A TOPOLOGICAL TOOLBOX FOR NEUROSCIENCE

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This handout is designed to support an introductory lecture on algebraic topology specifically geared towards applications in neuroscience. Concerning current and potential applications of algebraic topology to neuroscience, these notes are neither comprehensive nor complete. My aim here is to introduce just about enough mathematical background to make my collaborative work with the Blue Brain Project [1] understandable to a wider audience. The lecture is particularly aimed at scientists without comprehensive mathematical background, mathematicians who are not topologists, and mathematics or science students at all levels with interest in the subject. Hence the only prerequisite is working knowledge in linear algebra and an open mind. As algebraic topology goes, these notes are a speck of dust on the tip of an iceberg. An extensive basic course is available in [6] or [4], and a good reference for topological techniques applicable to science can be found in [3].

I will start with introducing *simplicial complexes*. These are geometric objects which are in a sense a manageable approximation to the "universe" of topological spaces. Another advantage of simplicial complexes is how closely related they are to *graphs*. Indeed graphs are our access point into neuroscience, bearing in mind that the brain, any brain for that matter, is made out of neurons connected to each other in an immensely complicated network that can be modelled as a graph. Section 2 will therefore be dedicated to a short introduction to the mathematical concept of graphs, and more specifically *directed graphs*. In Section 3 we prepare the background for relating graphs to simplicial complexes and more specifically directed graphs to *ordered simplicial complexes* - a slight modification of the original concept of a simplicial complex, specifically designed to deal with directed phenomena, such as the directed network of a neural system. In Section 4 we introduce the main objects that will allow us an analysis of neural systems - the *flag complex* and the *directed flag complex*. These are simplicial complexes and ordered simplicial complexes that arise from graphs and directed graphs, respectively. In Section 5 we discuss some basic topology on a very intuitive level and some properties of topological spaces that are invariant under deformation. With the same intuitive approach we also explain the concept of *"holes"* or *"cavities"* in topological spaces, which in the appropriate sense characterise the space they exist in. Finally in Section 6 we introduce one of the main mathematical tools used in algebraic topology - *homology* - an algebraic object one can associate with topological spaces that in the appropriate sense detects the existence of cavities in the space, or more generally, informs on the way in which the building blocks of the space fit together.

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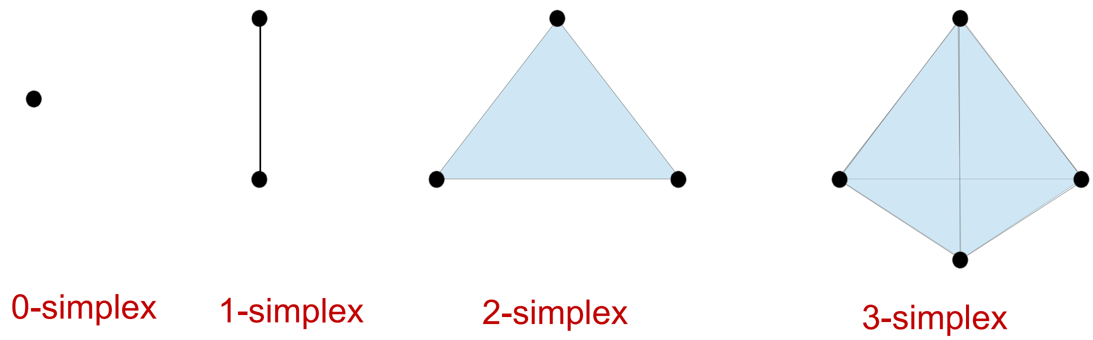
1. Simplicial complexes

Topology as a concept includes an enormous variety of objects. We shall however satisfy ourselves with a rather restricted collection of topological objects, that nonetheless is more than enough for most practical and even most theoretical purposes. These objects are called *simplicial complexes*.

Imagine a child building a castle out of building blocks. The building blocks can be very simple, yet an imaginative kid can build quite impressive constructions by putting the building blocks together in various ways. This is the idea behind simplicial complexes. The building blocks are called *simplices*, or in singular *simplex*, and they are indeed very simple. A 0-dimensional simplex is just a single point. A 1-dimensional simplex is a line segment. A 2-dimensional simplex is a triangle. A 3-dimensional simplex is a tetrahedron.



Beyond dimension 3 one can still define simplices, although drawing them could be a bit tricky. Higher dimensional simplices live comfortably in Euclidean space of the appropriate dimension, totally oblivious to the fact that we can't draw them or imagine what they look like. Formally the *standard n-simplex* is the collection of all points in $(x_0, x_1, \ldots x_n) \in \mathbb{R}^{n+1}$, where $x_i \geq 0$ for all i, and such that they satisfy the equation

$$x_0 + x_1 + \cdots x_n = 1.$$

Another way to define an n-simplex is as the convex hull of $n+1$ points in $\mathbb{R}^n$ that are not all on the same $n-1$ dimensional hyperplane (affinely independent points). Explicitly if $v_0, v_1, \ldots v_n$ is such a collection of points, then the n-simplex they span is the set of all points in $\mathbb{R}^n$ of the form

