



”FROM KNOTS TO GENES: EXPLORING THE INTERSECTION OF KNOT THEORY AND DNA BIOLOGY”

Zewail City

Math 205:Discrete Mathematics Project

By: Mohammed Ayman

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Abstract

Knot theory is an exciting area of study with numerous applications in various sciences. This paper explores the application of knot theory in molecular biology, particularly in understanding DNA topology. We begin by discussing the history of knot theory and covering basic definitions. We then delve into the property of tricolorability and its use in determining whether a given knot is equivalent to the unknot.

Recent developments have shown that knot theory provides a valuable tool for modeling DNA recombination. The relationship between mathematics and DNA began in the 1950s with the discovery of the helical Crick-Watson structure of duplex DNA. This discovery opened the door for mathematical analysis of DNA, leading to models such as the Tangle

Model for Site-Specific Recombination introduced by De Witt Sumner's. This model uses knot theory to study enzyme mechanisms involved in DNA recombination.

DNA, the genetic material of all cells, consists of two polynucleotide strands twisted around each other in a double helix. Replication and transcription of DNA require it to unpack itself from highly tangled knots. Enzymes play a crucial role in this process by slicing through individual knots and reconnecting strands in a more orderly manner.

This paper aims to provide an overview of the mathematical tools and concepts used in the study of DNA topology, including definitions, theorems, and the structure of DNA molecules from biological and biochemical perspectives. By bridging the gap between mathematics and biology, we hope to inspire further interdisciplinary research in this fascinating field.

Keywords: Knot theory, DNA biology, molecular biology, topology, mathematical modeling, enzyme mechanisms, site-specific recombination, tangle model, DNA supercoiling, topoisomerases, recombinases

1 .introduction

Knot theory is a subset of a larger branch of mathematics called topology. Topology is an area of mathematics which involves studying the properties of geometric figures which are unaltered by elastic deformations such as stretching or twisting so, Knot Theory is a section of topology which focuses on the study of mathematical knots. Similar to knots we see around us, like the knots in shoelaces, for example, mathematical knots are 3-dimensional and are made of crossing strands of a string. However, a mathematical knot, unlike the knots we see in day-to-day life, is composed of a theoretical string, with its two ends attached to one another permanently. The most basic knot in knot theory is known as the "unknot". In its simplest form, the unknot is simply a ring. Two knots are considered equivalent if one can be made into a perfect replica of the other through a series of deformations known as ambient isotopies. These are deformations that do not alter the knot by cutting, gluing, or passing the string through itself.

In recent years, exciting new applications of mathematics to the field of molecular biology have been developed. In particular, knot theory gives a very nice way to model DNA recombination. The relationship between mathematics and DNA began in the 1950s with the discovery of the helical Crick-Watson structure of duplex DNA. The discovery of this model opened the door for mathematical analysis of DNA. One such mathematical model is the Tangle Model for Site-Specific Recombination, which was first introduced by De Witt Sumner's. This model uses knot theory to study enzyme mechanisms.

The purpose of this project is to explain the details of this application of knot theory to DNA recombination. Of course, we are all aware that DNA are long, thin molecules found inside the nucleus of a cell; these molecules are nature's way of encoding biological traits and are the mechanism for reproduction. To get a sense of the scale of things, imagine the cell nucleus as the size of a basketball.



Figure 1: An enzyme (E) induced supercoil

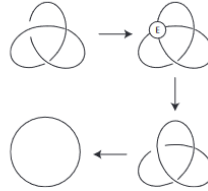


Figure 2: An enzyme (E) induced crossing change in a DNA trefoil knot



Figure 3: Recombination

Inside a nucleus of that size, you would find that the DNA would resemble thin fishing line with 200 km packed inside. Because the DNA is so tightly packed into such a confined space, it is not surprising that it is a tangled and knotted mess. DNA must be topologically manipulated in order for vital processes such as replication, transcription, and recombination to take place.

Nature's answer to the tangling problem is "enzymes". Enzymes act by manipulating DNA in several different ways. They may cause coiling up of DNA (supercoiling – Figure 1). They may switch a crossing of nearby strands of DNA (transient enzyme-bridged break – Figure 2), or they may break apart a pair of strands and recombine them to different ends (recombination – Figure 3) above.

We can gain insight into the unknotting of DNA by using principles of topology. Topologists study the invariant properties of geometric objects, such as knots. Tightly packed DNA in the genes must quickly unknot itself in order for replication or transcription to occur. This is a topological problem, and the Question is : How can knot theory help us understand DNA packing? How can we estimate the rates at which enzymes unknot DNA?

2 How our Math 205 course have been applied in our project ?

In our project on DNA and knot theory, discrete mathematics is applied in several ways:

Topological Analysis: The analysis of the topology of knots and links in DNA and understanding how DNA strands are intertwined and how enzymes manipulate DNA topology.

Graph Theory: Graph theory is used to model and analyze various aspects of DNA structure and manipulation and the representation of the topology of DNA molecules, with vertices representing crossings and edges representing DNA strands.

Combinatorics: we used Combinatorial methods to study the possible configurations of DNA strands and the ways in which enzymes can manipulate these configurations. This involves counting the number of possible knot and link types that can arise in DNA.

Algorithm Design: designing algorithms for analyzing DNA topology and enzyme actions, for example : algorithms for identifying knot and link types in DNA structures and for simulating enzyme actions on DNA molecules.

Network Theory: we used it to model the interactions between enzymes and DNA molecules as a network of nodes (enzymes) and edges (DNA interactions) which will help us to understand how enzymes recombine DNA strands to achieve specific biological functions.

3 what is the main problem that we aim to solve?

Knot theory in DNA biology provides a framework for understanding the topology and spatial arrangements of DNA molecules, in the context of DNA recombination and replication. One of the main biological problems that knot theory addresses is the formation and resolution of DNA knots and tangles that arise during cellular processes.

DNA molecules are long and highly twisted, and they can become tangled like a knotted rope. This tangling can interfere with important cellular processes such as replication, transcription, and recombination. Knot theory helps biologists understand how enzymes called topoisomerases and recombinases act to manage and resolve these DNA knots as DNA knots can lead to genetic instability, which can result in genetic abnormalities. Resolving knots helps maintain the stability of the genetic material and reducing the risk of genetic diseases and abnormalities. if the humans have a genetic instability this may lead to cancers and uncontrolled cell growth and the formation of tumors. Also it can impact the function of the immune system, leading to be caught by infections and autoimmune diseases.

4 Background: History of Knot Theory

Knot theory, now a branch of topology, originated not in mathematics, but in chemistry during the late 1800s. Lord Kelvin and his physicist colleagues speculated that atoms might correspond to knots in the ether, a substance believed to fill all space. To catalog different kinds of knots, they embarked on a trial-and-error process. However, the Michelson-Morley experiment of the late 19th century, which showed the non-existence of ether, dashed their hopes. As a result, chemists lost interest in the theory, and it was abandoned in favor of newer atomic models.

