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Computing homology of subcomplexes of the 3-torus

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Summary

Suppose one has a collection of large geometric objects and one wishes to differentiate between them. When taking measurements on an object, one can probably only get a finite approximation of the object. It is not always possible to fully reconstruct what the original object looked like from this approximation. However, we can compute certain characteristics of the object.

This thesis deals with computing some of these characteristics, called homology groups. The approximations we use are simplicial complexes. We use a fast incremental algorithm by Delfinado and Edelsbrunner for computing simplicial homology over $\mathbb{Z}_2$ for subcomplexes of the 3-sphere. These complexes include simplicial approximations of objects realized in ordinary 3-dimensional space. The algorithm outputs the Betti numbers of a complex. These numbers are the ranks of the homology groups, and they uniquely identify the homology group.

Many approximating data sets, however, are periodic. We therefore adapt the algorithm to work with subcomplexes of the 3-torus. To use the algorithm, we need to expand subcomplexes of the 3-torus to complete triangulations of the 3-torus. A method is developed to accomplish this.

The adapted algorithm is shown to be approximately correct: the true first and second Betti numbers can be at most three higher than the computed ones. For large simplicial complexes this incremental algorithm might be more practical than the already available slower methods which provide a more accurate output.

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Contents

1 Introduction **1**

2 Simplicial complexes **3**
2.1 Foundations . . . 3
2.2 Combinatorial manifolds . . . 5

3 Homology **11**
3.1 Construction . . . 11
3.2 Relative homology . . . 14
3.3 Duality . . . 16

4 Computing homology **19**
4.1 Arbitrary simplicial complex . . . 19
4.2 Subcomplexes of $\mathbb{S}^3$ . . . 20
4.3 Tetrahedralizing $\mathbb{S}^3$ . . . 22
4.4 Time complexity . . . 22

5 The 3-torus **25**
5.1 Introduction . . . 25
5.2 Adapting the algorithm . . . 26
5.3 Triangulating the torus . . . 28
5.4 Extending to the 3-torus . . . 30
5.5 Other work . . . 31

6 Conclusions and future work **33**

Chapter 1

Introduction

Suppose one has a collection of large geometric objects and one wishes to differentiate between them. When taking measurements on an object, one can probably only get a finite approximation of the object. It is not always possible to fully reconstruct what the original object looked like from this approximation. However, we can compute certain characteristics of the object.

In this thesis, we will deal with computing the homology groups of such finite approximations. These homology groups are topological invariants. Topology essentially captures 'what an object looks like' when we forget all notion of distance. We call the resulting object a *topological space*. A topological invariant is the same for two spaces which are topologically equivalent. Here, for such topologically equivalent (or *homeomorphic*) spaces, the homology groups are necessarily the same. For two objects, we can therefore not positively determine if two objects have the same topology. But, if their homology groups are different, we are sure that they are topologically different.

The approximations we use are simplicial complexes, which use triangles and their higher- and lower-dimensional analogues to construct finite representations of objects. There are algorithms which compute the homology of arbitrary simplicial complexes. However, for large complexes these algorithms might be computationally infeasible. In 1995, Delfinado and Edelsbrunner [4] published a faster algorithm to compute the homology groups for simplicial complexes which are realized in ordinary 3-dimensional space.

In this thesis, we will adapt this algorithm to use it in computing the homology groups of periodic simplicial complexes. This would allow us to differentiate between possibly infinitely large geometric objects, which are composed of repeating structures. Take for example a collection of polymers. In fact, lots of data sets are periodic [2]. The advantage of using periodic data sets is that effects which occur at the boundaries of the object can be avoided. The result is a simpler approach that is more focused on the structural part of the data than the exceptions to the structure.

We assume that the periodic complexes are realized as subcomplexes of the 3-torus. The 3-torus can be represented as a solid cube in 3-dimensional space with its opposite facets identified. This means that we can start at a point in the cube and travel in any direction, and when we reach its boundary, we can go through it and emerge at the opposite side.

We start with a formal introduction of simplicial complexes in chapter 2. Then, we deal with homology groups in chapter 3. Chapter 4 will discuss the algorithm for computing homology of subcomplexes of the 3-sphere. These subcomplexes include complexes which are realized in ordinary three-dimensional space. Then, chapter 5 will introduce periodic spaces and adapt the algorithm from the chapter 4 to compute the homology of subcomplexes of the 3-torus. The adapted algorithm doesn't necessarily provide us with a correct output. However, we will prove it to be approximately correct.

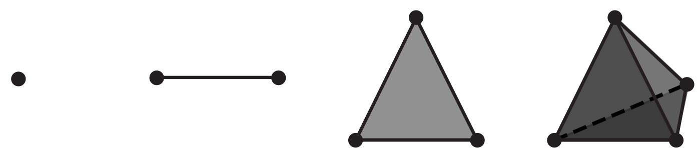
Chapter 2

Simplicial complexes

We can represent many topological objects by a finite set of points we call the *vertices* of the object and the points that lie 'between' two or more of these vertices. We call this representation a simplicial complex. One feature of a simplicial complex is that we can forget about the locations of the vertices once we know its structure. Section 2.1 will deal with the formal foundations of simplicial complexes. In section 2.2 we will expand this to certain triangulations of manifolds, for use in chapter 3.

2.1 Foundations

We call the k-dimensional analogue of a 2-dimensional triangle or a 3-dimensional tetrahedron a *k-simplex*. Formally, a k-simplex will be the convex hull of a set of $k+1$ affinely independent points in $\mathbb{R}^n$. Points $\{x_0, x_1, \ldots, x_k\}$ are affinely independent iff $\{x_1 - x_0, \ldots, x_k - x_0\}$ are linearly independent. So, a set of points is affinely independent if we can choose one point (any point will do) as the origin, and the remaining points are linearly independent with respect to this origin. The convex hull of these points is the set of all combinations $\sum_{i=0}^{k} \lambda_i x_i$, with each $\lambda_i \geq 0$ and the λ_i summing to 1. We have special names for the simplices of dimensions up to 3 (see figure 2.1).



(a) Vertex (b) Edge (c) Triangle (d) Tetrahedron

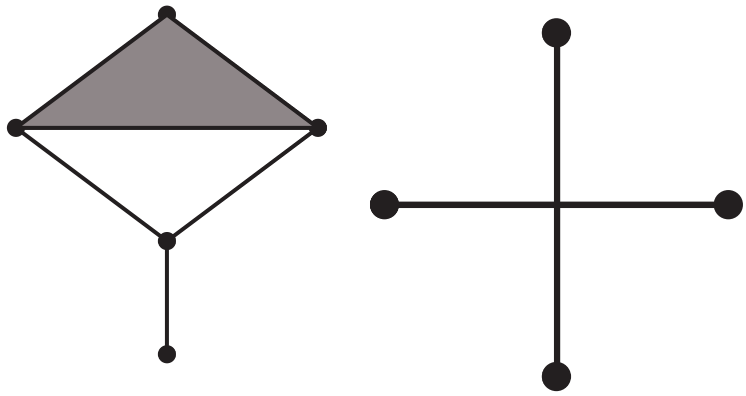
Figure 2.1: Simplices of dimension 0 through 3

For a k-simplex σ defined by the points $S = \{x_0, x_1, \ldots, x_k\}$, we define a *face* of σ to be a simplex τ defined by a subset T of S. A *coface* of σ is a simplex ρ defined by a superset R of S. We write $\tau \leq \sigma$ and $\rho \geq \sigma$ to express these relations. We call a face or coface of σ *proper* if it is not equal to σ, and we write $\tau < \sigma$ and $\rho > \sigma$, respectively. Note that if τ is a face of σ, then τ has σ as a coface.

Now we combine a collection of simplices such that they fit nicely together. We call a collection $K = \{\sigma_1, \ldots, \sigma_m\}$ of simplices a *simplicial complex* if it satisfies the following requirements:

1. if σ is a simplex in K, then all faces of σ are also in K,
2. if σ and τ are intersecting simplices in K, then their intersection $\sigma \cap \tau$ is a face of both.

Figure 2.2a shows an example of a simplicial complex. The collection of simplices depicted in figure 2.2b is not a simplicial complex, because the intersection of the two edges is not a vertex in the complex.



(a) a simplicial complex (b) not a simplicial complex

We can use such a simplicial complex to represent a topological space. We define the *underlying space* $|K|$ of K to be the union of all its simplices. Because we took the points of our simplex to be in the Euclidean space $\mathbb{R}^n$, the underlying space inherits the Euclidean topology. We call K a *triangulation* of a topological space X if its underlying space $|K|$ is homeomorphic to X. Not all topological spaces admit such a triangulation, though for example all differentiable manifolds do.

Thus, assuming a topological space X admits a triangulation, we are able to represent it by a simplicial complex K. We now go even further by forgetting the locations of the vertices in $\mathbb{R}^n$. What remains is a collection of sets of vertices. If k-simplex $\sigma_i \in K$ was the convex hull of vertices $x_0, x_1, \ldots, x_k$ then we now represent σ_i by just the set of vertices $[x_0, x_1, \ldots, x_k]$. The use of brackets instead of curly braces follows from a more general approach where the order of the vertices in the simplex is fixed. This is discussed in more detail in section 3.1. For our purposes, we just regard simplices as unordered sets and use the brackets for notational clarity.

We call the resulting set of simplices an *abstract simplicial complex*.

Definition An abstract simplicial complex is a non-empty finite set A such that for each element σ of A all subsets of σ are also in A. We call the union of all singleton sets $\{x_i\}$ in A its *vertex set*, denoted $\operatorname{Vert} A$. We call the elements of A its simplices. The dimension of an abstract simplicial complex is the maximum dimension (cardinality) of its simplices. A *realization* of an abstract simplicial complex A is a simplicial complex K such that there are functions $f : \operatorname{Vert} A \to \mathbb{R}^n$ and $g : A \to K$ such that $g([x_0, \ldots, x_n]) = \operatorname{conv}\{f(x_0), \ldots, f(x_n)\}$.

An abstract simplicial complex is much easier to manipulate in computations. Where a simplicial complex consists of infinite sets of points between vertices, an abstract simplicial complex is only a finite set of combinations of its vertices. It is clear that we can produce an abstraction of a given simplicial complex. The following theorem shows we can also produce a realization of an arbitrary abstract simplicial complex if the dimension of the ambient space is sufficiently large.

Theorem 2.1 *An abstract simplicial complex A of dimension d has a realization in $\mathbb{R}^{2d+1}$.*

In proving this theorem we find image points in $\mathbb{R}^{2d+1}$ for the vertex set of A. These points need to be in *general position*, that is, if we take $2d+2$ points or fewer they must be affinely independent. The following lemma states that we can do this (for proof, see [9, Theorem 1.6.7]):

Lemma 2.2 *There is a countable dense subset in $\mathbb{R}^n$ of points in general position, for an arbitrary n.*

We now prove the theorem.