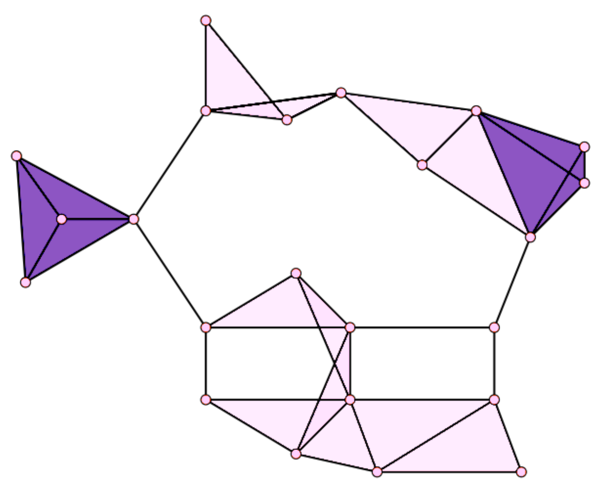
$$x = \lambda_0 v_0 + \lambda_1 v_1 + \cdots \lambda_n v_n, \qquad \text{where} \quad \sum_{i=0}^{n} \lambda_i = 1.$$

This definition is a bit more flexible than that of the standard n-simplex, but the resulting shapes are in the appropriate sense equivalent. Indeed if one takes for v_i the point corresponding to the $(i+1)$-st standard basis vector in $\mathbb{R}^{n+1}$, having a 1 in the i-th coordinate and 0 everywhere else, then the convex hull of these points is precisely the standard n-simplex. One nice advantage this formalism allows is that we can denote a simplex by the sequence of vertices that determine it. The standard notation is $\sigma = [v_0, v_1, \ldots, v_n]$ which means: σ is the n-simplex determined by the set of vertices $\{v_0, v_1, \ldots v_n\}$. Notice that in spite of having indexed the vertices of a simplex by integers from 0 to n, the ordering of the vertices plays no role in the definition. Later, when we talk about ordered simplicial complexes this will no more be the case.

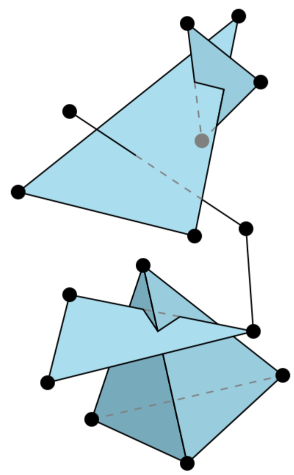
A very pleasant aspect of working with simplices is that they have *boundary faces* that are also simplices of dimension one below their own. For instance a 1-simplex as as its boundary two 0-simplices. The boundary of a 2-simplex is formed out of three 1-simplices. In general the boundary of an n-simplex is made out of $n+1$ simplices of dimension $n-1$. With the notation $\sigma = [v_0, v_1, \dots v_n]$ it is easy to see what is meant by the boundary simplices of an n-simplex. Those are the $(n-1)$-simplices determined by removing one point from the simplex σ. For instance the simplex $[v_0, v_1, \dots, v_{n-1}]$ is a face of σ as is $[v_0, v_2, v_3, \dots, v_n]$, or in general $[v_0, \dots, \hat{v}_i, \dots v_n]$, where $\hat{v}_i$ means that v_i was removed from the collection.

Obviously one can remove more than one vertex from an n-simplex, thus obtaining lower dimensional faces.

Now that we have our building blocks, we shall use them to build topological castles. There is only one rule in this game: *Any two simplices of any dimension can be attached along a face of the same dimension*. The picture below shows a simplicial complex made out of 0, 1, 2 and 3 simplices.



In general a finite simplicial complex is said to be n-dimensional if the highest dimension of a simplex in it is n. Hence the complex in the picture above is 3-dimensional. The following example is not a simplicial complex although it is made of simplices, because simplices are not always attached along faces.



We will sometimes refer to simplicial complexes as *geometric simplicial complexes*. This will become necessary when we define an abstract analog that will be called *abstract simplicial complexes*.

2. Graphs

One common way in which simplicial complexes arise, particularly in applications, is from graphs. Informally, a graph is just a collection of points (vertices) and line segments connecting them (edges). Normally we don't allow more than one edge connecting any two vertices. We will also work only with finite graphs, i.e., graphs that only have finitely many vertices and edges.

Mathematically a *graph* is a triple $\mathcal{G} = (V, E, \beta)$, where V and E are called the set of vertices and edges of the graph, respectively, and β is a function from E to the set of (unordered and distinct) pairs of elements in V. So if $e \in E$ is an edge and $\beta(e) = \{u, v\}$, it means that the vertices that e connects are u and v. The requirement that u and v are distinct means that we don't allow self-loops in our graphs, i.e., edges both of whose incident vertices are the same one.

If $\mathcal{G}$ is a graph, then an *n-clique* in $\mathcal{G}$ is a subgraph containing n vertices, and where every vertex in it is connected to any other vertex. An n-cliques is also referred to sometime as a *full graph on n vertices*. The notion of a clique is fundamental in graph theory, and in particular allows thinking about graphs in topological terms. One very important feature of cliques is that they define collections of vertices of the ambient graph with the following property:

If the set of vertices $\{v_1, v_2, \ldots v_n\}$ form an n-clique in $\mathcal{G}$, then every (nonempty) subset of k vertices $\{v_{i_1}, \ldots v_{i_k}\}$ spans a k-clique.

This means simply that if Δ is a fuIl graph on n vertices $v_1, v_2, \ldots, v_n$, then for any subset of vertices $v_{i_1}, \ldots, v_{i_k}$ the subgraph of Δ whose vertices are exactly those and is maximal with this property is also a full graph. It is exactly this property of cliques which allows us to associate a geometric object with every graph.

