

Lower Bounds for Betti Numbers in Vietoris–Rips Complexes of Hypercubes

by

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Abstract

This thesis serves as a comprehensive introduction and elucidation of Henry Adams and Žiga Virk's seminal work [6] on new lower bounds on the Betti numbers for Vietoris–Rips complexes of hypercube graphs across all dimensions and scales. Specifically, for a hypercube graph of dimension n with vertex set Q_n comprising 2^n vertices and equipped with the shortest path metric, we examine its Vietoris–Rips complex $\text{VR}(Q_n; r)$ at any given scale parameter $r \geq 0$. Here, $\text{VR}(Q_n; r)$ includes Q_n as its vertex set and considers all subsets with a maximum diameter of r as its simplices. Given integers $r < r'$, the inclusion $\text{VR}(Q_n; r) \hookrightarrow \text{VR}(Q_n; r')$ is found to be nullhomotopic, indicating that persistent homology bars do not extend beyond a unit length. Consequently, the study concentrates on the individual spaces $\text{VR}(Q_n; r)$. By succinctly presenting the foundational definitions and correcting minor inaccuracies in their formulation, we aim to make Adams and Virk's work more accessible and understandable. And we introduce Adams and Virk's work on lower bounds for the ranks of a specific dimensional homology group on these complexes. Utilizing cross-polytopal generators, for instance, we ascertain that the rank of $H_{2^r-1}(\text{VR}(Q_n; r))$ is no less than $2^{n-(r+1)} \binom{n}{r+1}$.

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Chapter 1

Introduction

Define Q_n as the vertex set of the n -dimensional hypercube graph with the shortest path metric. Equivalently, Q_n is the set of all 2^n binary strings, using the Hamming distance, or as $\{0, 1\}^n \subset \mathbb{R}^n$ with the ℓ^1 metric.

The study of *Vietoris–Rips simplicial complexes*, denoted as $\text{VR}(X; r)$, forms the core of this paper, focusing on their topology within the context of Q_n . For a metric space X and a given scale $r \geq 0$, $\text{VR}(X; r)$ is defined with X serving as the vertex set and a finite subset $\sigma \subseteq X$ constitutes a simplex if and only if its diameter does not exceed r . Initially developed for algebraic topology [9] and geometric group theory [8, 11] these complexes have since become pivotal in applied and computational topology for approximating dataset shapes [10, 14].

Significant findings reveal that Vietoris–Rips complexes facilitate the approximation of metric spaces through persistent homology barcodes, proving their utility in discerning the topological nuances of data [13, 12]. Further, they have been instrumental in retrieving the homotopy types of manifolds [18, 19, 24, 20] and in the efficient computation of persistent homology barcodes [7]. However, the understanding of Vietoris–Rips complexes, especially regarding manifolds or simple graphs at expansive scale parameters, remains limited. Notable exceptions include analyses on circular manifolds [3], cycle graphs [1, 2] and studies confined to 1-dimensional homology [23, 17].

The Vietoris–Rips complex $\text{VR}(Q_n; r)$ of the n -dimensional hypercube’s vertex set, with scale parameter r , presents intriguing homotopy characteristics, some of which are delineated up to $r \leq 3$, with further cases largely unexplored. For $r = 0$, $\text{VR}(Q_n; 0)$ manifests as a disjoint union of 2^n vertices, rendering it homotopy equivalent to a $(2^n - 1)$ -fold wedge sum of zero-dimensional spheres. At $r = 1$, $\text{VR}(Q_n; 1)$ evolves into a connected graph, specifically, the hypercube graph. Utilizing a straightforward computation of the Euler characteristic, it is shown to be homotopy equivalent to a $((n - 2)2^{n-1} + 1)$ -fold wedge sum of circles. When r is incremented to 2, Adams and Adamaszek [4] demonstrated that $\text{VR}(Q_n; 2)$ aligns with the homotopy type of a wedge sum of 3-dimensional spheres. For $r = 3$ and $n \geq 5$, Shukla’s findings

[22] illuminate the homology of $\text{VR}(Q_n; 3)$, specifying that the q -dimensional homology is nontrivial exclusively for $q = 7$ or $q = 4$. For $r = 3$, Feng’s pivotal work [15], predicated on earlier research by Feng and Nukula [16], establishes that $\text{VR}(Q_n; 3)$ invariably exhibits homotopy equivalence to a wedge sum of 7-spheres and 4-spheres. When the scale parameter is set to $r = n - 1$, $\text{VR}(Q_n; n - 1)$ transforms into a structure isomorphic to the boundary of a cross-polytope encompassing 2^n vertices. For $r \geq n$, $\text{VR}(Q_n; n)$ morphs into a complete simplex, rendering it contractible. Despite these advancements, a substantial region within the parameter space, defined by $r \geq 4$ and $r \leq n - 2$, remains uncharted in terms of understanding the homotopy types of $\text{VR}(Q_n; r)$. This “infinite triangle” of parameters represents a frontier in the study of Vietoris–Rips complexes, inviting further exploration and discovery within the field.

In this work, we extend the analysis of the Vietoris–Rips complexes $\text{VR}(Q_n; r)$ to encompass all values of r , presenting new lower bounds for the ranks of their homology groups. Theorem 1 establishes that $\text{rank}H_{2r-1}(\text{VR}(Q_n; r)) \geq 2^{n-(r+1)} \binom{n}{r+1}$.

For integers $r < r'$, a straightforward argument demonstrates that the inclusion $\text{VR}(Q_n; r) \hookrightarrow \text{VR}(Q_n; r')$ is nullhomotopic. Consequently, persistent homology bars exceed a length of one, implying all homological insights from the filtration $\text{VR}(Q_n; \bullet)$ are encapsulated by $\text{VR}(Q_n; r)$ for individual integer values of r . While our results have been articulated for $Q_n = \{0, 1\}^n$ with the ℓ^1 metric, it is pertinent to note that these findings are applicable across any ℓ^p metric for $1 \leq p < \infty$. Given $x, y \in Q_n$, the difference in the i -th coordinates of x and y is either 0 or 1 for each $1 \leq i \leq n$, leading to the equivalence $\text{VR}((Q_n, \ell^p); r) = \text{VR}((Q_n, \ell^1); r^p)$. This observation facilitates the translation of our results to any ℓ^p metric through a straightforward reparametrization of scale.