Proof: We choose an injective function f which realizes the vertices in A in $\mathbb{R}^{2d+1}$ in a way such that all points in its image are in general position. According to lemma 2.2, we can find countably many of these points. For an abstract simplex $\sigma \in A$ we call the convex hull of its image in $\mathbb{R}^{2d+1}$, $\operatorname{conv} f(\sigma)$, its realization. We only need to show that if σ and τ are two abstract simplices in A, then the intersection of their realizations in $\mathbb{R}^{2d+1}$ will either be empty or a face of both. The dimension of both simplices is at most d, so their union will contain at most $2d+2$ points. Because of the construction of f, these points will be affinely independent when realized in $\mathbb{R}^{2d+1}$. Now, suppose there exists a point x in the intersection of the realizations of σ and τ. Then $x \in (\operatorname{conv} f(\sigma) \cap \operatorname{conv} f(\tau)) \subseteq (\operatorname{conv} f(\sigma) \cup \operatorname{conv} f(\tau)) \subseteq \operatorname{conv}(f(\sigma) \cup f(\tau))$. The last set is a convex hull of affinely independent points, and x is therefore uniquely represented by a sum $\sum_i \lambda_i x_i$, where the x_i lie in $f(\sigma) \cup f(\tau)$. However, the same holds for $\operatorname{conv} f(\sigma)$ and $\operatorname{conv} f(\tau)$. It follows that all x_i in the sum must be in both $f(\sigma)$ and $f(\tau)$. Therefore, x is in the realization of a face of both σ and τ. $\square$

For a set of simplices S in an abstract simplicial complex A we can define some operators which relate the set to the simplicial complex (see e.g. [10]).

Definition The *closure* of S, denoted $\overline{S}$, is the smallest simplicial subcomplex of A containing the simplices in S. The *star* of S, denoted $\operatorname{St} S$, is the set of all cofaces in A of the simplices in S. The *link* of S, which we denote $\operatorname{Lk} S$, is the boundary of the star, or $\operatorname{Lk} S = \overline{\operatorname{St}} S \setminus \operatorname{St} \overline{S}$.

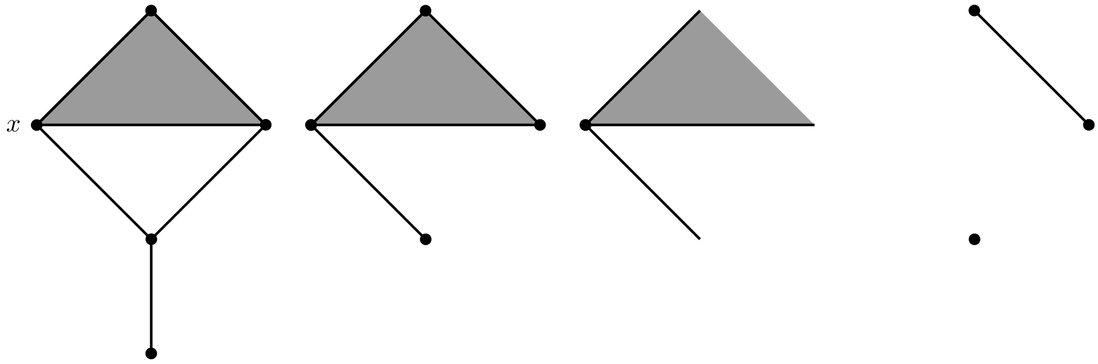
For notational clarity, we refrain from including the empty set as an element in the link.

One can easily verify that the link is closed under the taking of subsets. Therefore, the link of a set of simplices is always a simplicial complex. For a simplex $\sigma \in A$, the link of σ will be all simplices τ in A disjoint from σ such that $\sigma \cup \tau \in A$. For an example, see figure 2.2.

For a simplicial complex K, we define its *k-skeleton* to be all its simplices of dimension at most k. We denote this by $K^{(k)}$. See for example figure 2.3a.

2.2 Combinatorial manifolds

In this section our simplicial complexes will be ones that triangulate a spaces locally homeomorphic to Euclidean space. We start with the formal condition of such *combinatorial*



(a) the entire complex (b) $\overline{\mathrm{St}}\{[x]\}$ (c) $\mathrm{St}\,\overline{\{[x]\}}$ (d) $\mathrm{Lk}\{[x]\}$

Figure 2.2: The link of a 0-simplex $[x]$

manifolds, and will then associate a dual form with it: its *dual block decomposition*. We need these dual forms when discussing duality in section 3.3.

Definition A *combinatorial d-manifold* is 2-tuple (M, K), where K is a triangulation of a d-dimensional manifold M such that for each k-simplex $\sigma \in K$ the link of σ triangulates $\mathbb{S}^{d-k-1}$.

The condition implies that the closed star of each simplex σ is homeomorphic to the closed d-ball $\mathbb{B}^d$. Note that there are triangulations of a manifold that do not satisfy the condition on the links.

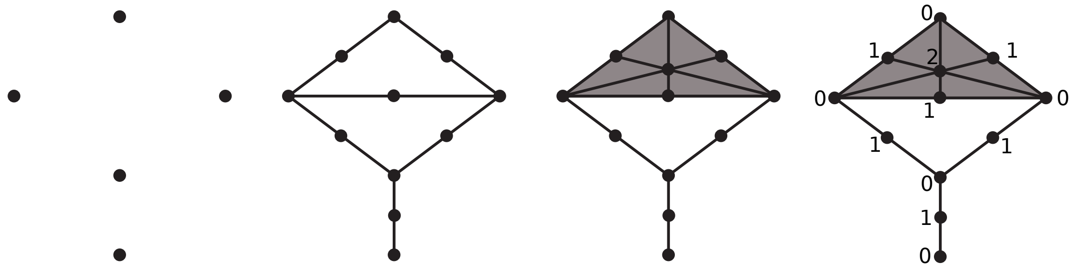
We will now introduce a way to subdivide simplicial complexes to facilitate constructing a dual form. This subdivision applies to all simplicial complexes.

Definition For a simplex $\mathrm{conv}\{x_0, \ldots, x_k\} = \sigma \in K$, we define its *barycentre* $\mathrm{Byc}(\sigma)$ to be the average of its vertices, $\mathrm{Byc}(\sigma) := \sum_{i=0}^{k} \frac{1}{i} x_i$. We construct the *barycentric subdivision* $\mathrm{Sd}\, K$ of K by adding the barycentre of each simple in K as a vertex and connect the vertices appropriately. We describe this process inductively:
To start, the 0-skeleton of the barycentric subdivision is the same as the vertices of the complex: $(\mathrm{Sd}\, K)^{(0)} = K^{(0)}$. For any $j > 0$, define $(\mathrm{Sd}\, K)^{(j)}$ to be $(\mathrm{Sd}\, K)^{(j-1)}$ with for each j-simplex σ in K its barycentre $\mathrm{Byc}(\sigma)$ added as a vertex. Furthermore, we add all simplices τ of dimension $k \leq j$ which have vertices $\{\mathrm{Byc}(\sigma)\} \cup \mathrm{Vert}\, \rho$, where ρ is a simplex in $(\mathrm{Sd}\, K)^{(j-1)}$ in the boundary of σ. For a d-dimensional simplicial complex K we define $\mathrm{Sd}\, K := (\mathrm{Sd}\, K)^{(d)}$.

For an illustration to help clarify the inductive process, see figure 2.3. In this example, we have one triangle in K. It is important to realize that $\mathrm{Sd}\, K$ no longer includes this large triangle as a simplex, but just the six small triangles which are a result of the subdivision process.

Note that the barycentric subdivision has an underlying space homeomorphic to the underlying space of the original complex.

In the inductive construction of $\mathrm{Sd}\, K$, we can associate a number with every vertex we add: the step at which it is added. We call this the *rank* of the vertex, denoted $r(x)$ for a vertex x. The rank corresponds to the dimension of the simplex of which x is the barycentre. The following proposition allows us to associate a vertex with each simplex in the barycentric subdivision:



(a) $K^{(0)} = (\operatorname{Sd} K)^{(0)}$ (b) $(\operatorname{Sd} K)^{(1)}$ (c) $(\operatorname{Sd} K)^{(2)} = \operatorname{Sd} K$ (d) $\operatorname{Sd} K$ with the ranks of the vertices

Figure 2.3: Constructing $\operatorname{Sd} K$

Proposition 2.3 *Each simplex in the barycentric subdivision has a unique vertex with minimal rank.*

Proof: The proof follows from the inductive construction of the barycentric subdivision. Let K be a simplicial complex and regard $(\operatorname{Sd} K)^{(k)}$. The proposition follows from the statement that for all k, each simplex in $(\operatorname{Sd} K)^{(k)}$ has a unique vertex with minimal rank. For $(\operatorname{Sd} K)^{(0)}$, we know that all simplices are 0-simplices and thus consist of only one vertex. Therefore, the statement holds for $k = 0$. Now suppose the statement holds for $k = j - 1$. From the inductive construction we know that $(\operatorname{Sd} K)^{(j)}$ consists of all simplices whose vertices are a combination of the barycentre of a j-simplex σ and the vertices of a simplex in $(\operatorname{Sd} K)^{(j-1)}$. Because of this construction, we know that the rank of the vertices in $(\operatorname{Sd} K)^{(j-1)}$ is at most $j - 1$. The rank of $\operatorname{Byc}(\sigma)$ is j, by definition, and therefore the added simplex still has a unique vertex with minimal rank. $\square$

This proposition defines a mapping $v : \operatorname{Sd} K \to \operatorname{Vert} K$, which maps each simplex in the barycentric subdivision of K to its associated vertex with minimal rank.

Definition The *dual block* of a simplex $\sigma \in K$, denoted $\hat{\sigma}$, is the simplicial complex consisting of all simplices $\tau \in \operatorname{Sd} K$ such that $v(\tau) = \operatorname{Byc}(\sigma)$. The dual block decomposition of K is the collection of all dual blocks of simplices in K. For a subcomplex $S \subseteq K$, the *complementary dual complex* consists of the dual blocks of all simplices in K that do not belong to S.

If (M, K) is a combinatorial d-manifold, then so is $(M, \operatorname{Sd} K)$.

We will now look at a subcomplex of a combinatorial manifold and its complementary dual complex. We will expand both these complexes to d-manifolds with a shared boundary.

Definition (M, K) is a combinatorial d-manifold with boundary if K triangulates M, which is a d-dimensional manifold with boundary, and for each k-simplex $\sigma \in K$ the link of σ either triangulates $\mathbb{S}^{d-k-1}$ or $\mathbb{B}^{d-k-2}$.

Let (M, K) be a combinatorial d-manifold with subcomplex S, and let T be the complementary dual complex of S. We are going to create combinatorial d-manifolds S'' and T'' of $\operatorname{Sd}^2 K$ with a shared boundary, such that they can be continuously deformed into S and T.

We call a subspace $A \subseteq X$ a *deformation retract* if there is a continuous function $F : X \times [0,1] \to X$ such that

$$\begin{aligned} F|_{X\times\{0\}} &= \operatorname{id} X, \\ F|_{A\times\{1\}} &= \operatorname{id} A, \\ F(X \times \{1\}) &= A \end{aligned}$$

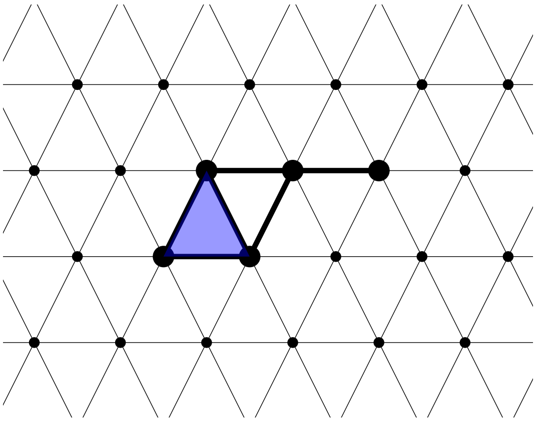
A nice property of deformation retracts is that their homology groups are isomorphic to the ones of the larger space (see [8]).

