eta})$ is an injective multiset map and, by the triangle inequality, $d(p_j, \sigma_{\bar{\delta}, \bar{\delta} + \eta} \circ \sigma_{\bar{\delta}}(p_j)) \leq \bar{\delta} + \eta$ for $1 \leq j \leq k$, implying that $\bar{\delta} + \eta \in A$. This would contradict the fact that $\bar{\delta} = \sup A$. Therefore, $\varepsilon = \max A$, and hence $\varepsilon \in A$. $\square$

The following result extends to the points at infinity Proposition 38. We omit the proof, which is quite analogous to the proof of Proposition 38.

Proposition 39. *If $\|\varphi - \psi\|_\infty \leq \varepsilon$, then for any finite multiset of cornerlines $X' \subseteq \text{Dgm}(\varphi)$, there exists an injective multiset map $\sigma : X' \rightarrow \text{Dgm}(\psi)$ such that $d(x, \sigma(x)) \leq \varepsilon$ for every $x \in X'$.*

Now we can prove that it is possible to injectively match all the points of $\text{Dgm}(\varphi)$ with points of $\text{Dgm}(\psi)$, making a maximum displacement not greater than $\|\varphi - \psi\|_\infty$.

Proposition 40. *If $\|\varphi - \psi\|_\infty \leq \varepsilon$, then there exists an injective multiset map $\tau : \text{Dgm}(\varphi) \rightarrow \text{Dgm}(\psi)$ such that $d(x, \tau(x)) \leq \varepsilon$ for every $x \in \text{Dgm}(\varphi)$.*

Proof. Set $X_1 := \{p \in \text{Dgm}(\varphi) : d(p, \Delta) > \varepsilon\}$ and $X_2 := \{p \in \text{Dgm}(\varphi) : d(p, \Delta) \leq \varepsilon\}$. The cardinality of X_1 is finite, according to Proposition 30 and Proposition 31. Therefore, Proposition 38 and Proposition 39 guarantee the existence of an injective multiset map τ_1 from the multiset X_1 to $\text{Dgm}(\psi)$, such that $d(x, \tau(x)) \leq \varepsilon$ and $\tau(x) \neq \Delta$ for every $x \in X_1$.

We can now consider an injective multiset map τ_2 from the multiset X_2 to the multiset containing just the point Δ with infinite multiplicity.

The map τ that coincides with τ_1 on X_1 and with τ_2 on X_2 is the wanted injective multiset map τ . $\square$

We now recall the following well-known result ⁸.

Theorem 10 (Cantor-Bernstein Theorem). *Let A and B be two sets. If two injections $f : A \rightarrow B$ and $g : B \rightarrow A$ exist, then there is a bijection $h : A \rightarrow B$. Furthermore, we can assume that the equality $h(a) = b$ implies that either $f(a) = b$ or $g(b) = a$ (or both).*

⁸ K. Kuratowski and A. Mostowski. *Set theory*. PWN—Polish Scientific Publishers, Warsaw; North-Holland Publishing Co., Amsterdam, 1968. Translated from the Polish by M. Maczyński

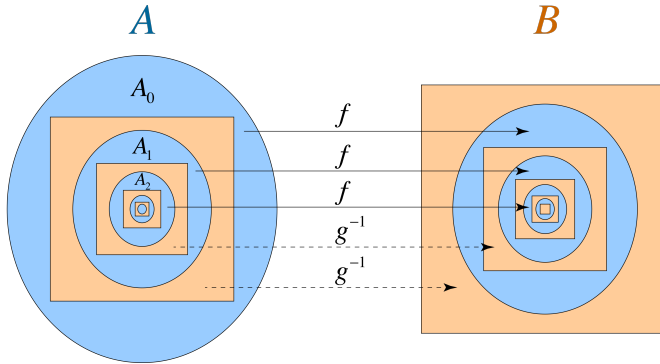


Figure 28: The classical construction used to prove the Cantor-Bernstein Theorem. Each arrow denotes a local bijection.

We are now ready to prove a key result in TDA.

Theorem 11 (Matching Distance Stability Theorem). ⁹

$$d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\psi)) \leq \|\varphi - \psi\|_\infty.$$

⁹ David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Stability of persistence diagrams. *Discrete Comput. Geom.*, 37(1):103–120, 2007. ISSN 0179-5376. DOI: 10.1007/s00454-006-1276-5. URL <http://dx.doi.org/10.1007/s00454-006-1276-5>

Proof. Proposition 40 implies that there exist an injective multiset map $\tau : \text{Dgm}(\varphi) \rightarrow \text{Dgm}(\psi)$ such that $d(x, \tau(x)) \leq \varepsilon$ for every $x \in \text{Dgm}(\varphi)$, and an injective multiset map $\tau' : \text{Dgm}(\psi) \rightarrow \text{Dgm}(\varphi)$ such that $d(y, \tau'(y)) \leq \varepsilon$ for every $y \in \text{Dgm}(\psi)$. Then the claim follows from the Cantor-Bernstein Theorem, by setting A equal to a realization of $\text{Dgm}(\varphi)$ and B equal to a realization of $\text{Dgm}(\psi)$. $\square$

Corollary 4. *Assume $\varphi, \psi : \text{Vert } K \rightarrow \mathbb{R}$ and G is a group of isomorphisms from K to K . Then*

$$d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\psi)) \leq d_G(\varphi, \psi).$$

Proof. From Proposition 29 and Theorem 11 it follows that

$$\begin{aligned} d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\psi)) &= d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\psi \circ g)) \\ &\leq \|\varphi - \psi \circ g\|_{\infty} \end{aligned}$$

for every $g \in G$. This implies the wanted inequality. $\square$

Definition 56. *If $\bar{\sigma}$ is a matching from $\text{Dgm}(\varphi)$ to $\text{Dgm}(\psi)$ and the equality $\max_{p \in \text{Dgm}(\varphi)} d(p, \bar{\sigma}(p)) = d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\psi))$ holds, then we say that $\bar{\sigma}$ is an **optimal matching**.*

We observe that for each pair $(\text{Dgm}(\varphi), \text{Dgm}(\psi))$ of persistence diagrams at least an optimal matching $\bar{\sigma} : \text{Dgm}(\varphi) \rightarrow \text{Dgm}(\psi)$ exists.

Exercise 19. *Find a simplicial complex K and two continuous functions $\varphi, \psi : \text{Vert } K \rightarrow \mathbb{R}$ such that*

$$0 = d_{\text{match}}(\text{Dgm}(\varphi), \text{Dgm}(\psi)) < d_G(\varphi, \psi).$$

Non-expansive equivariant operators

Until now, we focused on data, ignoring the role of observers. However, it is well-known that different observers can have different reactions in the presence of the same data, and this suggests that we should study the pairs *(data, observer)* rather than just the data.

If data analysis were not dependent on the chosen observer, then physicians' diagnoses would always be identical, scientists would always see the same causes for each phenomenon, and all people would agree in judging who the heroes and villains in a movie or a political event are.

In this chapter we will refer to the epistemological setting described by the following assumptions.