We initiate with preliminaries in Chapter 2. Chapter 3 is dedicated to reviewing contractions and establishing that $\text{VR}(Q_n; \bullet)$ exhibits no persistent homology bars exceeding a length of one. In Chapter 4, cross-polytopal generators are employed to demonstrate $\text{rank}H_{2r-1}(\text{VR}(Q_n; r)) \geq 2^{n-(r+1)} \binom{n}{r+1}$.

Chapter 2

Preliminaries and geometry of hypercubes

2.1 Hypercubes

A *simple graph* is a graph having no loops or multiple edges. *Hypercubes* are the simple graph whose vertices are the n -tuples with entries in $\{0, 1\}$ and whose edges are the pairs of n -tuples that differ in exactly one position.

Definition 1. Given $n \in \{1, 2, \dots\}$, the hypercube graph Q_n is the metric space $\{0, 1\}^n$, equipped with the ℓ^1 distance, also known as **Hamming distance** or **taxicab distance**, is defined as

$$d((a_1, a_2, \dots, a_n), (b_1, b_2, \dots, b_n)) = \sum_{i=1}^n |a_i - b_i|.$$

In other words, the distance between two n -tuples is the number of coordinates in which they differ.

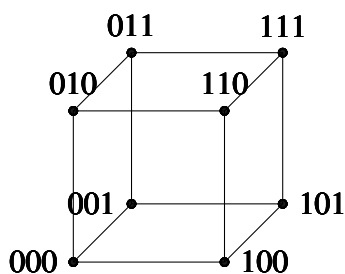


Figure 2.1: The Hamming distance $d(000, 101) = 2$

2.2 Homology

In the realm of Homology, we begin by understanding the fundamental notion of geometric independence and the construction of simplices.

Definition 2. Given a set $\{a_0, \dots, a_n\}$ of points of \mathbb{R}^N , this set is said to be **geometrically independent** if for any (real) scalars

$$\sum_{i=0}^n t_i = 0 \quad \text{and} \quad \sum_{i=0}^n t_i a_i = 0$$

imply that $t_0 = t_1 = \dots = t_n = 0$. We define the **n -simplex** σ spanned by a_0, \dots, a_n to be the set of all points x of \mathbb{R}^N such that

$$x = \sum_{i=0}^n t_i a_i, \quad \text{where} \quad \sum_{i=0}^n t_i = 1$$

and $t_i \geq 0$ for all i .

Definition 3. A **simplicial complex** K in \mathbb{R}^n is a collection of simplices in \mathbb{R}^n satisfying the following conditions:

1. If a simplex σ is in K , then each face of σ is also in K ,
2. Any two simplices in K are either disjoint or their intersection is a face of each.

Specifying a polyhedron X through a collection of simplices forming X proves impractical for detailed polyhedral analysis, entangling one in analytic geometry complexities and the cumbersome task of ensuring simplex accuracy and intersection integrity. A more efficient approach involves defining X via an “abstract simplicial complex,” a concept we will now introduce.

Definition 4. An **abstract simplicial complex** is a collection \mathcal{S} of finite nonempty sets, such that if A is an element of \mathcal{S} , so is every nonempty subset of A .

Definition 5. Let $|K|$ be the subset of \mathbb{R}^N that is the union of the simplices of K . Giving each simplex its **natural topology** as a subspace of \mathbb{R}^N , we then topologize $|K|$ by declaring a subset A of $|K|$ to be closed in $|K|$ if and only if $A \cap \sigma$ is closed in σ , for each $\sigma \in K$.

Now we introduce the notion of a “simplicial map” of one complex into another. Let K and L be simplicial complexes.

Definition 6. A **simplicial map** $f : K \rightarrow L$ is an assignment $K^{(0)} \rightarrow L^{(0)}$ of vertices to vertices which sends simplices to simplices, where $K^{(0)}$ is all vertices of K . So for each simplex $\sigma = [v_0, \dots, v_n]$ of K , the image $f(\sigma) = [f(v_0), \dots, f(v_n)]$ must be a simplex of L . And if simplicial map f is bijection, then it is called **simplicial isomorphism**.

A ***p-chain*** on K is a function c from the set of oriented p -simplices of K to the integers such that:

- $c(\sigma) = -c(\sigma')$, if σ and σ' are opposite orientations of the same simplex;
- $c(\sigma) = 0$, for all but finitely many oriented p -simplices σ .

We add p -chains by adding their values; the resulting group is denoted $C_p(K)$ and is called the *group of (oriented) p -chains* of K . If $p < 0$ or $p > \dim K$, let $C_p(K)$ be the trivial group.

Definition 7. We now define a homomorphism

$$\begin{aligned} \partial_p : C_p(K) &\longrightarrow C_{p-1}(K) \\ \sigma &\longmapsto \sum_{i=0}^p (-1)^i [v_0, \dots, \hat{v}_i, \dots, v_p] \end{aligned}$$

, where \hat{v}_i means that the vertex v_i is to be deleted from the array. The map ∂_p is called the ***boundary operator***.

Additionally, we say that two p -chains c and c' are ***homologous*** if $c - c' = \partial_{p+1}d$ for some $p + 1$ chain d . In particular, if $c = \partial_{p+1}d$, we say that c is ***homologous to zero***.

