On Persistent Homotopy, Knotted Complexes and the Alexander Module

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Abstract

In this paper techniques from persistent homology are generalized to homotopy groups and to algebraic invariants from knot theory. We define the persistent Alexander module, which can be used to detect knotting in a complex and determine when the knotting changes when viewed from different scales. Algorithms that use the persistent Alexander module are also presented and applied to examples including protein structures. While the basic definition of persistent homotopy is known, this is the first work to use it successfully for computations.

1 Introduction

The motivation behind topological persistence [8] is to studying features of shapes at a variety of scales. Often, small scale topological features can be caused by noise in a data set or are not of interest when studying larger scale features. In spirit, many invariants from geometry and topology can be generalized to incorporate persistence. To date, most work in topological persistence has used homological information. This is primarily due to the fact that efficient algorithms exist for working with homology, and a wealth of information can be obtained from the persistent homology groups.

In this paper, persistence is extended to homotopy groups and Alexander modules. Homotopy groups contain far more information than homology groups; however, they are far more difficult to perform calculations with. In particular, general homotopy groups have unsolvable word and isomorphism problems [25] making them impossible to work with algorithmically. For submanifolds of $\mathbb{R}^3$, these problems are solvable, but there are no practical algorithms to do calculations with these groups. This has stood in the way of the use of homotopy in topological persistence. Fortunately, the Alexander module [17], which has its origins in knot theory, can be used to calculate invariants of these homotopy groups. This makes it a natural candidate to generalize using persistence.

Persistent homology has been studied extensively and used in a variety of applications, see [7] for a survey of results. It has been used to study protein structures [1, 21], brain imaging [4], image processing [20], sensor networks [5] and statistics [2]. It will be shown that persistent homotopy carries all of the information that persistent homology does. This additional topological information could be applied to all of these application domains and provide new analysis tools.

A major focus of our work will be applying persistence to detect if a complex is knotted and if that knotting can be "undone" in a larger complex. Homotopy groups can be extremely useful for this. Dehn's lemma [26] implies that a circle is knotted in $\mathbb{R}^3$ if and only if its complement has trivial homotopy group. So, in classical knot theory, homotopy can always detect knotting. Furthermore, homotopy groups are a complete invariant for knots; that is, distinct knots will never have the same homotopy group. This makes homotopy an extremely powerful topological invariant. The Alexander module and Alexander polynomial can be calculated from these homotopy groups in a nice algorithmic manner and can determine if a complex is knotted; however, they do not aways detect knotting [13].

There have been many generalizations of the Alexander module and polynomial beyond knots in S^3, including the study of knotted graphs [30], virtual knots [16], twisted Alexander polynomials [23] and knotting in protein backbones [32]. From an applications perspective, knotting in proteins is of particular interest as it has potential applications to protein folding and stability of protein structures [35]. When applied to proteins, our new invariants can detect types of knotting that existing methods cannot. Furthermore, the persistence information gives information about the topological stability of the knotted structure is.

In Section 2, a brief overview of knotting and persistent homology is presented followed by a generalization to knot theory in section 3. A discussion of homotopy and persistent homotopy follows in section 4. Section 5 develops the persistent Alexander modules and polynomials, and Section 6 gives algorithms to calculate them. In Section 7, applications of this theory to the study of protein structures will be discussed.

2 Background

Before we can define persistent homotopy and Alexander module we review some background information on knotting and persistent homology.

2.1 Knotting

A knot can be thought of an embedded circle in $\mathbb{R}^3$. To study a knot it is necessary to consider its complement as knotting is not inherit in a shape but how that shape is embedded in a larger space. In order to have a compact complement, we will add a point at infinity to $\mathbb{R}^3$ to get the 3-sphere S^3. A knot $K \subset S^3$ is said to be *unknotted* if the complement of regular neighborhood of K is a solid torus. Further, any knot in S^3 can be homotoped to be unknotted. Fox addresses what happens for general submanifolds of the sphere. This motivates the definition of a submanifold being unknotted.

Theorem 2.1 (**Fox's re-embedding theorem** [10])**.** *If $f : M \to S^3$ is an embedding for a compact, connected manifold M then there exists another embedding $g : M \to S^3$ such that the closure of $S^3 - g(M)$ is the union of handlebodies. Furthermore, f and g are homotopic.*

Definition 2.2. *A connected submanifold $X \subset S^3$ is* unknotted *if $S^3 - X$ of unions of handlebodies.*

If X is not connected then it may or may not be possible to "pull the components of X apart" so that they are contained in disjoint balls. Components that can be "pulled apart" are referred to as separable.

Definition 2.3. *The components, $X_1, \dots, X_k$, of $X \subset S^3$ are* separable *if there exists disjoint embedded* 2*-spheres $S_1, \dots, S_k \subset S^3$ bounding disjoint balls, each containing one of the X_i.*

If X is not connected then it can be homotoped so that each component is unknotted and its components are separable. Unknotted, separable embeddings are unique up to isotopies of the sphere.

2.2 Persistent homology

Starting with any triangulation of S^3, we can consider a *filtration* $\{X_i\}$ or sequence of subcomplexes of the triangulation $X_0 \subset X_1 \subset \ldots \subset X_n \subset S^3$. Note that we could use a cell complex or any other decomposition of the space instead of a triangulation, and our index set does not have to be the integers. Often these sequences are built from alpha shapes [9]; they could also come from a filtration that has been simplified using the techniques like those in [8]. In a very general sense persistent homology counts the number of holes in the some X_i that remain, or persist, in X_{i+p}. For a full treatment of persistent homology, its applications and algorithms for computing it see [7, 8, 37].

Given a simplicial complex, or some other cell structure, K, with orientations defined on each of its cells, define the j-chains $C_j(K)$ to be the space of all integral linear combinations of the j-dimensional cells of K. The boundary of any j-dimensional cell can be thought of as a linear combination of $(j-1)$ cells. This notion can be used to define a linear map, $\partial_{j+1} : C_{j+1}(K) \to C_j(K)$, called the *boundary operator*. The *j-cycles*, $Z_j(K)$, is the kernel of ∂_j and the *j-boundary*, $B_j(K)$, is the image of ∂_{j+1}. It can be shown that $\partial_j \circ \partial_{j+1} = 0$, so $B_j(K) \subset Z_j(K)$. The j-th *homology group*, $H_j(K)$, is the quotient $Z_j(K)/B_j(K)$. For any p, the *p-persistent homology group* is defined as

$$H_j^p(X_i) = Z_j(X_i)/B_j(X_{i+p}) \cap Z_j(X_i)$$

Since $B_j(X_i) \subset B_j(X_{i+p})$, we are quotienting by a larger space so the persistent homology groups get smaller as p increases.

Since knot detection requires looking at complements of spaces, we often examine the complementary sequence

$$S^3 - X_0 \supset S^3 - X_1 \supset \ldots \supset S^3 - X_n$$

We will define the persistent homology of this complementary sequence $H_i^p(S^3 - X_{i+p})$ to the cycles in $S^3 - X_{i+p}$ modulo the boundaries in $S^3 - X_i$.

3 Persistent knotting

Persistent homology measures non-trivial loops in X_{i+p} that were also present in X_i. Knot persistence is similar; in some sense it measures knotting in X_{i+p} that was also present in X_i.

Definition 3.1. *Knotting of X_i is* p-transient *if it homotoped in X_{i+p} to be unknotted. If it is not p-transient it will be called* p-persistent.

Recall that X_i can always be homotoped in S^3 to be unknotted, so if $X_n = S^3$ then any knotting of X_i is always p-transient. Notice that is X_i is unknotted then it is also transiently unknotted. The generalization of separability of disconnected X_i to persistence is similar.

Definition 3.2. *If X_i is not connected then its components are* p-transiently linked *if it can be homotoped in X_{i+p} so that its components are separable. Otherwise, it is* p-persistently linked.

Separable components of X_i are also transiently unlinked. We will also be examining graphs and subcomplexes in S^3. We can consider their knotting behavior by considering their closed regular neighborhoods, which are compact manifolds.

