Computing Homology Groups of Simplicial Complexes in $\mathbf{R}^3$ [1]

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Abstract

Recent developments in analyzing molecular structures and representing solid models using simplicial complexes have further enhanced the need for computing structural information about simplicial complexes in $\mathbf{R}^3$. This paper develops basic techniques required to manipulate and analyze structures of complexes in $\mathbf{R}^3$.

A new approach to analyze simplicial complexes in Euclidean 3-space $\mathbf{R}^3$ is described. First, methods from topology are used to analyze triangulated 3-manifolds in $\mathbf{R}^3$. Then it is shown that these methods can, in fact, be applied to arbitrary simplicial complexes in $\mathbf{R}^3$ after (simulating) the process of thickening a complex to a 3-manifold homotopic to it. As a consequence considerable structural information about the complex can be determined and certain discrete problems solved as well. For example, it is shown how to determine the homology groups, as well as concrete representations of their generators, for a given complex in $\mathbf{R}^3$.

Keywords. Topology, homotopy, homology, generators, simplicial complexes, d dimensions.

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1 Introduction

Classification of topological spaces and functions is a primary goal in algebraic topology. The homology groups of a topological space T are invariants that are often computed in order to classify T. Given a continuous function $f : T_1 \to T_2$ between topological spaces the induced homomorphisms between corresponding homology groups help classify f. It is therefore important not only to compute the homology groups of a topological space, but also a representation of the elements of these groups that in turn allows representation of the induced homomorphisms.

Of particular significance in computational sciences are subspaces of Euclidean 3-space $\mathbf{R}^3$ because of their ubiquitous presence in applications such as solid modeling, molecular biology, computer aided manufacturing. Such subspaces are of course realizable in the real world and, further, the zeroth, first, and second Betti numbers (ie., ranks of the corresponding homology groups) have intuitive geometric interpretations as the number of components, tunnels, and voids, respectively. A typical discrete representation of such a subspace is as a simplicial complex embedded in $\mathbf{R}^3$, and of a function is as a simplicial map between complexes.

There is a classical algorithm to compute the homology groups of an arbitrary simplicial complex, see [13], based on reducing certain matrices to a canonical form, called Smith normal form. Unfortunately, the reduction of a matrix to its Smith normal form has a worst-case upper bound that is computationally prohibitive [10]. For recent improvements along this approach see [9].

Delfinado and Edelsbrunner [2] describe an algorithm, avoiding the computational bottleneck of reduction to Smith normal form, that computes the Betti numbers of a simplicial complex in $\mathbf{R}^3$. They assemble the complex incrementally simplex by simplex, and at each step update the Betti numbers of the current complex. The algorithm runs optimally in time and space linear in the size of the complex. However, they do not describe computing representations of generators of the homology groups.

We describe here a new approach to analyze complexes in $\mathbf{R}^3$. Our approach is based on first using methods from topology to derive algorithms for compact triangulated 3-manifolds (with boundary necessarily) in $\mathbf{R}^3$. Because of the relative niceness of compact 3-manifolds in $\mathbf{R}^3$ as topological objects we are able to apply classical results. However, theorems in Section 3 that form the basis of our algorithms for 3-manifolds do not seem to have appeared in the literature on the subject. Perhaps this omission is due to the greater emphasis in traditional mathematics on general theory, rather than on the specific case of 3-manifolds in $\mathbf{R}^3$. Such manifolds, on the other hand, are most relevant from the applications view point. Besides computational results, therefore, a contribution of this paper is useful topological results for 3-manifolds in $\mathbf{R}^3$.

The algorithms developed for 3-manifolds can apply to simplicial complexes as well, after thickening a given complex to a topological 3-manifold that is homotopic to it, so retaining identical homology. Actually, we simulate such a thickening as we never need to compute an explicit triangulation of the thickened manifold. We describe algorithms to:

1. Determine the ranks of homology groups (Betti numbers) of a complex K in $\mathbf{R}^3$ optimally in time and space linear in the size n of K. Although this algorithm is of the same complexity as that of [2] our new insight into the generators of the homology groups allows a somewhat simpler non-incremental algorithm that is different from [2].

2. Compute geometric realizations of a set of generators that form a basis of the first and second homology groups of K (for the zeroth homology group this is trivial) in $O(n^2\overline{g})$ and $O(n)$ time (and space), respectively, where $\overline{g}$ is an invariant of K such that always $\overline{g} < n$.

   In particular, $\overline{g}$ is the maximum genus of the component surfaces of the boundary of the 3-manifold obtained through thickening of K.

It is appealing and instructive how geometric insights often help improve the efficiency of our algorithms.

Further, our methods allow greater understanding of the structure of a simplicial complex in $\mathbf{R}^3$ than earlier ones as geometric realizations of the generators of the first and second homology groups allow "visualization" of tunnels and voids. Consequent applications are probable in such areas as solid modeling, molecular modeling, and alpha-shapes [5, 6, 7, 8].

In molecular biology, for example, homology of structures of polypeptide chains is often examined to determine similarities. A recent development in the work on alpha-shapes is the formalization by Edelsbrunner, Facello, and Liang [7] of the notion of "pockets" or imperfect voids in the three-dimensional structures of macromolecules, which is used in molecular docking. They model the molecules as a union of three-dimensional balls that represent atoms. It is shown in [5, 7] that the space generated by this union is homotopic to a simplicial complex, called alpha-complex, which is a subcomplex of the Delaunay complex that is a dual of the weighted Voronoi diagram of the balls. The definition and the algorithm for pockets are based on this Delaunay complex. Consequently, it is hoped that enhancements in understanding simplicial complexes in $\mathbf{R}^3$ would benefit the computational aspects of molecular structures.

We begin with necessary definitions from topology in Section 2. We prove results for 3-manifolds in Section 3 and develop algorithms in Section 4. We show how these results apply to simplicial complexes in Section 5 and finally conclude in Section 6.

2 Definitions

In the following we discuss some of the prerequisite mathematics that include elementary algebraic topology, simplicial homology, and manifold theory. Excellent sources for such material include [13, 15, 16] and we shall point to others as we proceed. Most of the definitions are taken from the survey paper [3], where a collection of relevant definitions from topology are presented concisely.

TOPOLOGICAL SPACES AND MAPS. A topological space X is *compact* if every *open cover of* X (ie., a collection of open sets of X whose union is X) has a finite subcover; X is *connected* if the only sets both open and closed in X are the empty set and X itself. A *component* of X is a maximal connected subset.

Suppose A and X are topological spaces such that $A \subseteq X$. Then the *interior* of A in X, denoted $\mathrm{int}\,(A)$ (assuming X is understood from the context), is the largest open set in X that is contained in A. The *closure* of A in X, denoted $\mathrm{cl}\,(A)$ (again assuming X is understood from the context), is the smallest closed set in X that contains A.

The *product* $X \times Y$ of two topological spaces has a natural topology defined on it with a basis consisting of sets of the form $A \times B$, where A is open in X and B is open Y.

A function $f : X \to Y$ from one topological space to another is *continuous* if the preimage of every open set in Y is open in X. A *map* is a continuous function. A *homeomorphism* is a bijective map whose inverse is also continuous. X and Y are *homeomorphic* or *topologically equivalent*, denoted $X \approx Y$, if there is a homeomorphism between them. A map $f : X \to Y$ is an *embedding* if it maps X homeomorphically onto its image $f(X)$ in Y.

Particular topological spaces that are useful in this paper are d-dimensional Euclidean space, $\mathbf{R}^d$, and its subspaces, the d-dimensional real halfspace $\mathbf{R}^d_{\geq}$ whose points have non-negative first coordinate, the closed d-ball $\mathbf{B}^d = \{x \in \mathbf{R}^d \mid \|x\| \leq 1\}$, and the $(d-1)$-sphere $\mathbf{S}^{d-1} = \{x \in \mathbf{R}^d \mid \|x\| = 1\}$, where $\|x\|$ denotes the usual Euclidean norm. We shall often loosely use $\mathbf{B}^d$ and $\mathbf{S}^d$ to refer to spaces homeomorphic to $\mathbf{B}^d$ and $\mathbf{S}^d$, respectively, when the spaces in question are clear from the context. For example, we may write $\mathbf{B}^3 \subseteq \mathbf{S}^3$ to indicate that the first space is a subspace of $\mathbf{S}^3$ homeomorphic to $\mathbf{B}^3$, eg., a closed hemisphere. A subspace X of $\mathbf{R}^d$ is *bounded* if $\|x\| \leq k$, for all $x \in X$, where k is a positive constant.