Before we define the ***homology group***, we need the following lemma:

Lemma 1. $\partial_{p-1} \circ \partial_p = 0$

Proof. Let $[v_0, \dots, v_p]$ be a p -simplex. we compute $\partial_{p-1} \circ \partial_p = 0$ by definition,

$$\begin{aligned} \partial_{p-1} \partial_p [v_0, \dots, v_p] &= \sum_{i=0}^p (-1)^i \partial_{p-1} [v_0, \dots, \hat{v}_i, \dots, v_p] \\ &= \sum_{j < i} (-1)^i (-1)^j [\dots, \hat{v}_j, \dots, \hat{v}_i, \dots] + \sum_{j > i} (-1)^i (-1)^{j-1} [\dots, \hat{v}_i, \dots, \hat{v}_j, \dots]. \end{aligned}$$

The terms of two summations cancel in pairs. □

Example 1. Compute $\partial_1(\partial_2(\Delta))$, where Δ defined as the following figure,

$$\begin{aligned}
\partial_1(\partial_2(\Delta)) &= \partial_1(e_1 + e_2 + e_3) \\
&= \partial_1(v_1, v_0) + \partial_1(v_2, v_1) + \partial_1(v_0, v_2) \\
&= (v_0 - v_1) + (v_1 - v_2) + (v_2 - v_0) \\
&= 0
\end{aligned}$$

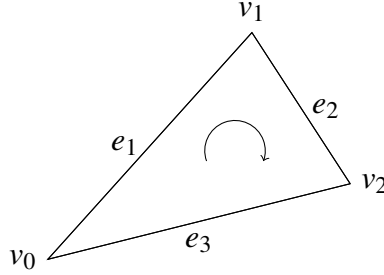


Figure 2.2: Let Δ be a 2-simplex, where $\Delta = [v_0, v_1, v_2]$.

The kernel of ∂_p is called the group of ***p-cycles*** and denoted as $Z_p(K)$, and the image of ∂_{p+1} is called the group of ***p-boundaries***, denoted as $B_p(K)$. And we can observe that each boundary of a $p + 1$ chain is automatically a p -cycle, i.e. $B_p(K) \subset Z_p(K)$.

Definition 8. Since $B_p(K)$ is a subgroup of $Z_p(K)$, we can form the quotient group $H_p(K) = Z_p(K)/B_p(K)$ and call it the ***p*th homology group of K** . The rank of homology group $H_p(K)$ is ***p*th Betti number β_p** , is the number of distinct p dimensional holes.

2.3 Cohomology

If A and G are abelian groups, then the set $\text{Hom}(A, G)$ of all homomorphisms of A into G becomes an abelian group if we add two homomorphisms by adding their values in G . That is, for $a \in A$ we define $(\phi + \psi)(a) = \phi(a) + \psi(a)$. The map $\phi + \psi$ is a homomorphism, because $(\phi + \psi)(0) = 0$ and

$$\begin{aligned}
(\phi + \psi)(a + b) &= \phi(a + b) + \psi(a + b) \\
&= \phi(a) + \psi(a) + \phi(b) + \psi(b) \\
&= (\phi + \psi)(a) + (\phi + \psi)(b).
\end{aligned}$$

The identity element of $\text{Hom}(A, G)$ is the function mapping A to the identity element of G . The inverse of the homomorphism ϕ is the homomorphism that maps a to $-\phi(a)$, for each $a \in A$.

Definition 9. A homomorphism $f : A \rightarrow B$ gives rise to a **dual homomorphism**

$$\text{Hom}(A, G) \xleftarrow{\tilde{f}} \text{Hom}(B, G)$$

going in the reverse direction. The map \tilde{f} assigns to the homomorphism $\phi : B \rightarrow G$, the composite

$$A \xrightarrow{f} B \xrightarrow{\phi} G.$$

That is, $\tilde{f}(\phi) = \phi \circ f$.

The map \tilde{f} is a homomorphism, since $\tilde{f}(0) = 0$ and

$$\begin{aligned} [\tilde{f}(\phi + \psi)](a) &= (\phi + \psi)(f(a)) = \phi(f(a)) + \psi(f(a)) \\ &= [\tilde{f}(\phi)](a) + [\tilde{f}(\psi)](a). \end{aligned} \tag{2.1}$$

Building on dual homomorphisms, we next introduce their application in the context of simplicial complexes, demonstrating the bridge between algebra and topology.

Definition 10. Let K be a simplicial complex; let G be an abelian group. The group of **p -dimensional cochains** of K , with coefficients in G , is the group $C^p(K; G) = \text{Hom}(C_p(K), G)$. The **coboundary operator** δ is defined to be the dual of the boundary operator $\partial : C_{p+1}(K) \rightarrow C_p(K)$. Thus $C^{p+1}(K; G) \xleftarrow{\delta} C^p(K; G)$, so that δ raises dimension by one.

$$0 \longrightarrow C^0 \xrightarrow{\delta^0} C^1 \xrightarrow{\delta^1} C^2 \xrightarrow{\delta^2} \dots \xrightarrow{\delta^{k-1}} C^k \xrightarrow{\delta^k} C^{k+1} \xrightarrow{\delta^{k+1}} \dots$$

We define **cocycles** $Z^p(K; G)$ to be the kernel of this homomorphism, **coboundaries** $B^{p+1}(K; G)$ to be its image, and noting that $\delta^2 = 0$, since $\partial^2 = 0$ by Lemma 1, so we can define the cohomology group:

Definition 11. For each dimensional $p \geq 0$, the **p -th cohomology group** is the quotient space

$$H^p(K; G) = Z^p(K; G) / B^p(K; G).$$

Before we define cap product, let denote $\sigma_{\leq i} = [v_0, \dots, v_i]$ as the ***i*-front face** and $\sigma_{\geq i} = [v_i, \dots, v_n]$ as the ***i*-back face**, where $\sigma = [v_0, \dots, v_n]$

Definition 12. Let X be a topological space and coefficient ring R . Consider p -cochain ξ as element of the cohomology group $H^p(X; R)$ and $(p+q)$ -chain $\gamma = \sum_{\sigma} \gamma_{\sigma} \cdot \sigma$ in $H_{p+q}(X; R)$, where σ ranges over oriented $(p+q)$ -simplices and each γ_{σ} is an element of the coefficient ring R . Define the **cap product** $\frown: H^p(X; R) \times H_{p+q}(X; R) \rightarrow H_q(X; R)$ by setting

$$\xi \frown \gamma = \sum_{\sigma} \gamma_{\sigma} \cdot \xi(\sigma_{\leq i}) \cdot \sigma_{\geq i}.$$

Then we have a new q -chain $\xi \frown \gamma$ in $H_q(X; R)$.