Despite the chemists' disinterest, mathematicians found knot theory intriguing, and it continued to be studied as a part of topology. In a twist of fate, chemists later renewed their interest in knots after realizing their importance in DNA and synthetic molecules. This rekindled involvement led to the exploration of knot theory's applications in various fields such as physics and chemistry.

Knot theory's early roots can be traced back to 1867 when scientists were trying to understand the fundamental nature of matter. Scottish mathematician and physicist Peter Guthrie Tait demonstrated a device for generating smoke rings to his friend Sir William Thomson (later Lord Kelvin). Thomson, fascinated by the rings' shapes and stability, proposed that atoms might be knotted vortex rings in the luminiferous ether, the medium through which light was believed to propagate.

This idea, although ultimately proven incorrect, spurred the study of knots as a way to understand the properties of different chemical elements. Tait and others began tabulating different types of knots, hoping to create a table similar to the periodic table of elements. This early work laid the foundation for knot theory as a mathematical field.

While the original theory linking knots to atoms was discarded due to the non-existence of the ether, mathematicians continued to study knots as purely abstract mathematical objects. Knot theory has since evolved into a rich and active area of research, with applications in physics, chemistry, biology, and beyond. Today, knot theory is used to study the structure of DNA, the behavior of knotted molecules, and even in the study of fluid dynamics and quantum computation. Mathematicians have been gracious about allowing chemists to reap from the results of their interim century of study, and knot theory is now an active and intriguing field of research, as much for its many applications to physics and chemistry as for its beautiful and fascinating theory.

5 Why studying Knot Theory is important?

Knot theory is one of the most active areas of research in mathematics today, and its techniques can be found in such wide-ranging areas as fluid dynamics, solar physics, DNA research, and quantum computation, and we have even found fish (called Myxine, or slime eels) that deliberately tie themselves up into knots to help escape from predators! Knots have a huge impact in understanding the

biochemistry of DNA, the synthesis of new materials, and the geometry of three-dimensional spaces. For example, in DNA, enzymes disentangle strands of linked DNA by manipulating them as if they were knots. Understanding knot theory can lead to advancements in medicine, such as developing chemotherapy drugs, helping us to understand DNA packing, estimating the rates at which enzymes unknot DNA which may lead to prevent the genetic instability which may be led to cancers and tumors if it was happened! or even, helping mathematicians solve complex problems related to higher-dimensional spaces. So, When we finally understand the deepest nature of knots, profound physical applications will blossom. And it will be beautiful!

6 introduction to Knot Theory:

6.1 Fundamentals and Definitions

So what exactly is a knot? There are a number of possible definitions that could formalize what we mean, and we'll work with an easy one:

DEFINITION 1: A **knot** is a simple, closed, non-self-intersecting curve in \mathbb{R}^3 .

For physical intuition, you can think of a knot as constructed from a string glued together at the ends, perhaps tangled in the middle. Thus your shoelaces' knot wouldn't count, but it would if you connected the loose ends together. We won't concern ourselves with the thickness of our string – its cross-section will be just a point. One way of graphically representing knots, called a knot diagram or projection, shows the curve as a black line on the page. Formally, the projection is the image of a function from the \mathbb{R}^3 in which the knot lives to the plane of the page, taking the triple (x, y, z) to the pair (x, y) . Two further definitions will be helpful:

DEFINITION 2: A **crossing** in a knot diagram is a place where the knot curve crosses – going over or under – itself.

DEFINITION 3: An **arc** in a knot diagram is a piece of the curve going between two undercrossings. Overcrossings are allowed along the way. Figure 2 shows the three simplest knots – the kinds that can be drawn with the least number of crossings. The leftmost is the unknot, or trivial knot, which can be drawn with no crossings. The middle is a trefoil knot, the simplest nontrivial knot, with a minimum of three crossings. The rightmost picture is of a figure-eight knot, so called because of the 8 shape in the middle, which can be drawn with a minimum of four crossings.

Of course, there are arbitrarily many ways of drawing a knot's diagram, with as many more crossings as you'd like, given our allowance of deformations. In Figure 3 you can see three equivalent diagrams of a figure-eight knot: Perhaps it's not too difficult to see how the three diagrams are of the same knot in figure 3, but sometimes it can be a much harder task.

when is one knot the same as another knot (often known as the comparison problem)? We begin by defining an equivalence relation between knots, Using

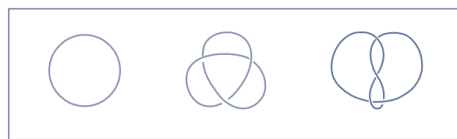


Figure 1: Three fewest-crossing knots: the unknot (0 crossings), a trefoil knot (3 crossings), and the figure-eight knot (4 crossings)

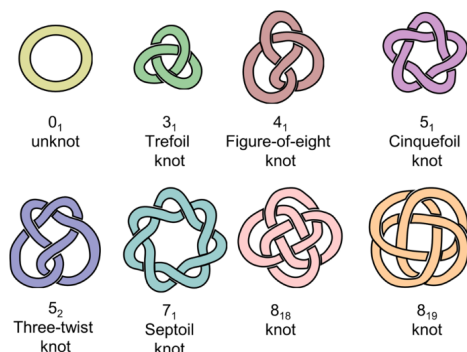


Figure 2: A Few Simple Knots

ambient isotopy, an ambient isotopy of a space $X \subset R^3$ is an isotopy of R^3 that carries X with it. We are required to use ambient isotopy (as opposed to homotopy, or isotopy for example), as we do not want the curve that forms our knot to be able to pass through itself, or be able to ‘shrink’ away.

Definition: Two knots K_1 and K_2 are equivalent (ambient isotopic) if there is an isotopy $h : R^3 \times [0, 1] \rightarrow R^3$ such that $h(K_1, 0) = K_1$ and $h(K_1, 1) = K_2$. We then say that two knots are equivalent if they can be deformed into each other using this ambient isotopy. From now on, when we say a ‘knot’ we are generally referring to a whole equivalence class, so if we say two knots are different, we mean they are in different equivalence classes. In the same way, if we want to know if one knot is the same as another knot, we are in fact asking whether they are in the same equivalence class.

The comparison problem now becomes a case of finding ambient isotopies (or showing there are none) between knots. As is the case in most of topology however, trying to define specific maps is very difficult; it would be virtually

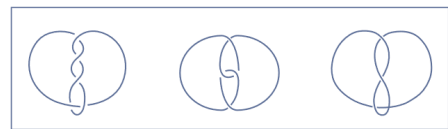


Figure 3: Three diagrams of a figure-eight knot , (figure by : MIT OCW)

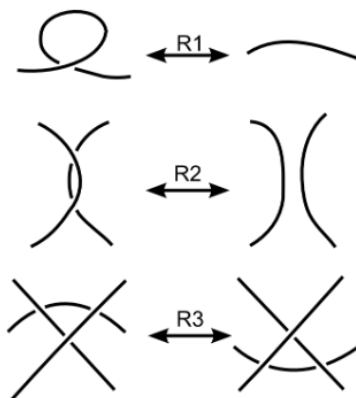


Figure 4: The Reidemeister moves.

impossible to define a specific ambient isotopy between most knots.