Let $S' := \operatorname{Sd}^2 S$ and $T' := \operatorname{Sd} T$. These are both subcomplexes of $\operatorname{Sd}^2 K$. We expand these complexes to make their union cover K (see figure 2.4):

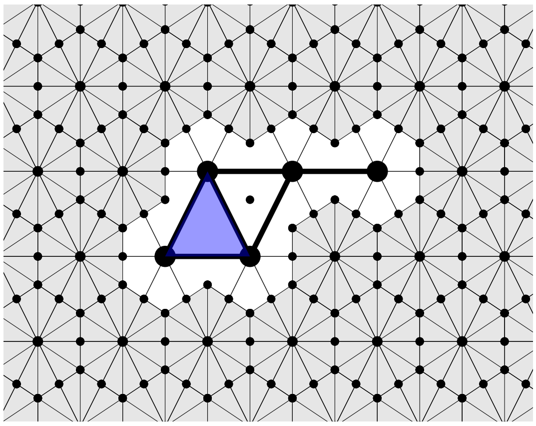
$$\begin{aligned} S'' &:= \bigcup_{\sigma\in S'} \overline{\operatorname{St}}\,\sigma \\ T'' &:= \bigcup_{\tau\in T'} \overline{\operatorname{St}}\,\tau \end{aligned}$$

Here, we take the star in the second barycentric subdivision of K. By the definition of the complementary dual complex, we have for a simplex $\sigma \in K$: $\sigma \in S \iff \hat{\sigma} \notin T$. Therefore, for a vertex $x \in \operatorname{Sd} K$ which is the barycentre of a simplex $\sigma \in K$ we have either $\sigma \in S \Rightarrow x \in \operatorname{Sd} S \subset S'$ or $\hat{\sigma} \in T \Rightarrow x \in T \subset T'$. So, a vertex in $\operatorname{Sd} K$ belongs to either S' or T', hence the closed stars of the vertices cover $\operatorname{Sd}^2 K$.

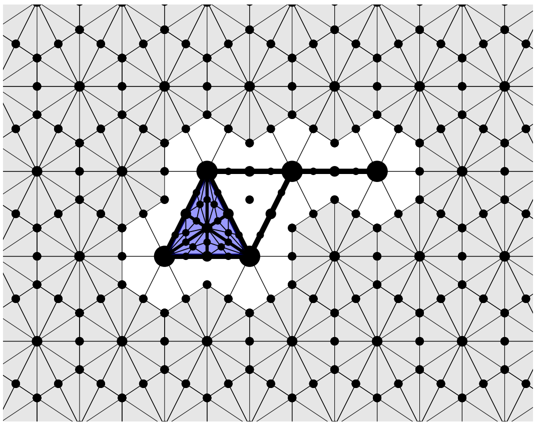
Since (M, K) is a combinatorial manifold, so is $(M, \operatorname{Sd}^2 K)$ and therefore S' and T' also form combinatorial d-submanifolds of M in their interiors. Their intersection is precisely their joint boundary $S' \cap T' = \partial S' = \partial T'$, since their interiors are disjoint and M doesn't have a boundary. All k-simplices in $\operatorname{Sd}^2 K$ have a link that triangulates a sphere of dimension $d - k - 1$. And so, a k-simplex $\sigma \in S' \cap T'$ will have a link $\operatorname{Lk}\sigma$ that triangulates a ball of dimension $d - k - 2$ when taking the link in S' or T', since the link in $\operatorname{Sd}^2 K$ will not be completely in either S' or T'.



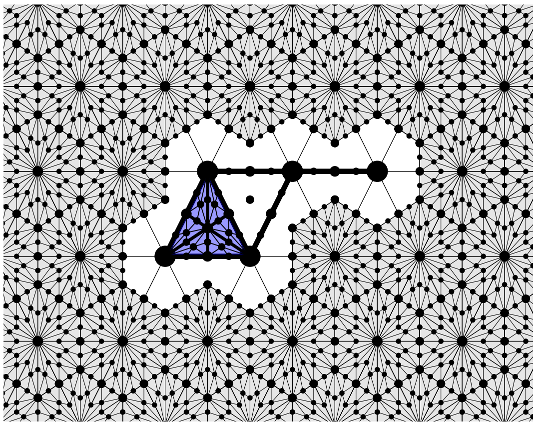
(a) A subcomplex S of a hexagonal complex K



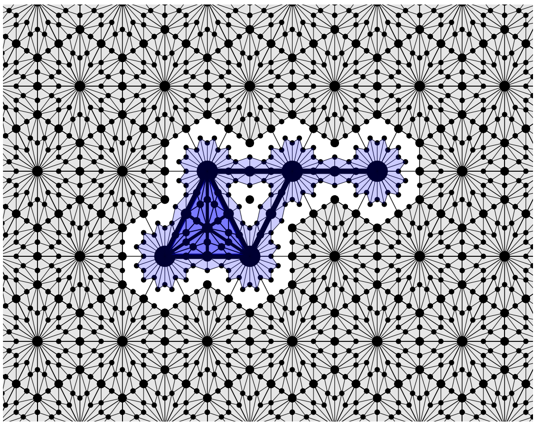
(b) The complementary dual complex T



(c) The second barycentric subdivision S'



(d) The barycentric subdivision T'



(e) S''

Figure 2.4: Constructing S'' and T''

Chapter 3

Homology

The homology of a topological space can tell us something about what a space looks like. Homology is a topological invariant, which means that homeomorphic spaces have the same homology. It can therefore also help us to distinguish between spaces. Section 3.1 will start off by constructing the homology groups. Section 3.2 will then continue by relating the homology of a subcomplex to the full space by introducing relative homology. Finally, in section 3.3 we will lay down some of the mathematical basis for the algorithms in chapters 4 and 5.

3.1 Construction

We define a *k-chain* to be a formal sum of k-simplices, denoted $c = \sum_i a_i \sigma_i$. This sum has no specific meaning; at this point, we just combine simplices. In algebraic topology this is usually regarded as an additive abelian group with the coefficients a_i in $\mathbb{Z}$. However, for our computational purposes it is easiest to work with these coefficients modulo 2. We denote this group of integers modulo 2 by $\mathbb{Z}_2$. A k-chain is then just a list of simplices with coefficient 1. We will write $[x_0, \ldots, x_k]$ for the simplex spanned by the vertices $x_0, \ldots, x_k$. The brackets denote an element in which the order is fixed. This is a convention from working with other coefficients, such as $\mathbb{Z}$. Usually, we orient the simplices. However, as our coefficients lie in $\mathbb{Z}_2$, the negatively oriented simplex is the same as the positively oriented one, seeing as $-1 = 1$ in $\mathbb{Z}_2$. We therefore won't bother ourselves with orienting the simplices.

The k-chains with simplices from a simplicial complex K form an additive abelian group, which we denote $C_k(K)$. When adding two chains one simply adds their coefficients. For a simplicial complex K of dimension d, we will have a maximum of $d + 1$ nontrivial groups of k-chains. For notational purposes, we will usually abbreviate $C_k(K)$ to C_k, where the simplices are understood to come from some finite simplicial complex.

Example Take for example the simplicial complex K_6 in figure 3.1. We have 7 vertices, so the zeroth chain group is generated by 7 simplices. An element in $C_0(K_6)$ is any combination or formal sum of $x_0, \ldots, x_6$, e.g. $x_0 + x_2 + x_3 \in C_0(K_6)$. There are 9 edges, so the first chain group is generated by 9 edges, in a way analogous to $C_0(K_6)$. One of the 1-chains is for example $[x_0, x_2] + [x_5, x_6]$. There is just one triangle, which is the sole generator of $C_2(K_6)$.

We now construct homomorphism between the chain groups.

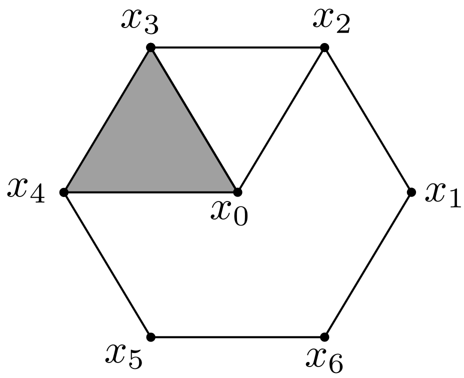


Figure 3.1: Example simplicial complex K_6

Definition The *boundary map* $\partial_k : C_k \to C_{k-1}$ is given by the linear extension of $\partial[x_0, \ldots, x_k] = \sum_i [x_0, \ldots, \hat{x_i}, \ldots, x_k]$, where the hat denotes an element that is removed. It is easy to see the linear extension is well-defined, which makes the map a homomorphism by construction.

Example Take the example simplicial complex K_6 from figure 3.1 again. For the edge $[x_0, x_2]$, the boundary $\partial_1[x_0, x_2]$ will be x_0+x_2. For the only triangle the boundary $\partial_2[x_0, x_3, x_4]$ is $[x_0, x_3] + [x_3, x_4] + [x_4, x_0]$.

Connecting the groups of k-chains through the boundary maps, we get the following sequence:

$$0 \to C_d \xrightarrow{\partial_d} C_{d-1} \xrightarrow{\partial_{d-1}} C_{d-2} \to \cdots \to C_0 \to 0 \tag{3.1}$$

The following proposition holds:

Proposition 3.1 *For any k, $\partial_{k-1} \circ \partial_k = 0$.*

Proof: Note that linearity of ∂_k implies that it is sufficient to prove the proposition for a chain c composed of a single k-simplex $\sigma = [x_0, \ldots, x_k]$. By definition of ∂_k, $\partial_k c = \sum_i [x_0, \ldots, \hat{x_i}, \ldots, x_k]$ and therefore $\partial_{k-1} \partial_k c = \sum_{j \neq i} \sum_i [x_0, \ldots, \hat{x_i}, \ldots, \hat{x_j}, \ldots, x_k]$, where x_i and x_j aren't necessarily in this order. i and j are interchangable in the sum, therefore all simplices appear exactly twice. Since the coefficients of our chains are in $\mathbb{Z}_2$, these simplices cancel. Therefore, $\partial_{k-1} \partial_k c = 0$. □

The boundary maps give rise to interesting subgroups of chains. For k-chains, we are interested in the image of ∂_{k+1} and the kernel of ∂_k. We call a k-chain which is in the kernel of ∂_k a *k-cycle*, and we denote the kernel by Z_k. Similarly, we call a k-chain which is in the image of ∂_{k+1} a *k-boundary*, and we denote this image by B_k. Remember that both the image and the kernel of a homomorphism are subgroups, in this case, of C_k. Because C_k is abelian, both B_k and Z_k are normal subgroups.

Example Returning to our example complex K_6 from figure 3.1, we can see that there are 7 different 1-cycles. These can by generated by three 1-cycles, for example the 1-cycle of length six around the hexagon, and the 1-cycles around the two triangles (by triangle we here mean 3 points with edges between them, not necessarily a 2-simplex). There is only one 1-boundary, that is the 1-cycle around the 2-simplex.