See Figure 1 for six examples. The first is a trefoil knot in a larger solid torus. Since all of the crossings occur inside the solid torus, the knot can be homotoped to remove this crossing while staying inside the larger torus; so it a transient knot. In the second example, a connected sum of a trefoil knot and a figure eight knot inside a solid torus that is tied into a trefoil knot. This is a persistent knot as it cannot be unknotted in the solid torus. All of the crossing on the right hand side (the figure eight knot) can be removed but the other three crossing cannot be removed. So the knot cannot be unknotted in the solid torus. In the third and fourth examples, there is a trefoil knot is transient in a handlebody of genus two and a handlebody of genus three, respectively. In the later case, the handlebody is knotted in S^3, but it is still large enough for the trefoil to unknot itself. The fifth example is a Whitehead double of a figure eight knot. This knot is transient in the larger figure eight knot as the two parts of its "clasp" can pass through each other and the knot can be shrunk to a point. The final example is a Whitehead link embedded in a neighborhood of a Hopf link; like the previous example the clasp can be undone and the two components can be undone implying that this link is transiently linked. One way to show that knotting and linking is transient is to show that the space is contained in an larger unknotted one.

Proposition 3.3. *If X_i is a handlebody (neighborhood of a graph) and there exists a connected and unknotted manifold Y such that $X_i \subset Y \subset X_{i+p}$ then X_i is p-transiently knotted. And if X_i is not connected then it is also p-transiently linked.*

Proof. With out loss of generality, we can assume that X_i is a closed neighborhood of a graph $G \subset X_{i+p}$. Furthermore, we can assume that each component of G is a wedge of circles without changes its neighborhood, so it has a single vertex. We can perform an isotopy so that Y is a neighborhood of a graph is a plane, see Figure 2.

Suppose that the edges of G are $e_1, \ldots, e_k$ and parametrize each one arbitrarily. Homotoping G to be unknotted will use a similar process to proving that any classical knot can be unknotted through a series of crossing changes [22]. We will perform homotopies to swap some of the crossings. If an edge e_i crosses above and edge e_j for $i < j$ we can perform a small homotopy to reverse the crossing, this homotopy is contained in Y so it is permissible. Similarly, any self-crossing of an edge E_i will be reversed if the over crossing appears earlier in the parametrization of E_i.

After these crossing changes, G is unknotted. If we replace the vertex of the graph with a vertical edge, we can perform an isotopy so each edge has monotonically increasing z coordinates with edges of higher index

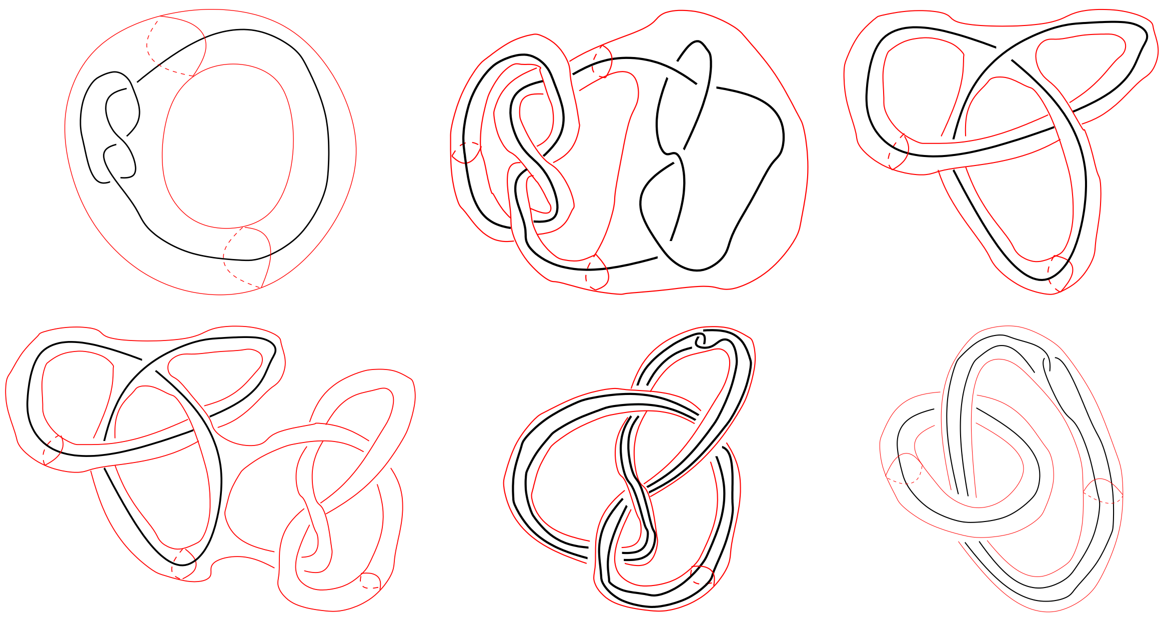

Figure 1: Six knots and links embedded in handlebodies. All but the second are transiently knotted and the final link is transiently linked.

above those with lower. Each edge is completely above all edges with lower indices, so they can be isotoped so they have disjoint projections to the plane. Finally, since each edge is going upwards monotonically, they can be isotoped to have no crossings. This yields a planar unknotted graph with components separated, see the final image in Figure 2. □

The converse of this proposition is not true. In fact, the final two examples in Figure 1 are counter-examples. In both cases, they are transiently knotted and linked but there are no unknotted submanifolds containing the knot and link, respectively, that are contained in the larger space.

4 Persistent homotopy

Persistent homotopy is defined for homotopy groups in a manner very similar to how persistent homology is a generalization of homology. First, a few definitions of homotopy. See [24] for a complete discussion of the definition of the fundamental group. Suppose that X is a path-connected space and $x_0 \in X$ is an arbitrary point. Consider the set of curves $\gamma : [0,1] \to X$ with $\gamma(0) = \gamma(1) = x_0$. The *fundamental group* or first *homotopy group* of X is the set of equivalence classes of these loops. $\gamma_1 \sim \gamma_2$ if there exists a homotopy $H : [0,1] \times [0,1] \to X$ such that $H(0,t) = \gamma_1(t)$, $H(1,t) = \gamma_2(t)$, and $H(s,0) = H(s,1) = x_0$. The equivalence classes forms a group

$$\pi_1(X, x_0) = \{\gamma : [0,1] \to X \mid \gamma(0) = \gamma(1) = x_0\}/_\sim$$

where the product of two loops is the following the first loop and then their second and the inverse of a loop is that loop traveled in reverse. It is well known that a different choice of base point x_0 will result in an isomorphic group. Since we do not care what the base point is, we will suppress it and use the notation $\pi_1(X)$ for the first homotopy group. Like persistent homology, persistent homotopy uses the generators in one space X_i along with the larger equivalence relation coming from X_{i+p}.

Definition 4.1. *The* first persistent homotopy group *or* persistent fundamental group *is defined for connected* X_i *as*

$$\pi_1^p(X_i) = \{\gamma : [0,1] \to X_i \mid \gamma(0) = \gamma(1) = x_0\}/_\approx$$

where $\gamma_1 \approx \gamma_2$ *if there exists a homotopy between the two curves in* X_{i+p} *that fixes* $x_0 \in X_i$.

If X_i is not connected then we will calculate its persistent homotopy groups on each component separately. We can also define higher persistent homotopy groups. These are abelian groups, but cannot be easily calculated so in the most of this work we will only be using $\pi_1^p(X_i)$ unless otherwise specified.

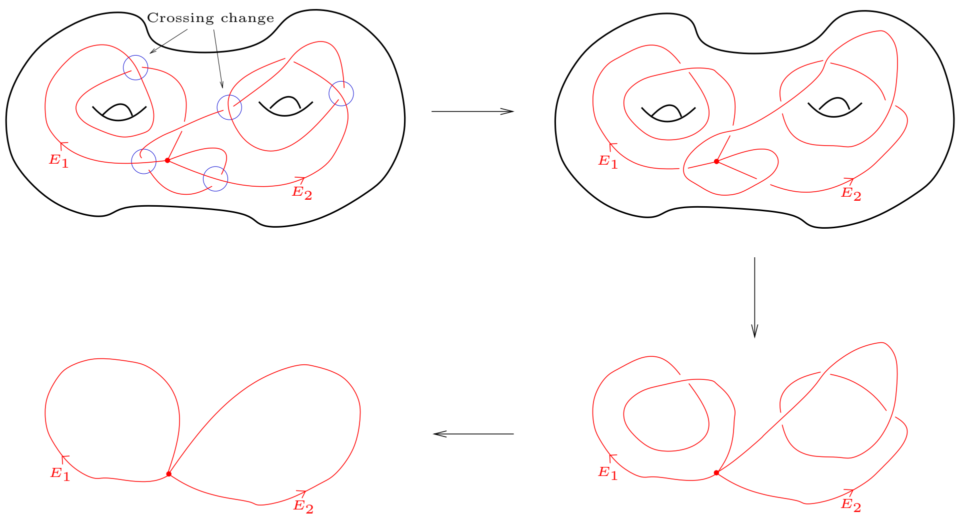

Figure 2: A wedge of circle in a neighborhood of a graph in a plane.