So far we did not discuss any directionality of the edges in a graph, which for the purpose of neuroscience is very important. The generalisation is rather simple. A *directed graph* or a *digraph* is again a triple $\mathcal{G} = (V, E, \beta)$ where V and E are finite sets called the vertices and edges of $\mathcal{G}$ respectively, and $\beta\colon E \to V \times V$ is a function that is required to be injective (i.e., 1–1: no two edges are allowed to "hit" the same pair of vertices). Thus if $e \in E$ is an edge in $\mathcal{G}$, and $\beta(e) = (v, u)$, where $v, u \in V$ are vertices in $\mathcal{G}$, then we think of e as a *directed edge* from v to u. Notice that the injectivity requirement implies that no two vertices are connected by more than one edge in the same direction, but it is possible that two vertices are connected reciprocally. Also, we generally require that the function β "avoids" the diagonal in $V \times V$, i.e., there is no edge $e \in E$, such that $\beta(e) = (v, v)$ for some $v \in V$. Geometrically this means that there are no self-loops in the graph.

The analog of cliques in a digraph is a *directed clique*. That is a collection of n vertices that are connected all to all, just like the case or an ordinary clique in an undirected graph, but where in every sub-clique (including the clique itself) there is a unique vertex that is a *source*, i.e. all directed edges in the sub-clique are pointing out of it, and a unique vertex that is a *sink*, i.e. all directed edges in the sub-clique are pointing into it. In other words, a set of n all-to-all connected vertices forming a subgraph in a graph $\mathcal{G}$ is a directed n-clique if its vertices can be ordered linearly $v_1, v_2, \ldots, v_n$, such that for every $i < j$ there is a directed edge in the subgraph from v_i to v_j.

3. Abstract and ordered simplicial complexes

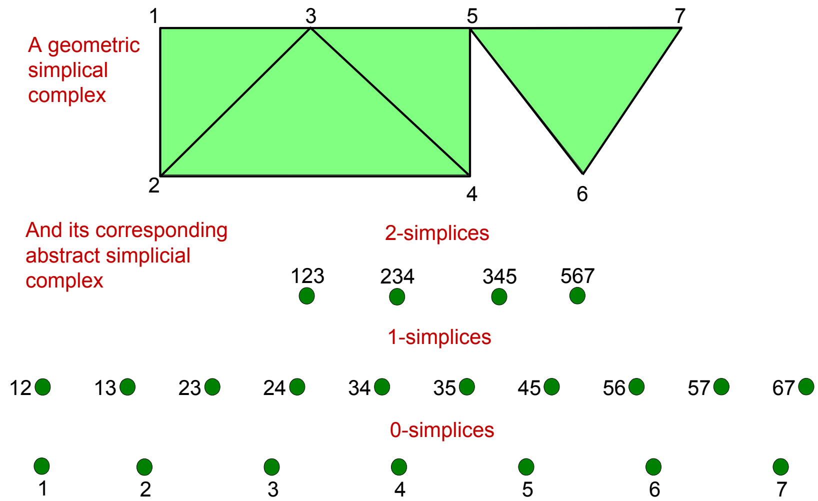
We now prepare for relating graphs to simplicial complexes, and more importantly to the definition of a geometric object that takes the directionality in a digraph into account. To do so we now describe simplicial complexes as abstract combinatorial objects. This new concept is equivalent to that of a geometric simplicial complex, as we will soon make clear. Once we have done that the generalisation that could take direction or order into account is rather straight forward.

Definition 3.1. *An abstract simplicial complex is a collection X of finite sets called* simplices *with the property that if $\sigma \in X$ is a simplex and $\tau \subseteq \sigma$ is a subset, then τ is also a simplex in X.*

Relating this back to geometric simplicial complexes defined above, notice that in a geometric simplicial complex every simplex is uniquely determined by its vertices, and every face of a simplex is itself a simplex that is in turn determined by some subset of vertices. In other words, every geometric simplicial complex automatically gives rise to an abstract simplicial complex.

If $\sigma \in X$ is a simplex and $\tau \subseteq \sigma$ is a subset, then τ is said to be a *face of σ*. If σ is a set of cardinality $n + 1$, then we say that σ is an *n-simplex*. Thus a 0-simplex is a singleton, a set of elements is a 1-simplex, etc. Every n-simplex has $n + 1$ faces that are themselves $(n - 1)$-simplices. For every $0 \leq k \leq n$, an n-simplex has $\binom{n+1}{k+1}$ faces that are k-simplices, better referred to as k-faces.

And now back to geometry. Given an abstract simplicial complex X, the *geometric realisation* of X is the geometric simplicial complex obtained by associating with every n-simplex $\sigma \in X$ a standard n-simplex, and if $\sigma, \tau \in X$ are any two simplices with a nonempty intersection, then we identify the corresponding faces in the two simplices. It is not hard to see that abstract and geometric simplicial complexes are in 1–1 correspondence, if one is willing to consider all geometric simplices as equivalent.