Homology Due to proposition 3.1, all k-boundaries are necessarily k-cycles, or $B_k \subseteq Z_k$ (in fact B_k is a subgroup of Z_k). This motivates us to look at the cycles that aren't boundaries, or, *non-bounding cycles*. In fact, we will regard the quotient group Z_k/B_k. In this group, we call k-cycles equivalent if they differ by a k-boundary. All k-boundaries are equivalent to the identity 0. Since B_k is a subgroup, which is normal by the fact that C_k is abelian, this quotient group is well-defined. We denote the group by H_k and call it the k-th *homology group*.

With each homology group we can associate a nonnegative integer, namely, its number of generators. It is easy to see that C_k and all of its subgroups and factor groups are generated by a finite set S of generators. This is a maximal set of different non-zero simplices. Each element of the group is then uniquely represented by a subset of S consisting of the simplices with coefficient 1 in the formal sum. We call the cardinality of S the *rank* of the group. We give the rank of the k-th homology a special name: we call it the k-th *Betti number*, denoted β_k.

These Betti numbers capture certain intuitive properties of the topological space. The zeroth Betti number β_0 captures the number of generating non-bounding 0-cycles in the space that do not differ by a boundary. Every vertex is a 0-cycle and a single vertex is never a boundary. Therefore, β_0 is just the number of generating nonequivalent (in the quotient group) vertices in the simplicial complex. Vertices are equivalent if there is a boundary between them. The 0-boundaries are exactly the endpoints of edges. Therefore, if there is a succession of edges connecting vertices to each other, they are equivalent. Therefore, β_0 measures the number of edge-connected components in a simplicial complex.

The first Betti number β_1 does the same for the 1-cycles. Edges however, are not trivially cycles. A 1-cycle is a succession of edges that starts and end at the same vertex. A non-bounding 1-cycle is one that isn't the boundary of a triangle. β_1 therefore measures the 'number of different ways' we can go through the space from a single vertex and arrive at the same point.

The second Betti number β_2 measures the number of generators for non-bounding 2-cycles. A 2-cycle that is not a boundary encloses a space in $\mathbb{R}^3$. Therefore, β_2 is equal to the number of enclosed spaces or *voids*.

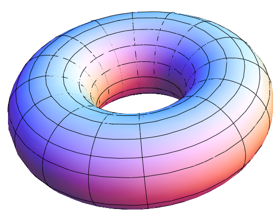


Figure 3.2: The 2-torus: the boundary of the doughnut

Example Take for example the 2-torus (see figure 3.1). It consists of one component, and therefore $\beta_0 = 1$. If we start on a point on the torus, we can go in two nonequivalent directions are arrive at the same point: through the 'gap' in the middle and around the torus through the horizontal plane. Hence $\beta_1 = 2$. The torus encloses one space or void: the interior of the doughnut. Thus $\beta_2 = 1$.

Reduced homology When using the Betti numbers, sometimes β_0 behaves differently than we expect with respect to the others. This is because all 0-simplices are cycles, and a single 0-simplex is never a boundary. The result is that a nonempty simplicial complex always has $\beta_0 \geq 1$. To correct this, we introduce what we call the *augmentation map* $\varepsilon : C_0(K) \to \mathbb{Z}_2$ as the linear extension of $\varepsilon = 1$ for every single vertex. Then, we define $\tilde{H}_0(K) := \ker \varepsilon / \operatorname{im} \delta^1$. This entails that a 0-cycle should now contain an even number of vertices. Effectively, we're decreasing the rank of H_0 by 1. We call the homology groups that use the augmentation map the *reduced homology group* and denote them by $\tilde{H}_k(K)$. Note that $H_k(K) = \tilde{H}_k(K)$ for all $k > 0$. The reduced homology groups give rise to the reduced Betti numbers, which we denote $\tilde{\beta}_k$. The main reason we introduce these reduced homology groups is that some theorems such as Alexander's duality theorem in section 3.3 allow an easier statement this way.

Singular homology Most of the proofs relating homology to the topology of a space is done through another branch of homology than we use here: singular homology. There, instead of convex hulls of points in $\mathbb{R}^n$, the simplices are mappings from the standard k-simplex Δ^k. The standard k-simplex has a vertex at the origin and has vertices at the origin translated by each of the first k unit vectors. We will not delve further into the subject, but note that for simplicial complexes the two kinds of homologies can be shown to be equivalent.

3.2 Relative homology

Relative homology is a useful tool which allows us to study the differences in homology groups between a simplicial complex and a subcomplex thereof.

Let K be a simplicial complex and L a subcomplex.

Definition The *relative chain group* $C_k(K, L)$ is the quotient group of the chain groups of the complexes: $C_k(K)/C_k(L)$. Chains in this group will be equivalent if their coefficients are equal for simplices in $K \setminus L$. The coefficients of simplices in L may differ. The boundary map $\partial_k : C_k(K, L) \to C_{k-1}(K, L)$ is induced by the one on K, which is still linear and equals 0 when applied twice. We can therefore define relative cycles, boundaries and the homology group in the usual way:

$$\begin{aligned} Z_k(K, L) &= \ker \partial_k \\ B_k(K, L) &= \operatorname{im} \partial_{k+1} \\ H_k(K, L) &= Z_k(K, L)/B_k(K, L) \end{aligned}$$

A relative k-chain $c + C_k(L)$ is a cycle iff its boundary is completely in $C_k(L)$.

Exact sequences are a useful tool in proofs related to homology:

Definition Consider the following sequence:

$$A_1 \xrightarrow{\eta_1} A_2 \xrightarrow{\eta_2} A_3 \to \cdots \to A_{n-1} \xrightarrow{\eta_{n-1}} A_n$$

Here, the A_i are abelian groups and the $\eta_i : A_i \to A_{i+1}$ are homomorphisms between them. We will call the sequence *exact* if for $1 \leq i < n$ $\operatorname{im} \eta_i = \ker \eta_{i+1}$.

Theorem 3.2 *For a subcomplex L of a simplicial complex K, there is an exact sequence:*

$$\cdots \to H_k(L) \xrightarrow{\eta_1} H_k(K) \xrightarrow{\eta_2} H_k(K,L) \xrightarrow{\phi} H_{k-1}(L) \xrightarrow{\eta_4} H_{k-1}(K) \to \ldots$$

Proof: The map $\eta_1 : H_k(L) \to H_k(K)$ is the canonical map induced by the inclusion of L in K. The map $\eta_2 : H_k(K) \to H_k(K,L)$ is also a natural map induced by the canonical map on the factor group $C_k(K,L)$. However, the next map $\phi : H_k(K,L) \to H_{k-1}(L)$ is an important map. We call it the *connecting homomorphism*. Let $c+C_k(L)$ be a relative k-cycle in $H_k(K,L)$. Then $\partial_k c \in C_{k-1}(L)$, so c is also in $H_{k-1}(L)$. Since $\partial_{k-1}\partial_k c = 0$, $\partial_k c$ is a cycle in $H_{k-1}(L)$, which needn't be bounding. To see that the map is well-defined, pick a boundary $b \in B_k(K)$ and a chain $l \in C_k(L)$. Then,

$$\partial_k(c+b+l) = \partial_k(c) + \partial_k(b) + \partial_k(l) = \partial_k c + 0 + \partial_k l \ \sim \ \partial_k c$$

under the equivalence relation $\sim$ in the factor group $Z_k(L)/B_k(L)$.

To show that the sequence is exact: $\operatorname{im}\eta_1$ consists of all k-cycles in L that do not bound in K. $\ker\eta_2$ consists of all non-bounding k-cycles in K that are completely in L. Therefore, $\operatorname{im}\eta_1 = \ker\eta_2$. The kernel of ϕ is composed of all relative k-cycles c such that $\partial_k c$ bounds in $C_{k-1}(L)$. This is precisely the image of η_2: all k-cycles $c + C_k(L)$ such that $\partial_k c \in C_{k-1}$. The kernel of η_4 is generated by the non-bounding generating cycles in L that disappear in K, that is, those generating cycles that bound in K. This kernel agrees with the image of ϕ, since ϕ maps $c + C_k(L)$, $c \in C_k(K \setminus L)$, $\partial_k c \in C_{k-1}(L)$ to $\partial_k c \in C_{k-1}(L)$. This covers all $(k-1)$-boundaries in K. □

We have two lemmas for exact sequences that consist of only five groups:

Lemma 3.3 *If we have the following exact sequence:*

$$A_1 \xrightarrow{\eta_1} A_2 \xrightarrow{\eta_2} A_3 \xrightarrow{\eta_3} A_4 \xrightarrow{\eta_4} A_5$$

then

$$0 \xrightarrow{\mu_1} A_2/\operatorname{im}\eta_1 \xrightarrow{\mu_2} A_3 \xrightarrow{\mu_3} \ker\eta_4 \xrightarrow{\mu_4} 0$$

is also exact. This last sequence is what we call a short exact sequence*, where the sequence consists of five groups of which the first and last are trivial.*

Proof: $A_2/\operatorname{im}\eta_1 = A_2/\ker\eta_2$, so $\ker(A_2/\ker\eta_2 \to A_3) = 0 = \operatorname{im}\mu_1$. Since $A_2/\ker\eta_2 \cong A_3$, and therefore $\operatorname{im}\mu_2 = \operatorname{im}\eta_2 = \ker\eta_3$, and furthermore $\ker\mu_3 = \ker(A_3 \to \ker\eta_4) = \ker(A_3 \to \operatorname{im}\eta_3) = \ker eta_3$, we have $\operatorname{im}\mu_2 = \ker\mu_3$. For $\operatorname{im}\mu_3$, we have $\operatorname{im}(A_3 \to \operatorname{im}\eta_3) = \operatorname{im}\eta_3$. Since $\ker\mu_4 = \ker\eta_4 = \operatorname{im}\eta_3$, the final condition for exactness of the sequence is met. □

Lemma 3.4 *If we have a short exact sequence:*

$$0 \to A_2 \xrightarrow{\eta_2} A_3 \xrightarrow{\eta_3} A_4 \to 0$$

then $\operatorname{rank}(A_3) = \operatorname{rank}(A_2) + \operatorname{rank}(A_4)$.

Proof: We have $\operatorname{im}\eta_3 = \ker(A_4 \to 0) = A_4$. Furthermore $\ker\eta_2 = \operatorname{im}(0 \to A_2) = 0$ so $A_2 \cong \operatorname{im} A_2 = \ker\eta_3$. For any homomorphism $\varphi : G \to G'$, a standard isomorphism theorem in group theory states that $G/\ker\varphi \cong \operatorname{im}\varphi$. We combine this with the fact that for the quotient G/H of a finitely-generated abelian group G and subgroup H we have $\operatorname{rank} G - \operatorname{rank} H = \operatorname{rank} G/H$. Hence we get $\operatorname{rank}(\operatorname{im}\eta_3) + \operatorname{rank}(\ker\eta_3) = \operatorname{rank}(A_3)$, so the lemma follows. □

The relative homology of two simplicial complexes is related only to their difference. That is, for a simplicial complex K and a subcomplex S, we can cut out a subcomplex $T \subset S \subset K$ from K and S such that their relative homology groups remains the same. This is formulated in the *excision theorem*, as found along with its proof in [5, p. 119]

Theorem 3.5 (Excision theorem) *Given subcomplexes $T \subset S \subset K$, the inclusion $(K \setminus T, S \setminus T) \hookrightarrow (K, S)$ induces isomorphisms $H_k(K \setminus T, S \setminus T) \to H_k(K, S)$ for all k.*

3.3 Duality

This section will present theory to allow us to give a proof of Alexander's duality theorem. This is the main duality we use in our algorithms for classifying simplices in the 3-sphere and 3-torus in the next two chapters.