Definition 4.2. *The* k-th persistent homotopy group *is defined as*

$$\pi_k^p(X_i) = \{\gamma : S^k \to X_i \mid \gamma(s_0) = x_0\}/\approx$$

where s_0 *and* x_0 *are fixed point in* S_k *and* X*, respectively, and two maps are equivalent if there is a homotopy between them in* X_{i+p} *that fixes the image of* s_0.

Theorem 4.3. *Given a filtration* $\{X_i\}$ *with each* X_i *connected,* $\pi_1^p(X_i)$ *satisfies the following properties*

1. $\pi_1^p(X_i)$ *is a group where multiplication is concatenation of curves.*
2. *For* $k > 1$, $\pi_k^p(X_i)$ *is an abelian group where multiplication is is the usual multiplication in higher homotopy groups.*
3. *The map* $\pi_k(X_i) \to \pi_k^p(X_i)$ *that sends equivalence classes of maps from the sphere to* X_i *to their larger equivalence classes in* X_{i+p} *is a group homomorphism.*
4. $\iota_* : \pi_k(X_i) \to \pi_k(X_{i+p})$ *is the map induced by inclusion, then* $\pi_k^p(X_i)$ *is isomorphic to the image of* ι_*.
5. $H_k^p(X_i) \cong h(\pi_k^p(X_i))$*, where* $h : \pi_k(X_{i+p}) \to H_k(X_{i+p})$ *is the Hurewicz map [24].*

Proof. To prove $\pi_1^p(X_i)$ is a group we must show that if f is homotopic to f' and g is homotopic in X_{i+p} to g' then fg is homotopic in X_{i+p} to $f'g'$ and f^{-1} is homotopic in X_{i+p} to f'^{-1}. These proofs follow exactly as those for the fundamental group. See any introductory topology text, such as [24], for a proof.

To show $f : \pi_1(X_i) \to \pi_1^p(X_i)$ is a group homomorphism, we need to show $f(\alpha\beta) = f(\alpha)f(\beta)$ and $f(\alpha^{-1}) = f(\alpha)^{-1}$. Suppose, $\alpha, \beta : [0,1] \to X_i$ with $\alpha(0) = \alpha(1) = \beta(0) = \beta(1) = x_0$. $f(\alpha)$ and $f(\beta)$ can be represented by the same curves as α and β. So $f(\alpha\beta)$ and $f(\alpha)f(\beta)$ are identical curves and hence homotopic. Similarly $f(\alpha)^{-1}$ and $f(\alpha^{-1})$ can be represented by the same curve.

Next, we will show that $\iota_*(\pi_k(X_i)) \cong \pi_k^p(X_i)$. Loops in X_i that are homotopic in X_{i+p} clearly have the same image in $\pi_k(X_{i+p})$. The converse is also true, proving the statement.

The final statement follows from examining the commutative diagram

$$\begin{tikzcd}
\pi_k(X_i) \arrow[r, "\iota_*"] \arrow[d] & \pi_k(X_{i+p}) \arrow[d] \\
H_k(X_i) \arrow[r, "\iota_*"] & H_k(X_{i+p})
\end{tikzcd}$$

The horizontal maps are induced by the inclusion $i : X_i \to X_{i+p}$ and the vertical maps are the Hurewicz maps that abelianize the homotopy groups. The Hurewicz maps are surjective and the image of $\iota_* : H_1(X_i) \to H_1(X_{i+p})$ is $H_1^p(X_i)$ implying the statement. □

The final statement implies that persistent homotopy carries all of the information of the persistent homology group and uses the Herewicz map. When $k = 1$, the map h abelianizes the fundamental group to obtain the first homology group.

Like homotopy groups, persistent homotopy groups can detect features that persistent homology cannot. In particular, homology is not capable of detecting knotting. However, if all of the X_i and their complements are assumed to be connected, then it is conjectured that persistent homotopy groups and the maps between them completely determine the filtration $X_1 \subset X_2 \subset \cdots \subset X_n$ up to isotopy. This is similar to the result in classical knot theory that any knot is characterized by the fundamental group of its complement.

Unfortunately, calculating the persistent homotopy groups can be very difficult in general. In particular, it can be difficult to write down a presentation for the group. Furthermore, even if we could find a nice presentation, the word problem and group triviality problems are undecidable for arbitrary groups. However, if we are working with submanifold of S^3, these problems are algorithmically decidable [33] but impractical. Fortunately, we will show in the next section that there are invariants coming from persistent homotopy that can be effectively calculated.

5 Alexander modules

Given a surjective map $\phi : \pi_1(X) \to G$ for some abelian group G, it is possible to define a module, called the *Alexander module* that captures some of the features of the group $\pi_1(X)$. Furthermore, a presentation matrix for this module can be easily calculated. These modules will provide an invariant for $\pi_1(X)$ that contains significantly more information than $H_1(X)$. The Alexander module was studied by Fox as an invariant that could be used to study the isomorphism problem for groups [12]. It also provides a theoretical basis for the Alexander knot polynomial, see [17] for a discussion.

5.1 Algebraic definitions

Before defining the Alexander module, we will recall some definitions for several algebraic structures. For more on these definition see an introductory algebra text, for example [14]. A *module* over a commutative ring R, or an R-module, is an abelian group with scalar multiplication $R \times M \to M$ that satisfies several associate laws. If the ring R is a field, e.g. $\mathbb{Q}$ or $\mathbb{R}$, then an R-module is a vector space. Any finite dimensional vector space can be written as a direct sum of some number of copies of its base field. This is not true for modules in general. A *free module* is a module that is isomorphic to $R^k = R \oplus R \oplus \ldots \oplus R$.

Every finitely presented R-module can be described by a presentation matrix, $A \in R^{m\times n}$. Each column represents a generator and each row a relation. The module, M, defined by the matrix $A = (a_{ij})$ is

$$M \cong \{(x_1, \ldots, x_n) \in R^n \mid \sum_{j=1}^{n} a_{ij}x_j = 0 \ \forall i\}$$

This matrix is a *presentation* of the module M.

In many applications the base ring R will be a Euclidean domain, that is a ring where greatest common divisors can be found using the Euclidean algorithm. Examples include $\mathbb{Z}$ and $\mathbb{Q}[x]$ the ring of polynomials with rational coefficients. The structure theorem for finitely generated modules [19] says that any finitely generated module, M, over such an R can be uniquely written in the form:

$$M \cong R \oplus \ldots \oplus R \oplus R/(d_1) \oplus R/(d_2) \oplus \ldots \oplus R/(d_n)$$

where each $d_i \neq 0$ or a unit, and d_i divides d_{i+1}. The $\{d_i\}$ are called the elementary divisors of M and are unique up to multiplication by a unit. This decomposition can be found by putting a presentation matrix of M into Smith normal form [29].

In our case, the rings we will be dealing with are group rings. Given a group G, the *group ring* $\mathbb{Z}G$ is the ring consisting of finite sums $a_1g_1 + a_2g_2 + \ldots a_kg_k$ for $a_i \in \mathbb{Z}$ and $g_i \in G$ with addition and multiplication defined in the obvious manner. For a free abelian group $G \cong \mathbb{Z}^n$, $\mathbb{Z}G$ is isomorphic to the ring of n-variable Laurent polynomials, that is polynomials in the variables $x_1, \ldots, x_n$ and their inverses. The group ring $\mathbb{Q}G$ is similarly defined as rational linear combinations of elements of G. To avoid confusion, we will write the product of two elements in an abelian group multiplicatively. These group rings are not Euclidean domains, so matrices with coefficients in these rings cannot, in general, be put in Smith normal form; this will be discussed further in Section 6.

5.2 Alexander module

Given any surjective map $\phi : \pi_1(X_i) \to G$ with G abelian, a covering space X_ϕ of X can be built with $\pi_1(X_\phi) \cong \ker \phi$. The covering transformations of X_ϕ are precisely the group G. So G acts on $\pi_1(X_\phi)$. This action puts a $\mathbb{Z}G$-module structure on $H_1(X_\phi)$, see [17, 22] for a full discussion of this construction. This module is called the *Alexander module* and will be denoted M_ϕ.