1. Data are represented as functions defined on topological spaces, since only data that are stable with respect to a certain criterion (e.g., with respect to some kind of measurement) can be considered for applications, and stability requires a topological structure.
2. Data cannot be studied in a direct and absolute way. They are only knowable through acts of transformation made by an agent that observes the data. From the point of view of data analysis, only the pair (data, observer) matters. In general terms, observers are not necessarily endowed with purposes or goals: they are just ways and methods to transform data. Acts of measurement are a particular class of acts of transformation, that can or not be at the service of a global goal quantified by a loss or a reward function.
3. Observers are described by the way they transform data while respecting some kind of invariance. In other words, any observer can be seen as a group equivariant operator acting on a function space.
4. Data similarity depends on the output of the considered observer.

In other words, in this chapter we will assume that the analysis of data is replaced by the analysis of the pair (data, observer). Since an observer can be seen as a group equivariant operator, from the

mathematical viewpoint our purpose consists in presenting a good topological theory of suitable operators of this kind, representing observers. For more details, we refer the interested reader to ¹⁰.

Data representation. Let K be a simplicial complex. In our mathematical model, each space of data is represented as a function space, that is, as a set Φ of real-valued functions $\varphi : \text{Vert } K \rightarrow \mathbb{R}$. We assume that Φ is endowed with the distance

$$D_{\Phi}(\varphi_1, \varphi_2) := \|\varphi_1 - \varphi_2\|_{\infty}. \quad (3)$$

We can think of K as the space where one makes measurements, and of Φ as the set of admissible measurements.

The set $\text{Vert } K$ is endowed with the pseudo-metric $D_{\text{Vert } K}$ which distinguishes points only if they are seen as different by some measurement:

$$D_{\text{Vert } K}(v_1, v_2) = \sup_{\varphi \in \Phi} |\varphi(v_1) - \varphi(v_2)| \quad (4)$$

for every $v_1, v_2 \in \text{Vert } K$. We recall that a pseudo-metric is just a distance d without the property that $d(a, b) = 0$ implies $a = b$.

We will assume that the metric space Φ is large enough to imply that $D_{\text{Vert } K}$ is a distance.

Transformations on data and equivariance. We assume that data can be transformed through Φ -preserving isomorphisms. The set of these isomorphisms will be denoted by the symbol $\text{Iso}_{\Phi}(K)$. This set is a group with respect to the composition of maps.

Proposition 41. *If $g \in \text{Iso}_{\Phi}(K)$, then g is an isometry (and hence a bijective maps) with respect to $D_{\text{Vert } K}$.*

Proof. Let us fix two arbitrary vertexes v, v' in X . Obviously, the map $R_g : \Phi \rightarrow \Phi$ taking each function φ to $\varphi \circ g$ is surjective, since $\varphi = R_g(R_{g^{-1}}(\varphi))$. Hence $R_g(\Phi) = \Phi$. Therefore, g preserves the distance $D_{\text{Vert } K}$:

$$\begin{aligned} D_{\text{Vert } K}(g(v), g(v')) &= \sup_{\varphi \in \Phi} |\varphi(g(v)) - \varphi(g(v'))| \\ &= \sup_{\varphi \in \Phi} |(\varphi \circ g)(v) - (\varphi \circ g)(v')| \end{aligned} \quad (5)$$

$$\begin{aligned} &= \sup_{\varphi \in R_g(\Phi)} |\varphi(v) - \varphi(v')| \\ &= \sup_{\varphi \in \Phi} |\varphi(v) - \varphi(v')| = D_{\text{Vert } K}(v, v'). \end{aligned} \quad (6)$$

Since g is bijective, it follows that g is an isometry w.r.t. $D_{\text{Vert } K}$. $\square$

¹⁰ P. Frosini. Towards an observer-oriented theory of shape comparison: Position paper. In *Proceedings of the Eurographics 2016 Workshop on 3D Object Retrieval*, 3DOR '16, page 5–8, Goslar, DEU, 2016. Eurographics Association. ISBN 9783038680048

Let us now consider a subgroup G of the group $\text{Iso}_\Phi(K)$. G represents the set of transformations on data for which we require equivariance to be respected. We already know that G is endowed with the pseudo-metric defined by setting

$$D_G(g_1, g_2) := \sup_{\varphi \in \Phi} D_\Phi(\varphi \circ g_1, \varphi \circ g_2) \quad (7)$$

for every $g_1, g_2 \in G$. D_G measures the distance between two isomorphisms as the difference of their actions on the set Φ of possible measurements.

Proposition 42. D_G is a metric, provided that $D_{\text{Vert } K}$ is a metric.

Exercise 20. Prove Proposition 42.

As we know, the pair (Φ, G) is called a *perception pair*. The group G of transformations can be either learned, or fixed as part of prior knowledge.

Group Equivariant Non-Expansive Operators. If two perception pairs $(\Phi, G), (\Psi, H)$ are given, together with a map $F : \Phi \rightarrow \Psi$ and a homomorphism $T : G \rightarrow H$ such that $F(\varphi \circ g) = F(\varphi) \circ T(g)$ for every $\varphi \in \Phi, g \in G$, the pair (F, T) is said to be a **group equivariant operator** (GEO) from (Φ, G) to (Ψ, H) .

We observe that the functions in Φ and the functions in Ψ are defined on domains that are generally different from each other, and the equivariance groups G, H can be different from each other as well.

Definition 57. If (F, T) is a group equivariant operator from (Φ, G) to (Ψ, H) and F is non-expansive (i.e., $D_\Psi(F(\varphi_1), F(\varphi_2)) \leq D_\Phi(\varphi_1, \varphi_2)$ for every $\varphi_1, \varphi_2 \in \Phi$), then (F, T) is called a **Group Equivariant Non-Expansive Operator** (GENEO).

Example 5. Let K be the set of all vertexes and edges of a regular hexagon, with the natural incidence relation, Φ be the set of all functions from $\text{Vert } K$ to $[0, 1]$, and G be the group of all rotations that take the hexagon to itself. Analogously, let L be the set of all vertexes and edges of a regular triangle, with the natural incidence relation, Ψ be the set of all functions from $\text{Vert } L$ to $[0, 1]$, and H be the group of all rotations that take the triangle to itself. Let $v_0, \dots, v_5$ be the vertexes of the hexagon and w_0, w_1, w_2 be the vertexes of the triangle. Now, let us consider the map $F : \Phi \rightarrow \Psi$ taking each function $\varphi \in \Phi$ to the function $\psi \in \Psi$ defined by setting $\psi(w_i) = \frac{\varphi(v_i) + \varphi(v_{i+3})}{2}$, where the sum $i + 3$ is intended modulo 6. Let $T : G \rightarrow H$ be the homomorphism taking each rotation of α degrees to the rotation of 2α degrees. We can easily check that (F, T) is a GENEO from (Φ, G) to (Ψ, H) .

The following statement makes clear how GENEOS act on the natural pseudo-distances.

Proposition 43. *If (F, T) is a GENEOS from (Φ, G) to (Ψ, H) , then F is a contraction with respect to the natural pseudo-distances d_G, d_H .*

Proof. Since F is a GENEOS, it follows that

$$\begin{aligned} d_H(F(\varphi_1), F(\varphi_2)) &= \min_{h \in H} D_\Psi(F(\varphi_1), F(\varphi_2) \circ h) \\ &\leq \min_{g \in G} D_\Psi(F(\varphi_1), F(\varphi_2) \circ T(g)) \\ &= \min_{g \in G} D_\Psi(F(\varphi_1), F(\varphi_2 \circ g)) \\ &\leq \min_{g \in G} D_\Phi(\varphi_1, \varphi_2 \circ g) = d_G(\varphi_1, \varphi_2). \end{aligned} \tag{8}$$

□

Compactness and convexity of the space of GENEOS. We can prove that if the function spaces are compact and convex, then the space of GENEOS is compact and convex too. The compactness guarantees that the space of GENEOS can be approximated by a finite set. The convexity implies that new GENEOS can be obtained by convex combinations of pre-existing GENEOS.