Theorem 3.6 (Alexander duality theorem) *Let (M, K) be a d-dimensional combinatorial manifold where $M = \mathbb{S}^d$, S be a subcomplex of K with T as its complementary dual complex. For reduced homology groups over $\mathbb{Z}_2$, the following holds: $\tilde{H}_k(S) \cong \tilde{H}_{d-k-1}(T)$.*

We will establish the tools we need to prove this theorem. Some of the groundwork has already been done in section 2.2.

Definition We define a *k-cochain* to be a homomorphism $\gamma : C_k \to \mathbb{Z}_2$. The k-th cochain group will be the group of all such homomorphisms under the composition operation, $C_k^* := \mathrm{Hom}(C_k, \mathbb{Z}_2)$. This is the dual group of C_k. The dual of the boundary map, $\delta^k : C_k^* \to C_{k+1}^*$ is given by $\gamma \mapsto \gamma \circ \partial_{k+1}$. We call this the *coboundary map*.

One readily verifies that $\delta^{k+1} \circ \delta^k = 0$, and therefore we can define the homology groups of the cochains as we did with the regular chains. We call $H^k := (H_k)^* = \ker \delta^k / \operatorname{im} \delta^{k-1}$ the *k-th cohomology group*.

Earlier, when introducing k-chains, we discussed that the coefficients of our chains lie in $\mathbb{Z}_2$. Here, we could've also taken another group or even any module. It turns out that for coefficients in $\mathbb{Z}_2$ the cohomology groups are isomorphic to the homology groups (for a proof, see e.g. [5, p. 195]).

Theorem 3.7 (Universal coefficient theorem for cohomology in $\mathbb{Z}_2$) *For any simplicial complex K and $k \geq 0$, $H^k(K) \cong H_k(K)$.*

The result absolves the need for introducing cohomology groups in $\mathbb{Z}_2$, but the following main duality theorem used in the proof of Alexander duality relates relative homology to absolute cohomology. We will not give its full proof, because doing so would require a fair amount of additional material involving dual blocks. For a proof, see [8].

Theorem 3.8 (Lefschetz duality) *For a combinatorial d-manifold (M, K) with boundary, and nonnegative integers p, q such that $p + q = d$, the following groups are isomorphic: $H_p(M, \partial M) \cong H^q(M)$.*

We will now prove Alexander duality using the results established in this section along with earlier results on combinatorial manifolds (section 2.2) and relative homology (section 3.2).

Proof: Let (M, K) be a d-dimensional combinatorial manifold, $M = \mathbb{S}^d$, S be a subcomplex of K with T as its complementary dual complex. We can construct S'' and T'' as in section 2.2 as expansions of S and T which are combinatorial d-manifolds with a shared boundary $S'' \cap T'' = \partial S'' = \partial T''$. S'' and T'' are deformation retracts of S and T, respectively, and therefore have isomorphic homology groups.

First, suppose $0 \leq k < d-1$. We get the following sequence of isomorphisms and identities:

$$\begin{aligned}
\tilde{H}_k(S) &\cong \tilde{H}_k(S'') && (3.2)\\
&\cong \tilde{H}_{k+1}(\mathrm{Sd}^2 K, S'') && (3.3)\\
&= H_{k+1}(\mathrm{Sd}^2 K, S'') && (3.4)\\
&\cong H_{k+1}(T'', \partial T'') && (3.5)\\
&\cong H^{d-k-1}(T'') && (3.6)\\
&= \tilde{H}^{d-k-1}(T'') && (3.7)\\
&\cong \tilde{H}^{d-k-1}(T) && (3.8)\\
&\cong \tilde{H}_{d-k-1}(T) && (3.9)
\end{aligned}$$

We have equation 3.2 because S is a deformation retract of S''. Next, we have the exact reduced homology sequence

$$\cdots \to \tilde{H}_{k+1}(\mathrm{Sd}^2 K) \to \tilde{H}_{k+1}(\mathrm{Sd}^2 K, S'') \to \tilde{H}_k(S'') \to \tilde{H}_k(\mathrm{Sd}\, K^2)$$

Since K triangulates $M = \mathbb{S}^d$ so does $\mathrm{Sd}^2 K$. For the d-sphere the reduced homology groups are trivial except for $k = d$, where it has rank 1. Equation 3.3 follows. Next, because $k + 1 > 0$, the reduced homology group equals the standard homology group (3.4). The isomorphism 3.5 follows from the excision theorem (theorem 3.5). We excise the interior of S'' from $(\mathrm{Sd}^2 K, S'')$ to get $(T'', \partial T'')$, since S'' and T'' cover $\mathrm{Sd}^2 K$ and are disjoint but for their boundary. Equation 3.6 follows directly from the application of Lefschetz duality (theorem 3.8). Since $k < d-1$, reduced cohomology is again the same as standard cohomology. Since T is a deformation retract of T'', we have (3.8). Theorem 3.7 tells us cohomology and homology are isomorphic, hence we get (3.9).

Now, for $k = d - 1$ we have a similar sequence of isomorphisms. Here, we get:

$$\begin{aligned}
\tilde{H}_{d-1}(S) \oplus \mathbb{Z}_2 &\cong \tilde{H}_{d-1}(S'') \oplus \mathbb{Z}_2 \\
&\cong \tilde{H}_d(\mathrm{Sd}^2 K, S'') && (3.10)\\
&= H_d(\mathrm{Sd}^2 K, S'') \\
&\cong H_d(T'', \partial T'') \\
&\cong H^0(T'') \\
&\cong \tilde{H}^0(T'') \oplus \mathbb{Z}_2 && (3.11)\\
&\cong \tilde{H}^0(T) \oplus \mathbb{Z}_2 \\
&\cong \tilde{H}_0(T) \oplus \mathbb{Z}_2
\end{aligned}$$

We have equation 3.10 because the reduced homology sequence now looks like

$$0 \to \mathbb{Z}_2 = H_d(\mathrm{Sd}^2 K) \to H_d(\mathrm{Sd}^2 K, S'') \to H_{d-1}(S'') \to 0$$

and using lemma 3.4 for short exact sequences the isomorphism follows. In dimension 0, reduced homology differs from homology by one copy of $\mathbb{Z}_2$, hence we have isomorphism 3.11.

□

Chapter 4

Computing homology

This chapter will deal with algorithmically computing the homology of simplicial complexes embeddable in the 3-sphere $\mathbb{S}^3$. First, an incremental algorithm for computing the Betti numbers of an abstract simplicial complex will be given in section 4.1. Then, a classification algorithm for subcomplexes of $\mathbb{S}^3$ will be presented in section 4.2. Next, a triangulation algorithm to extend subcomplexes of $\mathbb{S}^3$ to a full triangulation of $\mathbb{S}^3$ will be given in section 4.3. Finally, we will briefly discuss the time complexity of the algorithm in section 4.4 and provide a motivation for adapting this algorithm for use in the 3-torus.

4.1 Arbitrary simplicial complex

In this section we will present an incremental algorithm for computing the Betti numbers of an abstract simplicial complex due to Delfinado and Edelsbrunner [4]. This algorithm isn't directly applicable to an abstract simplicial complex. We will need an additional algorithm to help us determine additional properties of the simplices, which we will introduce in a short while.

Suppose we have an abstract simplicial complex K_i. We will look what happens when we add a single k-simplex σ to it, $K_{i+1} = K_i \cup \{\sigma\}$. Using theorem 3.2 we have the exact sequence:

$$\cdots \to H_k(K_i) \xrightarrow{\varphi} H_k(K_{i+1}) \to H_k(K_{i+1}, K_i) \to H_{k-1}(K_i) \xrightarrow{\psi} H_{k-1}(K_{i+1}) \ldots$$

Since the dimension of σ is k, all $H_p(K_{i+1}, K_i)$ are trivial except for $p = k$. Here, there is a single non-bounding generating relative cycle , which is the one generated by σ. This is because we add one simplex and we know its boundary is in K_i, otherwise K_{i+1} wouldn't be a complex. So, the rank of the relative homology group is 1.

Using lemmas 3.3 and 3.4, we have the following equation for the Betti numbers:

$$1 = \tilde{\beta}_k(K_{i+1}, K) = \operatorname{rank}[\tilde{H}_k(K_{i+1})/\operatorname{im}\varphi] + \operatorname{rank}\ker\psi$$

φ is the inclusion map (see the proof of 3.2). In adding a k-simplex to K_i, no k-boundaries can arise, since $B_k(K) = \operatorname{im}\partial_{k+1}(K)$ which depends on the $k+1$-chains. Therefore, $\operatorname{im}\varphi = \tilde{H}_k(K_i)$ and $\operatorname{rank}[\tilde{H}_k(K_{i+1})/\operatorname{im}\varphi] = \tilde{\beta}_k(K_{i+1}) - \beta_k(K_i)$ (see proof of lemma 3.4), which is 1 if adding σ introduced a new k-cycle, or 0 if σ didn't. ψ is also an inclusion map, though following the observation above about k-boundaries, there is the possibility of a new $(k-1)$-boundary. We're looking at the kernel of ψ, and its rank is 1 iff a new $k-1$-boundary originated. Because the rank of $H_k(K_{i+1}, K_i)$ is always 1, one and only one of these cases must be true. In the first case, when σ introduces a k-cycle, we call σ a *positive simplex*. $\tilde{\beta}_k(K_{i+1})$ will then increase by 1. In the second case, σ destroys a $(k-1)$-cycle, and we call σ a *negative simplex*. Here, $\tilde{\beta}_{k-1}(K_i)$ will decrease by 1.

This construction yields the following algorithm. We assume here that we are given a sequence of simplicial complexes $K_1, \ldots, K_m$, such that for each i, $K_i = \{\sigma_1, \ldots, \sigma_i\}$.

Algorithm 4.1 Incremental algorithm for computing the Betti numbers of an abstract simplicial complex

---

```
∀(k > −1)(β̃_k = 0), β̃_{−1} = 1
for i := 1 to m
   k := dim(σ);
   if σ is positive
      then
            β̃_k := β̃_k + 1;
      else
            β̃_{k−1} := β̃_{k−1} − 1;
   fi
end
```

4.2 Subcomplexes of $\mathbb{S}^3$

Now, to actually use the algorithm in the preceding section we have to find a way to determine whether a simplex σ is positive or negative. Delfinado and Edelsbrunner published in 1995 a method to accordingly classify simplices in a subcomplex K of $\mathbb{S}^3$ [4]. The algorithm first marks all simplices in the 1-skeleton $K^{(1)}$ positive or negative, and then transverses all dual blocks of the full triangulation of $\mathbb{S}^3$ backwards to find 2- and 3-cycles.

First, we shall concern ourselves with the 1-skeleton to find 0- and 1-cycles. To keep track of the 1-skeleton when we add simplices, we introduce a data structure called the *union-find structure*. This data structure holds a partition of vertices into components, and has 3 operations:

Add(x) Add a vertex to the structure

Find(x) Find the component in which the vertex lies

Union(x, y) Join two components

We shall not concern ourselves with the inner workings of this data structure. Two vertices are in the same component of the structure iff they are connected by a succession of edges.