A presentation matrix for the Alexander module can be constructed using Fox's free differential calculus [11]. Suppose that $\pi_1(X)$ has a finite presentation

$$\langle g_1, \ldots, g_m \mid R_1 = \ldots = R_n = 1\rangle$$

The presentation matrix will have n rows and m columns. The (i, j)-th entry will be equal to $\phi\left(\frac{\partial R_i}{\partial g_j}\right)$. The derivative is Fox's free derivative defined by the following properties:

1. $\frac{\partial 1}{\partial g_i} = 0$
2. $\frac{\partial g_j}{\partial g_i} = \delta_{ij}$, where δ_{ij} is the Kronecker delta.
3. $\frac{\partial uv}{\partial g_i} = \frac{\partial u}{\partial g_i} + u\frac{\partial v}{\partial g_i}$
4. $\frac{\partial u^{-1}}{\partial g_i} = -u^{-1}\frac{\partial u}{\partial g_i}$

A module has many presentations; however, any two differ by a sequence of basic moves

Theorem 5.1 ([36]). *Any two presentations of the same module are equivalent through a sequence of the following moves*

1. *Permute the rows or columns.*
2. *Add a multiple of one row/column to another.*
3. *Multiply a row/column by a unit in R.*
4. *Add or remove a row consisting only of zeros:*
$$(A) \leftrightarrow \begin{pmatrix} A \\ 0 \end{pmatrix}$$
5. *Add (or remove) a new row and column where all of the entries are* 0 *except the new corner entry which is equal to* 1
$$(A) \leftrightarrow \begin{pmatrix} A & 0 \\ 0 & 1 \end{pmatrix}$$

The algorithm to put a matrix in Smith normal form can be thought of as a sequence of these moves.

The ring of Laurent polynomials in n variables is not a Euclidean domain, but it is an unique factorization domain [19]. This means that any polynomial can be factored uniquely up to multiplication by a unit. This implies that the gcd of any two polynomials exists even if we cannot compute it easily. Recall that *unit* is a (multiplicatively) invertible element of a ring; in the ring of Laurent polynomials over the integers a unit is a plus or minus a monomial. Two ring elements $x, y \in R$ will be considered equivalent, denoted $x \equiv y$, if $x = uy$ for some unit $u \in R$.

Since it is not possible to reduce a presentation matrix to a canonical form for these matrices, we will find invariants of the presentation. The d-elementary ideal of M, $E_d(M)$ is the ideal of R generated by the $n - d$ minors of M or the determinants of all of $(n - d) \times (n - d)$ submatrices of M. It can be shown that the above moves do not change this ideal only its generators and relations. Since we are working in a unique factorization domain, the gcd of these minors exists. The d-th *characteristic polynomial* of M, $\Delta_d(M)$ is the gcd of all of the elements of $E_d(M)$ and is defined to be zero if $E_d(M)$ is empty. This is the same as the gcd of the minors. In a Euclidean domain, calculating these characteristic polynomials is equivalent to finding the elementary divisors. Note that these gcds and characteristic polynomials are only defined up to multiplication by a unit. Furthermore, the module and its characteristic polynomials do not depend on choice of presentation and therefore are invariants of the module.

5.3 Persistent Alexander module

In classical knot theory, the Alexander module for a knot is defined to be M_h where where $h : \pi_1(S^3 - K) \to H_1(S^3 - K) \cong \mathbb{Z}$ is the Hurewicz map that abelianizes homotopy. The Alexander polynomial $\Delta(K)$ is defined to the first characteristic polynomial of M_h. Note that the homotopy groups involved are for the knot's complement as knotting is determined by the complement not by the space itself.

Given a sequence of spaces $X_0 \subset X_1 \subset \ldots \subset X_n \subset S^3$, we will consider their complements $S^3 - X_0 \supset S^3 - X_1 \supset \ldots \supset S^3 - X_n \supset \emptyset$. The persistent Alexander module is not an invariant of homotopy groups; instead it is defined as an invariant of the map $\pi_1(S^3 - X_{i+p}) \to \pi_1(X_i)$ which has image equal to $\pi_1^p(S^3 - X_{i+p})$.

To define the persistent Alexander module, consider the commutative diagram below. The horizontal maps are the maps induced by inclusion on homotopy and homology, respectively. Their images are the persistent homotopy group $\pi_1^p(S^3 - X_{i+p})$ and the persistent homology group $H_1^p(S^3 - S_{i+p})$, respectively. The vertical maps are the Hurewicz maps which abelianize the groups by quotienting out by their commutators.

$$\begin{tikzcd}
\pi_1(S^3 - X_i) \arrow[d, "h"'] & \pi_1(S^3 - X_{i+p}) \arrow[l, "\iota_*"'] \arrow[d, "h"] \arrow[dl, dashed, "\phi"'] \\
H_1(S^3 - X_i) & H_1(S^3 - X_{i+p}) \arrow[l, "\iota_*"]
\end{tikzcd}$$

The map ϕ can be the composition of either $h \circ \iota_*$ or $\iota_* \circ h$ as they are equal.

The map ϕ will be used to build a module over the ring $\mathbb{Z}H_1^p(S^3 - X_i)$. In general this ring could be difficult to use for calculations; however, the following lemma shows that the persistent homology groups are torsion free so the group ring on persistent homology is the ring of integral Laurent polynomials $\mathbb{Z}[x_1^{\pm 1}, \ldots, x_k^{\pm 1}]$ for some k.

Lemma 5.2. *If $X_i \subset X_{i+p} \subset S^3$ are manifolds then both $H_k^p(X_i)$ and $H_k^p(S^3 - X_i)$ are torsion free.*

Proof. First consider a submanifold Y of S^3. Fox's re-embedding theorem [10] says that Y can he homotoped so that its complement is a union of handlebodies. This homotopy does not change the homology groups, so $H_k(S^3 - Y)$ is free for all k. Starting with an embedding of $S^3 - Y$ into S^3 and using the same argument shows that $H_k(Y)$ is free.

$H_k^p(X_i)$ is a subgroup of $H_k(X_{i+p})$, which is free. Any subgroup of a finitely generated free group is also free. Thus $H_k^p(X_i)$ is free. A similar argument shows that $H_k^p(S^3 - X_i)$ is also free. □

We could define the Alexander module as M_ϕ. However, for several technical reasons we would prefer the base ring to consist of Laurent polynomials with rational coefficients. Instead, we will define the persistent Alexander module as $M_\phi \otimes \mathbb{Q}H_1^p(S^3 - X_i)$ which is the ring over $\mathbb{Q}H_1^p(S^3 - X_i) \cong \mathbb{Q}[x_1^{\pm 1}, \ldots, x_k^{\pm 1}]$ with the same presentation matrix as M_ϕ.

Definition 5.3. *Given a filtration $X_0 \subset \cdots \subset X_n \subset S^3$, the p-*persistent Alexander module *at i is defined as $\mathcal{A}^p(X_i) = M_\phi \otimes \mathbb{Q}H_1^p(S^3 - X_i)$, where $\phi : \pi_1(S^3 - X_{i+p}) \to H_1^p(S^3 - X_i)$ is the composition of the Hurewicz map and the map induced by inclusion.*

Similarly, the Alexander modules for the complements can be defined using the original filtration $\{X_i\}$ as $\mathcal{A}^p(S^3 - X_i) = M_\phi \otimes \mathbb{Q}H_1^p(X_i)$, where $\phi : \pi_1(X_i) \to H_1^p(X_{i+p})$. The base ring for this module would be $\mathbb{Q}H_1^p(X_i)$. The definition of the polynomial invariants from the Alexander module follows the same as in classical knot theory.

Definition 5.4. *The p-persistent Alexander polynomial, $\Delta_k^p(X_i)$, is defined to be the k-th characteristic polynomial of $\mathcal{A}^p(S^3 - X_i)$.*

The Alexander polynomials do not completely determine the module structure. So, the polynomials form a weaker invariant than the Alexander module but they are easier to work with.

In classical knot theory Alexander modules and polynomial are unchanged by ambient isotopy. Their persistent analogues are preserved under homotopies in the space they are embedded in.