If $\mathcal{F}^{\text{all}} := \text{GENEOS}((\Phi, G), (\Psi, H))$ is the set of all GENEOS (F, T) from (Φ, G) to (Ψ, H) , then the following theorem holds:

Theorem 12. *If Φ and Ψ are compact with respect to D_Φ and D_Ψ , respectively, then $\mathcal{F}^{\text{all}}$ is compact with respect to the metric*

$$D_{\text{GENEOS}}(F_1, F_2) := \sup_{\varphi \in \Phi} D_\Psi(F_1(\varphi), F_2(\varphi)). \tag{9}$$

Proof. We know that $(\mathcal{F}^{\text{all}}, D_{\text{GENEOS}})$ is a metric space. Therefore it will suffice to prove that $\mathcal{F}^{\text{all}}$ is sequentially compact. In order to do this, let us assume that a sequence (F_i) in $\mathcal{F}^{\text{all}}$ is given. Given that Φ is a compact (and hence separable) metric space, we can find a countable and dense subset $\Phi^* = \{\varphi_j\}_{j \in \mathbb{N}}$ of Φ . By means of a diagonalization process, we can extract a subsequence (F'_i) from (F_i) , such that for every fixed index j the sequence $(F'_i(\varphi_j))$ converges to a function in Ψ with respect to D_Ψ . Now, let us consider the function $\bar{F} : \Phi^* \rightarrow \Psi$ defined by setting $\bar{F}(\varphi_j) := \lim_{i \rightarrow \infty} F'_i(\varphi_j)$ for each $\varphi_j \in \Phi^*$.

We extend $\bar{F}$ to Φ as follows. For every $\varphi \in \Phi$ we choose a sequence (φ_{j_r}) in Φ^* , converging to $\varphi \in \Phi$, and set $\bar{F}(\varphi) := \lim_{r \rightarrow \infty} \bar{F}(\varphi_{j_r})$. We claim that such a limit exists in Ψ and does not depend on the sequence that we have chosen, converging to $\varphi \in \Phi$. In order to prove

that the previous limit exists, we observe that $\bar{F} : \Phi^* \rightarrow \Psi$ is non-expansive. We have indeed that for every $a, b \in \mathbb{N}$

$$\begin{aligned} D_\Psi(\bar{F}(\varphi_a), \bar{F}(\varphi_b)) &= D_\Psi\left(\lim_{i \rightarrow \infty} F'_i(\varphi_a), \lim_{i \rightarrow \infty} F'_i(\varphi_b)\right) \\ &= \lim_{i \rightarrow \infty} D_\Psi(F'_i(\varphi_a), F'_i(\varphi_b)) \\ &\leq \lim_{i \rightarrow \infty} D_\Phi(\varphi_a, \varphi_b) = D_\Phi(\varphi_a, \varphi_b), \end{aligned}$$

because each F'_i is non-expansive.

Since the sequence (φ_{j_r}) converges to $\varphi \in \Phi$, it follows that $(\bar{F}(\varphi_{j_r}))$ is a Cauchy sequence with respect to D_Ψ . The compactness of Ψ implies that $(\bar{F}(\varphi_{j_r}))$ converges in Ψ .

If another sequence (φ_{k_r}) is given in Φ^* , converging to $\varphi \in \Phi$, then $D_\Psi(\bar{F}(\varphi_{j_r}), \bar{F}(\varphi_{k_r})) \leq D_\Phi(\varphi_{j_r}, \varphi_{k_r})$ for every index $r \in \mathbb{N}$.

Since both (φ_{j_r}) and (φ_{k_r}) converge to φ , then it follows that $\lim_{r \rightarrow \infty} \bar{F}(\varphi_{j_r}) = \lim_{r \rightarrow \infty} \bar{F}(\varphi_{k_r})$. Therefore the definition of $\bar{F}(\varphi)$ does not depend on the chosen sequence (φ_{j_r}) , converging to φ .

Now we have to prove that $\bar{F} \in \mathcal{F}^{\text{all}}$, i.e., that $\bar{F}$ verifies the properties defining this set of operators. We have already seen that $\bar{F} : \Phi \rightarrow \Psi$.

For every φ, φ' we can consider two sequences $(\varphi_{j_r}), (\varphi_{k_r})$ in Φ^* , converging to φ and φ' , respectively. Due to the fact that the operators F'_i are non-expansive, we have that

$$\begin{aligned} D_\Psi(\bar{F}(\varphi), \bar{F}(\varphi')) &= D_\Psi\left(\lim_{r \rightarrow \infty} \bar{F}(\varphi_{j_r}), \lim_{r \rightarrow \infty} \bar{F}(\varphi_{k_r})\right) \\ &= D_\Psi\left(\lim_{r \rightarrow \infty} \lim_{i \rightarrow \infty} F'_i(\varphi_{j_r}), \lim_{r \rightarrow \infty} \lim_{i \rightarrow \infty} F'_i(\varphi_{k_r})\right) \\ &= \lim_{r \rightarrow \infty} \lim_{i \rightarrow \infty} D_\Psi(F'_i(\varphi_{j_r}), F'_i(\varphi_{k_r})) \\ &\leq \lim_{r \rightarrow \infty} \lim_{i \rightarrow \infty} D_\Phi(\varphi_{j_r}, \varphi_{k_r}) \\ &= \lim_{r \rightarrow \infty} D_\Phi(\varphi_{j_r}, \varphi_{k_r}) \\ &= D_\Phi(\varphi, \varphi'). \end{aligned}$$

Therefore, $\bar{F} : \Phi \rightarrow \Psi$ is non-expansive. As a consequence, it is also continuous.

We can now prove that the sequence (F'_i) converges to $\bar{F}$ with respect to D_{GENEO} . Let us consider an arbitrarily small $\varepsilon > 0$.

Since Φ is compact and Φ^* is dense in Φ , we can find a finite subset $\{\varphi_{j_1}, \dots, \varphi_{j_n}\}$ of Φ^* such that for every $\varphi \in \Phi$, there exists an index $r \in \{1, \dots, n\}$, for which $D_\Phi(\varphi, \varphi_{j_r}) < \varepsilon$.