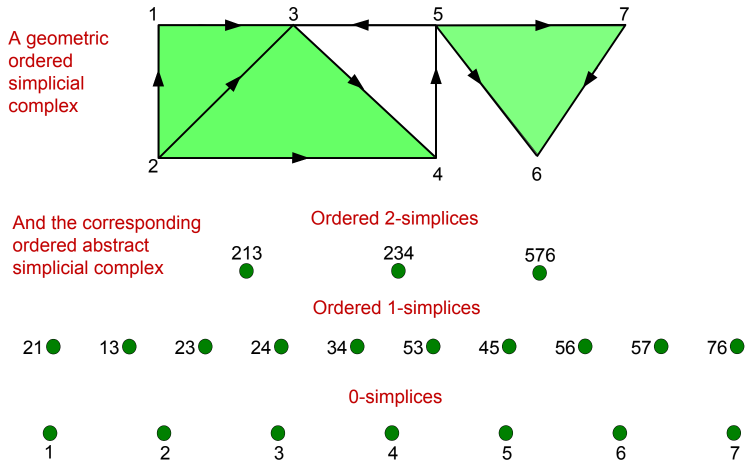


We now describe an ordered version of abstract simplicial complexes. It is a slight but very important variation.

Definition 3.2. *An* ordered abstract simplicial complex *is a collection X of finite* ordered *sets called* ordered simplices*, or simply* simplices*, with the property that if $\sigma \in X$ is an ordered simplex and $\tau \subseteq \sigma$ is a subset ordered by the induced ordering, then τ is also an ordered simplex in X.*

The major difference between ordinary and ordered simplicial complexes is that in an ordinary simplicial complex a simplex is determined uniquely by its set of vertices. In an ordered simplicial complex, by contrast, this is not true. A set of $n+1$ vertices could support as many as $(n+1)!$ distinct n-simplices, corresponding to all possible orderings of the set of vertices. For example a set of two vertices x and y, and two edges e and f with $\beta(e) = (x, y)$ and $\beta(f) = (y, x)$ is an ordered simplicial complex, but it is not an ordinary abstract simplicial complex.

The *geometric realisation* of an ordered simplicial complex X is carried out in a similar fashion to that of an ordinary abstract simplicial complex. One associates an n-simplex with every ordered n-simplex in X and glues together simplices along common intersections. The picture below is an example of an abstract ordered simplicial complex (bottom) and its geometric realisation (top). In the picture of the geometric complex the arrows are include only for illustration of the ordering. Notice that the vertices 3, 4 and 5 do not form a 2-simplex because they are not ordered linearly. Notice also that the ordering in this example does not correspond to the natural order in the natural numbers.



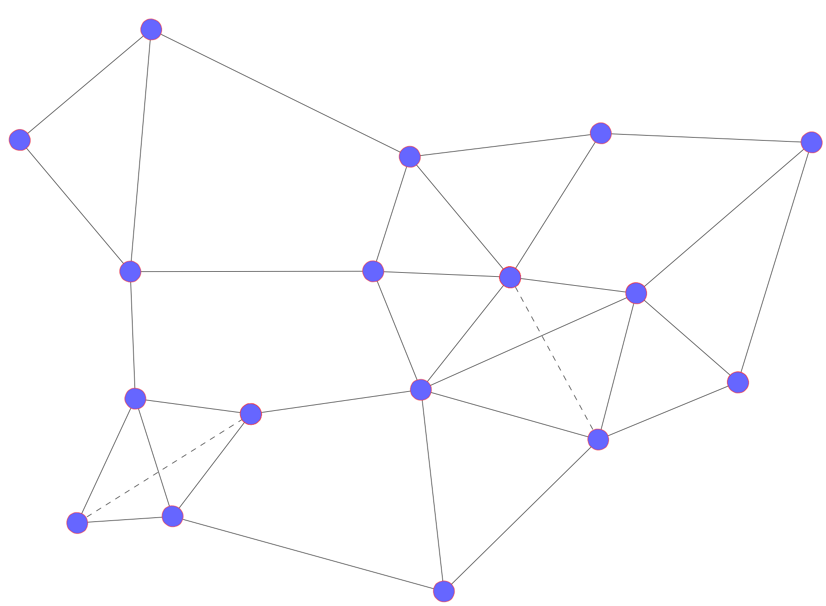
4. Flag complexes

Next we consider a way in which graphs give rise to abstract simplicial complexes and then how directed graphs give rise to ordered simplicial complexes.

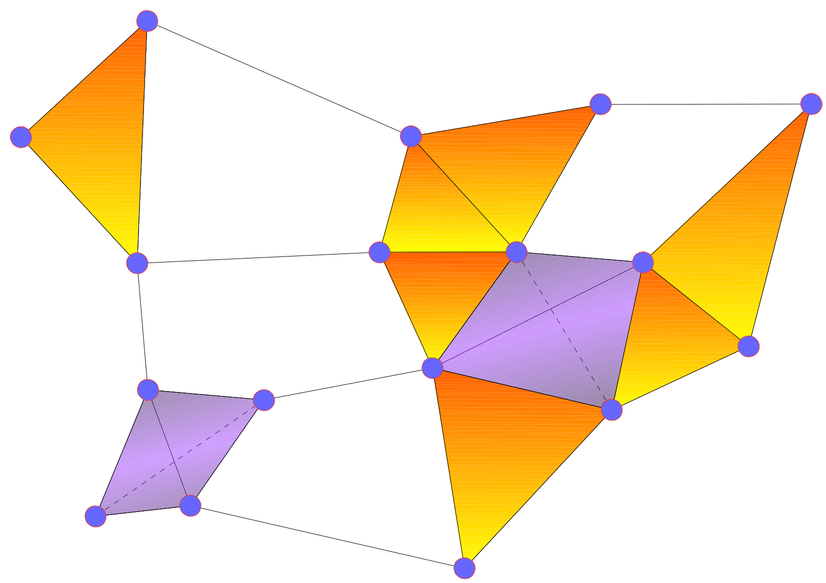
Definition 4.1. *Let $\mathcal{G} = (V, E, \beta)$ be a graph. The* flag complex *associated to $\mathcal{G}$ is the abstract simplicial complex whose n-simplices are the $(n+1)$-cliques in $\mathcal{G}$.*

Notice that by definition any subset of vertices in a clique spans a sub-clique. Hence the condition which defines an abstract simplicial complex is satisfied.