Theorem 5.5. *If $X_i \cong X_i'$ are homotopic in X_{i+p} then $\mathcal{A}^p(X_i) \cong \mathcal{A}^p(X_i')$ and $\Delta_k^p(X_i) \equiv \Delta_k^p(X_i')$.*

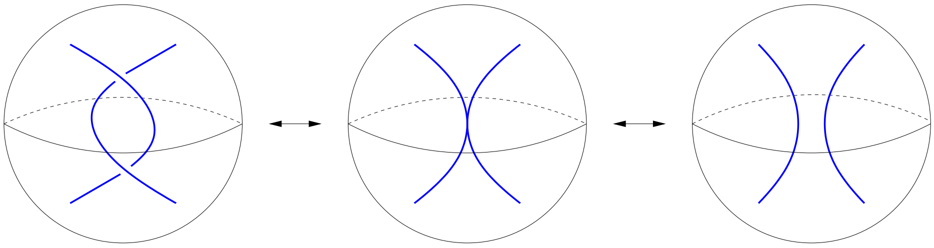

Figure 3: A crossing change in a small ball.

Proof. We will first assume that X_i is a handlebody and will think of it as the closure of a very small neighborhood of a graph. Since X_i is a transient knot, there is a homotopy in X_{i+p} that takes X_i to an unknotted graph. If necessary we can perturb this homotopy so the graph passes through itself in isolated points that avoid the vertices of the graph. We will show that as the homotopy passes through each of these points that the persistent Alexander module is unchanged.

Consider a small ball, B, where two edges cross through each other. In this small ball the change is as seen in Figure 3. Assume there is only one crossing change and X_i' be identical to X_i outside this ball, but have the crossing changed inside B. We now have two inclusion sequences

$$S^3 - X_{i+p} \subset S^3 - (X_i \cup B) = S^3 - (X_i' \cup B) \subset S^3 - X_i$$

$$S^3 - X_{i+p} \subset S^3 - (X_i \cup B) = S^3 - (X_i' \cup B) \subset S^3 - X_i'$$

We can compare how the two Alexander modules are calculated. They both begin with the same matrix of Fox derivatives. Consider the maps on their first homology groups induced by inclusion. Consider the final inclusion map on these sequences. For both a single loop becomes null homotopic, this loop separates the endpoints of one arc in B from the other. In particular, they both send the same loop to zero implying that they induce the same maps on homology. This implies that they have the same persistent Alexander module. The same procedure can be repeated for each crossing change to show that homotopies in X_{i+p} do not change the Alexander module of X_i.

If X_i is not a handlebody consider a cell decomposition for X_i. Then the homotopy between X_i and X_i' restricts to homotopy one-skeleton of the cell decomposition. Let S_i and S_i' be the one skeleton of X_i and X_i', respectively. The previous argument implies that $\mathcal{A}^p(S_i) \cong \mathcal{A}^p(S_i')$. We only need to understand how the Alexander module for X_i compares to the Alexander module for its one-skeleton. Since $X_i - S_i$ is a union of two-cells, $S^3 - S_i$ is obtained from $S^3 - X_i$ by a series of compressions. This implies that $\pi_1(S^3 - S_i) \cong \pi_1(S^3 - X_i) * F_g$ where F_g is the free group on g generators. So $\mathcal{A}^p(S_i) \cong \mathcal{A}^p(X_i) \oplus (\mathbb{Q}H_1^p(X_i))^g$. Similarly, $\mathcal{A}^p(S_i') \cong \mathcal{A}^p(X_i') \oplus (\mathbb{Q}H_1^p(X_i'))^g$. Since the Alexander modules for the one-skeletons agree this shows that $\mathcal{A}^p(X_i) \cong \mathcal{A}^p(X_i')$. $\square$

The following theorem shows how the persistent Alexander module can be used as an invariant to detect if X_i is persistently knotted in X_{i+p}. In a similar fashion, the persistent Alexander polynomials can also be used to detect this knotting behavior

Theorem 5.6. *If X_i is p-transiently knotted and linked then $\mathcal{A}^p(X_i)$ is a free module over $\mathbb{Q}H_1^p(S^3 - X_{i+p})$ and $\Delta_k^p(X_i)$ is either 0 or a unit for all $k \geq 0$.*

Proof. We can homotopy X_i in X_{i+p} to be unknotted and separable and apply theorem 5.5 to knot that the persistent Alexander module is unchanged. So we will assume that X_i is unknotted and all of its components are separable. After performing an isotopy we can assume that X_i is a neighborhood of one or more wedges of circle in a plane, see Figure 4(a). We can extend X_i to X_{i+p} by adding in some edges, E, followed by two-cells and taking a small neighborhood. Let Y be X_i union these edges. When projected to the plane, these edges can cross over or under X_i and also has crossing between these edges.

First, we will show that any crossing between edges in E can be changed without affecting the Alexander module. Consider the Wirtinger presentation for $\pi_1(S^3 - Y)$. It was two types of generators: g_i that loop around the edges in X_i and h_i that loop around the edges in E. Note that the inclusion map $S^3 - Y \to S^3 - X_i$ maps each g_i to a generator of $H_1(S^3 - X_i)$ and each h_i to the trivial element of $H_1(S^3 - X_i)$. In Figure 4(b), shows a crossing before and after it changes. Both have the same four generators $\{h_1, h_2, h_3, h_4\}$. The first diagram

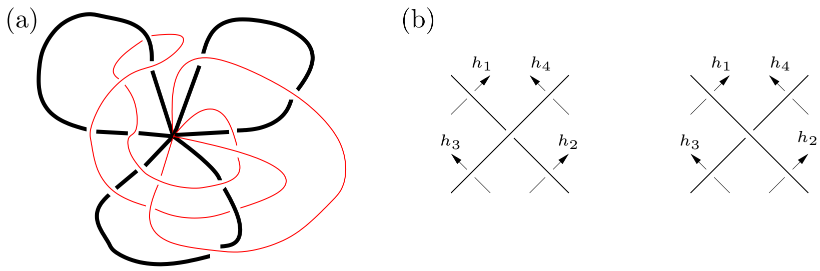

Figure 4: (b)A unknotted handlebody with extra (possibly) knotted and linked edges and (b) crossing changes that leave the Alexander module unchanged.

has the pair of relations $\{h_3h_1h_4^{-1}h_2^{-1}, h_3h_4^{-1}\}$ and the second $\{h_3h_1h_4^{-1}h_2^{-1}, h_1h_2^{-1}\}$. A quick calculation shows that the portions of the presentation matrix for the persistent Alexander module are

$$\begin{pmatrix} 1 & -1 & 1 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix} \text{ and } \begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & -1 & 0 & 0 \end{pmatrix}$$

These two matricies are equivalent after adding the second row to the first in each and interchanging the rows. This shows that crossing changes among the edges in E do not change the Alexander module.

Next we will show that we can make changes to that no edge in E crosses X_i as happens in Figure 4. Consider one of the edges starting from the first until it first crosses X_i. By changing crossings with the other edges in E we may assume it always goes under the other edges. We can the homotope the edge to remove a crossing between E and X_i, see Figure 4(c). We can repeat this until there are no crossing between E and edges in X_i. Finally, we can arrange the crossing in the edges the same way it was done in the proof of theorem 4.3 to ensure that the edges in E are unknotted and unlinked. After these changes $X_i \cup E$ is an unknotted handlebody and the persistent Alexander module has not changed. This shows that the persistent Alexander module for the including $S^3 - (X_i \cup E) \to S^3 - X_i$ must be free since it is same as the persistent Alexander module of an unknotted handlebody.

As in the proof of theorem 5.5, since X_{i+p} if obtained from $X_i \cup E$ by adding two-cells, the persistent Alexander module for the inclusion $S^3 - (X_i \cup E) \to S^3 - X_i$, which is free, is equal to $\mathcal{A}^p(X_i)$ summed with a free module. The solution to Serre's problem [31] implies that $\mathcal{A}^p(X_i)$ is also a free module, completing the proof. $\square$

As a consequence of the previous theorem, we have invariants that when non-trivial demonstrate that the knotting or linking in X_i persists in X_{i+p}. However, if they are trivial, then they tell you nothing. So if $\mathcal{A}^p(X_i)$ is free then we cannot tell if X_i can be unknotted in X_{i+p}. This follows from the fact the classical Alexander polynomial can be trivial for non-trivial knots [13]. The same applies to the persistent Alexander polynomial.

Here are a few basic properties of the persistent Alexander polynomial that can be used too speed up calculations.