A *homotopy* between two maps $f, g : X \to Y$ is a map

$$F : X \times [0,1] \to Y$$

for which the *initial map* $F(x,0) = f(x)$ and the *end map* $F(x,1) = g(x)$ for all $x \in X$. Two maps f and g are *homotopic* if such an F exists. Two topological spaces, X and Y, are *homotopy equivalent*, denoted $X \simeq Y$, if there are maps $f : X \to Y$ and $g : Y \to X$ with $g \circ f$ homotopic to the identity map 1_X and $f \circ g$ homotopic to 1_Y.

<u>Simplices</u>. A *k-simplex* is the convex hull of $k+1$ affinely independent points. We call a 0-simplex a *vertex*, a 1-simplex an *edge*, a 2-simplex a *triangle*, and a 3-simplex a *tetrahedron*. Let $V = \{p_0, p_1, \dots, p_k\}$ be affinely independent. Then $\sigma = \operatorname{conv} V$, the convex hull of V, is a k-simplex with vertex set $\{p_0, p_1, \dots, p_k\}$. A *face* of σ is a simplex $\tau = \operatorname{conv} U$ with $U \subseteq V$, denoted $\tau \leq \sigma$; it is *proper* if U is a proper subset of V, denoted $\tau < \sigma$. The *barycentric coordinates* of a point $x \in \sigma$ are real numbers ϕ_i with

$$x = \sum_{i=0}^{k} \phi_i p_i \quad \text{and} \quad 1 = \sum_{i=0}^{k} \phi_i.$$

The *barycenter* of σ is the point $b(\sigma)$ with barycentric coordinates $\phi_i = \frac{1}{k+1}$ for all i.

If σ is a k-simplex with vertex set $\{p_0, p_1, \dots, p_k\}$, two orderings of the vertex set are said to be *equivalent* if they differ by an even permutation. Each such equivalence class is called an *orientation* of σ. If σ is a 0-simplex there is only one orientation of σ; if σ is a k-simplex, $k > 0$, there are exactly two orientations of σ. An *oriented simplex* is a simplex σ together with an orientation. Denote by $[p_0, p_1, \dots, p_k]$ the simplex σ together with the orientation corresponding to the equivalence class of the particular ordering $p_0, p_1, \dots, p_k$ of its vertex set. The orientation of a $(k-1)$-face *induced* by σ is

$$\tau \quad = \quad (-1)^i [p_0, \dots, p_{i-1}, p_{i+1}, \dots, p_k],$$

where a leading minus reverses orientation.

<u>Simplicial Complexes</u>. A *simplicial complex* is a collection K of simplices with the following two properties:

(i) if $\sigma \in K$ and τ is a face of σ then $\tau \in K$, and

(ii) if $\sigma, \sigma' \in K$ then $\sigma \cap \sigma'$ is empty or a face of both.

The *vertex set* of K is $\operatorname{Vert} K = \{\sigma \in K \mid \dim \sigma = 0\}$. The *underlying space* of K is $|K| = \bigcup_{\sigma \in K} \sigma$. The *dimension* of K is $\dim K = \max\{\dim \sigma \mid \sigma \in K\}$. A *subcomplex* of K is a simplicial complex $L \subseteq K$. A simplicial complex L with $|L| = |K|$ is a *subdivision* of K if every simplex in L is contained in a simplex in K. A *simplicial map* $f : |K| \to |L|$ from the underlying space of one simplicial complex to another is a continuous function that maps each simplex of K linearly onto a simplex of L.

Let K be a simplicial complex. The *barycentric subdivision* of K is defined by

$$\operatorname{Sd} K \quad = \quad \{\operatorname{conv}(\{b(\sigma_0), b(\sigma_1), \dots, b(\sigma_r)\}) \mid \sigma_0 < \sigma_1 < \dots < \sigma_r \text{ and } \sigma_0, \sigma_1, \dots, \sigma_r \in K\}.$$

$\operatorname{Sd} K$ is indeed a simplicial complex and a subdivision of K.

A topological space X is said to be *triangulable* if it is homeomorphic to the underlying space of some simplicial complex. The homeomorphism in this case represents a *triangulation*.

<u>MANIFOLDS</u>. A topological space M is a *d-manifold* if every point $x \in M$ has a neighborhood homeomorphic either to $\mathbf{R}^d$ or $\mathbf{R}^d_{\geq}$ (note that some authors prefer to call such an object a "manifold with boundary").

The *boundary* of M, $\mathrm{bd}\,(M)$, is the subset of points with neighborhoods homeomorphic to $\mathbf{R}^d_{\geq}$. If M has empty boundary then M is said to be a *manifold without boundary* or, equivalently, a *closed manifold*. An arbitrary d-manifold is either without boundary, or its boundary is a $(d-1)$-manifold without boundary.

We make some observations about 3-manifolds in $\mathbf{R}^3$, objects of greatest interest to us. If M is a compact 3-manifold in $\mathbf{R}^3$, then, necessarily, $\mathrm{bd}\,(M) \neq \emptyset$. Furthermore, $\mathrm{int}\,(M) = M - \mathrm{bd}\,(M)$ and $\mathrm{cl}\,(\mathrm{int}\,(M)) = M$ (closures and interior are, of course, taken with respect to $\mathbf{R}^3$).

<u>GROUPS AND HOMOMORPHISMS</u>. A function $f : \mathsf{G} \rightarrow \mathsf{H}$ from one group to another is a *homomorphism* if $f(a * b) = f(a) \circ f(b)$, for all $a, b \in \mathsf{G}$, where $*$ and $\circ$ denote the group operations in G and H, respectively. A homomorphism that is one-to-one (onto) is called a *monomorphism* (*epimorphism*). An *isomorphism* is a homomorphism that is both a monomorphism and an epimorphism.

Suppose the group G is *Abelian*, in other words, $a * b = b * a$, for all $a, b \in \mathsf{G}$. Say H is a *subgroup* of G, ie., $\mathsf{H} \subseteq \mathsf{G}$, such that H itself is a group with the inherited group operation $*$. The quotient group G/H consists of *cosets* of H in G, ie., equivalence classes of of elements in G modulo the relation $a \sim b$ if $a * b^{-1} \in \mathsf{H}$. Denoting the coset of a by $[a]$, the group operation in G/H is defined by $[a] \circ [b] = [a * b]$.

A group G is *cyclic* if it is *generated* by a single element $a \in \mathsf{G}$, in other words, every element of G is of the form a^k, for some $k \in \mathbf{Z}$.

<u>HOMOLOGY GROUPS AND BETTI NUMBERS</u>. We consider only simplicial homology with integer coefficients. This is justified, in particular, as all spaces that we consider in this paper are triangulable. Let K be a simplicial complex and $K^j \subseteq K$ be the set of oriented j-simplices of K. A *j-chain* is a function $c : K^j \rightarrow \mathbf{Z}$ which vanishes on all but finitely many oriented j-simplices. We write the chain as a formal sum with finitely many non-vanishing terms:

$$c \;=\; \sum_{\sigma \in K^j} c(\sigma) \cdot \sigma.$$

Two j-chains are added component-wise. The j-chains together with addition form the group of j-chains, C_j. The *boundary operator* maps an oriented j-simplex $\sigma = [p_0, p_1, \ldots, p_j]$ to a $(j-1)$-chain

$$\partial_j \sigma \;=\; \sum_{i=0}^{j} (-1)^i [p_0, \ldots, p_{i-1}, p_{i+1}, \ldots, p_j].$$

The *boundary homomorphism*, $\partial_j : \mathsf{C}_j \rightarrow \mathsf{C}_{j-1}$, is defined by $\partial_j(\sum c(\sigma) \cdot \sigma) = \sum c(\sigma) \cdot \partial_j \sigma$. The *chain complex* is the sequence of chain groups connected by boundary homomorphisms:

$$\ldots \xrightarrow{\partial_{j+2}} \mathsf{C}_{j+1} \xrightarrow{\partial_{j+1}} \mathsf{C}_j \xrightarrow{\partial_j} \mathsf{C}_{j-1} \xrightarrow{\partial_{j-1}} \ldots$$

The *image* and *kernel* of the boundary homomorphism are

$$\begin{aligned} \mathrm{Im}\,\partial_j &= \{c \in \mathsf{C}_{j-1} \mid c = \partial_j c' \text{ for some } c' \in \mathsf{C}_j\} \text{ and} \\ \mathrm{Ker}\,\partial_j &= \{c \in \mathsf{C}_j \mid \partial_j c = 0\}. \end{aligned}$$

We term $c \in \mathsf{C}_j$ a *j-cycle* if $c \in \mathrm{Ker}\,\partial_j$, and a *j-boundary* if $c \in \mathrm{Im}\,\partial_{j+1}$. A j-boundary is sometimes called a *null-homologous* j-cycle. The j-cycles form a group Z_j and the j-boundaries form a group B_j.