Since the sequence (F'_i) converges pointwise to $\bar{F}$ on the set Φ^* , an index $\bar{i}$ exists, such that $D_\Psi(\bar{F}(\varphi_{j_r}), F'_i(\varphi_{j_r})) < \varepsilon$ for any $i \geq \bar{i}$ and any $r \in \{1, \dots, n\}$. Therefore, for every $\varphi \in \Phi$ we can find an index $r \in \{1, \dots, n\}$ such that $D_\Phi(\varphi, \varphi_{j_r}) < \varepsilon$ and the following inequalities

hold for every index $i \geq \bar{i}$, because of the non-expansivity of $\bar{F}$ and F'_i :

$$\begin{aligned} D_{\Psi}(\bar{F}(\varphi), F'_i(\varphi)) &\leq D_{\Psi}(\bar{F}(\varphi), \bar{F}(\varphi_{j_r})) + D_{\Psi}(\bar{F}(\varphi_{j_r}), F'_i(\varphi_{j_r})) + D_{\Psi}(F'_i(\varphi_{j_r}), F'_i(\varphi)) \\ &\leq D_{\Phi}(\varphi, \varphi_{j_r}) + D_{\Psi}(\bar{F}(\varphi_{j_r}), F'_i(\varphi_{j_r})) + D_{\Phi}(\varphi_{j_r}, \varphi) < 3\varepsilon. \end{aligned}$$

We observe that $\bar{i}$ does not depend on φ , but only on ε and on the set $\{\varphi_{j_1}, \dots, \varphi_{j_n}\}$. It follows that $D_{\Psi}(\bar{F}(\varphi), F'_i(\varphi)) < 3\varepsilon$ for every $\varphi \in \Phi$ and every $i \geq \bar{i}$.

Hence, $\sup_{\varphi \in \Phi} D_{\Psi}(\bar{F}(\varphi), F'_i(\varphi)) \leq 3\varepsilon$ for every $i \geq \bar{i}$. Therefore, the sequence (F'_i) converges to $\bar{F}$ with respect to D_{GENEO} .

The last thing to show is that $\bar{F}$ is group equivariant. Let us consider a $\varphi \in \Phi$, and a $g \in G$. We have that

$$\begin{aligned} \bar{F}(\varphi \circ g) &= \lim_{i \rightarrow \infty} F'_i(\varphi \circ g) \\ &= \lim_{i \rightarrow \infty} (F'_i(\varphi) \circ T(g)) \\ &= \left(\lim_{i \rightarrow \infty} F'_i(\varphi) \right) \circ T(g) \\ &= \bar{F}(\varphi) \circ T(g). \end{aligned}$$

This proves that $\bar{F}$ is group equivariant, and hence a GEO. In conclusion, $\bar{F}$ is a GENEIO. From the fact that the sequence F'_i converges to $\bar{F}$ with respect to D_{GENEO} , it follows that $(\mathcal{F}^{\text{all}}, D_{\text{GENEO}})$ is sequentially compact. $\square$

Exercise 21. Prove that the statement of Theorem 12 does not hold for group equivariant operators, by giving a counterexample where Φ, Ψ, X, Y, G and H are compact, but the space of GEOs is not compact with respect to the metric $D_{\text{GEO}}(F_1, F_2) := \sup_{\varphi \in \Phi} D_{\Psi}(F_1(\varphi), F_2(\varphi))$.

Let us now assume that $(F_1, T), (F_2, T), \dots, (F_n, T) \in \mathcal{F}^{\text{all}}$. If $(a_1, a_2, \dots, a_n) \in \mathbb{R}^n$ with $\sum_{i=1}^n |a_i| \leq 1$ and Ψ is convex, then we set

$$F_{\Sigma}(\varphi) := \sum_{i=1}^n a_i F_i(\varphi) \tag{10}$$

The following theorem holds.

Proposition 44. If $F_{\Sigma}(\Phi) \subseteq \Psi$, then (F_{Σ}, T) is a GENEIO from (Φ, G) to (Ψ, H) .

Proof. First we prove that (F_{Σ}, T) is a GEO. Since every (F_i, T) is a GEO we have that:

$$F_{\Sigma}(\varphi \circ g) = \sum_{i=1}^n a_i F_i(\varphi \circ g)$$

$$\begin{aligned}
&= \sum_{i=1}^n a_i (F_i(\varphi) \circ T(g)) \\
&= \left(\sum_{i=1}^n a_i F_i(\varphi) \right) \circ T(g) \\
&= F_\Sigma(\varphi) \circ T(g).
\end{aligned}$$

Since every F_i is non-expansive, F_Σ is non-expansive:

$$\begin{aligned}
D_\Psi(F_\Sigma(\varphi_1), F_\Sigma(\varphi_2)) &= \left\| \sum_{i=1}^n a_i F_i(\varphi_1) - \sum_{i=1}^n a_i F_i(\varphi_2) \right\|_\infty \\
&= \left\| \sum_{i=1}^n a_i (F_i(\varphi_1) - F_i(\varphi_2)) \right\|_\infty \\
&\leq \sum_{i=1}^n |a_i| \|F_i(\varphi_1) - F_i(\varphi_2)\|_\infty \\
&\leq \sum_{i=1}^n |a_i| \|\varphi_1 - \varphi_2\|_\infty \leq D_\Phi(\varphi_1, \varphi_2).
\end{aligned}$$

Therefore (F_Σ, T) is a GENEIO. $\square$

Theorem 13. *If Ψ is convex, then the set of all maps F such that (F, T) is a GENEIO from (Φ, G) to (Ψ, H) is convex.*

Proof. It is sufficient to apply Proposition 44 for $n = 2$, by setting $a_1 = t$, $a_2 = 1 - t$ for $0 \leq t \leq 1$, and observing that the convexity of Ψ implies $F_\Sigma(\Phi) \subseteq \Psi$. $\square$

In our model, the observers are represented by GEO and GENEIOs. Indeed, each observer can be seen as a black or white box that receives and transforms data. If a nonempty subset $\mathcal{F}$ of $\text{GENEIO}((\Phi, G), (\Psi, H))$ is fixed, a simple pseudo-distance $D_{\mathcal{F}, \Phi}(\varphi_1, \varphi_2)$ to compare two admissible functions $\varphi_1, \varphi_2 \in \Phi$ can be defined by setting $D_{\mathcal{F}, \Phi}(\varphi_1, \varphi_2) := \sup_{F \in \mathcal{F}} \|F(\varphi_1) - F(\varphi_2)\|_\infty$. This definition expresses our assumption that data comparison strongly depends on the choice of the observers. However, we note that the computation of $D_{\mathcal{F}, \Phi}(\varphi_1, \varphi_2)$ for every pair (φ_1, φ_2) of admissible functions is computationally expensive. In the next section, we will see how persistent homology allows us to replace $D_{\mathcal{F}, \Phi}$ with a pseudo-metric $\mathcal{D}_{\text{match}}^{\mathcal{F}, k}$ that is computationally more efficient, stable and, above all, strongly invariant with respect to the action of G .

Pseudo-metrics induced by persistent homology. Let us consider a subset $\mathcal{F} \neq \emptyset$ of $\mathcal{F}^{\text{all}}$. To compare data under the action of $\mathcal{F}$, one could simply define the pseudo-metric $D_{\mathcal{F}, \Phi}$ by setting, for $\varphi_1, \varphi_2 \in \Phi$,

$$D_{\mathcal{F}, \Phi}(\varphi_1, \varphi_2) := \sup_{F \in \mathcal{F}} \|F(\varphi_1) - F(\varphi_2)\|_\infty. \quad (11)$$

Though, the computation of $D_{\mathcal{F},\Phi}(\varphi_1, \varphi_2)$ for every pair (φ_1, φ_2) of admissible functions is computationally expensive. Persistent homology allows us to replace $D_{\mathcal{F},\Phi}$ with a pseudo-metric $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ computationally more efficient, stable and, above all, strongly invariant with respect to the action of G . We recall that a pseudo-metric $\hat{d}$ on Φ is *strongly G -invariant* if it is invariant under the action of G with respect to each variable, i.e., if

$$\hat{d}(\varphi_1, \varphi_2) = \hat{d}(\varphi_1 \circ g, \varphi_2) = \hat{d}(\varphi_1, \varphi_2 \circ g) = \hat{d}(\varphi_1 \circ g, \varphi_2 \circ g)$$

for every $\varphi_1, \varphi_2 \in \Phi$ and every $g \in G$.