To aid us in solving this problem, we try to simplify how we can represent knots.

6.2 Knot diagrams

A very natural and useful way to look at knots is by using knot diagrams. As we have seen, we define a knot as a closed curve in space, therefore we may look at the projection of this curve onto a plane; the knot is thus represented by a planar curve. Where one part of the projection passes over another we include crossings, making a break in the strand that corresponds to the lower part of the curve in space. A few examples of knot diagrams are shown in Figure 2

In some regards the comparison problem now becomes very easy. A knot corresponds to a regular presentation (knot diagram), so the problem is simplified to just comparing the relevant knot diagrams. Unfortunately any knot can have many different diagrams. In the 1920s however, Kurt Reidemeister proved a theorem, which theoretically solves everything:

Theorem 1 (Theorem of Reidemeister): If two knots (or links) are equivalent, their diagrams are related by a sequence of Reidemeister moves

Where the Reidemeister moves (R1, R2 and R3) are three pairs of possible changes to a knot diagram, assuming with each move that you only change the diagram locally as shown, leaving the rest of the diagram alone.

Now, to show that two knots are equivalent, all we have to do is find a sequence of Reidemeister moves that turn the diagram of the first knot into the diagram of the second. An example of a sequence of such moves is shown in Figure 5.

Unfortunately, there are a few problems. Suppose we have two different diagrams of a knot. How do we go about finding the sequence of Reidemeister moves that will turn one diagram into the other? Where do we start? Perhaps



Figure 5: Example showing the Reidemeister moves that change the first diagram into the standard diagram of the unknot. The red circles indicate where each move takes place.

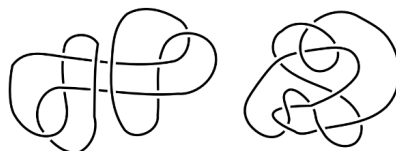


Figure 6: Two diagrams of the unknot, where a sequence of Reidemeister moves relating these to the standard unknot diagram requires us to first increase the number of crossings.

if we start by trying any move that does not increase the number of crossings? But if there are many different moves we could choose, how do we know which one to do first? Even if this doesn't matter, will we simplify a knot as much as possible if we only apply these kinds of moves?

The answer to this last question is unfortunately, no. There are cases where we must first increase the number of crossings before we can simplify the diagram further. Two examples of such a diagram are shown in Figure 6. the diagrams shown are both in fact the unknot, but to find a sequence of Reidemeister moves from this diagram to the standard unknot diagram, as seen in figure 2, would require us to first perform a Reidemeister move that would increase the number of crossings. Therefore, although in principle we can find a sequence of Reidemeister moves between two equivalent diagrams, there is no obvious way of knowing which moves we should actually perform. Even harder is trying to distinguish two different knots using just Reidemeister moves; we would need to show that there is no sequence of moves between the two diagrams, but as there are so many possible changes to a diagram how would we even know if we had exhausted all possibilities, and is it even possible? Clearly we need a quicker way to distinguish knots.

6.3 Knot Invariants

Luckily there is a much easier way to show two knots are distinct, through the use of "knot invariants".

Definition: A knot invariant is any function i of knots which depends only on their equivalence classes. Thus, if K and K' are two equivalent knots, $K \cong K'$, then $i(K) = i(K')$. Therefore, if $i(K) \neq i(K')$ then $K \not\cong K'$.

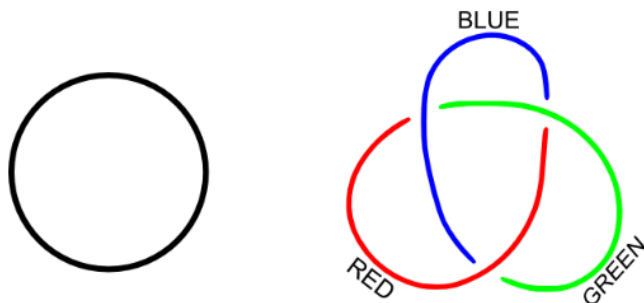


Figure 7: The unknot (not 3-colourable) and a diagram of a 3-colouring of the standard trefoil knot.

However, a complete invariant of knots has yet to be found, that is for all known invariants the reverse does not hold: if $i(K) = i(K')$ then K need not be equivalent to K' .

When (or perhaps if) a complete invariant is ever found, we will have a way of distinguishing all knots. For now, we will look at a number of examples of (incomplete) knot invariants, starting with 3-colourability, which gives us our first easy way of distinguishing many knots from the unknot.

Definition (3-colourability): A knot diagram is called 3-colourable if each arc can be assigned one of three colours, satisfying the following rules:

- at least two of the colours are used,
- at any crossing, either all three colours appear, or only one appears.

(Where an arc is an unbroken section of the knot diagram).

Example: The standard unknot diagram is not 3-colourable. But the standard diagram for the trefoil knot is 3-colourable, an example of such a colouring is shown in figure 7.

We now need to show this is a knot invariant.

Theorem 2 (Invariance of 3-colourability) If a diagram of a knot K is 3-colourable, then every diagram of K is 3-colourable. Hence, we may say the knot K itself is 3-colourable. (From the example above, this proves that the trefoil knot is indeed not the unknot).

There is a natural way to generalize this idea of colouring: instead of

using three colours for our 3-colourability invariant, we may instead label arcs with integers, 0, 1 and 2 - this way the relationship between arcs at a crossing (previously: all being the same colour, or all different) becomes an algebraic condition on integers (mod 3). The natural question then is whether we can look at similar relationships, but working in a different modulo.

We now look at two invariants (the crossing number, and the unknotting number), which both share the idea of looking at the minimal value of a property

of a knot. As we will see, both are quite obviously invariant by their definition, but both are very much more difficult to compute than other invariants, such as 3-colourability.

Definition (Crossing number): The crossing number $c(K)$ of a knot (or link) K is the minimum number of crossings in any diagram D of K . So if $c(D)$ is the number of crossings in a diagram D .

$$c(K) = \min\{c(D) : D \text{ is a diagram of } K\}.$$

Definition (Unknotting number): The unknotting number $u(K)$ of a knot K is the minimum, over all diagrams D of K , of the minimal number of crossing changes required to turn D into a diagram of the unknot, $u(D)$.

$$u(K) = \min\{u(D) : D \text{ is a diagram of } K\}.$$

These are both clearly invariants, as for a given knot all possibilities of isotopies are already taken into account in the definitions. This is also exactly why they are so difficult to compute. Suppose we have a diagram of a knot, how do we know if this particular diagram has minimal crossing number? Much like the problems surrounding the Reidemeister moves, technically we would have to check all possible diagrams.

Perhaps the most interesting invariants however, are polynomial valued knot invariants, known as knot polynomials. We will look at these in the next section.