The fact that every j-boundary is also a j-cycle is most important and follows from $\partial_j \partial_{j+1} c = 0$, for every $c \in \mathsf{C}_{j+1}$. This implies that $\mathsf{B}_j \subseteq \mathsf{Z}_j \subseteq \mathsf{C}_j$. The *$j$-th homology group* is the quotient of the cycle group over the boundary group:

$$\mathsf{H}_j \quad = \quad \mathsf{Z}_j / \mathsf{B}_j.$$

We often write $\mathsf{H}_j(K)$ to indicate H_j of the simplicial complex K. If $c \in \mathsf{Z}_j$, the coset $[c](\in \mathsf{H}_j)$ is called the homology class of c.

Homology groups are always Abelian. Furthermore, for spaces that we consider they are finitely generated. The fundamental theorem for finitely generated Abelian groups implies that H_j can be written as the direct sum of two subgroups, $\mathbf{Z}^{\beta_j}$ and T, where $\mathbf{Z}^{\beta_j} = \mathbf{Z} \oplus \ldots \oplus \mathbf{Z}$ (β_j times), and T is the direct sum of finitely many finite cyclic groups. We call β_j the *rank* of H_j. T is the *torsion* subgroup of H_j.

It is an important fact that H_j is invariant over all simplicial complexes triangulating the same topological space $X \approx |K|$. It is therefore meaningful to call H_j the j-th homology group of X. Similarly, the *j-th Betti number*, β_j, and the *Euler characteristic*,

$$\chi \quad = \quad \sum (-1)^j \beta_j,$$

are invariant over all triangulations of X. The Euler characteristic of every compact d-manifold with odd d is 0, which follows from Poincaré duality [13].

A simplicial map $f : |K| \to |L|$ induces a homomorphism $f_* : \mathsf{H}_j(K) \to \mathsf{H}_j(L)$ in each dimension.

Mayer-Vietoris Sequences. An *exact* sequence is a (possibly infinite) sequence of group homomorphisms

$$\ldots \to \mathsf{G}_{q+1} \stackrel{\phi_{q+1}}{\to} \mathsf{G}_q \stackrel{\phi_q}{\to} \mathsf{G}_{q-1} \stackrel{\phi_{q-1}}{\to} \ldots$$

such that $\mathrm{Im}\, \phi_{q+1} = \mathrm{Ker}\, \phi_q$, for every index q.

If K_1, K_2, and L are subcomplexes of a simplicial complex T such $K_1 \cup K_2 = T$ and $K_1 \cap K_2 = L$, then there is an exact sequence

$$\ldots \to \mathsf{H}_{q+1}(T) \stackrel{\delta}{\to} \mathsf{H}_q(L) \stackrel{\phi}{\to} \mathsf{H}_q(K_1) \oplus \mathsf{H}_q(K_2) \stackrel{\theta}{\to} \mathsf{H}_q(T) \to \ldots,$$

called the *Mayer-Vietoris sequence* of (K_1, K_2). For definitions of the homomorphisms δ, ϕ, and θ, and proof of exactness refer to [13].

Closed Complement in $\mathbf{S}^3$. For any space $P \subseteq \mathbf{R}^3$ ($\subset \mathbf{S}^3$), we use $\overline{P}$ to denote the closure of the complement of P in $\mathbf{S}^3$, ie., $\overline{P} = \mathrm{cl}\,(\mathbf{S}^3 - P)$. Another way of representing $\overline{P}$ is as a single point compactification of the closure of the complement of P in $\mathbf{R}^3$, ie., $\overline{P} = \mathrm{cl}\,(\mathbf{R}^3 - P) \cup p_\infty$, where p_∞ denotes the point at infinity.

Observe that if the compact 3-manifold $M \subset \mathbf{R}^3$, so that M has non-empty boundary $\mathrm{bd}\,(M)$, then $\mathrm{bd}\,(\overline{M}) = \mathrm{bd}\,(M)$.

Surfaces. Surfaces are compact and connected 2-manifolds without boundary. *Orientable* surfaces can be embedded in $\mathbf{R}^3$ with a distinct "inside" (bounded component) and an "outside" (unbounded component). More precisely, any surface S in $\mathbf{R}^3$ splits $\mathbf{R}^3$ into two connected manifolds, denoted U_S and V_S, such that $U_S \cup V_S = \mathbf{R}^3$, $U_S \cap V_S = \mathrm{bd}\,(U_S) = \mathrm{bd}\,(V_S) = S$, and U_S is bounded while V_S is unbounded. Notice that by our definition $\overline{U_S} = V_S \cup p_\infty$.

The *genus* of a surface is informally the number of "hollow handles" that must be "attached" to a sphere to form that surface. For example, a torus is of genus 1, while the surface S_3 in Figure 3.1 is of genus 2. See [17] for a more formal definition and a proof of the important fact that orientable surfaces are classified up to homeomorphism by their genus. If S is an orientable surface of genus g, then $\mathsf{H}_1(S) = \mathbf{Z} \oplus \ldots \oplus \mathbf{Z}$ ($2g$ terms), the free Abelian group of rank $2g$. A set of $2g$ generating cycles of $\mathsf{H}_1(S)$ consists of g *latitudinal* and g *longitudinal* generators as defined in the next section.

A *solid torus* is a 3-manifold homeomorphic to $\mathbf{S}^1 \times \mathbf{B}^2$.

A *handlebody* of genus g is a space obtained by attaching g distinct copies of $\mathbf{B}^1 \times \mathbf{B}^2$ (each called a handle) to a 3-ball $\mathbf{B}^3$ via $2g$ homeomorphisms that map the $2g$ disks $\{1, -1\} \times \mathbf{B}^2$ onto $2g$ disjoint disks on the boundary of $\mathbf{B}^3$, in such a way that the resulting 3-manifold is orientable.

A handlebody of genus g is homeomorphic to a *boundary connected sum* of g solid tori: the latter is the manifold obtained by taking g solid tori, say $T_i, i = 1, \ldots, g$, and, successively, connecting T_{i+1} to T_i, $i = 1, \ldots, g-1$, by identifying them along disks on their boundaries.

The following theorem (see [15, p. 107]) is crucial:

Theorem 2.1 (Solid torus theorem) Given a torus S in $\mathbf{R}^3$, either U_S or $\overline{U_S}$ is a solid torus.

Knots and Linking. A *knot* is a subspace of $\mathbf{R}^3$ that is homeomorphic to $\mathbf{S}^1$.

A homotopy $F : X \times [0, 1] \to X$ is an *ambient isotopy* if the initial map $F(x, 0)$ is the identity and $F(x, t)$ is a homeomorphism for each $t \in [0, 1]$. The map $F(x, 1)$ is called the *end map* of the ambient isotopy. Two knots K_1 and K_2 are called *equivalent* if there is a homeomorphism h of $\mathbf{R}^3$, which is the end map of an ambient isotopy of $\mathbf{R}^3$, such that $h(K_1) = K_2$. A knot equivalent to $\mathbf{S}^1$ is called *trivial*.

Two disjoint surfaces (or knots) S and T in $\mathbf{R}^3$ are *linked* if there is no ambient isotopy of $\mathbf{R}^3$ that can place them on different sides of a separating plane. Figure 3.1 illustrates two linked surfaces, S_1 and S_2. A surface S in $\mathbf{R}^3$ is said to be *knotted* if at least one of its generators is a non-trivial knot, or if a pair of its generators are linked. In Figure 3.1 S_2 is a knotted torus.

3 3-manifolds in $\mathbf{R}^3$

As we compute the homology groups of a simplicial complex embedded in $\mathbf{R}^3$ by first thickening the complex to a 3-manifold in $\mathbf{R}^3$, we begin with an investigation of the homological properties of compact 3-manifolds in $\mathbf{R}^3$.

Let M be a compact connected *triangulated* 3-manifold in $\mathbf{R}^3$ (any compact 3-manifold is triangulable, see [1, 12]). Say $M = |K|$, the underlying space of a simplicial complex K. M must necessarily be orientable with non-empty boundary $\mathrm{bd}\,(M)$, and $\mathsf{H}_j(M)$ does not have a torsion subgroup for any $j \geq 0$. The boundary $\mathrm{bd}\,(M)$ is a disjoint union of, say, r orientable surfaces S_i, $1 \leq i \leq r$, of genus g_i, respectively. A triangulation of $\mathrm{bd}\,(M)$ is obtained as a subcomplex ∂K of K. We shall henceforth often not distinguish between K and M.

At this point it may be useful to give an intuitive geometric description of M. It has an "enclosing" surface, say S_r (adjacent to the unbounded component of the complement of M in $\mathbf{R}^3$); M is then formed from the solid M', bounded by S_r, by excision to form $r - 1$ "voids" inside M' that are also bounded by surfaces, say S_i, $1 \leq i \leq r - 1$. The homeomorphic type of M of course depends not only on the S_i but also on their disposition inside S_r: they may be arbitrarily knotted and linked, see Figure 3.1.