For any fixed degree k , we define the pseudo-metric $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ on Φ :

$$\mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2) := \sup_{F \in \mathcal{F}} d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2))) \quad (12)$$

for every $\varphi_1, \varphi_2 \in \Phi$. Observe that this pseudo-metric is an optimal lower bound for the metric defined in (11). Then:

Proposition 45. $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is a strongly G -invariant pseudo-metric on Φ .

Proof. The Matching Distance Stability Theorem 11 and the non-expansivity of every $F \in \mathcal{F}$ imply that

$$\begin{aligned} d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2))) &\leq D_{\Psi}(F(\varphi_1), F(\varphi_2)) \\ &\leq D_{\Phi}(\varphi_1, \varphi_2). \end{aligned}$$

Therefore $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is a pseudo-metric, since it is the supremum of a family of pseudo-metrics that are bounded at each pair (φ_1, φ_2) . Moreover, for every $\varphi_1, \varphi_2 \in \Phi$ and every $g \in G$

$$\begin{aligned} \mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2 \circ g) &:= \sup_{F \in \mathcal{F}} d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2 \circ g))) \\ &= \sup_{F \in \mathcal{F}} d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2) \circ T(g))) \\ &= \sup_{F \in \mathcal{F}} d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2))) \\ &= \mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2) \end{aligned}$$

because of the equality $F(\varphi \circ g) = F(\varphi) \circ T(g)$ for every $\varphi \in \Phi$ and every $g \in G$ and the invariance of persistent homology under the action of the homeomorphisms. Since the function $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is symmetric, this is sufficient to guarantee that $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is strongly G -invariant. $\square$

Exercise 22. In the proof of Proposition 45 we have used the statement that the supremum of a family of bounded pseudo-metrics is still a pseudo-metric. Prove this statement.

The pseudo-distance $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is stable with respect to both the pseudo-metric d_G and the metric D_Φ . This fact guarantees that $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ can be used in the presence of noise as it is stated in the following result.

Theorem 14. *If $\mathcal{F}$ is a non-empty subset of $\mathcal{F}^{\text{all}}$, then*

$$\mathcal{D}_{\text{match}}^{\mathcal{F},k} \leq d_G \leq D_\Phi. \quad (13)$$

Proof. For every $F \in \mathcal{D}_{\text{match}}^{\mathcal{F},k}$, every $g \in G$ and every $\varphi_1, \varphi_2 \in \Phi$, we have that

$$\begin{aligned} & d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2))) \\ &= d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2) \circ T(g))) \\ &= d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2 \circ g))) \\ &\leq D_\Psi(F(\varphi_1), F(\varphi_2 \circ g)) \leq D_\Phi(\varphi_1, \varphi_2 \circ g). \end{aligned}$$

The first equality follows from the invariance of persistent homology under the action of $\text{Iso}_\Phi(K)$ (Proposition 29), and the second equality follows from the fact that (F, T) is a group equivariant operator. The first inequality follows from the Matching Distance Stability Theorem 11, while the second inequality follows from the non-expansivity of F . It follows that, if $\mathcal{F} \subseteq \mathcal{F}^{\text{all}}$, then for every $g \in G$ and every $\varphi_1, \varphi_2 \in \Phi$

$$\mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2) \leq D_\Phi(\varphi_1, \varphi_2 \circ g). \quad (14)$$

Hence, the inequality $\mathcal{D}_{\text{match}}^{\mathcal{F},k} \leq d_G$ follows, while $d_G \leq D_\Phi$ is a trivial consequence of the definition of d_G . $\square$

We stress that the definitions of the natural pseudo-distance d_G and the pseudo-distance $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ come from different theoretical concepts. The former is based on a variational approach involving the set of all homeomorphisms in G , while the latter refers only to a comparison of persistent homologies depending on a family of group equivariant non-expansive operators. Thus, the next result may appear unexpected. Indeed, the role of the group G is not explicitly expressed in the definition of $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$, but implicitly encoded in the GENEOS that are equivariant with respect to G . Moreover, the information contained in each single persistence diagram used in the definition of $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is generally much smaller than the one expressed by the natural pseudo-distance d_G .

Theorem 15. *Let us assume that $\mathcal{F}^{\text{all}} := \text{GENEO}((\Phi, G), (\Phi, G))$, T is the identity from G to G , every function in Φ is non-negative, the k -th Betti number of X does not vanish, and Φ contains each constant function c for which a function $\varphi \in \Phi$ exists such that $0 \leq c \leq \|\varphi\|_\infty$. Then $\mathcal{D}_{\text{match}}^{\mathcal{F}^{\text{all}},k} = d_G$.*

Proof. For every $\varphi' \in \Phi$ let us consider the operator $F_{\varphi'} : \Phi \rightarrow \Phi$ defined by setting $F_{\varphi'}(\varphi)$ equal to the constant function taking everywhere the value $d_G(\varphi, \varphi')$ for every $\varphi \in \Phi$ (i.e., $F_{\varphi'}(\varphi)(x) = d_G(\varphi, \varphi')$ for any $x \in X$). Our assumptions guarantee that such a constant function belongs to Φ .

We observe that

1. $F_{\varphi'}$ is a group equivariant operator associated with T , because the strong invariance of the natural pseudo-distance d_G with respect to the group G implies that if $\varphi \in \Phi$ and $g \in G$, then $F_{\varphi'}(\varphi \circ g)(x) = d_G(\varphi \circ g, \varphi') = d_G(\varphi, \varphi') = F_{\varphi'}(\varphi)(g(x)) = (F_{\varphi'}(\varphi) \circ g)(x) = (F_{\varphi'}(\varphi) \circ T(g))(x)$, for every $x \in X$.
2. $F_{\varphi'}$ is non-expansive on Φ , because for every $\varphi_1, \varphi_2 \in \Phi$

$$\begin{aligned} D_{\Psi} \left(F_{\varphi'}(\varphi_1), F_{\varphi'}(\varphi_2) \right) &= |d_G(\varphi_1, \varphi') - d_G(\varphi_2, \varphi')| \\ &\leq d_G(\varphi_1, \varphi_2) \leq D_{\Phi}(\varphi_1, \varphi_2). \end{aligned}$$

Therefore, $F_{\varphi'}$ is a GENEIO.

For every $\varphi_1, \varphi_2, \varphi' \in \Phi$ we have that

$$d_{\text{match}}(\text{Dgm}(F_{\varphi'}(\varphi_1)), \text{Dgm}(F_{\varphi'}(\varphi_2))) = |d_G(\varphi_1, \varphi') - d_G(\varphi_2, \varphi')|.$$

Indeed, $\text{Dgm}(F_{\varphi'}(\varphi_1)) \setminus \{\Delta\}$ contains only the point $(d_G(\varphi_1, \varphi'), \infty)$, while $\text{Dgm}(F_{\varphi'}(\varphi_2)) \setminus \{\Delta\}$ contains only the point $(d_G(\varphi_2, \varphi'), \infty)$. Both the points have the same multiplicity, which equals the (non-null) k -th Betti number of X .