6.4 Knot polynomials

Knot polynomials are particularly useful, as not only are they (relatively) simple to compute, but they also manage to distinguish large numbers of different knots. There are a number of different knot polynomials, the first of which was found by J. Alexander in 1928. We will begin by looking at the more recent Kauffman bracket polynomial, which was not discovered until 1987. What makes the bracket polynomial particularly interesting, is the way that it relates to state sums - an idea commonly used in physics and Biology. Its definition stems from the idea of splitting a knot diagram into a number of different states, by splicing crossings as shown in figure 8. In this way, a knot diagram can be decomposed into a number of states. The bracket polynomial is then defined as a particular summation over these states. An example is shown in figure 9. In this example we have decomposed a diagram of the figure eight knot into two states. This method can then be repeated to establish a complete family of state diagrams of trivial knots. **Definition (The bracket polynomial) :** The Kauffman bracket polynomial $\langle K \rangle$ of a knot (or link) K , is a Laurent polynomial defined by the rules:

- it satisfies the skein relation (shown below), which is a relation between the bracket polynomial of diagrams that are different only inside a small neighbourhood as shown in figure 10,

For this to be a knot invariant it is sufficient to ensure that the bracket polynomial remains invariant under the three Reidemeister moves. By imposing

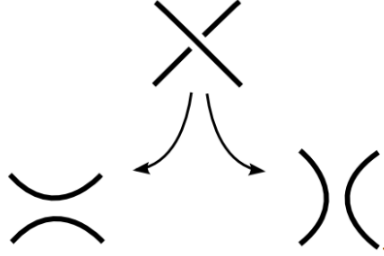


Figure 8:

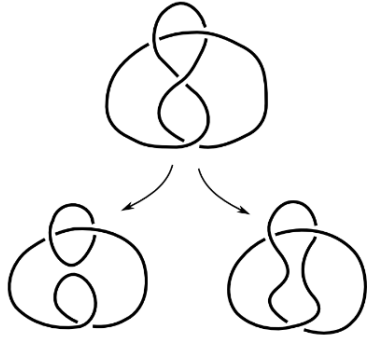


Figure 9:

$$\langle \text{crossing} \rangle = A \langle \text{two arcs facing} \rangle + B \langle \text{two arcs facing away} \rangle$$

- it satisfies:

$$\langle \bigcirc K \rangle = C \langle K \rangle$$

(where $\langle \bigcirc K \rangle$ is the disjoint union of a knot diagram K and the crossingless diagram of the unknot \bigcirc),

- and the normalisation:

$$\langle \bigcirc \rangle = 1$$

Figure 10:

$$\begin{aligned}
\langle \overline{\sigma} \rangle &= A \langle \overline{\sigma} \rangle + A^{-1} \langle \overline{\cup} \rangle \\
&= (-A^2 - A^{-2}) A \langle - \rangle + A^{-1} \langle - \rangle \\
&= -A^3 \langle - \rangle \\
\langle \overline{\sigma} \rangle &= A \langle \overline{\cup} \rangle + A^{-1} \langle \overline{\sigma} \rangle \\
&= A \langle - \rangle + (-A^2 - A^{-2}) A^{-1} \langle - \rangle \\
&= -A^{-3} \langle - \rangle
\end{aligned}$$

Figure 11: The bracket polynomial's 'failure' under R1 moves.

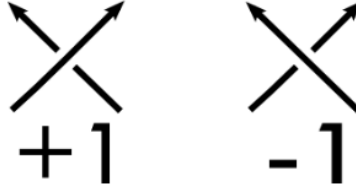


Figure 12: the crossing signs of an oriented knot diagram.

the fact that we want it to be invariant under Reidemeister move $R2$, we can determine that $B = A^{-1}$, and $C = -A^2 - A^{-2}$.

With these values for B and C the third Reidemeister move is also satisfied. However, although this is indeed invariant under $R2$ and $R3$ moves, $R1$ moves give different values for the bracket polynomial, see figure 11. Invariance under the second and third Reidemeister moves, but not the first, is known as regular isotopy, and has its own interpretation as an invariant of the topological embeddings of knotted, linked and twisted bands in three-dimensional space. In fact, it is usually possible to normalise a regular isotopy invariant to obtain an ambient isotopy invariant. The way we may normalise the bracket polynomial to be an ambient isotopy invariant of knot diagrams, requires the notion of an oriented knot and two definitions - the crossing sign, and the writhe.

Definition : A knot (or link) is said to be oriented if it has been given a direction along its curve. Equivalently each arc in its knot diagram is assigned a direction so that at each crossing the orientations appear as one of the two possibilities as seen in figure 12. The crossing sign (or crossing orientation) is the label $(+1)$ or (-1) to the crossing. **Definition** : The writhe of a diagram D , denoted $w(D)$, is the sum of the crossing signs $(+1$'s and -1 's) of all of the crossings in the given diagram.

It is easy to see that the writhe is invariant under $R2$ and $R3$ moves, and

each $R1$ move changes the writhe by ± 1 . We now have all of the ingredients to alter the bracket polynomial to make it an invariant for oriented knots and links. This new polynomial is often called the X polynomial:

Definition: The X polynomial of an oriented knot (or link) K is defined to be:

$$X(K) = (-A^3)^{-w(K)} \langle K \rangle.$$

Theorem 3 (Invariance of the X polynomial): The X polynomial is an invariant of oriented knot diagrams.

Proof: It is again sufficient to check that the X polynomial remains invariant under the three Reidemeister moves. We already know that the bracket and the writhe of a knot are invariant under $R2$ and $R3$ moves, and so $X(K)$ is also invariant under $R2$ and $R3$ moves. We thus only need to check $R1$ moves. If we denote a knot that includes a loop of one of the first two types as K^+ and a knot that includes a loop of one of the second two types as K^- , then:

$$\begin{aligned} X(K^+) &= (-A^3)^{-w(K^+)} \langle K^+ \rangle \\ &= (-A^3)^{-(w(K^+)-1)} (-A^{-3}) \langle K^+ \rangle \\ &= (-A^3)^{-(w(K^+)-1)} (-A^{-3}) (-A^3) \langle - \rangle \\ &= (-A^3)^{-(w(K^+)-1)} \langle - \rangle \\ &= X(-). \end{aligned}$$

Similarly, $X(K^-) = X(-)$.

Where $\langle - \rangle$ denotes the bracket polynomial of the knot K^+ after performing an $R1$ move at the given loop, and $X(-)$ denotes the X polynomial after performing an $R1$ move. Thus, the X polynomial is invariant under $R1$ moves.

The X polynomial is equivalent to another invariant knot polynomial, known as the Jones polynomial. Now that we have constructed the X polynomial, the Jones polynomial is easy to define by a simple change of variable:

Definition (Jones polynomial): The Jones polynomial of a knot K , denoted $V(K)$, is a polynomial in the variable t , obtained from the X polynomial via the transformation $A \rightarrow t^{-1/4}$. That is:

$$V(K)(t) = X(K)(t^{-1/4}).$$

When viewed in this way, the Jones polynomial looks like nothing more than a simple variation on the X polynomial (and hence the bracket polynomial). However, the importance of the Jones polynomial is really seen when we look at where its original definition came from.