Proposition 5.7. *For every i.k and p,*

1. $\Delta_k^p(X_i) = 0$ *for* $k < \beta_1(X_{i+p}) - \beta_0(X_{i+p}) + 1$, *where* $\beta_0(Z)$ *is the number of components in* Z *and* $\beta_1(Z) =$ *rank* $H_1(Z)$.
2. $\Delta_{k+1}^p(X_i)$ *divides* $\Delta_k^p(X_i)$.
3. $\Delta_k^{p+1}(X_{i-1})$ *divides* $i_*(\Delta_k^p(X_i))$
4. *If a presentation of* $\pi_1(S^3 - X_{i+p})$ *can be extended to a presentation of* $\pi_1(S^3 - X_{i+p-1})$ *with the addition of* g *generators then* $\Delta_{k+g}^{p-1}(X_i)$ *divides* $\Delta_k^p(X_i)$.

Proof. 1. This is theorem 1 from [18].

2. There are both gcd's of minors of the same matrix. $\Delta_k^p(X_i)$ is the gcd of all the determinants of all $(n-k) \times (n-k)$ submatrices. Expanding by minors we see that each of these determinants is a linear combination of the determinants of some $(n-k-1) \times (n-k-1)$ submatrices. Since, $\Delta_{k+1}^p(X_i)$ divides each of these determinants it must divide their linear combination.

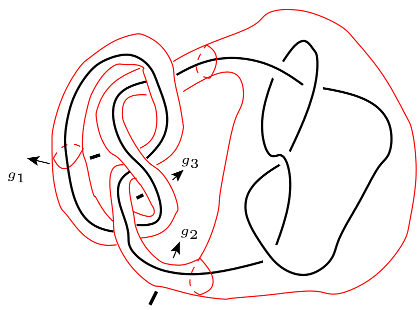

Figure 5: Connected sum of trefoil and figure eight knots in a knotted handlebody of genus two.

3. Note that for both polynomials we start with the same presentation matrix and $\Delta_k^{p+1}(X_{i-1})$ is the gcd of the same determinants after projecting them from $\mathbb{Q}H_1^p(S^3 - X_{i+p}))$ to $\mathbb{Q}H_1^{p+1}(S^3 - X_{i+p})$. The result follows since the projection of a gcd always divides the gcd of projections.

4. Let M be a presentation matrix for the Alexander module of $\pi_1(S^3 - X_{i+p})$. Entries in this matrix get mapped to $H_1(S^3 - X_i)$ to calculate $\Delta_k^p(X_i)$. For the a presentation matrix for the Alexander module of $\pi_1(S^3 - X_{i+p-1})$, M gets expanded by adding g extra columns and possibly some rows corresponding to additional relations. Call the expanded matrix M'. Note that entries in M' also get mapped to $H_1(S^3 - X_i)$ and the $(n-k)\times(n-k)$ minors of M are also $(n-k)\times(n-k)$ minors of M'. The gcds of this larger set of minors in M' are used to calculate $\Delta_{k+g}^{p+1}(X_i)$. Since the gcd is taken over a larger set, $\Delta_{k+g}^{p+1}(X_i)$ divides $\Delta_k^p(X_i)$.

$\square$

5.4 Example calculations

For two of the examples in Figure 1, the persistent Alexander module and polynomials will be calculated. For each of the X_1 will be the knot or link and X_2 the larger manifold containing X_1.

Example 1 The knot is a connected sum of a trefoil and a figure eight knot embedded in a larger solid torus in a trefoil knot. see figure 5. Using the Wirtinger presentation for $\pi_1(S^3 - X_2)$ we get a group with three generators $\{g_1, g_2, g_3\}$ and three relations $\{g_1g_2g_1^{-1}g_3^{-1}, g_2g_3g_2^{-1}g_1^{-1}, g_3g_1g_3^{-1}g_2^{-1}\}$.

So, the matrix of Fox derivatives is

$$\begin{pmatrix} 1 - g_1g_2g_1^{-1} & g_1 & -g_1g_2g_1^{-1}g_3^{-1} \\ -g_2g_3g_2^{-1}g_1^{-1} & 1 - g_2g_3g_2^{-1} & g_2 \\ g_1 & -g_3g_1g_3^{-1}g_2^{-1} & 1 - g_3g_1g_3^{-1} \end{pmatrix}$$

Let t be a generators of $H_1(S^3 - X_1) \cong \mathbb{Z}$. Then $\phi(g_i) = t$ for each of the generators. So the presentation for $\mathcal{A}^p(X_1)$ is

$$\begin{pmatrix} 1-t & t & -1 \\ -1 & 1-t & t \\ t & -1 & 1-t \end{pmatrix}$$

After performing simplification moves this presentation matrix is equivalent to $\begin{pmatrix} 1-t+t^2 & 0 \end{pmatrix}$ So $\mathcal{A}^1(X_1) \cong \mathbb{Z}[t^{\pm1}] \oplus \mathbb{Z}[t^{\pm1}]/(1-t+t^2)$ and

$$\Delta_k^1(X_1) = \begin{cases} 0 & \text{if } k = 0 \\ 1-t+t^2 & \text{if } k = 1 \\ 1 & \text{if } k > 1 \end{cases}$$

This demonstrates that X_1 is persistently knotted in X_2.

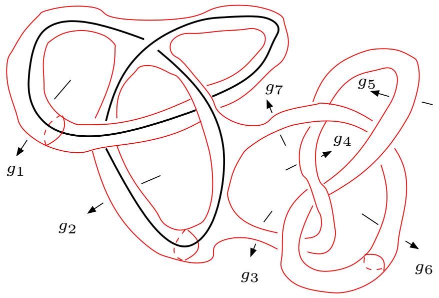

Figure 6: A trefoil in a genus two handlebody.

$$\begin{pmatrix} 0 & -g_3g_2^{-1} & -g_3g_2^{-1}g_3^{-1} & 1 & 0 & 0 & 0 & -g_3g_4^{-1}g_5^{-1}g_7^{-1} \\ 0 & 0 & 0 & 0 & -g_7g_5g_7^{-1}g_4^{-1} & g_7 & 0 & 1-g_7g_5g_7^{-1} \\ 0 & 0 & 0 & 0 & 0 & 1-g_5g_7g_5^{-1} & -g_5g_7g_5^{-1}g_6^{-1} & g_5 \\ 0 & 0 & 0 & 0 & 1-g_4g_5g_4^{-1} & g_4 & -g_4g_5g_4^{-1}g_6^{-1} & 0 \\ 0 & 0 & 0 & g_6 & -g_6g_3g_6^{-1}g_4^{-1} & 0 & 1-g_6g_3g_6^{-1} & 0 \end{pmatrix}$$

Figure 7: The presentation matrix for the Alexander module in example 2.

Example 2 This is a trefoil knot embedded in a genus two handlebody with one handle tied in a trefoil knot and the other in a figure eight knot, see figure 6. $\pi_1(S^3 - X_2)$ has generators $\{g_1, g_2, g_3, g_4, g_5, g_6, g_7\}$ relations $\{g_3g_2^{-1}g_3^{-1}g_7^{-1}, g_7g_5g_7^{-1}g_4^{-1}, g_5g_7g_5^{-1}g_6^{-1}, g_4g_5g_4^{-1}g_6^{-1}, g_6g_3g_6^{-1}g_4^{-1}\}$. The map ϕ sends g_1, g_2 to t and the other g_i to 1. The matrix of Fox derivatives can be found in figure 7 After applying the map ϕ a presentation matrix for $\mathcal{A}^p(X_1)$ is

$$\begin{pmatrix} 0 & -t^{-1} & -t^{-2} & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \end{pmatrix}$$

This simplifies to the matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

This shows that $\mathcal{A}^p(X_1) \cong \mathbb{Z}[t^{\pm 1}] \oplus \mathbb{Z}[t^{\pm 1}] \oplus \mathbb{Z}[t^{\pm 1}]$. We cannot conclude the X_1 is unknotted from this, but it suggests that it is a possibility.

6 Algorithms

The theoretical algorithm to find the persistent Alexander polynomials would not be very practical. First, the presentation matrices would be very large with a relation for each edge of the triangulation and a generator for every face of the triangulation. Second, once created every $k \times k$ submatrix would have to have its determinant calculated, which are exponentially many determinants to find. Finally, the gcd of these determinant must be found and they are multivariable polynomials so the Euclidean algorithm cannot be used. Instead the gcd's could be found using Grobner bases. This process is impractical for all but the smallest examples. There are two improvements to this process to make these calculations both theoretically and practically feasible. The first improvement is to simplify the group presentations involved to reduce the size of the presentation matrix. The second is to use probabilistic techniques to detect when a persistent Alexander polynomial is non-trivial.