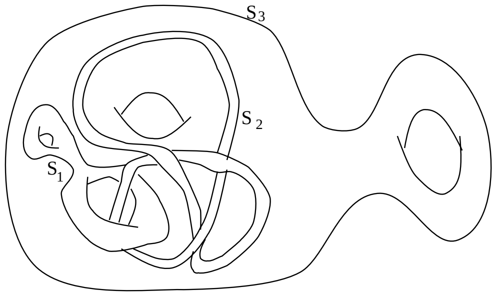


Figure 3.1: Knotted and linked surfaces.

3.1 Second homology group H_2

We investigate first the second homology group of M as it is straightforwardly determined by the bounding surfaces S_i as shown by the following theorem.

THEOREM 3.1 The homology classes of the surfaces, $[S_i], 1 \leq i \leq r-1$, form a basis of $\mathsf{H}_2(M)$.

PROOF. The $S_i, 1 \leq i \leq r-1$, represent $r-1$ independent 2-cycles as they do not bound a 3-chain (a solid) in M. Next, we show that the homology class of any 2-cycle is linearly dependent on $[S_i], 1 \leq i \leq r-1$.

For, any 2-cycle in M is just a "sum" of surfaces. Each such surface S must contain some (possibly empty) subset of $\{S_i : 1 \leq i \leq r-1\}$ in its interior. Suppose S contains $S_{i_1}, \ldots, S_{i_k}$ in its interior. Then, $S, S_{i_1}, \ldots, S_{i_k}$ together clearly bound a 3-chain (which is a solid with S as the enclosing surface, and the S_{i_j} bounding voids inside it), so that the equation in homology classes $[S] + [S_{i_1}] + \ldots + [S_{i_k}] = 0$ holds, with appropriate orientations of the S_{i_j}. The equation $[S] = -([S_{i_1}] + \ldots + [S_{i_k}])$ follows.

Thus, the $r-1$ homology classes, $[S_i], 1 \leq i \leq r-1$, indeed form a basis of $\mathsf{H}_2(M)$. $\square$

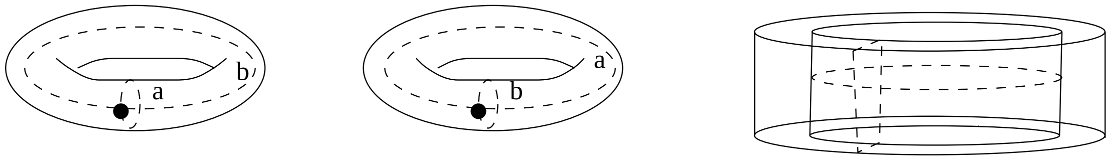
Eg., in Figure 3.1, $[S_1] + [S_2] + [S_3] = 0$, as S_1, S_2, S_3 together bound the 3-chain represented by M itself. The following corollary is an immediate consequence of the previous theorem.

COROLLARY 3.2 $\beta_2(M) = r-1$.

3.2 First homology group H_1

It is the first homology group of M which is more difficult to compute and requires greater insight into the structure of M. It is important to note that various homeomorphic copies of M may exist via non-homotopic embeddings. We shall attempt to investigate the structure of M through an understanding first of its bounding surface. Henceforth, by surface we shall always mean an orientable surface, equivalently, one which is embeddable in $\mathbf{R}^3$.

A surface, as well, may be embedded in $\mathbf{R}^3$ in many different ways. For example, Figure 3.2(a) and (b) show images of two embeddings $f, g : \mathbf{S}^1 \times \mathbf{S}^1 \to \mathbf{R}^3$ of a torus that swap its generators. These two embeddings are non-homotopic – one cannot be continuously deformed to the other.



(a) (b) (c)

Figure 3.2: Embeddings of a torus.

Defining and distinguishing between *longitudinal* and *latitudinal* generators of a surface is critical to our development. Doing this exactly requires care owing to certain subtleties, and we reserve this till after we prove Theorem 3.4. Informally, though, let us note that in each of the tori in Figure 3.2, the larger broken ellipse represents a longitudinal generator, while the smaller one represents a latitudinal generator. Figure 3.2(c), in particular, may motivate the observation that if a torus is imagined as the surface of an object formed by boring a cylindrical hole through a solid ball, then a generator (of the first homology group) of the cylinder bounding the hole is, in fact, a longitudinal generator of the torus. All this will be made precise after we prove Theorem 3.4. A similar observation holds for surfaces of higher genus: in Figure 3.3 the larger broken ellipses again represent longitudinal generators, and the smaller ones latitudinal generators.

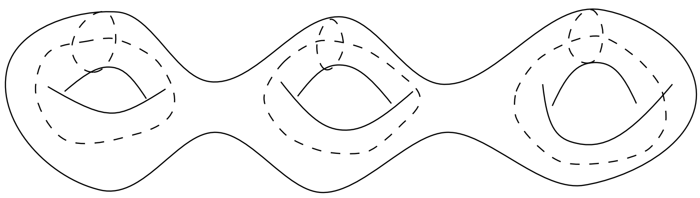


Figure 3.3: A surface of genus 3.

We begin now the computation of $\mathsf{H}_1(M)$. Our first theorem establishes a crucial relation between the genus of the surfaces of M and the first Betti number.

THEOREM 3.3 $\beta_1(M) = \sum_{i=1}^{r} g_i$.

PROOF. Consider the *doubling* of M, the manifold M_d obtained by taking a homeomorphic copy M' of M and identifying corresponding points on their boundaries, see [12, 16]. Then, M_d is a compact connected orientable *and closed* (ie., boundaryless) 3-manifold, no longer embeddable in $\mathbf{R}^3$ of course. A triangulation K_d of M_d can be obtained by correspondingly doubling K (or possibly a barycentric subdivision of K [12]).

The Euler characteristic of K_d, $\chi(K_d) = 2\chi(K) - \chi(\partial K)$, but the Euler characteristic of a compact closed 3-manifold is 0 by Poincaré duality (see [13]). Therefore,

$$\chi(K_d) = 0 \Rightarrow \chi(\partial K) = 2\chi(K).$$

Further, given the relation between the Euler characteristic and genus of a surface (see [11]),

$$\chi(\partial K) = \sum_{i=1}^{r}(2 - 2g_i) = 2r - 2\sum_{i=1}^{r} g_i.$$

Therefore,

$$\chi(K) = r - \sum_{i=1}^{r} g_i.$$

But Euler's formula gives (see [13]), $\chi(K) = \beta_0(K) - \beta_1(K) + \beta_2(K) - \beta_3(K)$. We know $\beta_0(K) = 1$ as K is connected, and $\beta_3(K) = 0$ as there exists no non-trivial 3-cycle in $\mathbf{R}^3$. Therefore,

$$\begin{aligned}
\beta_1(K) &= 1 + \beta_2(K) - \chi(K) \\
&= 1 + \beta_2(K) - (r - \sum_{i=1}^{r} g_i) \\
&= \sum_{i=1}^{r} g_i + \beta_2(K) - (r-1) \\
&= \sum_{i=1}^{r} g_i \text{ (from Corollary 3.2)}
\end{aligned}$$

Thus, $\beta_1(M) = \sum_{i=1}^{r} g_i$. □

The previous theorem gives the size of a basis, equivalently, rank, of $\mathsf{H}_1(M)$. We shall next attempt to identify a set of actual generators that form a basis of $\mathsf{H}_1(M)$, and design an algorithm to compute a description of these generators. Interestingly, a first step in that direction turns out to be to investigate $\overline{M}$, which is a disjoint union of compact 3-manifolds in $\mathbf{R}^3$, each bounded by a single surface.

We proceed, therefore, to determining the first homology group and its generators for a compact 3-manifold in $\mathbf{R}^3$ bounded by a single surface.

3.2.1 Manifolds bounded by a single surface

First, we show that the structure of a 3-manifold M in $\mathbf{R}^3$ bounded by a single surface (ie., with boundary consisting of a single component) may be described in a particularly efficient manner.

Define a *3-ball with wormholes* to be a manifold Q constructed as follows:

Choose $2g$ distinct points $\{p_i, q_i : i = 1 \dots g\}$ on the boundary $\mathbf{S}^2$ of the 3-ball $\mathbf{B}^3$ in $\mathbf{R}^3$. Choose arcs d_i joining p_i to q_i such that, except for its endpoints p_i and q_i, d_i lies in the interior of $\mathbf{B}^3$, and such that the d_i are pairwise disjoint. Choose pairwise disjoint closed tubular neighborhoods N_i of the arcs d_i. Each N_i is homeomorphic to $d_i \times \mathbf{B}^2$.

Set $Q = \mathrm{cl}\,(\mathbf{B}^3 - \cup_{i=1}^{g} N_i)$. In particular, we say that Q is a 3-ball with g wormholes. Informally, we shall often say that Q is obtained by removing the wormholes $N_i, i = 1, \dots, g$, from $\mathbf{B}^3$. See figure 3.4.