The Jones polynomial was discovered by Vaughan Jones in 1984, and is widely accepted to have reinvigorated the study of knot theory. Jones' original construction, however, came from studying operator algebras, braid theory, and statistical mechanics. The fact that it can so easily be defined as an invariant of knots, as we have done here, suggests a significant connection between all of these (previously, very different) branches of mathematics and physics.

$$v^{-1}P(\text{X}) - vP(\text{X}) = zP(\text{O})(\text{O})$$

Figure 13:

$$\begin{aligned}
vP(\text{Trefoil}) &= v^{-1}P(\text{Trefoil}) - zP(\text{Trefoil}) \\
P(\text{Trefoil}) &= v^{-2}P(\text{O}) - v^{-1}zP(\text{Trefoil}) \\
&= v^{-2} - v^{-2}z(v^{-1}P(\text{Trefoil}) - zP(\text{Trefoil})) \\
&= v^{-2} - v^{-3}zP(\text{OQ}) + v^{-2}z^2P(\text{Q}) \\
&= v^{-2} - v^{-3}z(v^{-1} - v)z^{-1}P(\text{O})P(\text{Q}) + v^{-2}z^2 \\
&= v^{-2} - v^{-4} + v^{-2} + v^{-2}z^2 \\
&= 2v^{-2} - v^{-4} + z^2v^{-2}
\end{aligned}$$

Figure 14: Example showing how to calculate the Homfly polynomial of the trefoil knot.

After the discovery that the Jones polynomial could be defined using skein relations (as in the definition of the bracket polynomial), many people tried to come up with a general case. The result of this was the Homfly polynomial, named after six researchers who all published their results in 1985 . This is a general form of a linear skein relation for oriented knots. There are a number of forms of the Homfly polynomial, but they only differ by a change of variables.

Definition (Homfly polynomial): The Homfly polynomial of an oriented knot K , denoted $P(K)$, is a polynomial in two variables v and z , defined by the following rules: - the skein relation: (where the diagram below is a relation between the Homfly polynomial of diagrams that are different only in small neighborhoods as shown in figure 13)

- $P(0) = 1$, where (0) denotes the diagram of the unknot with no crossings.
- $P(K_1 \cup K_2) = (v^{-1} - v)z^{-1}P(K_1)P(K_2)$, where $(K_1 \cup K_2)$ denotes the disjoint union of diagrams K_1 and K_2 .

The proof that this is a knot invariant is similar to that of the X polynomial. An example calculation can be seen in Figure 14.

6.5 Computing and Algorithms in Knot Theory

Now that we have a reasonable collection of knot invariants, we may feel that we are in a strong position to distinguish many different knots. However, although

this is true, the actual task of calculating many of these invariants by hand, in particular knot polynomials, is a labourious task. This section explores how computers can be used to speed up the process. We begin by the use techniques, we then construct our own algorithm that could be implemented in a computer program to calculate the Homfly polynomial of a knot. Our aim in this section is to find a way that a computer may aid someone to the Homfly polynomial of a knot diagram, which requires little work by the user.

6.5.1 Dowker notation

We first have to understand the limitations of computers. Although their abilities to calculate very specific tasks very quickly are far beyond that of a human being, they do not have the ability to think for themselves; it is up to the human programmer to provide complete instructions detailing exactly what the computer must do. We also require that the information input is in a format that the computer can do simple calculations, and answer true/false questions. Furthermore, a computer is not able to ‘see’ a knot, (unless perhaps it was using some specialized graphics program, but these are in general very intensive on a computer’s memory), instead they require lists of numbers and characters to be input in order to do any calculations on them. We therefore need a new notation for our knots that can be read by a computer. Although there are a few ways this could be achieved, a popular choice of notation is the Dowker notation. It also has the direct benefit of being very easy to compute given a knot diagram: Construction : Starting with a diagram of a knot, choose any point on the To determine the Dowker notation for a knot, begin by choosing a point on the knot to be the ‘origin’. From the origin, choose a direction along the knot, and move around the diagram in that direction. The construction will be completed when you have made one full circuit of the diagram and reached the origin again.

As you move along the diagram, assign to each of the x crossings a number, $1, \dots, n$, (where $n = 2x$) in order each time you encounter it (thus assigning two different numbers to each crossing, one as you reach the crossing through an overcrossing arc, and one as an undercrossing arc).

Once this is done for all crossings (that is, you have reached the origin again), form ordered pairs (U_x, O_x) for each crossing x , where U_x is the number assigned to the undercrossing, and O_x is the number assigned to the overcrossing.

The set of ordered pairs is the Dowker notation for the particular knot presentation.

We begin by choosing an origin (represented by the black dot) in figure 15 and a direction (shown by the arrow). As we move around the knot, we assign numbers, in order, to the crossings (see centre diagram). When we arrive at each crossing for the second time, we form an ordered pair of the numbers assigned for the undercrossing arc and the overcrossing arc, where the first of the pair represents the undercrossing and the second the overcrossing (see diagram on right). The Dowker notation for this choice of origin and direction of the trefoil knot is therefore $T = \{(1, 4), (5, 2), (3, 6)\}$.

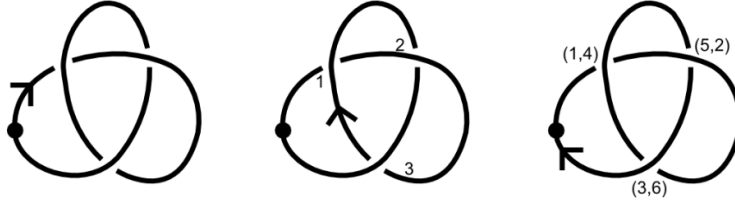


Figure 15: Example showing the calculation of a Dowker notation for the trefoil knot, T .

A given knot may have many different Dowker notations; however, once an origin and direction have been fixed, the knot has a unique Dowker notation.

It is worth noting here that it is also possible to draw a knot diagram given a Dowker notation, and so we do not lose any information by encoding a knot in this way. It is not true, however, that any Dowker notation represents a drawable knot diagram. For our purposes, we need not worry about this, as we will be assuming that we begin with a knot diagram and construct the Dowker notation from it. However, this fact could be used... within a program that implements our algorithm, in order to check that any Dowker notation input into the program does in fact represent a drawable knot - if it does not then the user must have made an error in calculating the Dowker notation of their knot diagram. Here, we will simply focus on calculating the Homfly polynomial. If we are now given a knot diagram we are able to calculate the Dowker notation, and therefore we have a way of storing the given knot onto a computer. The next section will look at how the Dowker notation can be implemented to calculate the Homfly polynomial using a computer algorithm.