Setting $\varphi' = \varphi_2$, we have that

$$d_{\text{match}}(\text{Dgm}(F_{\varphi_2}(\varphi_1)), \text{Dgm}(F_{\varphi_2}(\varphi_2))) = d_G(\varphi_1, \varphi_2).$$

As a consequence, we have that

$$\mathcal{D}_{\text{match}}^{\mathcal{F}^{\text{all}}, k}(\varphi_1, \varphi_2) \geq d_G(\varphi_1, \varphi_2). \quad (15)$$

By applying Theorem 14, we get

$$\mathcal{D}_{\text{match}}^{\mathcal{F}^{\text{all}}, k}(\varphi_1, \varphi_2) = d_G(\varphi_1, \varphi_2)$$

for every φ_1, φ_2 . □

We observe that if Φ is bounded, the assumption that every function in Φ is non-negative is not quite restrictive. Indeed, we can obtain it by adding a suitable constant value to every admissible function.

Here we show how $\mathcal{D}_{\text{match}}^{\mathcal{F}, k}$ can be approximated arbitrarily well with a finite subset of operators.

Proposition 46. Let $\mathcal{F}$ be a non-empty subset of $\mathcal{F}^{\text{all}} := \text{GENEO}((\Phi, G), (\Psi, H))$. For every $\varepsilon > 0$, a finite subset $\mathcal{F}'$ of $\mathcal{F}$ exists, such that

$$|\mathcal{D}_{\text{match}}^{\mathcal{F}',k}(\varphi_1, \varphi_2) - \mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2)| \leq \varepsilon$$

for every $\varphi_1, \varphi_2 \in \Phi$.

Proof. Let us consider the closure $\overline{\mathcal{F}}$ of $\mathcal{F}$ in $\mathcal{F}^{\text{all}}$. Let us also consider the covering $\mathcal{U}$ of $\overline{\mathcal{F}}$ obtained by taking all the open balls of radius $\frac{\varepsilon}{2}$ centered at points of $\mathcal{F}$, with respect to D_{GENEO} . Theorem 12 guarantees that $\mathcal{F}^{\text{all}}$ is compact, hence also $\overline{\mathcal{F}}$ is compact. Therefore we can extract a finite covering $\{B_1, \dots, B_m\}$ of $\overline{\mathcal{F}}$ from $\mathcal{U}$. We can set $\mathcal{F}'$ equal to the set of centers of the balls $B_1, \dots, B_m$.

Now, for every $F \in \mathcal{F}$, a $F' \in \mathcal{F}'$ exists such that $D_{\text{GENEO}}(F, F') < \frac{\varepsilon}{2}$. The definition of D_{GENEO} implies that $D_{\Psi}(F(\varphi), F'(\varphi)) < \frac{\varepsilon}{2}$ for every $\varphi \in \Phi$. From the Matching Distance Stability Theorem 11 it follows that

$$d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F'(\varphi_1))) < \frac{\varepsilon}{2}$$

and

$$d_{\text{match}}(\text{Dgm}(F(\varphi_2)), \text{Dgm}(F'(\varphi_2))) < \frac{\varepsilon}{2}$$

for every $\varphi_1, \varphi_2 \in \Phi$.

Therefore,

$$|d_{\text{match}}(\text{Dgm}(F(\varphi_1)), \text{Dgm}(F(\varphi_2))) - d_{\text{match}}(\text{Dgm}(F'(\varphi_1)), \text{Dgm}(F'(\varphi_2)))| < \varepsilon.$$

As a consequence, $\mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2) \leq \mathcal{D}_{\text{match}}^{\mathcal{F}',k}(\varphi_1, \varphi_2) + \varepsilon$.

Since $\mathcal{F}' \subseteq \mathcal{F}$, we know that $\mathcal{D}_{\text{match}}^{\mathcal{F}',k}(\varphi_1, \varphi_2) \leq \mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2)$.

From these two inequalities, the proof of our statement follows. $\square$

Proposition 46 states that the approximation of $\mathcal{D}_{\text{match}}^{\mathcal{F},k}(\varphi_1, \varphi_2)$ can be reduced to the computation of $\mathcal{D}_{\text{match}}^{\mathcal{F}',k}(\varphi_1, \varphi_2)$, i.e. the maximum of a finite set of bottleneck distances between persistence diagrams, which are well-known to be computable by means of efficient algorithms.

Finally, we observe that we can use persistent homology to define a computable and stable pseudo-metric between GENEOS. If $F_1, F_2 \in \mathcal{F}^{\text{all}} := \text{GENEO}((\Phi, G), (\Psi, H))$, for every fixed $k \in \mathbb{N}$, we can set

$$\Delta_{\text{GENEO}}(F_1, F_2) := \sup_{\varphi \in \Phi} d_{\text{match}}(\text{Dgm}(F_1(\varphi)), \text{Dgm}(F_2(\varphi))) \quad (16)$$

for which it holds $\Delta_{\text{GENEO}} \leq D_{\text{GENEO}}$.

As a final remark, we observe that the approach based on GENEOS and persistent homology can be used also when we wish to

have equivariance with respect to a *set* instead of a *group* of homeomorphisms. Indeed, whereas the definition of the natural pseudo-distance d_G requires that G has the structure of a group, the definition of $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ does not need this assumption.

Exercise 23. Assume that $F_1 \in \text{GENEO}((\Phi_1, G_1), (\Phi_2, G_2))$ with respect to a homomorphism $T_1 : G_1 \rightarrow G_2$, and $F_2 \in \text{GENEO}((\Phi_2, G_2), (\Phi_3, G_3))$ with respect to a homomorphism $T_2 : G_2 \rightarrow G_3$. Prove that $F_2 \circ F_1 \in \text{GENEO}((\Phi_1, G_1), (\Phi_3, G_3))$ with respect to $T_2 \circ T_1$.

Exercise 24. Assume that $F_1, F_2 \in \text{GENEO}((\Phi, G), (\Psi, H))$ with respect to a homomorphism $T : G \rightarrow H$. Prove that $\max(F_1, F_2) \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. T , provided that $\max(F_1, F_2)(\Phi) \subseteq \Psi$.

Exercise 25. Assume that $F_1, F_2 \in \text{GENEO}((\Phi, G), (\Psi, H))$ with respect to a homomorphism $T : G \rightarrow H$. Prove that $\min(F_1, F_2) \in \text{GENEO}((\Phi, G), (\Psi, H))$ w.r.t. T , provided that $\min(F_1, F_2)(\Phi) \subseteq \Psi$.