We transverse the simplices of the 1-skeleton of K in an order such that we never lose the structure of a simplicial complex when we add a simplex. When we're dealing with a 0-simplex, we automatically have a new component. This is because of the simplicial structure; there cannot have been an edge introduced containing a vertex before the vertex itself is introduced, and the vertex thus starts off isolated. We mark the simplex positive and Add the vertex to the structure. If, on the other hand, we're dealing with a 1-simplex, we check if the endpoints of the 1-simplex lie in different components (using FIND). If they do, we join the two components (UNION), and mark the simplex negative. If they are in the same component already, we have created a 1-cycle, and mark the simplex positive. See table 4.2 for an example.

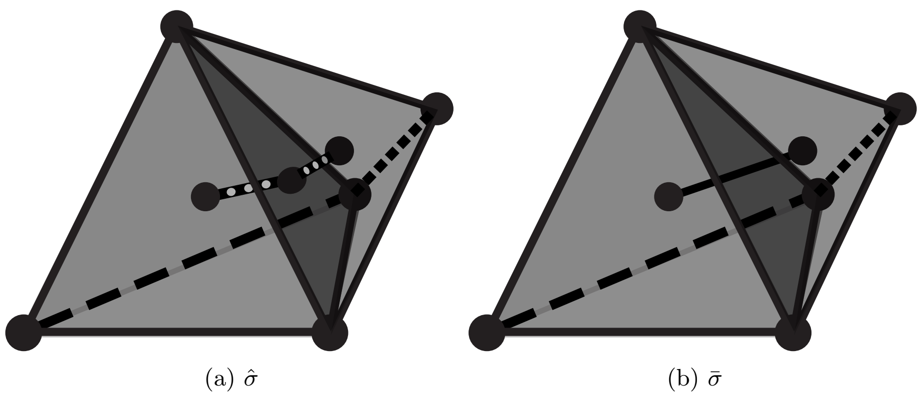
This part of the classification algorithm works for any simplicial complex regardless of the space in which it is embedded. Note though that correct classification of the 0- and 1-simplices only allows the correct computation of $\tilde{\beta}_0$, for it doesn't identify 1-boundaries.

Now, to find 2- and 3-cycles, we need $K = \{\sigma_1, \ldots, \sigma_m\}$ as a subcomplex of a triangulation $\{\sigma_1, \ldots, \sigma_n\}$ of $\mathbb{S}^3$. Let $K_i = \{\sigma_1, \ldots, \sigma_i\}$ and T_i be its complementary dual complex $T_i = \{\hat{\sigma} \mid \sigma \in K \setminus K_i\}$.

Applying the Alexander duality theorem (theorem 3.6) gives us $\tilde{H}_2(K_i) \cong \tilde{H}_0(T_i)$. Remember that the first part of the algorithm allowed us to correctly compute $\tilde{\beta}_0$ for any simplicial complex. Therefore, we can use this to compute $\tilde{H}_0(T_i)$.

Since K is a combinatorial 3-manifold, we know that the dual blocks of tetrahedra in K will be vertices. For a triangle, the dual block will consist of the closure of two connected edges between the dual vertices of the incident tetrahedra and the barycentre of the triangle (see figure 4.1). Since we're only concerned with the zeroth homology group, whose rank is solely determined by the number of connected components, we can identify this dual block with the edge directly between the barycentres of the tetrahedra (figure 4.1b).

Adding a triangle to K_i means removing its dual edge from T_i. Because our union-find structure only allows the addition of vertices, we transverse the simplices in backwards direction. We start with $T_n = \emptyset$ and keep track of the 1-skeleton of T_i in a union-find structure while processing the simplices in reverse. Thus, if for a triangle σ we have $K_{i+1} = K_i \cup \{\sigma\}$, then $T_i = T_{i+1} \cup \{\bar{\sigma}\}$ where $\bar{\sigma}$ is the edge identified with $\hat{\sigma}$. If doing this results in a union operation in the union-find structure for T_{i+1}, we know that $\tilde{\beta}_0(T_i) = \tilde{\beta}_0(T_{i+1}) - 1$, so $\tilde{\beta}_2(K_i) + 1 = \tilde{\beta}_2(K_{i+1})$, and the triangle gets marked positive. Otherwise, it is marked negative.



(a) $\hat{\sigma}$ (b) $\bar{\sigma}$

Figure 4.1: A triangle with its two incident tetrahedra

For tetrahedra, we know that $\tilde{\beta}_3(\mathbb{S}^3) = 1$. Since there are no 3-boundaries, the last 3-simplex must create this cycle. Thus, the last 3-simplex is positive, the others are negative.

4.3 Tetrahedralizing $\mathbb{S}^3$

The algorithm works on a simplicial complex $K_m = \{\sigma_1, \ldots, \sigma_m\}$ that already is a subcomplex of a triangulation $K_n = \{\sigma_1, \ldots, \sigma_n\}$ of $\mathbb{S}^3$. Suppose we just have the simplicial complex, how do we extend it to a triangulation of $\mathbb{S}^3$?

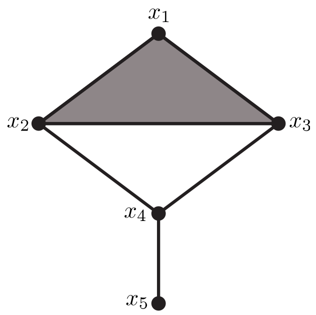
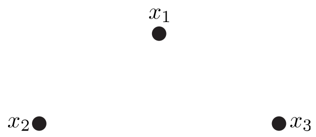
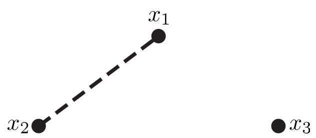
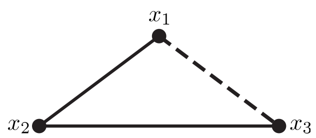
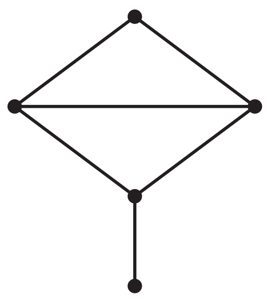
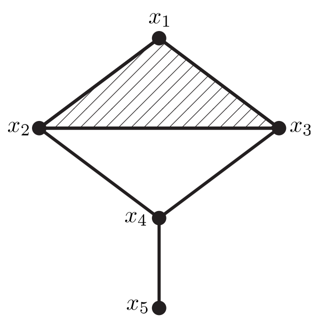
For this, we can use a combination of two algorithms. Starting, we split the complex into 'empty' regions that we wish to tetrahedralize. To emphasize that this is a 3-dimensional problem, we use the term *tetrahedralize* instead of triangulate. Then, for each region, we tetrahedralize the boundary such that a tetrahedralized solid seperates the outside from the inside, using an algorithm by Bern [1]. We do this because we cannot always tetrahedralize a set of points in space without adding points on the boundary, called *Steiner points*. These Steiner points wouldn't necessarily be compatible with our existing simplices, and adding them would destroy our simplicial structure. We then tetrahedralize the inside, using an algorithm by for example Chazelle and Palios ([3]). Finally, we extend the tetrahedralization to a full triangulation of $\mathbb{S}^3$ by connecting all vertices on the boundary to a new vertex at infinity and tetrahedralizing the whole. This tetrahedralization will be homeomorphic to $\mathbb{S}^3$.

4.4 Time complexity

The algorithm for computing the Betti numbers of a subcomplex $K_m = \{\sigma_1, \ldots, \sigma_m\}$ of a triangulation $K_n = \{\sigma_1, \ldots, \sigma_n\}$ presented in this chapter has a running time of $O(n\,\alpha(n))$ [4]. Here, $\alpha(n)$ denotes the inverse of the Ackermann function. This is due to the implementation of the union-find structure. This inverse is extremely slow-growing, and is constant for all practical purposes. The algorithm is therefore practically linear in the number of simplices. The time complexity for the tetrahedralization algorithm is $O(m^2)$ [1].

The use of this algorithm is limited to subcomplexes of the 3-sphere. While there are more generic algorithms which work for any abstract simplicial complex, see for example [10], there is a trade-off in speed. The algorithm presented in [10] has a worst case running time of $O(m^3)$. This is what motivates us to try to adapt the faster incremental algorithm for use in the 3-torus in chapter 5.

Table 4.1: Example

 The full complex. UF $= \emptyset$ $\tilde{\beta} = (-1, 0, 0)$	 We add three vertices. All vertices get marked positive and each adds their own component into the data structure. UF $= \{\{[x_1]\}, \{[x_2]\}, \{[x_3]\}\}$ $\tilde{\beta} = (2, 0, 0)$
 Adding the edge $[x_1, x_2]$. Since both endpoints are in different components, the edge joins them. The edge gets marked negative. UF $= \{\{[x_1], [x_2]\}, \{[x_3]\}\}$ $\tilde{\beta} = (1, 0, 0)$	 Adding the edge $[x_1, x_3]$. The endpoints are now in the same component, so the edge creates a 1-cycle and thus gets marked positive. UF $= \{\{[x_1], [x_2], [x_3]\}\}$ $\tilde{\beta} = (0, 1, 0)$
 The 1-skeleton of the complex. We have one component, with two 1-cycles. UF $= \{\{[x_1], [x_2], [x_3], [x_4], [x_5]\}\}$ $\tilde{\beta} = (0, 2, 0)$	 Adding the triangle $[x_1, x_2, x_3]$. We will see shortly how triangles are handled in this algorithm, but for now we just stick to the observation that the triangle introduces a 1-boundary and thus gets marked negative. UF $= \{\{[x_1], [x_2], [x_3], [x_4], [x_5]\}\}$ $\tilde{\beta} = (0, 1, 0)$

Chapter 5

The 3-torus

5.1 Introduction

The algorithm for computing homology of subcomplexes of $\mathbb{S}^3$ works for complexes which are realized in ordinary 3-dimensional space. $\mathbb{R}^3$ and $\mathbb{S}^3$ are closely related: $\mathbb{S}^3$ is just the 1-point compactification of $\mathbb{R}^3$, or, the 3-sphere is topologically equivalent to 3-dimensional space with a point added at infinity. Stereographic projection from the north pole of $\mathbb{S}^3$ to the equitorial plane readily confirms this. However, when we are dealing with periodic input data, a space such as the 3-torus might be more suitable for representing a simplicial complex. The 3-torus $\mathbb{T}^3$ is topologically equivalent to three copies of the circle. This is the same as the unit cube in $\mathbb{R}^3$ with opposite facets identified. The latter definition is probably the easiest to visualize.

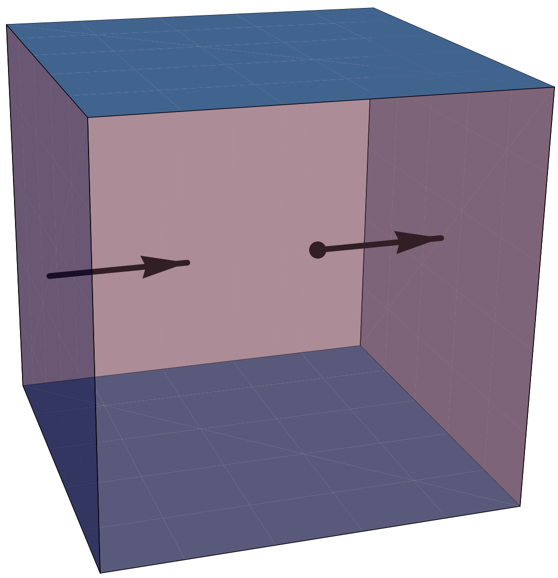


Figure 5.1: A representation of $\mathbb{T}^3$: a cube with its opposite facets identified. When we travel in one direction and pass through the boundary, we emerge at the opposite side.