2.4 Vietoris-Rips complexes

Definition 13. Given a metric space X and a finite subset $A \subseteq X$, the **diameter** of A is

$$\text{diam}(A) = \max_{a, b \in A} d(a, b)$$

The **local diameter** of A at a point $a \in A$ equals

$$\text{localDiam}(A, a) = \max_{b \in A} d(a, b).$$

Definition 14. Given $r \geq 0$ and a metric space X the **Vietoris-Rips complex** $\text{VR}(X; r)$ is the simplicial complex with vertex set X , and with a finite subset $\sigma \subseteq X$ being a simplex whenever $\text{diam}(\sigma) \leq r$.

2.5 Embeddings of hypercubes

An **isometric embedding** of a graph G into a metric space (X, d_X) is an injective map $f: V(G) \rightarrow X$ such that $d_G(x, y) = d_X(f(x), f(y))$, where $V(G)$ is the vertex set of graph G .

For k a positive integer, let $[k] = \{1, 2, \dots, k\}$. Given $p \in [n-1]$ there are many isometric copies of Q_p in Q_n . For any subset $S \subseteq [n]$ of cardinality p we can isometrically embed Q_p in Q_n , using set S as its variable coordinates, and leaving the rest of the entries fixed. In more detail, we define an isometric

embedding $\iota_S^b : Q_p \hookrightarrow Q_n$ associated to a subset $S = \{s_1, s_2, \dots, s_p\} \subseteq [n]$ of coordinates and an offset $(b_i)_{i \in [n] \setminus S} \in \{0, 1\}^{n-|S|}$, maps $(a_i)_{i \in [p]}$ to $(a'_i)_{i \in [n]}$ with

- $a'_{s_i} = a_i$ for $i \in [p]$, and
- $a'_i = b_i$ otherwise.

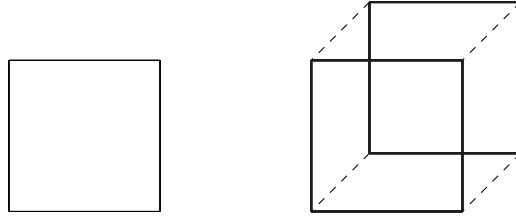


Figure 2.3: Example: For $n = 3, p = 2$, and $S = \{1, 2\}$, the element of offset b_3 can be either 0 or 1. When $b_3 = 0$, the square is embedded onto the front of the cube in blue; when $b_3 = 1$, it is embedded onto the back face of the cube, also in blue.

Given a fixed set S , there are 2^{n-p} such embeddings ι_S , each associated to a different offset b . Let $\pi_S : Q_n \rightarrow Q_p$ be the map projecting onto the coordinates in S . Then $\pi_S \circ \iota_S = id_{Q_p}$ for any map ι_S (i.e., for any choice of an offset b). Given an offset $(b_i)_{i \in [n] \setminus S}$, let Q_p^b denote the image of ι_S^b corresponding to the offset b , and let $\pi_S^b : Q_n \rightarrow Q_p^b$ be defined as $\iota_S^b \circ \pi_S$. Given $B \subseteq Q_n$ its **Cubic Hull** $\text{cHull}(B)$ is the smallest isometric copy of a cube (i.e., the image of Q_p^b via some map ι) containing B .

For our purposes we will only consider isometric embeddings $Q_p \hookrightarrow Q_n$ that retain the order of coordinates. With this convention of retaining the coordinate order, there are $\binom{n}{p} 2^{n-p}$ isometric embeddings $\iota : Q_p \hookrightarrow Q_n$ and $\binom{n}{p}$ projections $\pi : Q_n \rightarrow Q_p$.

Chapter 3

Contractions and the persistent homology of hypercubes

In this chapter, we aim to establish the following results. Initially, we set the scale $r > 0$ and choose p such that $p \leq n$ and consider an isometric embedding $Q_p \hookrightarrow Q_n$; this induces an inclusion $\text{VR}(Q_p; r) \hookrightarrow \text{VR}(Q_n; r)$ that preserves injectivity on homology across all dimensions. Moreover, for a fixed dimension n and integer scale parameters satisfying $r < r'$, we assert that the inclusion $\text{VR}(Q_n; r) \hookrightarrow \text{VR}(Q_n; r')$ is nullhomotopic. Consequently, the filtration $\text{VR}(Q_n; \bullet)$ has no persistent homology bars of length longer than one.

3.1 Contractions

A map $f : X \rightarrow A$ from a metric space (X, d) onto a closed subspace $A \subseteq X$ is a **contraction** if $f|_A = \text{id}_A$ and if $d(f(x), f(y)) \leq d(x, y)$ for all $x, y \in X$.

The foundation of our interest in contractions is based on a noteworthy property: if a contraction $X \rightarrow A$ exists, it guarantees that the homology of the Vietoris-Rips complex of A is mapped into injectively by the homology of the corresponding Vietoris-Rips complex of X .

Proposition 1. ([25]) *If $f : X \rightarrow A$ is a contraction, then the embedding $A \hookrightarrow X$ induces injections on homology $H_q(\text{VR}(A; r)) \rightarrow H_q(\text{VR}(X; r))$ for all integers $q \geq 0$ and scales $r \geq 0$.*

We prove that projections mapping from a higher-dimensional cube onto lower-dimensional cube in Section 2.5 are contractions:

Lemma 2. *Given fixed $p \in [n - 1]$, set $S \subseteq [n]$ of cardinality p , and offset b as in Section 2.5, the following hold:*

(1) *Maps π_S and π_S^b are contractions,*

(2) *For each $x \in Q_p^b$ and $y \in Q_n$, we have $d(x, y) = d(x, \pi_S^b(y)) + d(\pi_S^b(y), y)$.*

(3) For each offset b' :

(a) For each $x, y \in Q_p^{b'}$, we have $d(x, y) = d(\pi_p^{b'}(x), \pi_p^{b'}(y))$.