For example this graph:



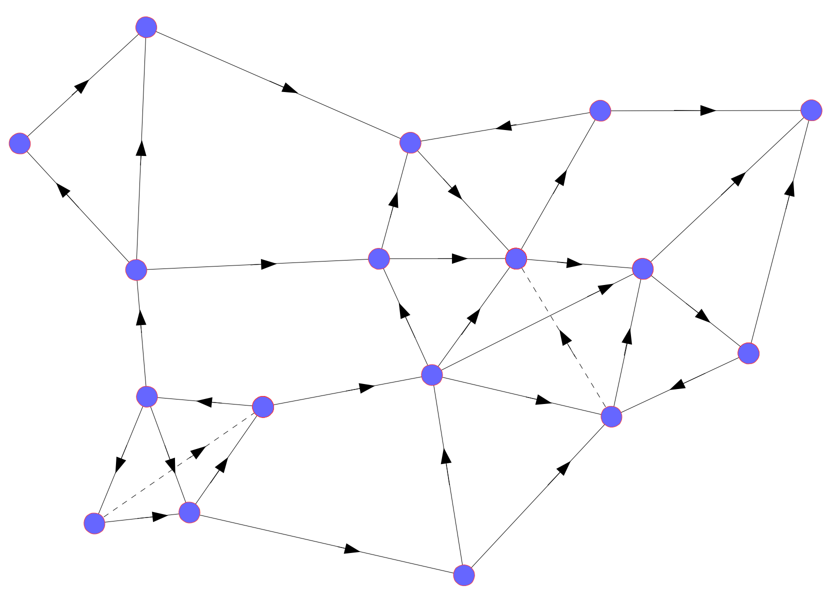
gives rise to an abstract simplicial complex whose geometric realisation is:



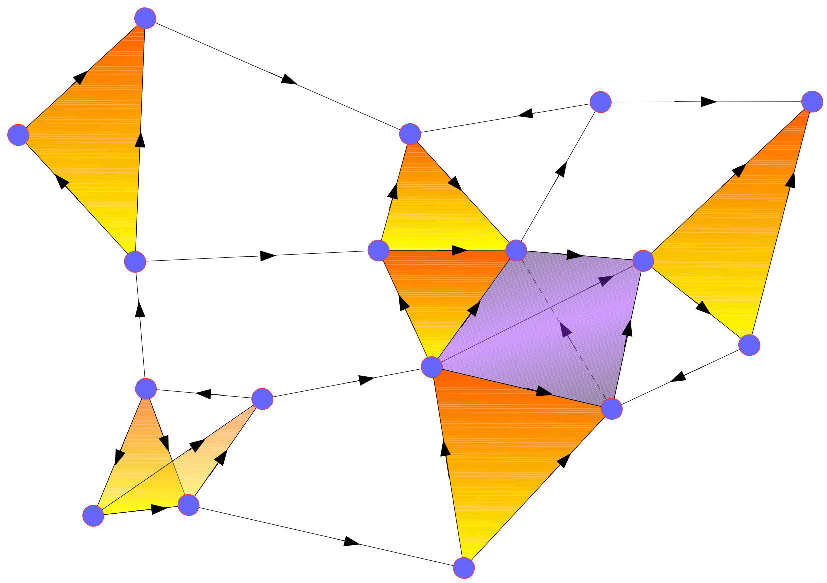
Next we consider the directed analog. If $\mathcal{G}$ is a digraph, then within it one finds directed cliques, as explained above. These can be used to form a directed simplicial complex. The definition is almost identical.

Definition 4.2. *Let $\mathcal{G} = (V, E, \beta)$ be a digraph. The* directed flag complex *associated to $\mathcal{G}$ is the abstract ordered simplicial complex whose n-simplices are the directed $(n+1)$-cliques in $\mathcal{G}$.*

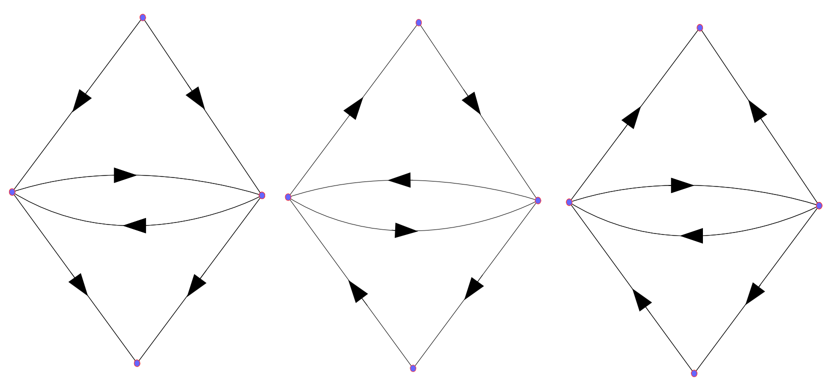
For example the digraph,



whose underlying undirected graph is precisely the same as in the former example, gives rise to the following directed flag complex:



Notice that the directed flag complex of the digraph in this example is a subcomplex of the flag complex in the previous undirected example. This is because with the prescribed directionality some of the cliques are not directed and therefore do not define simplices in the directed flag complex. However this is not always the case. In fact the directed flag complex associated to a digraph could be very different from the ordinary flag complex associated to the underlying undirected graph. Consider for instance the following three digraphs:



These three graphs have identical underlying undirected graphs, with the two reciprocal horizontal edges identified to a single edge between the left and right vertices (remember that we do not allow more than one edge between any two vertices in an undirected graph). The flag complexes of that undirected graph is simply two 2-simplices attached on an edge. On the other hand, if one looks carefully at the three digraphs, it is not too hard to see that the left graph has four ordered 2-simplices that enclose a 3D cavity, hence the caption "2-sphere". In the middle there are two ordered 2-simplices, in the top front and the bottom back. The other two triangles are not ordered, and so in the directed flag complexes these two triangles will not be filled. Since the 2-simplices are solid triangles, one can imagine them "squashed" onto their horizontal edge without tearing them, thus squashing the entire shape into a circle, whence the caption for this picture. Finally in the right graph all but the bottom back triangle are ordered 3-cliques. The missing one is like a "hole in a sphere". Hence one can imagine it as a punctured air balloon that can be shrank completely into a speck of rubber - a point - motivating the caption. The conclusion from this example is that at the presence of reciprocal connections one obtains a much larger variety of complexes that when direction is not considered.

This last remark has to be considered with caution. From a topological point of view almost any "reasonable" topological space can be "modelled" in the appropriate sense by a simplicial complex. Hence we are not claiming here that ordered simplicial complexes and directed flag complexes give a richer family of topological objects. All we claim is that directed flag complexes are better in capturing the structure of a digraph in a topological space, and hence are more suitable for the purpose of analysing them.

5. Topology, deformation and "holes"

Topology is the part of mathematics that studies abstract objects generally referred to as *topological spaces*. We will not go into the precise definition of what this means, but rather satisfy ourselves with the understanding that topology is a vast and far reaching generalisation of the much older and more intuitive concept of geometry. The word 'topology' first appeared in the mathematical literature in work of the German mathematician Listing in 1847, but topological ideas date back to Euler in his solution of the Königsberg Bridges problem. Topology as an abstract concept however had to wait till the early 1900 when it was introduced by Riesz and Hausdorff. Topological spaces in the full glory of their general definition form such a vast collection of objects, that mathematicians found it necessary to restrict attention to particularly nicely behaved topological spaces. Among those there were the classical geometric objects such as polyhedra and manifolds, which by themselves offer enough richness of mathematical structure to satisfy the mathematical community for the next few millennia, and possibly beyond. The geometric realisation of simplicial complexes and ordered simplicial complexes can be thought of as examples of polyhedra.

Even restricting to particularly nice spaces such as manifolds and polyhedra, studying these objects is a rather daunting task, and it turns out that many topological properties do not depend on the actual object but rather on its behaviour under a certain type of deformation called "homotopy". Algebraic topology is a part of mathematics that studies topological spaces by using a variety of algebraic tools, one of which we shall explore later. Most of those algebraic tools are sensitive to spaces and maps between them only "up to homotopy". We will not go into the formalities of what homotopy means. Instead we will only mention a few examples.

As a first example one could consider the euclidian space $\mathbb{R}^n$ for any $n \geq 0$. For any point $x \in \mathbb{R}^n$ one has a straight line segment connecting x to the origin. One can imagine sliding the point x along this line towards the origin. In fact one can imagine doing the same for all points in $\mathbb{R}^n$ at the same time. This process deforms all of $\mathbb{R}^n$ onto a single point - the origin. It is therefore one can refer to $\mathbb{R}^n$ as a *contractible* space. Similarly a line segment, a solid disk and more generally a solid ball of any dimension are contractible. On the other hand, circles, spheres of any dimension, tori and many other objects are not contractible. That is to say, they cannot be deformed into a single point without tearing them. *Very intuitively*, this is because these objects contain "holes". A circle is a 1-dimensional hole, a 2-sphere encloses a 2-dimensional hole, and so on for higher dimensional spheres. A torus can be thought of as having two 1-dimensional holes and one 2-dimensional hole.

The relation of two topological spaces being homotopy equivalent basically means that one space can be deformed into the other without tearing it, or more formally the deformation has to take the form of a continuous function. There is a corresponding concept for functions between topological space, but we will not dive any deeper. The interested reader can find instruction to basic topology in [5] or [2], and to basic algebraic topology in [4]. A good introduction to algebraic topology from the simplicial perspective is in [6].

6. HOMOLOGY

We now introduce one of the major vices in an algebraic topologist tool box - homology. Intuitively, homology is an algebraic object one can associate to any topological space, but with particular ease to simplicial complexes (ordered or not) that detects, in the appropriate sense, how many "holes" the space contains in each dimension. Homology is a homotopy invariant. Therefore it will not distinguish among a circle, an annulus and a solid torus. In the eyes of homology they are one and the same - a topological space with a single 1-dimensional hole.