Exercise 26. Assume that $F_1, \dots, F_n \in \text{GENEO}((\Phi, G), (\Psi, H))$ with respect to a homomorphism $T : G \rightarrow H$, and L is a 1-Lipschitz map from $\mathbb{R}^n$ to $\mathbb{R}$, where $\mathbb{R}^n$ is endowed with the max-norm. Consider the map $L^*(F_1, \dots, F_n) : \Phi \rightarrow C^0(X, \mathbb{R})$ defined as

$$L^*(F_1, \dots, F_n)(\varphi) := [L(F_1(\varphi), \dots, F_n(\varphi))],$$

where $[L(F_1(\varphi), \dots, F_n(\varphi))]$ is defined by setting

$$[L(F_1(\varphi), \dots, F_n(\varphi))](x) := L(F_1(\varphi)(x), \dots, F_n(\varphi)(x)).$$

Prove that $L^*(F_1, \dots, F_n) \in \text{GENEO}((\Phi, G), (\Psi, H))$ with respect to T , provided that $L^*(F_1, \dots, F_n)(\Phi) \subseteq \Phi$.

Exercise 27. Assume that $F_1 \in \text{GENEO}((\Phi_1, G_1), (\Psi_1, H_1))$ with respect to a homomorphism $T_1 : G_1 \rightarrow H_1$, and $F_2 \in \text{GENEO}((\Phi_2, G_2), (\Psi_2, H_2))$ with respect to a homomorphism $T_2 : G_2 \rightarrow H_2$. Prove that $F_1 \otimes F_2 \in \text{GENEO}((\Phi_1 \otimes \Phi_2, G_1 \otimes G_2), (\Psi_1 \otimes \Psi_2, H_1 \otimes H_2))$ with respect to the homomorphism $T_1 \otimes T_2 : G_1 \otimes G_2 \rightarrow H_1 \otimes H_2$.

Links between GENEOS and TDA

In this section we will list several links that exist between the theory of GENEOS and TDA.

The operator taking φ to $\text{Dgm}(\varphi)$ is a GENEOS. In some sense, the operator taking each continuous function to a suitable representation of its persistence diagram can be seen as a GENEOS. To show this, let us consider a space Φ of continuous functions $\varphi : X \rightarrow \mathbb{R}$ whose persistence diagrams are generic (in the sense that each point in

$\text{Dgm}(\varphi)$ has multiplicity equal to 1) and contain at least one point at infinity. Let us endow $\mathbb{P} := \{\text{Dgm}(\varphi) : \varphi \in \Phi\}$ with the Hausdorff distance d_H associated with the usual pseudo-distance d on the set $\bar{\Delta}^*$ (see Definition 54). We observe that each persistence diagram $D \in \mathbb{P}$ can be identified with the function $\psi_D : \bar{\Delta}^* \rightarrow \mathbb{R}$ that takes each $p \in \bar{\Delta}^*$ to its distance $d(p, D)$ from D . Moreover, if $\text{Dgm}(\varphi_1), \text{Dgm}(\varphi_2) \in \mathbb{P}$, then $d_H(\text{Dgm}(\varphi_1), \text{Dgm}(\varphi_2)) \leq \|\varphi_1 - \varphi_2\|_\infty$.

Let us now assume that

- G is the group of all self-homeomorphisms of X ;
- Ψ is the set of all continuous functions from $\bar{\Delta}^*$ to $\mathbb{R}$;
- H is the trivial group containing only the identity $\text{id} : \bar{\Delta}^* \rightarrow \bar{\Delta}^*$;
- $T : G \rightarrow H$ is the trivial homomorphism.

It is easy to prove that the operator taking each function $\varphi \in \Phi$ to $\psi_{\text{Dgm}(\varphi)}$ is a GENEIO from Φ to Ψ associated with T .

GENEIOs restrict the invariance of TDA. In this Chapter, we have seen that $\mathcal{D}_{\text{match}}^{\mathcal{F},k}$ is a stable and strongly invariant pseudo-distance with respect to G . It allows to restrict the invariance group of persistent homology from $\text{Homeo}_\Phi(X)$ to G . This is of use in applications.

GENEIOs interact with biparameter Persistent Homology. In the Section “??”, we have seen that the definition of the matching distance between two bifiltrations $\varphi, \psi : X \rightarrow \mathbb{R}^2$ of the topological space X can be seen as the supremum of the classical bottleneck distance between the persistence diagrams associated with the filtrations $F_{a,b}(\varphi), F_{a,b}(\psi) : X \rightarrow \mathbb{R}$, where the operator $F_{a,b}$ is defined by setting $F_{a,b}(\varphi) = \varphi_{(a,b)}^*$. It is interesting to observe that the operator $F_{a,b}$ is a GENEIO for any value of a and b (provided that we consider the natural extension of the concept of GENEIO to operators acting on vector-valued functions).

GENEIOs can be compared by means of TDA. As we have seen in this Chapter, Persistent Homology can indeed be used to define the computable and stable pseudo-metric Δ_{GENEIO} .

Remark 11. *Persistent Homology also gives a shortcut to compare elements of each equivariance group G , by the pseudo-distance*

$$\Delta_G(g_1, g_2) := \sup_{\varphi \in \Phi} d_{\text{match}}(\text{Dgm}_k(\varphi \circ g_1), \text{Dgm}_k(\varphi \circ g_2)).$$

Applications of Topological Data Analysis

In this chapter, we briefly illustrate two applications of TDA.

An application of persistence diagrams (from the book ¹¹)

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Multilocus sequence typing analysis. Within a single bacterial species there can be many genetically distinct strains. Different strains can have important functional differences. For example, some strains may be more virulent than others and some may be more susceptible to the immune responses generated by vaccines. [Multilocus sequence typing \(MLST\) is a method for detecting particular bacterial strains that does not require whole-genome sequencing.](#) It relies on the fact that strains can be identified from certain representative genomic loci selected from regions within housekeeping genes. Typically the size of each locus is about 500 base pairs. Curated MLST data from laboratories around the world is available in large online databases. Often there are thousands of strains identified within a single pathogenic species (over 10,000 in the case of *Neisseria* spp.). MLST data can be used to study horizontal exchange of genomic material in bacteria. Because different species have different loci, one can only examine horizontal exchange within species. Furthermore, because all of the selected loci exist within a few housekeeping genes, our analysis does not provide information about events involving genes other than these housekeepers. The data used here comes from PubMLST ¹². For each of twelve bacterial species, one can construct a pseudogenome by concatenating the typed sequence at each locus. Using the Hamming distance metric, one can calculate a pairwise distance matrix between strains and compute persistent homology on the resulting metric space. The persistence diagrams in degree 1 for the twelve bacterial species are displayed in Figure 29 (Source: ¹³). For the bulk of pathogens, there are three major scales of recombination: one short-lived scale at intermediate distances, another longer-lived scale at intermediate distances, and a third short-lived scale at longer distances. *Helicobacter pylori* is a clear outlier, tending to recombine at significantly lower scales than the other pathogens.

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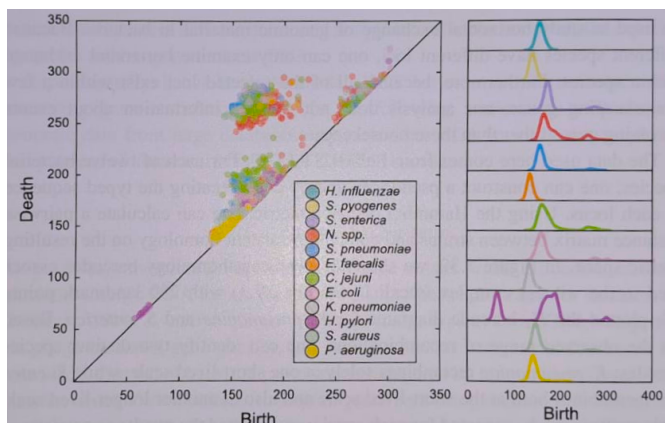


Figure 29: On the left, the persistence diagrams in degree 1 for the twelve strains of pathogens selected for this study MLST profile data. Observe three scales of recombination. On the right, the birth time distribution for each strain. There is an earlier scale of recombination present in *Helicobacter pylori* not observed in the other species.