THEOREM 3.4 A compact 3-manifold M in $\mathbf{R}^3$ bounded by a single surface L of genus g is homeomorphic to some 3-ball with g wormholes Q.

PROOF. We proceed by induction on the genus g of the surface L.

The start of induction at $g = 1$ follows by Theorem 2.1 (Solid Torus Theorem). In particular, when L is a torus, the Solid Torus theorem says that either one of M and $\overline{M}$ is a solid torus:

If M is a solid torus then it is homeomorphic to $\mathbf{S}^1 \times \mathbf{B}^2$, which itself is clearly homeomorphic to $\mathrm{cl}\,(\mathbf{B}^3 - N_1)$, where N_1 is any closed tubular neighborhood of, say, the straight-line arc d_1 joining the north and south poles of $\mathbf{B}^3$. In other words, M is homeomorphic to a 3-ball with an "unknotted" cylindrical wormhole through it.

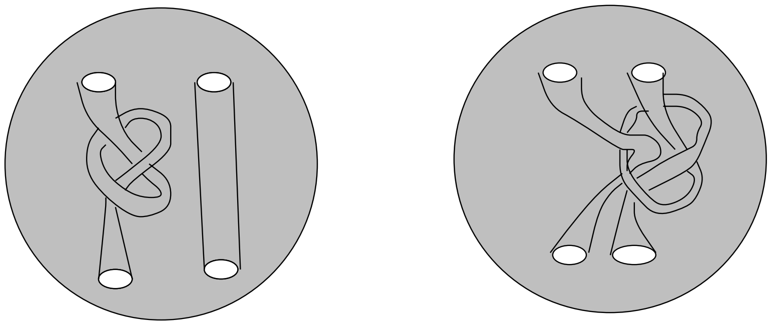


Figure 3.4: 3-balls with two wormholes each. The two wormholes are not linked in the left figure, while they are linked in the right figure.

If, on the other hand, $\overline{M}$ is a solid torus, say $\overline{M} = \mathbf{S}^1 \times \mathbf{B}^2$. Now, let I be a closed subarc of $\mathbf{S}^1$, ie., I is a subset of $\mathbf{S}^1$ that is homeomorphic to a closed unit interval. Consider the space $O = \text{int}\,(I \times \mathbf{B}^2) \subset \text{int}\,(\overline{M})$. O may be thought of as an open ball or open cylinder. Now,

$$\begin{aligned}
\mathbf{B}^3 &= \mathbf{S}^3 - O, \text{ as removing any open 3-ball from } \mathbf{S}^3 \text{ leaves a closed 3-ball} \\
&= (M \cup \overline{M}) - O \\
&= M \cup (\overline{M} - O) \\
&= M \,\cup\, (\text{cl}\,(\mathbf{S}^1 - I) \times \mathbf{B}^2) \,\cup\, (I \times \text{bd}\,(\mathbf{B}^2)) \\
&= M \,\cup\, (\text{cl}\,(\mathbf{S}^1 - I) \times \mathbf{B}^2), \text{ as } I \times \text{bd}\,(\mathbf{B}^2) \subset \text{bd}\,(\overline{M}) = \text{bd}\,(M) = L \\
&= M \,\cup\, N_1, \text{ denoting cl}\,(\mathbf{S}^1 - I) \times \mathbf{B}^2 \text{ by } N_1.
\end{aligned}$$

Now, N_1 is a closed tubular neighborhood of the arc $d_1 = \text{cl}\,(\mathbf{S}^1 - I) \times (0,0)$, where $(0,0)$ is the center of $\mathbf{B}^2$. The endpoints of d_1, which form the set $\text{bd}\,(\text{cl}\,(\mathbf{S}^1 - I)) \times (0,0) = \text{bd}\,(I) \times (0,0)$, lie on the boundary of $\mathbf{B}^3$; and, N_1 intersects M in exactly $\text{cl}\,(\mathbf{S}^1 - I) \times \text{bd}\,(\mathbf{B}^2) \subset \text{bd}\,(M)$. It follows, therefore, that $M = \text{cl}\,(\mathbf{B}^3 - N_1)$. Note that, in this case, N_1 may represent a knotted wormhole.

Assume now that the theorem is true for surfaces L of genus up to g. Suppose L has genus $g+1$. By an argument exactly as in proof of the Solid Torus theorem (see [15]) find an essential simple closed curve J in L that bounds a piecewise linear disk D in either M or $\overline{M}$.

First suppose D is in M. Let N be a tubular neighborhood of D in M. Then, clearly $X = \text{cl}\,(M - N)$ is bounded by a surface of genus g. By the inductive hypothesis X is homeomorphic to a ball with g wormholes. Now, $N = \mathbf{B}^1 \times D = \mathbf{B}^1 \times \mathbf{B}^2$, a cylindrical handle, is attached to X along the two discs $\{-1\} \times \mathbf{B}^2$ and $\{1\} \times \mathbf{B}^2$ to give M. The images of $\{-1\} \times \mathbf{B}^2$ and $\{1\} \times \mathbf{B}^2$, by the attaching map, are two disjoint discs, say, D_1 and D_2, on $\text{bd}\,(X)$. Imagine D_1 and D_2 to be "small and close together" on $\text{bd}\,(X)$, as indeed they can be made to be by a self-homeomorphism of X. It is not hard to see then that the manifold obtained by attaching any (possibly knotted) cylindrical handle to X at D_1 and D_2 is identical *up to homeomorphism* to that obtained by attaching an unknotted cylindrical handle to X at D_1 and D_2, which in turn is identical up to homeomorpism to attaching to X a 3-ball with an unknotted straight cylindrical hole through it. We conclude that M is homeomorphic to a 3-ball with $g+1$ wormholes.

Next suppose D is in $\overline{M}$. Let N be a tubular neighborhood of D in $\overline{M}$. Then, reasoning as before, $Y' = \text{cl}\,(\overline{M} - N)$ is bounded by some surface, say K, of genus g. It follows that $Y = M \cup N$, which is the closure of the complement of Y' in $\mathbf{S}^3$, is bounded by K as well. By the inductive hypothesis Y is homeomorphic to a 3-ball with g wormholes. Since $N = \mathbf{B}^1 \times D = \mathbf{B}^1 \times \mathbf{B}^2$, a (possibly knotted) cylinder in

Y, it follows that $M = \mathrm{cl}\,(Y - N)$ is homeomorphic to a 3-ball with $g+1$ wormholes. □

Another useful insight is the following:

LEMMA 3.5 If Q is a 3-ball with g wormholes, then $\overline{Q}$ is a handlebody of genus g.

PROOF. Now, $Q = \mathrm{cl}\,(\mathbf{B}^3 - \cup_{i=1}^{g} N_i)$. Therefore,

$$\overline{Q} = \mathrm{cl}\,(\mathbf{S}^3 - \mathrm{cl}\,(\mathbf{B}^3 - \cup_{i=1}^{g} N_i)) = \mathrm{cl}\,(\mathbf{S}^3 - \mathbf{B}^3) \bigcup \cup_{i=1}^{g} N_i,$$

which represents $\overline{Q}$ as a 3-ball with g handles $N_i, i = 1, \ldots, g$, attached. □

However, as noted before, a handlebody of genus g is a boundary connected sum of g solid tori. For a solid torus T, now, notions of longitude and latitude are well-defined. In particular, assume $h : \mathbf{S}^1 \times \mathbf{B}^2 \to T$ is a homeomorphism. Then, the images of $\mathbf{S}^1 \times (1,0)$ and $(1,0) \times \mathrm{bd}\,(\mathbf{B}^2)$ are called a *longitude* and a *latitude*, respectively, of the solid torus T. Note that longitudes and latitudes are not unique, and that by our definition they lie always on the boundary of T.

We are finally in a position to complete the definition of longitudinal and latitudinal generators of a surface S of genus g. Now, $S = \mathrm{bd}\,(U_S)$, where U_S is a compact 3-manifold in $\mathbf{R}^3$. By Theorem 3.4, U_S is homeomorphic to some 3-ball with g wormholes Q, and, therefore, S is homeomorphic to $\mathrm{bd}\,(Q)$. Let us restrict ourselves then to defining the longitudinal and latitudinal generators of the boundary $\mathrm{bd}\,(Q)$ of a 3-manifold with g wormholes Q. By Lemma 3.5, $\overline{Q}$ is a handlebody of genus g, which is a boundary connected sum of g solid tori, say $T_i, i = 1 \ldots g$. A longitude and a latitude may be chosen from each of the T_i such that the longitude and latitude from a given T_i intersect exactly at one point, and such that longitudes and latitudes from different T_i do not intersect at all. These $2g$ closed curves all lie on $\mathrm{bd}\,(\overline{Q}) = \mathrm{bd}\,(Q)$.