6.5.2 Constructing the algorithm

Our algorithm assumes that the user calculates the Dowker notation themselves, and then inputs this into the algorithm (or ultimately, the computer program). We then also ask that the user calculate the crossing orientations (also called the crossing signs) of each of the crossings. We will now look at how we may calculate the Homfly polynomial using just this information.

6.5.3 Skein Relation

Throughout the calculation, we will have to apply the skein relation for the Homfly polynomial, as stated before. This poses a few problems, as the skein relation may require us to change crossings, or remove them altogether.

Changing a crossing (from a positive crossing to a negative crossing, or vice versa) is achieved by simply swapping the numbers corresponding to the overcrossing and the undercrossing components. That is, (U_x, O_x) becomes (O_x, U_x) , and the crossing orientation is opposite.

The next problem we need to address is how we may alter the Dowker notation to denote removed crossings. A simple way to do this is by replacing the ordered pair (U_x, O_x) at the corresponding crossing with the unordered pair $\{U_x, O_x\}$. However, we need to think a little about how we may interpret this in order to draw the resulting knot or link. If we have a Dowker notation with removed crossings, it is possible to find the components of the knot or link. We start with some number in the Dowker notation, and continue through the proceeding numbers, until we reach a removed crossing - we then 'switch' to the other number in the removed pair, and continue from there. If we arrive at the highest number in the Dowker notation before returning back to the original number, we must return back to 1, and continue from there. This method continues until we return to the original number that we started with. The sequence of numbers that we have now found represents one component of the link. If we have exhausted all numbers in the notation, then the Dowker notation has only one component, and so must simply represent a knot, (if not then the notation must represent a link). If we have not come across all numbers yet, we then pick the lowest number not found in the first component, and continue in the same way to calculate the sequence of numbers that correspond to this next component of the link. This is done until all numbers have been exhausted, and thus, all components found. It is easiest to see how this works in an example, see figure 15.

6.5.4 Loops

Using this notation for removed crossings, we can simplify our diagrams and speed up calculation of our algorithm, by checking for loops where we may apply the first Reidemeister move. It is possible to find situations where this is possible, from the Dowker notation, as any crossing of the form $(n, n + 1)$ or $(n + 1, n)$ must cause a loop, see figure 17. In fact, any crossing that is made up from consecutive numbers in the same component must cause a loop. By looking for these in the algorithm, we can simply remove crossings. the first Reidemeister move. As the Homfly polynomial is invariant under the first Reidemeister move, this will still give the correct value

6.5.5 Trivial diagrams

We can simplify our calculation further by checking for diagrams of the unknot, as we know that the unknot U has Homfly polynomial $P(U) = 1$. So our first check is to see if we have a trivial diagram of the unknot. This is a simple matter of calculating the number of crossings, which may be done by calculating the number of ordered pairs in the Dowker notation. If there are no ordered pairs, then the Dowker notation must represent the trivial diagram of the unknot, and we are done.

We also know that any knot (but not link) with fewer than three crossings must be the unknot - this is easy to check. So, if our diagram only has one component (that is, it is a knot), then if the number of crossings is fewer than

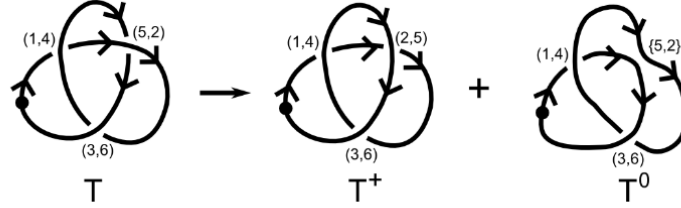


Figure 16: Example showing how the skein relation is applied to the Dowker notation of the trefoil knot

three, the diagram represents the unknot, and so $P(K) = 1$.

$$\begin{aligned} T &= \{(1, 4), (5, 2), (3, 6)\} \\ T^+ &= \{(1, 4), (2, 5), (3, 6)\} \\ T^0 &= \{(1, 4), \{5, 2\}, (3, 6)\} \end{aligned}$$

The left-hand diagram shows a Dowker notation for the trefoil knot T . Supposing we applied the skein relation for the Homfly polynomial on the crossing denoted $(5, 2)$, we would get: $vP(T) = v^{-1}P(T^+) - zP(T^0)$, where T^+ is the same diagram but with the crossing $(5, 2)$ changed to $(2, 5)$, and T^0 is the diagram with the crossing removed, $\{5, 2\}$, as shown. Notice that the crossing orientation of $(5, 2)$ in T was -1 (negative), and in T^+ the crossing orientation of $(2, 5)$ is $+1$ (positive). The components of T^0 are calculated as such: starting with 1, the next number is 2, which is part of a removed crossing, so we ‘switch’ to the other number in the removed pair, 5. The next number is then 6, which returns back to our original number 1, and so we have found a component of the link. The number 3 has not been used yet, and so must be part of a different component. This second component is found as we move on to 4, then to 5, which is part of a removed crossing, so we switch to 2, which returns us to 3. All numbers are used, so we conclude that there are 2 components in this diagram, $\{1, 6\}$ and $\{3, 4\}$.

To check for other diagrams of the unknot, it is useful to use the following lemma.

Lemma: A descending or ascending diagram always represents a trivial knot. Where a diagram is called ascending if it is possible to choose a starting point and a direction around the knot, so that each crossing is first encountered on the under-crossing strand. Similarly, a descending diagram is where each crossing is first encountered on the over-crossing strand.

If our diagram has only one component (so that it is a knot), then it is easy to check for an ascending or descending diagram; in this case, we have chosen to only look for ascending diagrams. To see if a knot diagram is ascending using only the Dowker notation, We only need to look at each crossing (each ordered pair) in turn. If the undercrossing number is less than the overcrossing

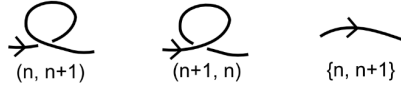


Figure 17: Diagrams showing how crossings of the form $(n, n + 1)$, and $(n + 1, n)$ form a loop, and can then be removed.

number for all crossings ($U_x < O_x$ for all crossings x), then our diagram is ascending. This is because using the origin and direction as decided in the construction of the Dowker notation as our starting point - $U_x < O_x$ signifies that we encounter the crossing x in the undercrossing component first. If this is true for all crossings, then this satisfies the definition of an ascending diagram, and so our diagram is trivial and has Homfly polynomial $P(K) = 1$.

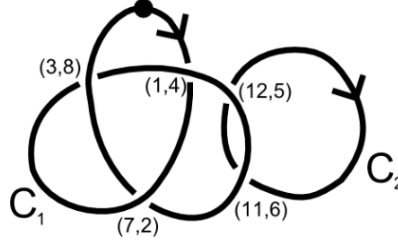
We now have two methods for checking if we have a trivial diagram of a knot, but we still need a way to use these methods if we are looking at a link diagram.