Starting with a triangulation for our filtration, we can build a presentation for $S^3 - X_{i+p}$ where the generators correspond to edges is the dual cell decomposition, so there is one for each face of the triangulation, and a relation for small loops going around each edge. Fox derivatives can be calculated efficiently using their definition. And finally the map $\phi : \pi_1(S^3 - X_{i+p}) \to H_1^p(S^3 - X_i)$ can be found at the same time persistent homology is calculated, which can be done in matrix multiply time [3].

Lemma 6.1. *The presentation matrix for $\mathcal{A}^p(X_i)$ can be found in polynomial time.*

6.1 Probabilistic techniques

If the base ring for the module was a Euclidean domain then we could quickly put the presentation matrix for $\mathcal{A}^p(X_i)$ in Smith normal form and simultaneously find $\Delta_k^p(X_i)$ for all k. However, the base ring is not a Euclidean domain. However, if we randomly project the entries in the presentation matrix to univariate polynomials, we would the be able to put the matrix in Smith normal form in polynomial time [34]. We will show that, with high probability, this algorithm will succeed in detecting if any of the persistent Alexander polynomials are non-trivial.

Theorem 6.2. *It can be determined if $\Delta_k^p(X_i) \equiv 1$ in randomized polynomial time.*

The effectiveness of this algorithm is based on constructing a random projection $r : \mathbb{Z}[x_1, \ldots, x_k] \to \mathbb{Q}[t]$. This projection is constructed by finding random numbers

$$a_2, \ldots, a_k, b_2, \ldots, b_k \in \mathbb{Q}$$

and defining $r(f(x_1, \ldots, x_k)) = f(t, a_2 + b_2t, \ldots, a_k + b_kt)$. It is shown in [15] that, with high probability, the projection r preserves many properties of polynomials. This allows the detection of non-trivial persistent Alexander polynomials in a fast reliable manner.

Theorem 6.3. *Suppose that M is a $\mathbb{Z}[x_1, \ldots, x_k]$-module with an $m \times n$ presentation matrix with every entry having degree at most d. If $a_2, \ldots, a_k, b_2, \ldots b_k$ are chosen randomly from $S \subset \mathbb{Q}$ and $r(M)$ is the matrix M with each polynomial entry $f(x_1, \ldots, x_n)$ replaced with $f(t, a_2 + b_2t, \ldots, a_k + b_kt)$ then with a probability of at least $1 - \frac{d^{n-k}(2d^{n-k}+3)}{|S|}$*

$$\Delta_k(r(M)) = ct^{p_1}(a_2 + b_2t)^{p_2} \cdots (a_k + b_kt)^{p_k}$$

for any $c \in \mathbb{Q} - \{0\}, p_i \in \mathbb{Z}^+ \Leftrightarrow \Delta_k(M) \equiv 1$

Corollary 6.4. *For a random projection, r, if*

$$\Delta_k(r(\mathcal{A}^p(X_i))) \neq ct^{p_1}(a_2 + b_2t)^{p_2} \cdots (a_k + b_kt)^{p_k}$$

for some k then, with high probability, X_i is a persistent knot in X_{i+p}.

Note that this theorem uses a very conservative bound on the degree of the $(n-k) \times (n-k)$-minors of d^{n-k}. If a better bound is known it can be used instead.

The proof of theorem 6.3 follows from arguments using probabilistic testing of polynomial identities. These results all rely on the Schwartz-Zippel lemma for probabilistically testing if a polynomial is zero. Recall that an integral domain is a commutative ring with $1 \neq 0$ and no zero divisors, for example $\mathbb{Z}$ or $\mathbb{Z}[x_1, \ldots, x_k]$.

Lemma 6.5 ([28])**.** *For any integral domain R and any non-zero polynomial $f \in R[x_1, \ldots, x_n]$ of degree d and for randomly chosen $p_1, \ldots, p_n \in S \subset R$*

$$Prob(f(p_1, \ldots, p_n) = 0) \leq \frac{d}{|S|}$$

This lemma allows bounding the probability that a non-zero polynomial will evaluate to zero at a random point.

Proof of theorem 6.3. The k-th characteristic polynomial, $\Delta_k(M)$ is the gcd of all of the $(n-k) \times (n-k)$-minors. Let $f_1, \ldots, f_l$ be the non-zero minors. Then $\Delta_k(M) = gcd(f_1, \ldots, f_l)$. Each of the entries in M have degree at most d, so each of the f_i have degree at most d^{n-k}.

Pick random elements $c_3, \ldots, c_l \in S$ and write $g = f_2 + \sum_{i=3}^{l} c_i f_i$. Lemma 2 of [6] implies that $gcd(f_1, \ldots, f_l) = gcd(f_1, g)$ with a probability of at least $1 - \frac{d^{n-k}}{|S|}$. Let $p : \mathbb{Q}[x_1, \ldots, x_k] \to \mathbb{Q}[t]$ be the projection $p(f) = f(t, a_2 + b_2t, \ldots, a_k + b_kt)$. The same lemma implies that, with probability at least $1 - \frac{d^{n-k}}{|S|}$, $gcd(p(f_1), \ldots, p(f_l)) = gcd(p(f_1), p(g))$.

Lemma of [6] implies that with probability at least $1 - \frac{2d^{2(n-k)}}{|S|}$, $p(gcd(f_1, g)) = gcd(p(f_1), p(g))$ Combining all of this, we see that

$$\begin{aligned} p(\Delta_k(M)) &= p(gcd(f_1, \ldots, f_l)) \\ &= p(gcd(f_1, g)) \\ &= gcd(p(f_1), p(g)) \\ &= gcd(p(f_1), \ldots, p(f_l)) \\ &= \Delta_k(M') \end{aligned}$$

with probability at least

$$1 - 2\frac{d^{n-k}}{|S|}2 - \frac{2d^{2(n-k)}}{|S|} = 1 - \frac{2d^{n-k}(d^{n-k}+1)}{|S|}$$

So, with high probability, the characteristic polynomial of the projected matrix is the projection of the characteristic polynomial of M.

Therefore, with probability at least $1 - \frac{2d^{n-k}(d^{n-k}+1)}{|S|}$, $\Delta_k(M') \neq \pm t^{p_1}(a_2 + b_2t)^{p_2} \dots (a_k + b_kt)^{p_k}$ for some $p_1, \dots, p_k$ implies $\Delta_k(M) \not\equiv 1$. This proves one direction of the theorem.

If $\Delta_k(M') = \pm t^{p_1}(a_2+b_2t)^{p_2} \dots (a_k+b_kt)^{p_k}$ it is possible, although unlikely, that $\Delta_k(M) \neq \pm x_1^{p_1} x_2^{p_2} \dots x_k^{p_k}$. To quantify how unlikely this is, consider the polynomials

$$\begin{aligned} h_1(y_2, \dots, y_k, z_2, \dots, z_k) &= \Delta_k(M)(t, y_2 + z_kt, \dots, y_k + z_kt) \\ &\quad + t^{p_1}(y_2 + z_2t)^{p_2} \dots (y_k + z_kt)^{p_k} \\ h_2(y_2, \dots, y_k, z_2, \dots, z_k) &= \Delta_k(M)(t, y_2 + z_kt, \dots, y_k + z_kt) \\ &\quad - t^{p_1}(y_2 + z_2t)^{p_2} \dots (y_k + z_kt)^{p_k} \end{aligned}$$

in the variables $y_2, \dots, y_k, z_2, \dots, z_k$ and coefficients in $\mathbb{Q}[t]$. Both of these are non-zero, but for some i we have

$$h_i(a_2, \dots, a_k, b_2, \dots, b_k) = 0$$

The Schwartz-Zippel lemma implies that this happens with probability at most $\frac{d^{n-k}}{|S|}$. So with a probability of at least $1 - \frac{2d^{n-k}(d^{n-k}+1)}{|S|} - \frac{d^{n-k}}{|S|} = 1 - \frac{d^{n-k}(2d^{n-k}+3)}{|S|}$, $\Delta_k(M') = \pm t^{p_1}(a_2 + b_2t)^{p_2} \dots (a_k + b_kt)^{p_k}$ implies that $\Delta_k(M) \equiv 1$. □

Algorithmically, these random projections give a huge improvement since $\Delta_k(r(M))$ can be found efficiently by putting the matrix $r(M)$ in Smith normal form. Assuming that the space of projections is large enough, we can control the probability of error. This yields a practical probabilistic algorithm to determine if any persistent Alexander polynomial is non-trivial. This can be used to determine, with high probability, that X_i is persistently knotted in X_{i+p}.