Now, let's get a bit more formal. When one talks about homology, one usually needs to specify "coefficients". Our coefficients for the purpose of these notes will be the field of 2-elements $\mathbb{F}_2$. It is indeed the simplest nontrivial algebraic object one can think of, and turns out to be very useful in algebraic topology in general and in applied topology in particular. Like with any field one can consider vector spaces over the field $\mathbb{F}_2$. (The elements of the field $\mathbb{F}_2$ may be denoted 0 and 1, with the when one adds or multiplies elements, one takes the result to be the remainder after dividing by 2. So, for instance $1 + 1 = 0$ in $\mathbb{F}_2$.) We note that homology can take as coefficients any abelian group, commutative ring or a field.

Let X be a simplicial complex and let X_n denote the set of its n-simplices. For $\sigma \in X_n$ and $0 \leq i \leq n$, let σ^i denote the i-th face of σ, as defined above. Define the *chain complex* $C_*(X, \mathbb{F}_2)$ to be the sequence $\{C_n = C_n(X, \mathbb{F}_2)\}_{n\geq 0}$, such that C_n is the $\mathbb{F}_2$-vector space whose basis elements are the n-simplices $\sigma \in X_n$, for each $n \geq 0$. In other words, the elements of C_n are formal linear combinations of n-simplices in X with coefficients in $\mathbb{F}_2$. For each $n \geq 1$, there is a linear transformation called a *differential*

$$\partial_n \colon C_n \to C_{n-1}$$

specified by $\partial_n(\sigma) = \sigma^0 + \sigma^1 + \cdots + \sigma^n$ for every n-simplex $\sigma \in C_n$. Having defined ∂_n on the basis, one extends the definition linearly to the entire vector space C_n.

The n-th mod 2 *homology group* of X is defined by

$$H_n(X, \mathbb{F}_2) = \mathrm{Ker}(\partial_n)/\mathrm{Im}(\partial_{n+1}).$$

For all $n \geq 1$, there is an inclusion of vector subspaces $\mathrm{Im}(\partial_{n+1}) \subseteq \mathrm{Ker}(\partial_n) \subseteq C_n$, and so the definition of homology makes sense. To complete the picture we may define $H_0(X, \mathbb{F}_2)$ to be $C_0/\mathrm{Im}(\partial_1)$.

Since every vector space is determined up to isomorphism by its dimension, it makes sense to associate numbers to the homology groups of a complex. The *mod-2 n-th Betti* *number* $\beta_n(X)$ of a simplicial complex X is the $\mathbb{F}_2$-vector space dimension of its n-th mod 2 homology group.

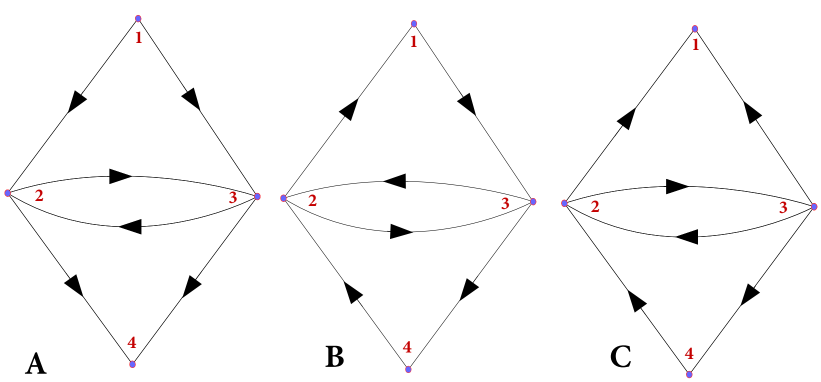
The n-the Betti number $\beta_n(X)$ gives an indication of "n-dimensional holes" in the geometric realisation of X. For instance $\beta_0(X)$ is the number of connected components of X, $\beta_1(X)$ is the number of 1-dimensional holes, and so on. Some topological phenomena that are visible to homology with coefficients in $\mathbb{F}_2$ will not be visible to homology with other coefficients, and vice versa. Furthermore, considering only the mod-2 Betti numbers of a simplicial complex only scratches the surface of what homology can reveal about the complex. There is in fact much more structure in homology that at this stage we will not touch at all, but which are crucial in theoretical algebraic topology and will almost certainly become useful in applications.

Computing the Betti numbers of a simplicial complex is conceptually very easy. Let $|X_n|$ denote the number of n-simplices in the simplicial complex X. If one encodes the differential ∂_n as a $\big(|X_{n-1}| \times |X_n|\big)$-matrix D_n with entries in $\mathbb{F}_2$, then one can easily compute its *nullity*, $\mathrm{null}(D_n)$, and its *rank*, $\mathrm{rk}(D_n)$, which are the $\mathbb{F}_2$-dimensions of the null-space and the column space of D_n, respectively. The *Betti numbers* of X are then a sequence of natural numbers defined by

$$\beta_0(X) = \dim_{\mathbb{F}_2}(C_0) - \mathrm{rk}(D_1), \quad \text{and} \quad \beta_n(X) = \mathrm{null}(D_n) - \mathrm{rk}(D_{n+1}).$$

Since $\mathrm{Im}(\partial_n) \subseteq \mathrm{Ker}(\partial_{n-1})$ for all $n \geq 1$, the Betti numbers are always non-negative.

We now demonstrate a computation on three examples of directed flag complexes of digraphs we already considered.



This time we labelled the vertices in order to have an easy way of naming the simplices.