An application of GENEOS

Finding pockets via GENEOS. GENEOnet¹⁴ is a shallow neural network that exploits the rationale behind GENEOS to solve the problem of protein pocket detection. The paradigm has been here declined for the specific application here considered, but, with the right adjustments, it could be extended and applied to many other situations.

The main reason for choosing this specific application is due to some characteristics that make it very suitable to be treated with GENEOS. First of all there is some important empirical knowledge that is hard to embed in the usual machine learning techniques, but can easily be exploited by a method based on GENEOS. For example it is known that binding sites tend to be in the lipophilic areas of the protein, otherwise they would continuously be filled with solvent, having thus no chances to interact with any other ligand. Another empirical rule says that if a pocket wants to host a binding site then it should be able to accept and donate some hydrogen bonds otherwise no ligand could find stable housing into that pocket. Secondly if we rotate or translate a protein, its pockets will be as well transformed in the same way, coherently with the entire protein. This clearly implies that pocket detection is equivariant with respect to the group of spatial isometries. We used these and some other pieces of information to design a pool of GENEOS able to identify promising binding sites. We first discretized the space surrounding the protein into voxels. Thus, GENEOnet falls in the group of grid-based computational methods. Our choice for the GENEOS fell on convolutional operators that process a set of “channels”, i.e., functions that reflect a reasoned selection of geometric, physical, and chemical properties of a protein. The convolutional kernels of these operators have been designed with a knowledge engineering process to exploit all the information

about the problem. Therefore, the final pool of GENEOnets is composed by families of operators, each parametrized by a shape parameter. These parameters directly influence the shape of the kernels of the operators belonging to the corresponding family and thus the action of each single operator. These families are then networked through a [convex combination](#) that allows us to explore a larger region of the space of GENEOnets. Indeed these second-level operators depend on all the shape parameters and the convex combination weights. A last parameter is needed to transform the output of the method pipeline into a binary function. This function assigns to each voxel of the space surrounding the protein the value 1 if it belongs to a pocket and 0 otherwise.

The parameters of the model are then identified during an optimization step, that employs the Adam optimizer. Optimization is aimed to maximize our accuracy function that expresses a weighted ratio of correct recognition of voxels lying either inside pockets or outside pockets. Since GENEOnet depends eventually on 17 unknown parameters only, the optimization is performed using a small training set of ligand-protein complexes, that proved to be sufficient to obtain a quite good accuracy in pocket identification. As a byproduct of our model we also obtained a druggability score for each identified pocket. In this way it is possible to rank the pockets on the same molecule by scoring them in decreasing order. As a consequence, a set of models trained on different training sets of the same (small) size have been compared on a validation set, and the model providing the best accuracy in the pocket ranking has been selected.

In Figure 30 an example of results of GENEOnet applied to the protein 2QWE is shown. The picture shows a relevant aspect of GENEOnet: the depicted protein is made up of four symmetrical units so that the true pocket is replicated four times. GENEOnet correctly outputs, among the others, four symmetrical pockets which get high scores. This happens thanks to [equivariance](#), because the results of the model on identical units are the same, with position and orientation coherently adjusted. Moreover this happens even if the model has been trained mainly on single chain examples.

In Figure 31 the results of a comparison of GENEOnet with other state-of-the-art methods are displayed. We see that GENEOnet has a better performance than all the other methods considered in the comparison; in particular if we look at T_3 , that is the fraction of proteins whose true pocket is identified within the three top-ranked predicted ones, we see that GENEOnet achieves a result of 0.941 which means that, with this data, we can expect that more than 90% of the times we will find the right pocket considering just the three pockets with

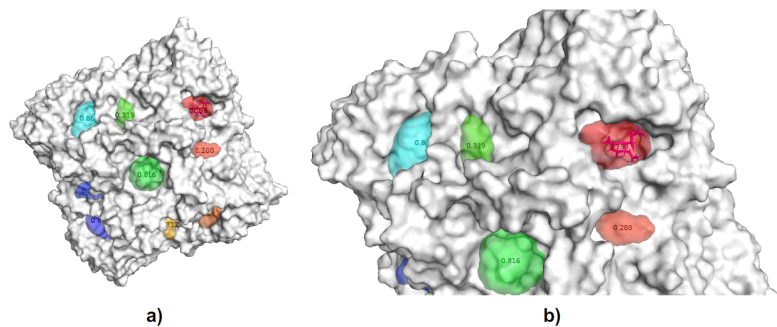
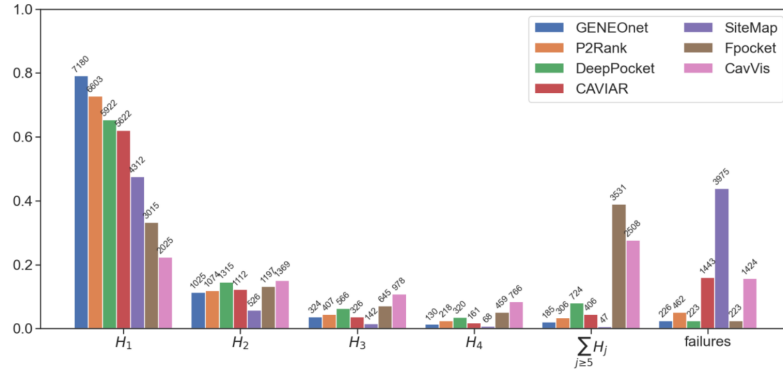
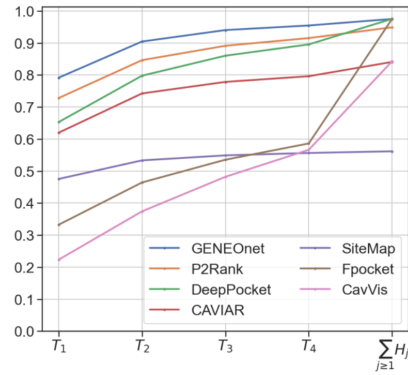


Figure 30: Model predictions for protein 2QWE. In Figure a) the global view of the prediction is shown, where different pockets are depicted in different colors and are labelled with their scores. In Figure b) the zoomed of the pocket containing the ligand is shown.

the highest score. All the other methods, instead, have a value of T_3 below 0.9.



a)



b)

$$H_j = \frac{\#(\text{proteins whose true pocket is hit by the } j\text{-th top ranked})}{\#(\text{proteins})}$$

$$T_j = \frac{\#(\text{proteins whose true pocket is hit within the } j\text{-th top ranked})}{\#(\text{proteins})} = \sum_{i=1}^j H_i$$

Figure 31: Results of comparison on the test set. Figure a) shows a bar chart of the H_j coefficients for the different methods, reporting also the absolute frequencies, while Figure b) shows cumulative frequency curves.

This is the first version of my lecture notes, and they could contain many misprints and errors. Please report them to me at this email address: patrizio.frosini@unipi.it.

PF

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