We define now the g latitudes of the T_i to be longitudinal generators and the g longitudes of the T_i to be latitudinal generators of $\mathrm{bd}\,(Q)$. Note, again, sets of longitudinal and latitudinal generators are not unique, and that each longitudinal generator may be paired with the latitudinal generator that lay on the boundary of the same T_i.

The following corollary of the definitions is not hard to verify (see [15]):

COROLLARY 3.6 If M is a compact 3-manifold in $\mathbf{R}^3$ bounded by a single surface L of genus g, and C_i, $i = 1, \ldots, g$, are g longitudinal generators of L and D_i, $i = 1, \ldots, g$, are g latitudinal generators of L, then

(a) the C_i and D_i, $i = 1, \ldots, g$, together form a basis $\mathsf{H}_1(L)$.

(b) the C_i, $i = 1, \ldots, g$, form a basis of $\mathsf{H}_1(M)$.

(c) the D_i, $i = 1, \ldots, g$, form a basis of $\mathsf{H}_1(\overline{M})$.

PROOF. Part (a) is classical [17].

For part (b), assume, by Theorem 3.4, that M is obtained by removing the wormholes N_i, $i = 1, \ldots, g$, from a 3-ball $\mathbf{B}^3$. Say N_i is the closed tubular neighborhood $d_i \times \mathbf{B}^2$ of an arc d_i in $\mathbf{B}^3$, $i = 1, \ldots, g$. Keeping in mind that $M \bigcup \cup_{i=1}^{g} N_i = \mathbf{B}^3$ and that $M \bigcap \cup_{i=1}^{g} N_i = \cup_{i=1}^{g} N_i'$, where $N_i' = d_i \times \mathrm{bd}\,(\mathbf{B}^2)$, the following is a portion of the Mayer-Vietoris sequence of the pair $(M, \cup_{i=1}^{g} N_i)$:

$$\mathsf{H}_2(\mathbf{B}^3) \to \mathsf{H}_1(\cup_{i=1}^{g} N_i') \xrightarrow{\phi} \mathsf{H}_1(M) \oplus \mathsf{H}_1(\cup_{i=1}^{g} N_i) \to \mathsf{H}_1(\mathbf{B}^3).$$

Since $\mathsf{H}_1(\mathbf{B}^3)$, $\mathsf{H}_2(\mathbf{B}^3)$, and $\mathsf{H}_1(\cup_{i=1}^{g} N_i)$ are all trivial, we deduce that ϕ gives an isomorphism from

$\mathsf{H}_1(\cup_{i=1}^{g} N_i')$ to $\mathsf{H}_1(M)$. The result then follows from observing that $\mathsf{H}_1(\cup_{i=1}^{g} N_i')$ is generated by a set of longitudinal generators of L.

Part (c) follows similarly. □

3.2.2 Manifolds not necessarily bounded by a single surface

Now we are ready to consider the case when M is not necessarily bounded with a single surface. So, assume $S_1, S_2, ..., S_{r-1}$ are the inner surfaces and S_r is the outer surface of M. Observe that $\overline{M}$ consists of r components, each a compact 3-manifold which is embeddable in $\mathbf{R}^3$ and which is bounded by a single surface. In particular,

$$\overline{M} = U_{S_1} \cup U_{S_2} ... \cup U_{S_{r-1}} \cup (\overline{U_{S_r}}),$$

Our description of the first homology group of M is contained in the following:

THEOREM 3.7 Let $C_1^i, \ldots C_{g_i}^i$ and $D_1^i, \ldots, D_{g_i}^i$ be g_i longitudinal and latitudinal generating cycles of S_i, respectively, $1 \leq i \leq r$.

Then, the set of $\sum_{i=1}^{r} g_i$ homology classes of cycles

$$\cup_{i=1}^{r-1} \{[D_1^i], \ldots [D_{g_i}^i]\} \cup \{[C_1^r], \ldots, [C_{g_r}^r]\}$$

forms a basis of $\mathsf{H}_1(M)$.

PROOF. Let $L = M \cap \overline{M}$ be the union of the set of surfaces that constitute $\mathrm{bd}\,(M)$ and $\mathrm{bd}\,(\overline{M})$. Certainly, $M \cup \overline{M} = \mathbf{S}^3$. The following is a portion of the Mayer-Vietoris sequence of the pair $(M, \overline{M})$:

$$\mathsf{H}_2(\mathbf{S}^3) \to \mathsf{H}_1(L) \xrightarrow{\phi} \mathsf{H}_1(M) \oplus \mathsf{H}_1(\overline{M}) \to \mathsf{H}_1(\mathbf{S}^3).$$

As $\mathsf{H}_1(\mathbf{S}^3)$ and $\mathsf{H}_2(\mathbf{S}^3)$ are both trivial, it follows that ϕ is an isomorphism.

Therefore, a basis of $\mathsf{H}_1(L)$ must split into two parts such that, by inclusion, ϕ maps one part to a basis of $\mathsf{H}_1(M)$ and the remainder to a basis of $\mathsf{H}_1(\overline{M})$.

Corollary 3.6 implies that a set of longitudinal generators of S_i forms a basis of $\mathsf{H}_1(U_{S_i}), i = 1, \ldots, r-1$, while a set of latitudinal generators of S_r forms a basis of $\mathsf{H}_1(\overline{U_{S_r}})$. Consequently, ϕ maps the longitudinal generators of $S_1, S_2, ..., S_{r-1}$ and the latitudinal generators of S_r to a basis of $\mathsf{H}_1(\overline{M})$. It follows, therefore, that ϕ must map the remaining generators in L, i.e., the latitudinal generators of $S_1, S_2, ..., S_{r-1}$ and the longitudinal generators of S_r, to a basis of $\mathsf{H}_1(M)$.

We conclude that

$$\cup_{i=1}^{r-1} \{[D_1^i], \ldots [D_{g_i}^i]\} \cup \{[C_1^r], \ldots, [C_{g_r}^r]\},$$

forms a basis of $\mathsf{H}_1(M)$. □

Figure 3.5 illustrates this theorem for different cases. In Figure 3.5(a) the surfaces S_i are not knotted or linked. In such cases the latitudinal generators of the $S_i, 1 \leq i \leq r-1$, and the longitudinal generators of S_r are not null-homologous (identity in $\mathsf{H}_1(K)$), while the remaining generators are null-homologous. Eg., in Figure 3.5(a) it is easy to imagine the longitudinal generators of S_1 and S_2 and the latitudinal generator of S_3 each bounding a distinct disc in K (in fact, Seifert surfaces [15], on which each can "contract" to a point),

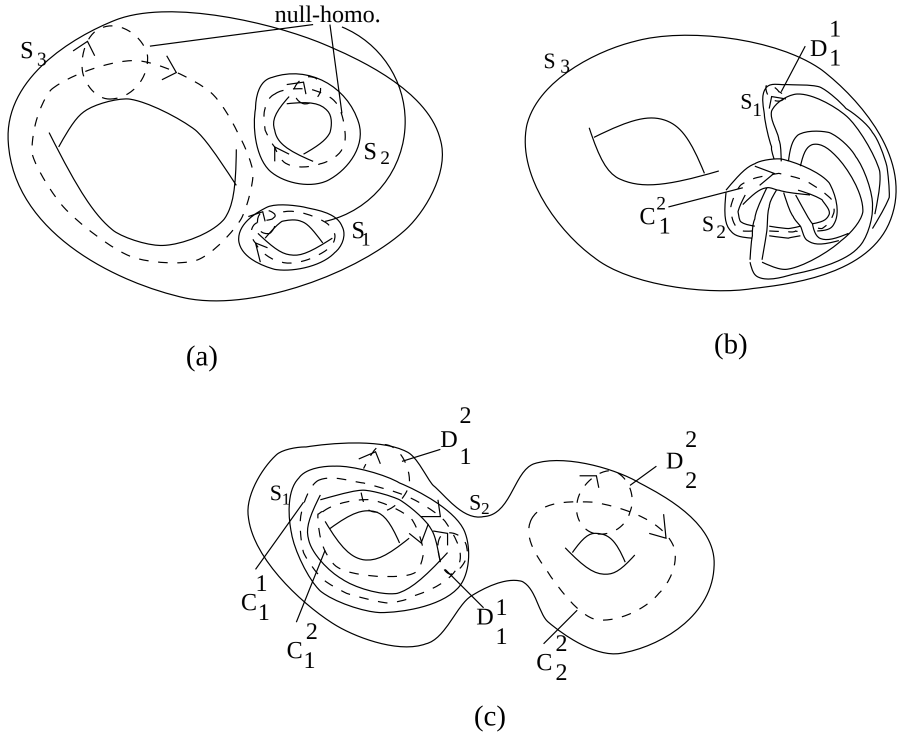


Figure 3.5: Basis of H_1.

while the other three generators do not. These three generators which are not null-homologous form a basis of $\mathsf{H}_1(K)$.