In this chapter, we will adapt this algorithm for use in the 3-torus. The resulting algorithm will not always yield a correct output, however, we prove it to be approximately correct.

Section 5.2 will establish that the classification method is approximately correct in $\mathbb{T}^3$. We still need to extend subcomplexes to triangulations of the 3-torus, however. In section 5.3 we will develop an algorithm to accomplish this with the 2-torus, which we will extend for use with the 3-torus in section 5.4. Finally, we will briefly discuss another recently published tetrahedralization algorithm for the 3-torus in section 5.5.

5.2 Adapting the algorithm

In section 4.2 we established a method for classifying simplices in subcomplexes of the 3-sphere. There, we established a generic method for classifying the 0- and 1-simplices, and relied on Alexander duality for classifying the triangles. Unfortunately, Alexander duality does not hold for subcomplexes of the 3-torus, because the homology groups of dimension $k < 3$ are not trivial. Therefore, the classification method doesn't necessarily yield a correct output for subcomplexes of the 3-torus.

For the 3-torus, we have the following Betti numbers:

$$\begin{aligned}\tilde{\beta}_0 &= 0\\ \tilde{\beta}_1 &= 3\\ \tilde{\beta}_2 &= 3\\ \tilde{\beta}_3 &= 1\end{aligned}$$

However, Alexander duality does hold to some degree. In this section we will establish a result which allows us to use the same classification method to yield an approximately correct output.

We are only interested in classifying the triangles. We therefore more closely examine the Alexander duality for $\tilde{H}_2(S) \cong \tilde{H}_0(T)$, for T the complementary dual complex of a subcomplex $S \subset K$. All steps in the proof hold for generic combinatorial manifolds, except equation 3.3. Here we relied on the trivial homology groups of the d-sphere.

We examine the exact sequence we used in proving Alexander duality in more detail for $k = 2$.

$$\cdots \to \tilde{H}_3(\mathrm{Sd}^2 K) \to \tilde{H}_3(\mathrm{Sd}^2 K, S'') \to \tilde{H}_2(S'') \to \tilde{H}_2(\mathrm{Sd}^2 K) \to \tilde{H}_2(\mathrm{Sd}^2 K, S'') \to \dots$$

Here, we take K to be a triangulation of the 3-torus, and S'' to be the expanded subcomplex of K as in the proof of theorem 3.6. Since K triangulates the 3-torus, so does $\mathrm{Sd}^2 K$ and we can substitute its absolute homology groups.

$$\cdots \to \mathbb{Z}_2 \to \tilde{H}_3(\mathrm{Sd}^2 K, S'') \to \tilde{H}_2(S'') \to (\mathbb{Z}_2)^3 \to \tilde{H}_2(\mathrm{Sd}^2 K, S'') \to \dots$$

Using lemmas 3.3 and 3.4, we know that:

$$\tilde{H}_2(S'') \cong \tilde{H}_3(\mathrm{Sd}^2 K, S'')/\operatorname{im}(\mathbb{Z}_2 \to \tilde{H}_3(\mathrm{Sd}^2 K, S'')) \oplus \ker((\mathbb{Z}_2)^3 \to \tilde{H}_2(\mathrm{Sd}^2 K, S''))$$

We know that for a homomorphism $\varphi : G \to G'$ the rank of the image or kernel can never exceed the rank of G, so we have:

$$\tilde{\beta}_2(S'') = \tilde{\beta}_3(\mathrm{Sd}^2 K, S'') - u + v$$

where $u \in \{0,1\}$ and $v \in \{0,1,2,3\}$. The value of u depends on the image of an inclusion map (see proof of theorem 3.2). In fact $u = 0$ iff the only 3-cycle in $\mathrm{Sd}^2 K$ is completely in S''. This can only be if all tetrahedra are in S, and $S = K$. Since in this case we know the Betti numbers of S, namely those of the 3-torus, we assume $S \neq K$ and therefore $u = 1$.

Since $k = d - 1$, with $d = 3$ the dimension of the 3-torus, we get $\tilde{H}_d(\mathrm{Sd}^2 K, S'') \cong \tilde{H}_0(T) \oplus Z_2$. So, we have $\tilde{\beta}_2(S) = \tilde{\beta}_0(T) + 1 - u + v = \tilde{\beta}_0(T) + v$.

We combine the incremental algorithm from section 4.1 and the classification method from section 4.2. We are interested in the Betti numbers of a subcomplex $K_m = \{\sigma_1, \ldots, \sigma_m\}$ of $K_n = \{\sigma_1, \ldots, \sigma_n\}$ with complementary dual complex T_m. If we let c_k denote the number of k-simplices in K_m and p_k and n_k denote the number of positive and negative k-simplices in K_m, respectively, the incremental algorithm gives us:

$$\begin{aligned}
\tilde{\beta}_0 &= -1 + p_0 - n_1 = -1 + c_0 - n_1 \\
\tilde{\beta}_1 &= p_1 - n_2 \\
\tilde{\beta}_2 &= p_2 - n_3 \\
\tilde{\beta}_3 &= p_3
\end{aligned}$$

The equation for $\tilde{\beta}_0$ follows because all 0-simplices are positive.

We assume $m < n$, so $p_3 = 0$ and $n_3 = c_3$. For any k, we have $n_k = c_k - p_k$. Applying this, we get:

$$\begin{aligned}
\tilde{\beta}_0 &= -1 + c_0 - c_1 + p_1 \\
\tilde{\beta}_1 &= p_1 - c_2 + p_2 \\
\tilde{\beta}_2 &= p_2 - c_3 \\
\tilde{\beta}_3 &= 0
\end{aligned} \tag{5.1}$$

The numbers c_k are trivially computable from K_m, and we use the classification method for computing p_1 and p_2. For subcomplexes of $\mathbb{S}^3$, we could've also computed $\tilde{\beta}_2(K_m) = \tilde{\beta}_0(T_m)$, instead of marking all the simplices directly, and then using equation 5.1 to yield a result for p_2.

Applied to a triangulation K_n of $\mathbb{T}^3$, this gives us an approximate result for the Betti numbers. We know that $\tilde{\beta}_2(K_m) = \tilde{\beta}_0(T_m) + v,\ 0 \leq v \leq 3$. Solving equation 5.1 for p_2, we get $p_2 = \tilde{\beta}_0(T_m) + v + c_3$, and so $\tilde{\beta}_1(K_m) = p_1 - c_2 + \tilde{\beta}_0(T_m) + v + c_3$. We know we can compute $\tilde{\beta}_0(T_m)$ and p_1, and all terms but for v are the same as in the case for subcomplexes of $\mathbb{S}^3$.

We have established the following result:

Theorem 5.1 *If for a proper subcomplex $K_m = \{\sigma_1, \ldots, \sigma_m\}$ of a triangulation $K_n = \{\sigma_1, \ldots, \sigma_n\}$ of the 3-torus we let $\tilde{\beta}^{\mathrm{c}}_i(K_m)$ denote the i-th computed Betti number obtained by running the algorithm with classification method as detailed in sections 4.1 and 4.2, we have:*

$$\begin{aligned}
\tilde{\beta}_0(K_m) &= \tilde{\beta}^{\mathrm{c}}_0(K_m) \\
\tilde{\beta}_1(K_m) &= \tilde{\beta}^{\mathrm{c}}_1(K_m) + v \\
\tilde{\beta}_2(K_m) &= \tilde{\beta}^{\mathrm{c}}_2(K_m) + v \\
\tilde{\beta}_3(K_m) &= \tilde{\beta}^{\mathrm{c}}_3(K_m)
\end{aligned}$$

for some $v \in \{0,1,2,3\}$.

5.3 Triangulating the torus

To see what a triangulation of the 3-torus looks like, we will first take a look at its lower dimensional variant: the 2-torus $\mathbb{T}^2$. The 2-torus is lower dimensional and has a triangulation with fewer vertices. On top of this, the space is embeddable in $\mathbb{R}^3$, and therefore easy to visualize.

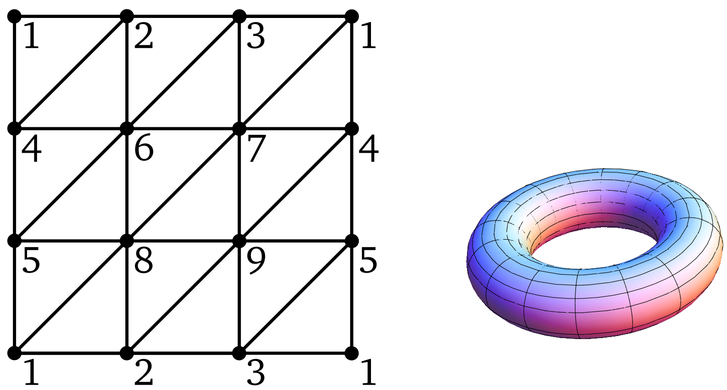


Figure 5.2: Basic triangulation of the 2-torus

We see that this triangulation of the 2-torus has 9 vertices. We will use this triangulation as a basis for constructing our algorithm which extends subcomplexes of the 2-torus to triangulations of the 2-torus. This is not a minimal triangulation (see for example [6]), but will make describing the algorithm easier. In this section we describe the algorithm for the 2-torus, which we extend in the next section to work for the 3-torus.

There are numerous methods for triangulating (or extending subcomplexes to) simplicial complexes embedded in $\mathbb{R}_3$ [1, 3, 7]. Our algorithm constructs an outline of the unit square, in a way such that if it is completed to a full triangulation of the square, identification of the appropriate boundaries will give a triangulation of the 2-torus.

The following theorem provides conditions for a triangulation of the unit square such that identification of appropriate boundary points will result in a triangulation of the 2-torus.