(b) For each $x \in Q_p^{b'}$ and $y \notin Q_p^{b'}$, we have $d(x, y) - 1 \geq d(\pi_p^b(x), \pi_p^b(y)) \geq d(x, y) - (n - p)$.

Proof. (1) Given two points $p_1, p_2 \in Q_n$, their Hamming distance $d(p_1, p_2)$ counts the differing components. The distance $d(\pi_S(p_1), \pi_S(p_2))$ represents the count of differing components restricted to the subset S , thus $d(\pi_S(p_1), \pi_S(p_2)) \leq d(p_1, p_2)$. This inequality also holds for π_S^b , indicating that both π_S and π_S^b function as contractions.

(2) The second item is evident from noting that:

- The distance $d(x, \pi_S^b(y))$ counts the differing components within S between x and y , and
- $d(\pi_S^b(y), y)$ tallies the differences of components in $[n] \setminus S$.

So $d(x, y) = d(x, \pi_S^b(y)) + d(\pi_S^b(y), y)$.

(3) (a) Since $x, y \in Q_p^{b'}$, then $d(x, y) = d(\pi_p^b(x), \pi_p^b(y))$, as their coordinates outside S agree.

(b) For $x \in Q_p^{b'}$ and $y \notin Q_p^{b'}$, we have $d(x, y) - d(\pi_p^b(x), \pi_p^b(y)) \geq 1$. This is because there is at least one coordinate outside the subset S where x and y differ, given that they do not belong to the same subspace $Q_p^{b'}$.

The maximum of $d(x, y) - d(\pi_p^b(x), \pi_p^b(y))$ can reach to $n - p$, considering all coordinates in S are different, then $d(x, y) - d(\pi_p^b(x), \pi_p^b(y)) \geq n - p$.

Hence, $d(x, y) - 1 \geq d(\pi_p^b(x), \pi_p^b(y)) \geq d(x, y) - (n - p)$.

□

Given that each projection $\pi : Q_n \rightarrow Q_p$ is a contraction by Lemma 2, it follows from Proposition 1 that the corresponding embeddings $Q_p \hookrightarrow Q_n$ induces an injective map on homology $H_q(\text{VR}(Q_p; r)) \rightarrow H_q(\text{VR}(Q_n; r))$ across all dimensions q .

3.2 Persistent homology of hypercubes

A primary focus within contemporary topology is the study of persistent homology, which arise from the application of the Vietoris-Rips filtration. However, when considering Vietoris-Rips complexes

associated with hypercubes, the persistent homology yields no additional insight beyond the homology groups at fixed scale parameters. Indeed, the subsequent proposition asserts that for any integers $r < r'$, the inclusion $\text{VR}(Q_n; r) \hookrightarrow \text{VR}(Q_n; r' + 1)$ induces a map that is trivial on homology.

Proposition 2. ([21]) *Let K be a simplicial complex and X an arbitrary space. If two maps $f, g : X \rightarrow |K|$ are contiguous then $f \simeq_K g$, we call f and g are homotopic; and when g is a constant map, it is said that f is nullhomotopic.*

Proposition 3. *For any positive integers n and r , the natural inclusion $\iota : \text{VR}(Q_n; r) \hookrightarrow \text{VR}(Q_n; r + 1)$ is nullhomotopic.*

Proof. We first claim that the inclusion $\iota : \text{VR}(Q_n; r) \hookrightarrow \text{VR}(Q_n; r + 1)$ is homotopic to the projection $\pi_{[n-1]} : \text{VR}(Q_n; r) \rightarrow \text{VR}(Q_{n-1}; r)$ in $\text{VR}(Q_n; r + 1)$. In order to prove the claim we will show that the two maps are contiguous in $\text{VR}(Q_n; r + 1)$. (i.e., for each simplex $\sigma \in \text{VR}(Q_n; r)$ the union $\sigma \cup \pi_{[n-1]}(\sigma)$ is contained in a simplex of $\text{VR}(Q_n; r + 1)$), which implies that the two maps are homotopic.

Let $\sigma \in \text{VR}(Q_n; r)$, there exists a simplex in $\text{VR}(Q_n; r + 1)$ such that $\iota(\sigma)$ and $\pi_{[n-1]}(\sigma)$ is contained in it. By the definition of Vietoris-Rips complexes, we have $\text{diam}(\sigma) \leq r$. As $\pi_{[n-1]}(\sigma)$ is obtained by dropping the final coordinate we also have $\text{diam}(\pi_{[n-1]}(\sigma)) \leq r$. Taking $x \in \sigma$ and $y \in \pi_{[n-1]}(\sigma)$, i.e. $y = \pi_{[n-1]}(y')$ for some $y' \in \sigma$, we see that

$$d(x, y) \leq d(x, y') + d(y', y) \leq r + 1$$

as $d(y, y') \leq 1$. This $\sigma \cup \pi_{[n-1]}(\sigma) \in \text{VR}(Q_n; r + 1)$, and the claim is proved.