It is instructive to study examples where the S_i are knotted and linked, and verify the theorem. Eg., consider Figure 3.5(b) where the torus S_1 "winds" twice through torus S_2. No longer is C_1^2 null-homologous, but $[C_1^2] = 2[D_1^1]$, as a disc bounded by C_1^2 is punctured twice by cycles homotopic to D_1^1. So, despite the linking, $\{[D_1^1],\ [D_1^2],\ [C_1^3]\}$ is still a basis of $\mathsf{H}_1(K)$.

In Figure 3.5(c) neither C_1^1 nor D_1^2 is null-homologous, but $[C_1^1] = [C_1^2]$ and $[D_1^2] = [D_1^1]$, as one can imagine two annular strips in K, one bounded by C_1^1 and C_1^2, and the other by D_1^2 and D_1^1, so that these pairs of cycles are co-homologous, respectively (one cycle can "transform" to the other of the pair along the annulus). Thus, $\{[D_1^1],\ [C_1^2],\ [C_2^2]\}$ is a basis of $\mathsf{H}_1(K)$.

4 Algorithms

4.1 Computing Betti numbers and generators

Assume the simplicial complex K is a triangulation of the compact 3-manifold M in $\mathbf{R}^3$. Since $\sum_{i=1}^{r} g_i = r - \chi(K)$ by the proof of Theorem 3.3, computing the Betti number reduces to detecting all $r > 0$ bounding surfaces of M followed by computing their genus. The bounding surfaces can be detected through any linear-time traversal through the data structure representing K: simply list those triangles visited that do not bound a tetrahedron on both sides. The genus of a bounding surface can be computed by counting simplices as $g_i = 2 - \chi(S_i)$ for any surface S_i.

Alternatively, after determining bounding surfaces, we could compute $\beta_1(K)$ by computing the Euler characteristic of K through a simplex counting and then using the relation $\chi(K) = \beta_0(K) - \beta_1(K) + \beta_2(K) - \beta_3(K)$ where $\beta_0(K) = 1$, $\beta_2(K) = r - 1$ and $\beta_3(K) = 0$. This eliminates the 1-cycle detection step from the algorithm of [2].

To find the generators for $\mathsf{H}_1(K)$, as is evident from theorem 3.7, there are two major computational questions that we must first answer:

1. Given an embedding of K, how do we decide which of the bounding surfaces is the enclosing surface S_r?
2. Given a set of $2g_i$ generating cycles of the surface S_i, computed, eg., by the method of Vegter and Yap [20], how do we distinguish between latitudinal and longitudinal ones? Recall that we do not necessarily have a triangulation of the ambient space, ie., any information about the disposition of S_i with respect to the rest of $\mathbf{R}^3$.

To resolve the first question shoot a ray $\vec{r}$ in an arbitrary direction from a point on any surface S_i. In linear time compute all intersection points along $\vec{r}$ with surfaces S_i. The last intersection point along $\vec{r}$ must necessarily be due to S_r, thus identifying the outer surface.

To resolve the second question we require the notion of the *linking number* $L(C_1, C_2)$ of two disjoint oriented polygonal knots C_1 and C_2 in $\mathbf{R}^3$. Intuitively, $L(C_1, C_2)$ counts the number of times one of C_1 and C_2 winds around the other. We give below two equivalent definitions (from [15]); the first one relates to homology groups, while the second suggests a method to compute the linking number:

1. As $\mathsf{H}_1(\mathbf{R}^3 - C_2) = \mathbf{Z}$, the integers, [15], we can choose a generator $[C']$ of this group (in fact, C' may be chosen to be a latitudinal generating cycle of a tubular toroidal neighborhood of C_2). Then, if the homology class $[C_1] = n[C']$ in $\mathsf{H}_1(\mathbf{R}^3 - C_2)$, define $L(C_1, C_2) = n$.
2. Consider a *regular* projection π of $C_1 \cup C_2$ on to a plane P that is below both C_1 and C_2. A projection $\pi : C_1 \cup C_2 \to P$ is regular if $|\pi^{-1}(p)| \leq 2, \forall p \in P$.

   For each point $p \in P$ at which $\pi(C_1)$ intersects $\pi(C_2)$, ie., a point such that both C_1 and C_2 cross directly over it, assign a crossing number of ± 1 or 0 according to the following rules :

   (a) If C_1 crosses under C_2, and, facing along the orientation of C_1, C_2 appears to cross from left to right, then assign a crossing number of 1.

   (b) If C_1 crosses under C_2, and, facing along the orientation of C_1, C_2 appears to cross from right to left, then assign a crossing number of -1.

   (c) If C_1 crosses over C_2, then assign a crossing numer of 0.

   See Figure 4.6. If the sum of all crossing numbers at intersection points on P is l, define $L(C_1, C_2) = l$. Eg., in Figure 4.6, $L(C_1, C_2) = 2$.

We use linking numbers and the method of *barycentric perturbation* to distinguish between latitudinal and longitudinal generators of a surface.

For each surface S_i, construct the generators C_k^i and D_k^i in longitudinal/latitudinal pairs by the method of Vegter and Yap [20, Lemma 4.3]. For each $k = 1, ..., g_i$, this method produces the pair of cycles C_k^i and D_k^i intersecting at a single point, where cycles from distinct pairs do not intersect. To do barycentric perturbation, we need as well to construct the the first barycentric subdivision K' of K.

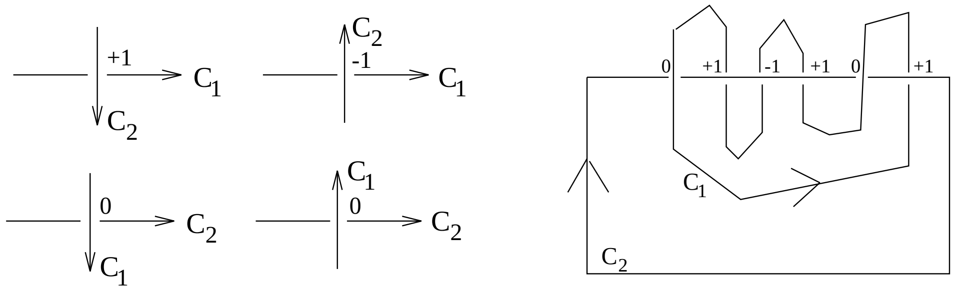


Figure 4.6: Linking number.

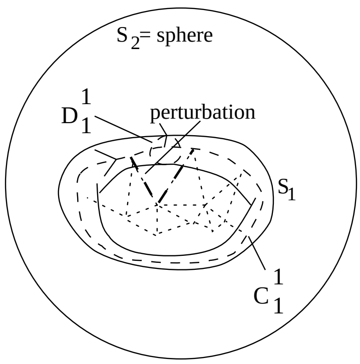


Figure 4.7: Perturbing generators.

Now, consider the longitudinal generating cycle C_k^i of an internal surface S_i. If C_k^i is *perturbed in* K', *minimally* to avoid intersecting D_k^i in K', then it is geometrically evident that the linking number of C_k^i and D_k^i (after perturbation) is 0. See Figure 4.7. However, if a latitudinal generating cycle D_k^i is similarly minimally perturbed in K', the linking number of D_k^i and C_k^i becomes ± 1. Choose orientations of the generating cycles so that this linking number, in fact, becomes 1.

The situation is symmetric for the enclosing surface S_r: a longitudinal generating cycle of a pair perturbs to link (with linking number ± 1) with its paired generating cycle, while the latitudinal generating cycle does not link with its paired generating cycle after minimal perturbation.

We should remark that the reason to go to the first barycentric subdivision K' to perform perturbations is that it is just fine enough that we can perturb (homotopically) a 1-cycle C to avoid intersections it originally had in K, without causing a new one.

A simple observation at this point suggests that we need not attempt at all to distinguish the enclosing surface:

It is exactly each of the longitudinal generators of the enclosing surface and each of the latitudinal generators of the interior surfaces that link non-trivially with the corresponding paired generator after perturbation. Therefore, we simply need to retain such sets of generators from each surface, without necessarily deciding if the given surface is enclosing or not.

4.2 Complexities

We assume that the triangulated manifold or complex is represented in a practical data structure, eg., as the one described in [8]. The counting of simplices for Betti number computations can be carried out through any linear-time traversal in this data structure. The only non-standard subroutines that are required to implement the algorithm for computing the generators are to:

1. *Compute the $2g_i$ generators of a triangulated surface S_i of size n_i.*

   For this we invoke the algorithm of Vegter and Yap [20] to obtain output as described in [20, Lemma 4.3]. Both the running time and space are $O(g_i n_i)$. Therefore, the total complexity is $O(n\overline{g})$ for r surfaces, where $\sum_{i=1}^{r} n_i = O(n)$ and $\overline{g} = \max_{1\leq i\leq r} g_i$.