	A	**B**	**C**
0-simplices	$1, 2, 3, 4$	$1, 2, 3, 4$	$1, 2, 3, 4$
1-simplices	[12], [13], [23], [32], [24], [34]	[13], [21], [23], [32], [34], [42]	[21], [31], [23], [32], [34], [42]
2-simplices	[123], [132], [234], [324]	[213], [342]	[231], [321], [342]

We will compute the differential matrices one case at a time, using the ordering of the simplices as indicated in the table above.

$$\mathbf{A}: \qquad D_1 = \begin{bmatrix} 1&1&0&0&0&0 \\ 1&0&1&1&1&0 \\ 0&1&1&1&0&1 \\ 0&0&0&0&1&1 \end{bmatrix} \qquad D_2 = \begin{bmatrix} 1&1&0&0 \\ 1&1&0&0 \\ 1&0&1&0 \\ 0&1&0&1 \\ 0&0&1&1 \\ 0&0&1&1 \end{bmatrix}$$

A quick computation by row reduction shows that $\mathrm{rk}(D_1) = 3$ and having 6 columns $\mathrm{null}(D_1) = 3$. Also $\mathrm{rk}(D_2) = 3$ and so $\mathrm{null}(D_2) = 1$, since it has 4 columns. We are ready to compute Betti numbers.

$$\beta_0(A) = \dim_{\mathbb{F}_2}(C_0) - \mathrm{rk}(D_1) = 1,\ \beta_1(A) = \mathrm{null}(D_1) - \mathrm{rk}(D_2) = 0,\ \beta_2(A) = \mathrm{null}(D_2) = 1.$$

$$\mathbf{B}: \qquad D_1 = \begin{bmatrix} 1&1&0&0&0&0 \\ 0&1&1&1&0&1 \\ 1&0&1&1&1&0 \\ 0&0&0&0&1&1 \end{bmatrix} \qquad D_2 = \begin{bmatrix} 1&0 \\ 1&0 \\ 1&0 \\ 0&1 \\ 0&1 \\ 0&1 \end{bmatrix}$$

Once more, by direct calculation using row reduction one shows that $\mathrm{rk}(D_1) = 3$, $\mathrm{null}(D_1) = 3$, and $\mathrm{rk}(D_2) = 2$ so $\mathrm{null}(D_2) = 0$. Hence

$$\beta_0(B) = \dim_{\mathbb{F}_2}(C_0) - \mathrm{rk}(D_1) = 1,\ \beta_1(B) = \mathrm{null}(D_1) - \mathrm{rk}(D_2) = 1,\ \beta_2(B) = \mathrm{null}(D_2) = 0.$$

$$\mathbf{C}: \qquad D_1 = \begin{bmatrix} 1&1&0&0&0&0 \\ 1&0&1&1&0&1 \\ 0&1&1&1&1&0 \\ 0&0&0&0&1&1 \end{bmatrix} \qquad D_2 = \begin{bmatrix} 1&1&0 \\ 1&1&0 \\ 1&0&0 \\ 0&1&1 \\ 0&0&1 \\ 0&0&1 \end{bmatrix}$$

And one last time $\mathrm{rk}(D_1) = 3$, $\mathrm{null}(D_1) = 3$, and $\mathrm{rk}(D_2) = 3$ so $\mathrm{null}(D_2) = 0$. Thus

$$\beta_0(C) = \dim_{\mathbb{F}_2}(C_0) - \mathrm{rk}(D_1) = 1,\ \beta_1(C) = \mathrm{null}(D_1) - \mathrm{rk}(D_2) = 0,\ \beta_2(C) = \mathrm{null}(D_2) = 0.$$

We now clearly see how Betti numbers distinguish the flag complexes of the three digraphs, and by implication the digraphs themselves.

A much weaker, but very important invariant of topological spaces is the Euler characteristic. If X is a simplicial complex and $|X_n|$ denotes the cardinality of the set of n-simplices in X, then the Euler characteristic of X is defined to be

$$\chi(X) = \sum_{n\geq 0} (-1)^n |X_n|.$$

There is a well known close relationship between Euler characterstic and Betti numbers [6, Theorem 22.2], which is expressed as follows. If $\{\beta_n(X)\}_{n\geq 0}$ is the sequence of Betti numbers for X, then

$$\chi(X) = \sum_{n\geq 0} (-1)^n \beta_n(X).$$

While computing Betti number is theoretically very easy, for large simplicial complexes it becomes rather challenging. For example, in the paper [1] one has to deal with a directed flag complex that contains up to 80 million 2-simplices and about 65 million 3-simplices. Clearly this cannot be done by hand and requires the aid of big computers and sophisticated programming. Advanced storage techniques allow a relatively economical storage of large sparse matrices, but the manipulation required in order to compute the rank and nullity is nonetheless extremely costly in memory and computation time.

References

[1] Reimann MW, Nolte M, Scolamiero M, Turner K, Perin R, Chindemi G, Dłotko P, Levi R, Hess K and Markram H (2017) *Cliques of Neurons Bound into Cavities Provide a Missing Link between Structure and Function*. Front. Comput. Neurosci. 11:48. doi: 10.3389/fncom.2017.00048
[2] M. A Armstrong; Basic Topology; Springer, 1983.
[3] R. Ghrist; Elementary Applied Topology; https://www.math.upenn.edu/ ghrist/notes.html. Also available through Amazon.co.uk
[4] A. Hatcher; Algebraic Topology; Cambridge University Press, 2002.
[5] K. Jänich; Topology; Springer, 1984.
[6] E. Munkres; Elements of algebraic topology; Addison-Wesley, 1984.