We proceed inductively, proving that each projection $\pi_{[k]} : \text{VR}(Q_n; r) \rightarrow \text{VR}(Q_k; r)$ is homotopic to the projection $\pi_{[k-1]} : \text{VR}(Q_n; r) \rightarrow \text{VR}(Q_{k-1}; r)$ in $\text{VR}(Q_n; r + 1)$, by the same argument as above. As a result, the embedding $\text{VR}(Q_n; r) \rightarrow \text{VR}(Q_n; r + 1)$ is homotopic to the projection $\pi_{[1]} : \text{VR}(Q_n; r) \rightarrow \text{VR}(Q_1; r)$. Since $\text{VR}(Q_1; r)$ is clearly contractible, this completes the proof. Therefore, embedding ι is contractible. □

Chapter 4

Homology bounds via cross-polytopes and maximal simplices

Let us fix a scale parameter $r \geq 2$ and consider an isometric embedding $\iota : Q_{r+1} \hookrightarrow Q_n$ for $n \geq r+1$. The objective of this chapter is to demonstrate that the induced map $\text{VR}(Q_{r+1}; r) \hookrightarrow \text{VR}(Q_n; r)$ is not only injective on $(2^r - 1)$ -dimensional homology, but also that distinct ordered embeddings ι give rise to independent generators of homology. We shall elucidate this in further detail.

Definition 15. *Regular polytope* is a shape with sides and vertices that are symmetrical; and if any line segment joining two points in the polytope is also contained in the polytope then we call it **convex polytope**. A **cross-polytope** is a regular, convex polytope that exists in n -dimensional Euclidean space.

Initial observations reveal that the Vietoris-Rips complex $\text{VR}(Q_{r+1}; r)$ is topologically equivalent to a $(2^r - 1)$ -dimensional sphere, denoted as S^{2^r-1} , i.e., $\text{VR}(Q_{r+1}; r) \cong S^{2^r-1}$. This homeomorphism arises due to the connectivity properties within Q_{r+1} , where each vertex x is linked by an edge in $\text{VR}(Q_{r+1}; r)$ to every other vertex except for \bar{x} , the antipodal vertex. Therefore, after taking the clique complex of this set of edges, we see that $\text{VR}(Q_{r+1}; r)$ is isomorphic (as simplicial complexes) to the boundary of the cross-polytope with 2^{r+1} vertices. This cross-polytope is a 2^r -dimensional ball in 2^r -dimensional Euclidean space, and therefore its boundary is a sphere of dimension $2^r - 1$. In particular, $\text{rank } H_{2^r-1}(\text{VR}(Q_{r+1}; r)) = 1$.

Since $\text{VR}(Q_{r+1}; r)$ is the boundary of a cross-polytope, there is a convenient $(2^r - 1)$ -dimensional cycle γ generating $H_{2^r-1}(\text{VR}(Q_{r+1}; r))$. Define the set of maximal antipode-free simplices as

$$\mathcal{A}_r = \{Y \subseteq Q_{r+1} \mid x \in Y \iff \bar{x} \notin Y\}.$$

The cycle γ is defined as the sum of appropriately oriented elements of \mathcal{A}_r . The space Q_{r+1} consists of 2^{r+1} points, which can be partitioned into 2^r pairs of mutually antipodal points. If a subset of Q_{r+1} contains exactly one point from each such pair, it is of cardinality 2^r . Thus \mathcal{A}_r consists of sets of cardinality

2^r . Given $x \in Q_{r+1}$, the only element Q_{r+1} which disagrees with x on all $r+1$ coordinates is \bar{x} . As a result each element of \mathcal{A}_r is a of diameter at most r and thus a simplex of $\text{VR}(Q_{r+1}; r)$. Observe also that any element of \mathcal{A}_r is a maximal simplex of $\text{VR}(Q_{r+1}; r)$: adding any point to such a simplex would mean the presence of an antipodal pair, and so the diameter would thus grow to $r+1$.

Recall that $2^{n-(r+1)} \binom{n}{r+1}$ is the number of different (ordered) embeddings $\iota : Q_{r+1} \hookrightarrow Q_n$. In the end of this chapter, we will use maximal simplices and pairing between homology and cohomology in order to prove that these $2^{n-(r+1)} \binom{n}{r+1}$ different embeddings provide independent cross-polytopal generators for homology.

Proposition 4. *Suppose K is a simplicial complex and σ is a maximal simplex of dimension p in K . If there is a p -cycle α in K in which σ appears with a non-trivial coefficient λ , then any representative p -cycle of $[\alpha]$ also contains σ with the same coefficient λ .*

Proof. Let $\alpha = \sum_i \gamma_i + n\sigma$ and $\alpha' = \sum_j \gamma'_j + n'\sigma$ be homologous p -cycle, where γ_i and γ'_j are p -dimensional simplices, and n and n' are the coefficients of the maximal simplex σ , indicating that both α and α' belong to the same homology class $[\alpha]$. The condition that α and α' are homologous implies that their difference $\alpha - \alpha'$ can be expressed as the boundary of some $(p+1)$ -chain d , specifically, $\alpha - \alpha' = \partial_{p+1}d$.

Given σ is a maximal simplex, it cannot appear in $\partial_{p+1}d$ since p -dimensional maximal simplex cannot appear in a $(p+1)$ -dimensional simplex. Consequently, when we express $\alpha - \alpha' = \sum_i \gamma_i - \sum_j \gamma'_j + (n - n')\sigma = \partial_{p+1}d$, the term involving σ must equate to zero to satisfy the condition that is part of a boundary. This leads to the conclusion that $n = n'$, thereby showing the coefficients of σ in both α and α' are identical. \square

Our attention now shifts to delineating the construction of maximal simplices within the Vietories-Rips complex $\text{VR}(Q_{r+1}; r)$, which are simultaneously maximal in $\text{VR}(Q_n; r)$. The following is a simple criterion identifying such a simplex as a maximal simplex in $\text{VR}(Q_n; r)$; see Figure 4.

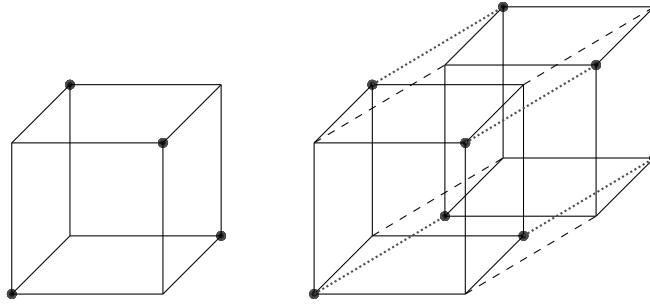


Figure 4.1: Left: Subcube Q_3 with a maximal simplex $\sigma \in \text{VR}(Q_3; 2)$ drawn in red, illustrating Proposition 5 and also Lemma 3 when r is even. An inclusion of σ in Q_4 also gives a maximal simplex $\iota_S^b(\sigma) \in \text{VR}(Q_4; 2)$. Right: Subcube Q_4 with a maximal simplex $\sigma \times \{0, 1\} \in \text{VR}(Q_4; 3)$ drawn in red, illustrating Lemma 3 when r is odd.