Proof of theorem 6.2. A presentation matrix, M, for $\mathcal{A}^p(X_i)$ can be found in polynomial time. The set S can be choose to be large enough to ensure that the probability bounds in theorem 6.3 exceed 1/2 and random projection r, can be chosen a new presentation matrix $r(M)$ built with entries in $\mathbb{Q}[t]$. Smith normal form of $r(M)$ can be found in polynomial time [34]. The k-characteristic polynomials of $r(M)$ is the product of the first $n-k$ entries on the diagonal of the matrix in Smith normal form. Let $f(t)$ be this characteristic polynomial. Factors of a_i+b_it can be removed from f by testing if $-\frac{a_i}{b_i}$ and dividing by the term. This simplification also runs in polynomial time. If the resulting polynomial is non-constant then we know that the persistent Alexander polynomial is non-trivial. Otherwise, with probability at least 1/2, the persistent Alexander polynomial is trivial. □

6.2 Practical improvements

Without simplification the size of the presentation matrix makes the algorithms completely impractical. Figure 8(b) show the size dimensions of the presentation matrices and the number of non-zero entries in the matrix both before and after simplification. Notice that as the number of vertices in the triangulation approach one hundred thousand the presentation matrix has over a million rows and a million columns. However, there is a lot of simplifications that can be done to reduce the dimensions of the matrix by approximately two orders of magnitude.

These simplifications include:

1. Any relation of the form $g_i = 1$ can be used the eliminate that generator from the presentation.
2. Relations of the form $g_ig_j = 1$ or $g_ig_j^{-1} = 1$ can be used to replace one of the generators by another in every relations, reducing the number of generators by one.
3. Remove any generator that appears in no relations.

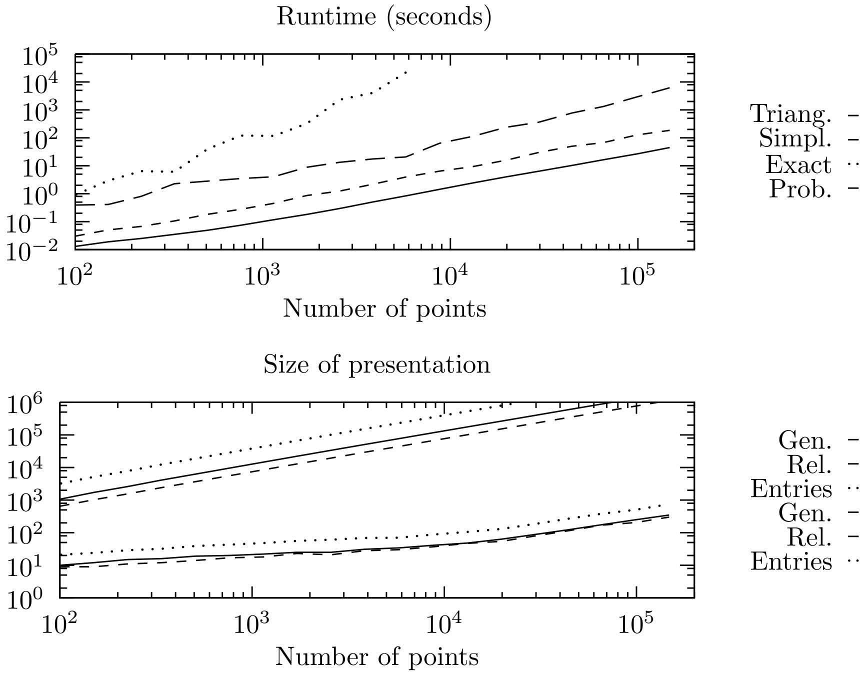

Figure 8: (a) Times for finding all of the persistent Alexander polynomials (b) The number of generators, relations and non-zero entries in the presentation matrix for the Alexander module both before and after simplification.

4. If a generator appears in in exactly one relations then both that generator can be removed.

5. If a generator appears exactly twice in all of the relations then the two relations can be combined reducing both the number of generators and relations by one.

In presentations coming from triangulations, each generator appears in at most three relations so these types of simplifications are extremely common and lead to the huge reduction in the size of the presentation matrices observed.

Figure 8 shows the total run time for two variations of these algorithms. Most of input triangulations come from protein structures obtain from the Protein Data Bank [27] and have between a thousand and 150 thousand atoms. Both use the same routines to build the triangulation and perform simplifications; the times for each of these steps is shown. Also, both algorithm perform their calculations on every persistent Alexander polynomial for the filtration. The exact algorithm takes the simplified group presentation to build the presentation matrix for the Alexander polynomial and attempts to put it in Smith normal form. Even though the Smith normal form algorithm is not guaranteed to work, in practice it simplifies the matricies significantly. When the algorithm fails, it resorts to brute force calculations of the characteristic polynomials of the presentation matrix. This algorithm calculates the persistent Alexander polynomials exactly. The probabilistic algorithm detects if the persistent Alexander polynomials are non-trivial with a probability of at least 99.5%. The timing shows that the probabilistic algorithm is efficient enough to be practical for proteins with up to a hundred thousand atoms in their structure.

7 Applications to Protein Structures

One of the primary applications of the techniques introduced in this paper is the analysis of protein, RNA and DNA structures. In [32] a technique was introduced to identify knotting in protein backbones. It relies on the fact that the protein termini are typically near the surface of a protein's structure. To create mathematical knots the termini are extended to the point at infinity and to calculate the Alexander polynomial of the resulting knot. The techniques in this paper find the knots but also are capable of finding knots in protein structures

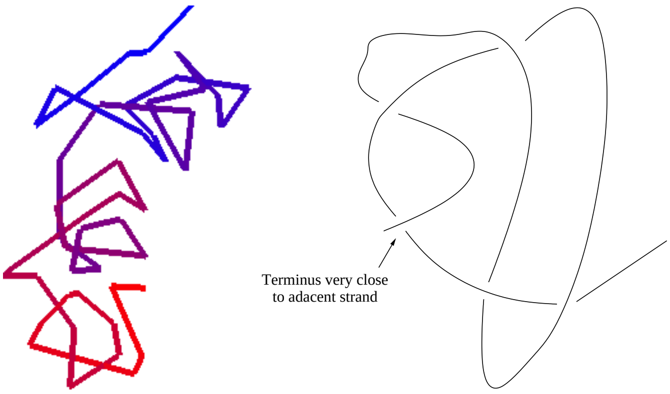

Figure 9: (a) A trefoil knot in the protein 1IPA. (b) The knotting structure of 1XD3 that is unstable due to the proximity of the terminus to another region of the protein.

that don't follow the protein's backbone. Additionally, it can be used in conjunction with these techniques to measure the stability of knotted structures.

Figure 9(a) shows a trefoil knot in the (simplified) backbone of the protein 1IPA [32]. The trefoil is clearly visible at the bottom of the knot. However, there is another type of knot detected by persistence in this example. It follows the trefoil at the bottom of the backbone until it reaches a pair of amino acids that are very close together and jumps to another portion of the backbone close to the original terminus. This new knot avoids most of the protein's backbone. This type of knotting or knots that follow disulphide bonds are not detectable by previous techniques. To date we have detected five proteins that have knots following their disulphide bonds that do not have knots in their backbones.

Persistence can also be used to detect knotting that has ambiguous structure when other techniques are applied. Figure 9(b) is a schematic picture of the backbone of the protein 1XD3 [35]. A five crossing knot is detected in its structure. However, one terminus of the protein is very close to another strand and if the structure is perturbed slightly this will turn into a trefoil knot. In either case it is knotted but the exact structure is unclear. From a persistent knotting perspective, if the neighborhood of the backbone is grown slightly the terminus merges with the strand and a knotted graph is formed that realizes the features of both of these candidate knots.

Another application is the linking of backbone structures. Our techniques are the first to computationally detect knotted between different strands in a protein complex.

8 Future Work

One of the next steps is to develop improved algorithms so these techniques can be applied to larger examples. With improved algorithms, we hope to catalog knotting and linking structures in proteins and RNA structures, measure their persistence and explore the biological significance of these knotted structures. In particular, how do knotting structures affect structural formation and stability. From a mathematical perspective, persistence knotting could be extended to other knot invariants that could detect structures that the Alexander polynomial is incapable of detecting.

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