2. *Compute the first barycentric subdivision and perform barycentric perturbation of a cycle.*

   The first barycentric subdivision is easily checked to be an $O(n)$ time and space procedure given a triangulation of size n. Observe that we need to perturb one of the cycles in a pair of longitudinal and latitudinal generator at the single point where they meet. This would seem to require traversing the cycle vertex by vertex, deciding for each vertex if it occurs on the other cycle also (possibly using binary search), and finally perturbing at the point of intersection. This can be made more efficient by perturbing all edges of the cycle *together*, so that intersections are avoided even without detecting where they originally occurred. The total time and space requirement is $O(k)$ for a cycle of length k.

3. *Compute the the linking number of two disjoint oriented polygonal cycles C and D in $\mathbf{R}^3$.*

   Assume C and D are of lengths k_1 and k_2, respectively. Project the cycles in linear time on an arbitrary plane (if the projection is not regular it can be perturbed slightly so that it is so) to obtain two closed polygonal curves C' and D' of lengths k_1 and k_2, respectively, on the plane. Compute all intersections of C and D using even the naive algorithm in $O(k_1 k_2)$ time and space (*any* algorithm would have a similar worst-case bound because of output size [14]). It is then possible to determine in constant time per intersection point p the crossing number at p by referring back to the points of C and D that lie above p. The complexity is $O(k_1 k_2)$ in time and space. Summing over all pairs of longitudinal and latitudinal generators we obtain a total complexity of $O(\sum k_i k_j) = O(n \sum k_j) = O(n^2\overline{g})$, since the size of the generators summed over all surfaces could be $O(n\overline{g})$. Observe that the complexity of this step dominates all others.

Considering all costs we have the following theorem:

THEOREM 4.1 Given a triangulated 3-manifold M of size n in $\mathbf{R}^3$, the Betti numbers of M can be computed in $O(n)$ time and space. A basis of $\mathsf{H}_1(M)$ and $\mathsf{H}_2(M)$ can be computed in time and space $O(n^2\overline{g})$ and $O(n)$, respectively.

5 Simplicial Complexes in $\mathbf{R}^3$

So far we have considered only triangulated 3-manifolds in $\mathbf{R}^3$. Of course, a simplicial complex K in $\mathbf{R}^3$ need not be a 3-manifold. In this section we show how K may be thickening to a 3-manifold M that is homotopic to K, so that results for 3-manifolds of the previous section can apply to analyze the structure of K. We first simplify the process of thickening K somewhat through a procedure called *collapsing*. A k-simplex $\sigma \in K$ is called *free* if it is incident on exactly one $(k+1)$-simplex σ'. Elimination of σ together with σ' constitute a collapsing of K to $K' = K - \{\sigma, \sigma'\}$. We first collapse K as long as it has free 0-simplices and 1-simplices. See Figure 5.8(a) for an illustration. At the end of this procedure each edge and vertex of K falls into one of two categories according as

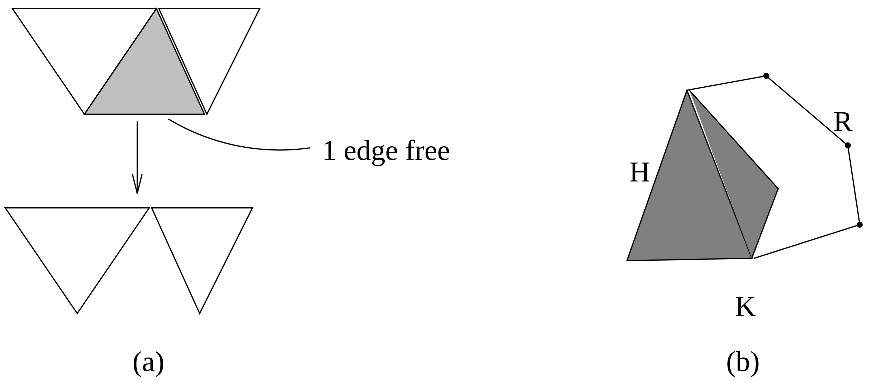


Figure 5.8: Collapsing.

i. it is not incident on any triangle.

ii. it is incident on two or more triangles.

For ease of presentation, we first excise all edges and vertices of K in the first category. The closure of the union of such edges and vertices forms a 1-dimensional simplicial complex (a graph), say R. See Figure 5.8(b). As R is a graph, it can be thickened straightforwardly in linear time to a tubular neighborhood, and attached back to the remainder of K. We consider next thickening this remainder, in fact, $H = \mathrm{cl}\,(K - R)$.

First, a definition: a *hive* is defined to be an at most 3-dimensional simplicial complex where every 1-simplex is the face of *two or more* 2-simplices (ie., triangles). Clearly, the remainder H forms a hive. It may be intuitively clear that a hive can be thickened to a 3-manifold M homotopic to it. We shall see that the process of thickening may, in fact, be "simulated" without computing an explicit triangulation of M. This procedure is similar to the one described in [2].

Consider a triangle t of H and choose a vector $\vec{n}$ normal to t (ie., a choice of a side of t), such that t is not the face of a tetrahedron on that side. Imagine thickening t by the width of a small ϵ in the direction of $\vec{n}$. For each edge e_i of t, $i = 1, 2, 3$, find the triangle t_i with e_i as edge that is adjacent to t by rotation around e_i in the direction $\vec{n}$. As H is a hive such t_i exist, and as the embedding of H in $\mathbf{R}^3$ is assumed known, each t_i may be found by a search through the linked list of triangles adjacent to e_i.

Now, imagine thickening each t_i correspondingly by a width of ϵ on the side that it is struck by the rotation around e_i as described above. We may continue this procedure at the remaining borders of the t_i, and further on through H in a breadth-first manner.

Finally, we shall indeed have a thickening of H to a 3-manifold M such that each bounding surface of M retracts homotopically on to a surface represented by a connected component of the graph G whose vertices are pairs $(t, \vec{n})$, where t ranges over triangles that do not face tetrahedrons on both sides and the $\vec{n}$ (at most 2 per t) indicate the sides of t not facing a tetrahedron. Adjacencies of vertices in G are defined as above (the method in [2] considers a similar graph as well). Thus, if T is a triangulation of M, we have then an explicit triangulation ∂T of the boundary $\mathrm{bd}\,(M)$ of M, except for the cases where these simulated surfaces meet at isolated vertices. The difficulty arises because of a shortcoming of our simulation process which does not thicken these vertices properly. To overcome this difficulty we replace such a vertex v with a small 3-ball represented by a regular tetrahedron σ centered at v. We triangulate the faces as necessary to take care of the intersections of σ with H, and let H' denote this new simplicial complex. Note that H' and H are homotopic and have sizes within a constant factor of each other. The surface simulation can now be applied to H' without

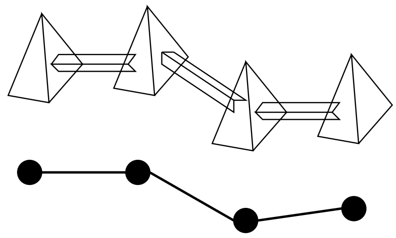


Figure 5.9: Thickening graphs.

any anomaly.

5.1 Complexity

It is not difficult to see that the simulation procedure is linear in the size of the complex being traversed if the triangles around edges are already sorted. Otherwise an extra log factor would appear in the complexity to sort the triangles around edges. Collapsing and explicit thickening of necessary edges and vertices adds at most a linear number of simplices and takes only linear time. Thus the entire simulation process adds an extra cost of $O(n)$ (or, $O(n \log n)$ if triangles are not sorted around edges) to the overall cost of computing Betti numbers and generators.

6 Conclusion

In this paper we have analyzed the homology groups of simplicial complexes in three dimensions. Theorems 3.1 and 3.7 are fundamental in that they characterize the generators of the second and first homology groups. These characterizations lead to efficient algorithms to compute actual sets of generators. Theorem 3.4 is a useful topological result.

There is considerable scope for further investigation:

- Find tight complexity bounds for the problems considered here. We do not know if our algorithms are optimal, except for ones that are trivially so.
- Find similar algorithms for the homotopy groups. This of course is much harder and one might therefore consider more restricted class of complexes that tend to arise naturally (see [4]).
- Extend these methods of analysis to topological objects, in particular simplicial complexes, in spaces of dimension higher than 3.
- Find real applications. There are various possibilities. Topology has long been applied in the physical sciences, and currently exciting applications are arising in molecular biology [7, 18]. See [3, 19] for a survey of related problems in the rapidly growing field of computational topology.

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