Proposition 5. *Let $n \geq r + 1$, let $S \subseteq [n]$, and let b be an associated offset. Let $\sigma \subseteq Q_{r+1}^b$, and suppose $\sigma \in \mathcal{A}_r$ as a subset of Q_{r+1} . If $\text{localDiam}(\sigma, w) = r$ for all $w \in \sigma$, then σ is a maximal simplex in $\text{VR}(Q_n; r)$.*

Proof. Assume, for contradiction, that σ is not a maximal simplex in $\text{VR}(Q_n; r)$. This implies there exists a point $x \in Q_n \setminus \sigma$ that can be added to σ to form a simplex. Consider the following cases:

- If $\pi_S^b(x) \notin \sigma$, then the antipode $\overline{\pi_S^b(x)}$ must be in σ . The distance between x and $\overline{\pi_S^b(x)}$ is given by

$$d(x, \overline{\pi_S^b(x)}) = d(x, \pi_S^b(x)) + d(\pi_S^b(x), \overline{\pi_S^b(x)}) \geq 0 + (r + 1) = r + 1.$$

- If $\pi_S^b(x) \in \sigma$, then $d(x, \pi_S^b(x)) \geq 1$. Since the $\text{localDiam}(\sigma, w) = r$ for all $w \in \sigma$, there exists $y \in \sigma$ such that $d(\pi_S^b(x), y) = r$. Consequently,

$$d(x, y) = d(x, \pi_S^b(x)) + d(\pi_S^b(x), y) \geq 1 + r.$$

Both cases lead to the conclusion that the diameter of σ exceeds r , contradicting the assumption that $\sigma \in \mathcal{A}_r$. □

Now by Proposition 5 we have that the maximal simplices σ in $\text{VR}(Q_{r+1}; r)$ is still maximal in $\text{VR}(Q_n; r)$. We recall that $\text{cHull}(\sigma)$ represents the smallest isometric copy of a cube containing σ .

Lemma 3. *If $r \geq 2$, then there exists a maximal simplex $\sigma \subseteq Q_{r+1}$ from \mathcal{A}_r with $\text{localDiam}(\sigma, y) = r$ for all $y \in \sigma$, and with $\text{cHull}(\sigma) = Q_{r+1}$.*

Proof. First, consider the case $r \geq 2$ to be even, making $r + 1$ is odd. Define σ as the collection of vertices in Q_{r+1} with an even number of 1s in their coordinates.

Given $r + 1$ is odd, each vertex x in σ has its antipode \bar{x} featuring an even number of 0s and an odd number of 1s, which implies that $\bar{x} \notin \sigma$. This confirms $\sigma \in \mathcal{A}_r$.

To assess the local diameter, consider any vertex y in σ and create y' by flipping one of \bar{y} 's coordinates. The new vertex y' remains in σ , given the preserved even count of 1's, and differs from y in exactly one coordinate, setting $d(y, y') = r$. Therefore, $\text{localDiam}(\sigma, y) = r$ for all $y \in \sigma$, establishing σ as maximal according to Proposition 5.

To demonstrate that $\text{cHull}(\sigma) = Q_{r+1}$, we first acknowledge that $\text{cHull}(\sigma) \subset Q_{r+1}$ as $\text{cHull}(\sigma)$ represents the minimum cube containing σ . To argue by contradiction, assume that $\text{cHull}(\sigma) \subsetneq Q_{r+1}$, implying all the vertices of σ share at least one fixed coordinate. However, given $r \geq 2$, any single coordinate can vary independently, and then fill in the rest of the coordinates to obtain a vertex of σ :

- If the chosen coordinate was 1, fill another coordinate as 1 and the rest as 0;
- If the chosen coordinate was 0, fill it and another coordinate as 1 and the rest as 0.

This point satisfies the coordinates contain an even number of value 1, which contradicts with σ as the collection of all vertices in Q_{r+1} whose coordinates contain an even number of value 1.

For the scenario where $r \geq 3$ is odd, we extend the argument as follows: Let τ be the maximal simplex in Q_r obtained in the proof of the even case. Define

$$\sigma = \tau \times \{0, 1\} \subseteq Q_{r+1}.$$

Formally speaking, $\sigma = \iota_{[r]}^{(0)}(Q_r) \cup \iota_{[r]}^{(1)}(Q_r)$, with the associated index set being $S = [r]$.

We first verify that $\sigma \in \mathcal{A}_r$. Consider a point $x \in \sigma$ is of the form $x = y \times \{i\}$ with $y \in \tau$, $i \in \{0, 1\}$. As antipode $\bar{x} = \bar{y} \times \{1 - i\}$ and $y \in A_{r-1}$, so $\bar{y} \notin \tau$, and $\bar{x} \notin \tau \times \{0, 1\}$. Hence we have $\sigma \in \mathcal{A}_r$ and Therefore $\text{localDiam}(\sigma, x) = r$.

We proceed by determining the local diameter. Given $x = y \times \{i\}$ with $y \in \tau$ and knowing $\text{localDiam}(\tau, y) = r - 1$, there exists $y' \in \tau$ such that $d(y, y') = r - 1$. Consequently, $y' \times \{1 - i\} \in \tau$ and $d(y \times \{i\}, y' \times \{1 - i\}) = r$.