Theorem 5.2 *Suppose we are given an abstract triangulation A of the unit square $[0,1]^2$ and a map $g : \operatorname{Vert} A \to \operatorname{Vert} A$ on the vertices of A such that vertices in the boundary opposite eachother get mapped to the same vertex by g. If let f be the map induced by g on the simplices of A, $[x_0, \dots, x_n] \mapsto [g(x_0), \dots, g(x_n)]$, then the image of f will be an abstract triangulation of the 2-torus if the following conditions hold:*

1. *For all pairs of simplices $\sigma \neq \tau$ in A such that $f(\sigma) = f(\tau)$, σ and τ are both mapped opposite eachother into the boundary of the unit square by the triangulation.*

2. *For all simplices $\sigma \in A$ that are mapped into the boundary of the unit square, there is a simplex $\tau \in A$ which gets mapped opposite σ.*

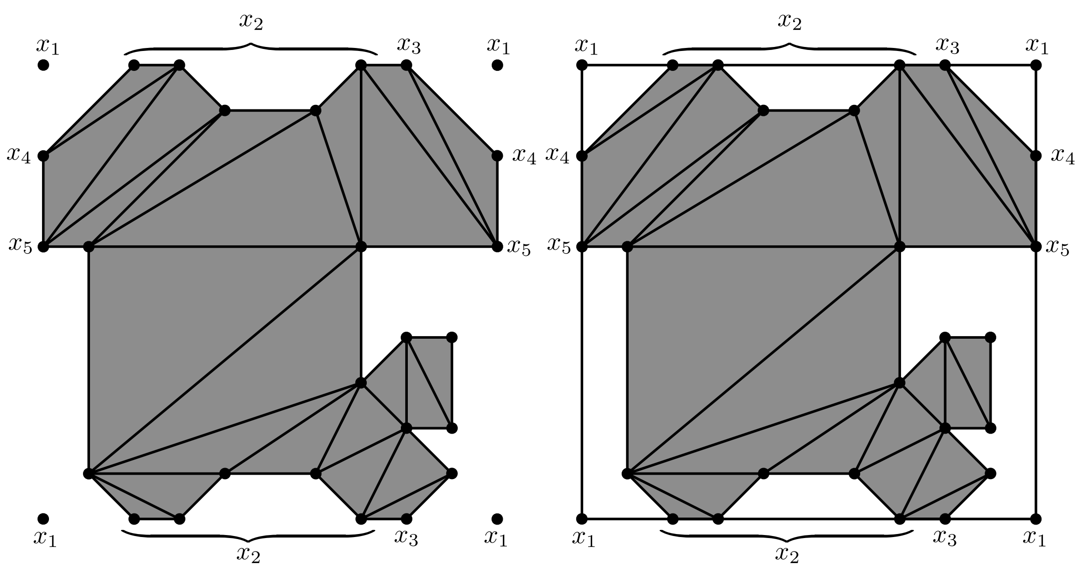
Proof: We denote the image of f by A'. Choose a realization K of A. Let $t : K \to [0,1]^2$ be a triangulation of the unit square. Identifying opposite boundary points on the unit square gives us an equivalence relation which we denote $\smile$. Let $p : [0,1]^2 \to [0,1]^2/\smile$ be the corresponding projection map. We define an equivalence relation $\frown$ on K compatible with

$\smile$, such that $x \frown y \iff t(x) \smile t(y)$. If we let $p' : K \to K/\frown$ be the projection map induced by $\frown$, then $K/\frown$ will be homeomorphic to the 2-torus. The composition of maps $p \circ t \circ p'^{-1}$ is a composition of maps which are necessarily continuous and have a continuous inverse. Bijectivity follows from the compatibility of the equivalence relations. The composition is therefore a homeomorphism.

$$\begin{array}{ccccc} A & \xrightarrow{r} & K & \xrightarrow{t} & [0,1]^2 \\ \big\downarrow f & & \big\downarrow p' & & \big\downarrow p \\ A' & & K/\frown & & [0,1]^2/\smile \end{array}$$

To show that $K/\frown$ is in fact the underlying space of a realization of A', we take K and glue its simplices together according to f. Let $r : A \to \operatorname{Vert} K$ be the map that realizes abstract simplices in A to convex hulls in K, the define $r' : A' \to \operatorname{Vert} K/\frown$ be the induced map $p' \circ r \circ f^{-1}$. We need to show that this is a true function, since the preimage f^{-1} of a simplex in A' may have multiple simplices in A. If this is the case, however, we know by the first condition that they both map opposite eachother into the boundary, hence their image under p' is a single simplex. To show that this realization is a valid simplicial complex in $[0,1]^2/\smile$, take two intersecting simplices σ, τ in the boundary of $K/\frown$. By the second condition, we know that there must be simplices $\sigma', \tau' \in K$ which are located in the same facet of the boundary. Since K is a simplicial complex, their intersection $\sigma' \cap \tau'$ must be a shared face of both. This intersection is mapped to $\sigma \cap \tau$. Thus, the theorem follows. $\square$

We start off with a simplicial complex K which is embedded in $\mathbb{T}^2$, which is defined by the unit square $[0,1]^2$ with its opposite edges identified. The idea is that we are going to expand K to a triangulation which is compatible with the triangulation in figure 5.2.



(a) Step 1: add boundary vertices (b) Step 2: connect boundary vertices

Figure 5.3: An example of how the extension algorithm works

Outlining the boundary First, we check if there are vertices of K which are on the boundaries of $[0,1]^2$. If not, we add them. We want x_1, x_2, x_3, x_4, x_5 to be nonempty disjoint sets of boundary vertices, relatively located as in figure 5.2. We demand that the second coordinates for x_1, x_2 and x_3 are $0 \sim 1$ and that the first coordinates for x_1, x_4 and x_5 are $0 \sim 1$ as well. x_1 is a fixed singleton, but the other vertices have one free coordinate. We require that the vertices are in the same order as in figure 5.2, with regards to the standard order on $[0, 1]$. We also order the vertices within each set of vertices.

Computationally, this step is not hard. We simply transverse all vertices and check if they are on the boundary. If they are, we put them in the appropriate set. We can just put all top boundary vertices (except for x_1, which is fixed) in x_2, and at the end move the rightmost vertex to x_3. We do the same for the left boundary. If any of the sets is empty, we create a vertex to put in it. For an example, see figure 5.3a.

Connecting the vertices We now connect adjacent vertices on the boundaries. This gives us an outline of $[0, 1]^2$, such as in figure 5.3b. Then, we connect the vertices on the boundary to vertices in the interior. We order the vertices in the interior and pick four (e.g. top-left, top-right, bottom-left, bottom-right) such that we can connect all vertices in the left boundary to the two left-vertices and the same for the other boundaries.

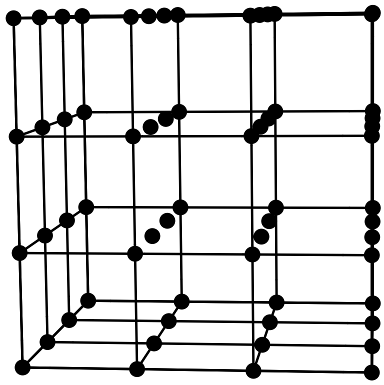
Filling in the gaps What remains now is to fully triangulate the complex. To do this, we can for example find the regions that are not yet triangulated (i.e., a closed edge path of length greater than 3 that doesn't have edges between its vertices other than those of the path itself). We can then find the Delaunay triangulation (cf. [7]) of these regions. Then we can fill all closed edge paths of length 3 (boundaries of triangles) with 2-simplices of which the boundary is the appropriate edge path.

5.4 Extending to the 3-torus

The algorithm for the 2-torus in the last section can be extended to the 3-torus. Now, however, the boundaries are no longer intervals but squares instead. We assume we have a subcomplex K of the 3-torus embedded in the unit cube. On each 3 unique boundaries (we identify opposite facets of the unit cube), we want nonempty 9 sets of vertices, set as in our triangulation of the 2-torus in figure 5.2. Note that some of these vertices are shared with other facets. We essentially subdivide the each boundary into a 4x4 lattice and use this to determine which vertices are shared.

Outlining the boundary We connect the vertices on the boundaries as in the triangulating the 2-torus. We then have a basic outline of the unit cube. Then, we simply tetrahedralize the inside of K in the same way as we would do for a subcomplex of $\mathbb{S}^3$ as described in section 4.3. First, we use a thickening algorithm to tetrahedralize the boundary. Then, we tetrahedralize the inside.

Connecting the vertices Now, we make sure that all vertices on the boundary are connected to a vertex in the interior of the unit cube. These need to be in order. We assume that the complex has enough vertices to allow edges from each vertex on the facet of the unit cube to the exterior boundary of the complex, without opposite vertices being joined by a single point.



(a) A 4x4x4 lattice for triangulating the 3-torus

Filling in the gaps We use the same construction as in the 2-torus, only now we need eight vertices (sides: top/bottom, front/back, left/right). What remains is tetrahedralizing the remaining space.

Correctness To prove this construction is correct, we note that theorem 5.2 can be directly extended to triangulations of the 3-torus, because dimension is nowhere mentioned (just the fact that the boundary consists of opposite faces). Thus, we need to show the conditions of the theorem hold for this construction. First off, since we constructed an outline of the cube and then tetrahedralized all space, we can establish that we indeed created a valid triangulation of $[0,1]^3$. Next, we need to make sure that there is no identification of simplices other than those on the boundary (the first condition). Under the assumption that we can actually use this method, the connections to the interior are constructed in such a way that between two opposite points on the boundary there is always a minimum of three edges. This is because the boundary vertices are connected to an interior point associated with that vertex, and points on the opposite boundary are necessarily connected to another vertex. The second condition follows from mirroring everything on one boundary to the opposite boundary.

5.5 Other work

In a recent tech report by Caroli and Teillaud ([2]), the authors established an algorithm to extend subcomplexes of the 3-torus to full triangulations using Delaunay triangulations. Their method is more focused on actual implementation; they present a detailed time and complexity analysis and conditions under which the triangulation is valid. The algorithm presented in section 5.4 relies on certain assumptions that would probably exclude some subcomplexes of $\mathbb{T}^3$. The paper defines the flat 3-torus as the quotient of $\mathbb{R}^3$ with the group of rectangular grid points for some set grid length. Operations such as taking the convex hull need help of an offset that locates vertices in $\mathbb{R}^3$ to be defined. We, instead, define the 3-torus as the fixed quotient of $[0,1]^3$ with points on its boundary appropriately identified. This allows us to work in $\mathbb{R}^3$ without the need for offsets.

Chapter 6

Conclusions and future work

The main challenge posed in writing this thesis was adapting the incremental algorithm by Delfinado and Edelsbrunner for use with subcomplexes of the 3-torus. For this, we developed an algorithm to extend subcomplexes to complete triangulations of the 3-torus. The algorithm then works for subcomplexes of the 3-torus, however, it does not always yield a correct output for $\tilde{\beta}_1$ and $\tilde{\beta}_2$. We have shown that the output is approximately correct however, and that for computed Betti numbers $\tilde{\beta}_1^{\mathrm{c}}$ and $\tilde{\beta}_2^{\mathrm{c}}$ we have $\tilde{\beta}_1 = \tilde{\beta}_1^{\mathrm{c}} + v$ and $\tilde{\beta}_2 = \tilde{\beta}_2^{\mathrm{c}} + v$ for some $v \in \{0, 1, 2, 3\}$.

Future work could focus on exactly determining v. Section 5.2 established that $v = \operatorname{rank}\ker(H_2(\operatorname{Sd}^2 K) \to H_2(\operatorname{Sd}^2 K, S))$ for the subcomplex $S \subset K$. This is precisely the number of generating 2-cycles in K that are completely in S.

Also, it might be possible to construct a faster algorithm specifically for the 3-torus based on the algorithms which work for any abstract simplicial complex, as referenced in section 4.4. Relative homology provides us with the following exact sequence:

$$\cdots \to H_k(I) \xrightarrow{\eta_k} H_k(K) \to H_k(K, I) \to H_{k-1}(I) \xrightarrow{\eta_{k-1}} H_{k-1}(K) \to \dots$$

Under some mild hypotheses, the relative homology group $H_k(K, I)$ is isomorphic to the absolute homology group of the quotient space $H_k(K/I)$. Using the exact sequence, the rank of the relative homology group might be computed if one can determine the images and kernels of the inclusions η_k. Using the incremental algorithm, Betti numbers for I and K can be quickly computed. It is harder to compute the ranks of the image and kernel of η_k, because one cannot tell which cycles get destroyed using the incremental algorithm. This might be solved using the generic algorithms.

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