It remains to prove that $\text{cHull}(\sigma) = Q_{r+1}$. Similarly as in the proof of the even case, if $\text{cHull}(\sigma) \subsetneq Q_{r+1}$, there would be a single coordinate shared by all the points of σ .

- If the chosen coordinate was the last one, i.e. $\sigma = \tau \times \{0\}$ or $\sigma = \tau \times \{1\}$, then let the last coordinate as 1 or 0;
- Any of the first r coordinates was chosen, we can construct it by the even case.

□

We have now reached a juncture where we are adequately equipped to prove the final theorem of this chapter.

Theorem 1. For $r \geq 2$,

$$\text{rank } H_{2^r-1}(\text{VR}(Q_n; r)) \geq 2^{n-(r+1)} \binom{n}{r+1}.$$

Proof. For notational convenience, let $k = 2^{n-(r+1)} \binom{n}{r+1}$. There are k isometric copies of Q_{r+1} in Q_n obtained via embeddings ι , which we enumerate as C_1, C_2, \dots, C_k . For each i :

- (1) Consider σ_i as the maximal simplex in C_i established by Proposition 5 and Lemma 3.
- (2) Let us denote by $[\alpha_i]$ the cross-polytopal generator consideration in the homology group $H_{2^r-1}(\text{VR}(C_i; r))$. The generator $[\alpha_i]$ is characterized more explicitly as a linear combination of the elements within the set \mathcal{A}_r , each oriented appropriately. In formal terms, the generator α_i can be expressed as $\alpha_i = \sum_{j \in J} n_j \gamma_j + n \sigma_i$, where each γ_j denotes a simplex of dimensional $(2^r - 1)$ and J is an index set. And we have same coefficients, i.e. $n_j = n$ for all $j \in J$, because $\alpha_i \in H_{2^r-1}(\text{VR}(C_i; r))$, so $\partial \alpha_i = 0$, therefore we have $n_j = n$. Hence $\alpha_i = n(\sum_{j \in J} \gamma_j + \sigma_i)$. And recall we have a standard $(2^r - 1)$ -dimensional cycle γ generating $H_{2^r-1}(\text{VR}(Q_{r+1}; r))$, which is defined as the sum of appropriately oriented elements of \mathcal{A}_r , so the coefficient of σ is 1 in γ . Therefore the coefficient of σ_i in all α_i is 1.

- (3) Let ω_i be the $(2^r - 1)$ -cochain on Q_n mapping σ_i to 1 and the rest of the $(2^r - 1)$ -dimensional simplices to 0. That is

$$\omega_i(\tau) = \begin{cases} 1, & \text{if } \tau = \sigma_i \\ 0, & \text{if } \tau \neq \sigma_i \end{cases},$$

where τ is a $2^r - 1$ dimensional simplex. And we can claim that the cochains ω_i are cocycles. Because σ_i is maximal simplex in C_i , there is no 2^r -dimensional simplex in C_i containing σ_i . Therefore $\partial^i(\omega_i) = 0$, which means ω_i are cocycles.

- (4) Observe that σ_i is not contained as a term in α_j for any $i \neq j$. We can prove it by contradiction, suppose that the maximal simplex σ_i in C_i , also lies in C_j . Since σ_i is part of both C_i and C_j , it follows that $\sigma_i \subseteq C_i \cap C_j$. Consequently, σ_i is a subset of the convex hull of σ_i , i.e. $\sigma_i \subseteq \text{cHull}(\sigma_i) \subseteq C_i \cap C_j$. However, according to Lemma 3, $\text{cHull}(\sigma_i) = C_i$ and $C_i \not\subseteq C_i \cap C_j$, leading to a contradiction. Next, we compute the following cap products $[\omega_i] \frown [\alpha_j]$ and $[\omega_i] \frown [\alpha_j]$ for $i \neq j$. Let $(2^r - 1)$ -dimensional simplex $\tau_j = \tau_j[v_0^j, \dots, v_{2^r}^j]$, by the definition of cap product,

$$\begin{aligned} [\omega_i] \frown [\alpha_i] &= \sum_{j \in J} 1 \cdot \omega_i(\tau_j[v_0^j, \dots, v_{2^r}^j]) \cdot \tau_j[v_{2^r}^j] \\ &= 1 \cdot \omega_i(\sigma_i[v_0^i, \dots, v_{2^r}^i]) \cdot \sigma_i[v_{2^r}^i] \\ &= 1 \cdot 1 \cdot \sigma_i[v_{2^r}^i] \neq 0 \end{aligned}$$

Similarly, we have $[\omega_i] \frown [\alpha_j] = 0$.

To demonstrate that the homology classes $[\alpha_i]$ in $H_{2^r-1}\text{VR}(Q_n; r)$ are linearly independent through the natural inclusion, consider a linear combination $\sum_{i=1}^k \lambda_i [\alpha_i] = 0$ for coefficients $\lambda_i \in \mathbb{Z}$. Applying the cap product with $[\omega_j]$, leading to $\lambda_j = 0$ by (4) above. Specifically, for each $j \in J$, we know $[\omega_j] \frown 0 = 0$, and instead of 0 as $\sum_{i=1}^k \lambda_i [\alpha_i]$, i.e. $[\omega_j] \frown \sum_{i=1}^k \lambda_i [\alpha_i] = 0$. Utilizing the bilinear property of the cap product, we obtain $[\omega_j] \frown \sum_{i=1}^k \lambda_i [\alpha_i] = \sum_{i=1}^k ([\omega_j] \frown \lambda_i [\alpha_i])$. Given that

$$[\omega_j] \frown \lambda_i [\alpha_i] = \begin{cases} \lambda_i \cdot \sigma_i[v_{2^r}^i], & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases},$$

It follows that $\lambda_i = 0$ for all $i \in \{1, 2, \dots, k\}$.

Therefore $H_{2^r-1}(\text{VR}(Q_n; r))$ contains at least k generators, that is $\text{rank} H_{2^r-1}(\text{VR}(Q_n; r)) \geq k = 2^{n-(r+1)} \binom{n}{r+1}$.

□

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