6.5.6 Link diagrams

The first thing we need to be able to check, is whether components in a link diagram are disjoint, or ‘linked together’. We can find out if a component is linked, by looking at where it crosses other components in the diagram. Assuming we have calculated which numbers in the Dowker notation correspond to which components (see section 6.5.3 for how this is done), then it is easy to know which crossings we should be looking at - simply discard any pairs that have both numbers in a single component, or both numbers in components other than the one we are looking at. The remaining crossings correspond to where this component crosses other components. Now that we have chosen the relevant crossings, we can check if the component is disjoint from the rest of the diagram, by seeing if it sits ‘above’ or ‘below’ the rest of the diagram. This is achieved by looking at the numbers within these crossings, that are elements of the component we are interested in. If all of these numbers are undercrossing parts, then the component must sit ‘below’ the rest of the diagram; if the numbers are all overcrossing parts then the component sits ‘above’. In either of these situations, the component we are looking at is disjoint from the rest of the diagram. If these numbers are a mixture of undercrossing and overcrossing parts, then we cannot deduce if it is disjoint. If we establish that the components are disjoint, we apply the third defining rule for the Homfly polynomial:

$$P(K_1 \cup K_2) = (v^{-1} - v)z^{-1}P(K_1)P(K_2),$$

(if the diagram can be separated into disjoint components K_1, K_2). If we cannot deduce if the components are disjoint, then we apply the skein relation again. Our next problem, however, is how to change the Dowker notation to distinguish these separate components K_1, K_2 .



$$L = \{(1, 4), (7, 2), (3, 8), (12, 5), (11, 6), \{9, 14\}, \{10, 13\}\}$$

Components: $C_1 = 1, 2, 3, 4, 5, 6, 7, 8$

$C_2 = 11, 12.$

Separated Dowker notations: $C_1 = \{(1, 4), (7, 2), (3, 8)\}$

$C_2 = \emptyset$

$L - C_1 = \{\{9, 14\}, \{10, 13\}\}$

$L - C_2 = \{(1, 4), (7, 2), (3, 8), \{9, 14\}, \{10, 13\}\}.$

Figure 18: Example showing how to separate the Dowker notations of disjoint components of a link L . The Dowker notation for the link L is shown above. From this we may calculate the components C_1 , C_2 as usual. The separated Dowker notations are then calculated by choosing the correct pairs of numbers from the Dowker notation of the link, as described in section 6.5.6, the results are shown above.

Supposing we find a disjoint component C_i of a link diagram L , we need a way to distinguish this component, and the link diagram without this component (which we denote $L - C_i$). To do this, we allow C_i to be represented by the pairs of numbers in the Dowker notation of L that are made up only from elements of C_i . The diagram $L - C_i$ is then made up from the Dowker notation of L without any pairs involving C_i . See the example in Figure 18. The only complication that we must face is that, by removing some crossings, we may remove some numbers in a sequence (for example, in Figure 18 the remaining trefoil knot, component C_1 , is described by numbers $\{1, 2, 3, 4, 7, 8\}$ - we are missing 5 and 6). This is overcome by simply ignoring any gaps in a sequence; if a number is not represented then simply move on to the next number until you arrive at a number that is represented, (starting again at 1 if you have reached the highest number in the notation), until you reach your original number again. There is no problem with doing this, as when separating components in this way, we only ever remove crossings between disjoint components and so the sequence of numbers should continue in the desired way.

6.5.7 Does the algorithm finish?

We now have all of the required techniques to make up the algorithm, however we need to ensure that the algorithm eventually stops and does not get stuck in a loop. Notice that when calculating the Homfly polynomial, and applying the skein relation, we must remove crossings and swap crossing orientations. Although removing crossings will always eventually lead to trivial components, swapping the crossing orientations does not guarantee that we simplify the diagram. To ensure that we always apply the skein relations in a way that will simplify our diagram, we aim to change the crossings so that they will lead to an ascending or descending diagram. In this way the diagram will always be simplified, ultimately resulting in trivial components. We have chosen here to aim for ascending diagrams, which may be achieved by only ever applying the skein relation to a crossing x , that has $U_x > O_x$ (or to crossings between separate components). In this way, we will always end up with a diagram where all crossings satisfy $U_x < O_x$, and is therefore ascending. We could equally have chosen to apply the skein relations in a way to ensure that we had descending diagrams. By constructing the algorithm in this way, although it may require that we run through the algorithm multiple times (for each new knot or link that the skein relation produces), we will always be simplifying our original diagram, and hence the algorithm will eventually finish. We will now see the completed algorithm in the form of a flow chart, and run through an example calculation.

6.5.8 Algorithm for calculating the Homfly polynomial

the next figure (19) showing our algorithm for calculating the HomFly polynomial:

Where:

$$(1) \quad P(L_+) = v^2 P(L_-) + zv P(L_0)$$

$$(2) \quad P(L_-) = v^{-2} P(L_+) - zv^{-1} P(L_0)$$

$$\delta = (v^{-1} - v)z^{-1}.$$

6.5.9 An example calculation

In this section, we see how the algorithm would work for the trefoil knot. Another example calculation can be found in Appendix C, where we use the algorithm to calculate the Homfly polynomial of the figure-eight knot. We have not attempted to lay these calculations out exactly how a computer program would calculate them, as this would not only depend greatly on the programming language used but would almost certainly be harder to follow. Instead, we lay them out within a table: in the left column, which step in the algorithm we have reached; in the center column, how this step may be evaluated; in the right-hand column, the result of this step. In this way, it should be relatively straightforward to follow the calculation through the flowchart in figure 19.

Step	Evaluation	Result
Read Dowker notation and crossing orientation.		$T = \{(1, 4), (5, 2), (3, 6)\},$ $\{-1, -1, -1\}$
Calculate number of crossings = k .	3 crossings	$k = 3$
Does $k = 0$?	$k = 3$	No.
Calculate components.	$1 \rightarrow 2 \rightarrow 3 \rightarrow$ $4 \rightarrow 5 \rightarrow 6.$	Components: $\{1, 2, 3, 4, 5, 6\}.$
Remove crossings with consecutive numbers from the same component.	No loops.	$k = 3$
Does $k = 0$?	$k = 3$	No.
Recalculate components. let n = number of components.	$1 \rightarrow 2 \rightarrow 3 \rightarrow$ $4 \rightarrow 5 \rightarrow 6.$	$n = 1$, components: $\{1, 2, 3, 4, 5, 6\}.$
Does $n = 1$?	$n = 1$.	Yes.
Is $k < 3$?	$k = 3$	No.
For each crossing x is $U_x < O_x$?	Crossing 1: $1 < 4$ Yes. Crossing 2: $5 > 2$ No.	No for $x = 2$.
Read orientation of crossing.	Crossing 2 is negative.	-1
Is crossing positive?	Negative.	No.
Apply (2).		$P(T) = v^{-2}P(L_+) - zv^{-1}P(L_0)$

Figure 20:

Step	Evaluation	Result
For L_0 change (U_x, O_x) to $\{U_x, O_x\}$	$(5, 2) \rightarrow \{5, 2\}.$	$L_0 = \{(1, 4), \{5, 2\}, (3, 6)\}$ Orientation: $\{-1, -1\}.$
For L_+ , change (U_x, O_x) to (O_x, U_x) and change orientation.	$(5, 2) \rightarrow (2, 5)$ $-1 \rightarrow +1$	$L_+ = \{(1, 4), (2, 5), (3, 6)\}$ Orientation: $\{-1, +1, -1\}.$

Figure 21:

We will use the Dowker notation for the trefoil knot that we calculated in Figure 15 : $T = \{(1, 4), (5, 2), (3, 6)\}$. We may also calculate that this has respective crossing orientations $\{-1, -1, -1\}$. We now have that the Homfly polynomial of the trefoil knot is:

$$P(T) = v^{-2}P(L^+) - zv^{-1}P(L^0),$$

and we have the Dowker notation of L^+ and L^0 . The program must now run through the algorithm again for both L^+ and L^0 . The order this is done does not matter - the order here was chosen simply to make the calculation easier. The Homfly polynomial of the trefoil knot is now:

$$P(T) = v^{-2}(1) - zv^{-1}P(L^0).$$

We now look at the algorithm computing the Homfly polynomial of L^0 . So the

Step	Evaluation	Result
Read Dowker notation and crossing orientation.		$L = \{(1, 4), (2, 5), (3, 6)\}, \{-1, +1, -1\}$
Calculate number of crossings = k	3 crossings	$k = 3$.
Does $k = 0$?	$k = 3$	No.
Calculate components.	$1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow 6$.	Components: $\{1, 2, 3, 4, 5, 6\}$.
Remove loops.	No loops.	$k = 3$
Does $k = 0$?	$k = 3$	No.
Recalculate components let n = number of components.	$1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow 6$	$n = 1$, components: $\{1, 2, 3, 4, 5, 6\}$.
Does $n = 1$?	$n = 1$.	Yes.
Is $k < 3$?	$k = 3$	No.
For each crossing x is $U_x < O_x$?	Crossing 1: $1 < 4$ Yes. Crossing 2: $2 < 5$ Yes. Crossing 3: $3 < 6$ Yes.	Yes for all x .
$P(L) = 1$		$P(L) = 1$.

Figure 22: first evaluating L^+ :

Homfly polynomial of the trefoil knot is:

$$\begin{aligned}
P(T) &= v^{-2} - zv^{-1}(v^{-2}(\delta(1)) - zv^{-1}) \\
&= v^{-2} - zv^{-3}(v^{-1} - v)z^{-1} + z^2v^{-2} \\
&= v^{-2} - v^{-4} + v^{-2} + z^2v^{-2} \\
&= 2v^{-2} - v^{-4} + z^2v^{-2}.
\end{aligned}$$

This is indeed the correct answer for the Homfly polynomial (see figure 14). If this algorithm were to be implemented by a computer program, it would only require that the user calculates the Dowker notation of their given knot diagram, and the crossing orientations. This is a much quicker, and easier task than calculating the Homfly polynomial by hand.

We have now seen some techniques that allow us to use computers to aid us in storing information and doing calculations on knots.

In the ext section we will discuss the Tangles and its relation to DNA Biology.....

6.6 Introduction To Tangles

article amsmath

This section relies on the literature and as well as the article . The closed 3-ball B^3 is bounded by the sphere S^2 . Fix two points on the sphere (say the north and south pole) and attach a curve between them embedded in B^3 . The

Step	Evaluation	Result
Read Dowker notation and crossing orientation		$L = \{(1, 4), \{5, 2\}, (3, 6)\}, \{-1, -1\}.$
Calculate number of crossings = k	2 crossings	$k = 2.$
Does $k = 0$?	$k = 2$	No.
Calculate components.	$1 \rightarrow (5) \rightarrow 6,$ $3 \rightarrow 4 \rightarrow (2).$	Components: $C_1 = \{1, 6\},$ $C_2 = \{3, 4\}.$
Remove loops.	No loops.	$k = 2$
Does $k = 0$?	$k = 2$	No.
Recalculate components, let n = number of components.	$1 \rightarrow (5) \rightarrow 6,$ $3 \rightarrow 4 \rightarrow (2).$	$n = 2$, components: $C_1 = \{1, 6\},$ $C_2 = \{3, 4\}.$
Does $n = 1$?	$n = 2.$	No.
Let $i = 1.$		$i = 1.$
Is $i > n$?	$i = 1, n = 2.$	No.
Look only at crossings involving elements from both C_1 and some other component.	$1 \in C_1$ and $4 \in C_2,$ so look at $(1, 4),$ $3 \in C_2$ and $6 \in C_1,$ so look at $(3, 6).$	Look at crossings: $\{(1, 4), (3, 6)\}.$
Of these, are all elements of C_1 under, or all over?	1 is under, 6 is over.	No.
Set $i = i + 1.$	Set $i = 1 + 1$	$i = 2$
Is $i > n$?	$i = 2, n = 2$	No.
Look only at crossings involving elements from both C_2 and some other component.	$1 \in C_1$ and $4 \in C_2,$ so look at $(1, 4),$ $3 \in C_2$ and $6 \in C_1,$ so look at $(3, 6).$	Look at crossings: $\{(1, 4), (3, 6)\}.$
Of these, are all elements of C_2 under, or all over?	3 is under, 4 is over.	No.
Set $i = i + 1.$	Set $i = 2 + 1$	$i = 3$
Is $i > n$?	$i = 3, n = 2.$	Yes.
Choose a crossing involving two different components.	First crossing: $(1, 4)$ involves C_1 and $C_2.$	$(1, 4).$
Read orientation.	$(1, 4)$ is negative.	-1
Is crossing positive?	Negative.	No.
Apply (2).		$P(L) = v^{-2}P(L_+) - zv^{-1}P(L_0)$

Figure 23: the algorithm computing the Homfly polynomial of (L_0)

Step	Evaluation	Result
For L_0 , change (U_x, O_x) to $\{U_x, O_x\}$	$(1, 4) \rightarrow \{1, 4\}$	$L_0 = \{\{1, 4\}, \{5, 2\}, (3, 6)\}$, Orientation: $\{-1\}$.
For L_+ , change (U_x, O_x) to (O_x, U_x) and change orientation.	$(1, 4) \rightarrow (4, 1)$ $-1 \rightarrow +1$	$L_+ = \{(4, 1), \{5, 2\}, (3, 6)\}$ $\{+1, -1\}$

The Homfly polynomial of the trefoil knot is now:

$$P(T) = v^{-2} - zv^{-1}(v^{-2}P(L_+) - zv^{-1}P(L_0)),$$

where we have the Dowker notation for these new L_+ and L_0 given in the table above, and must now calculate the Homfly polynomial of these using the algorithm. We start with L_0 :

Step	Evaluation	Result
Read Dowker notation and crossing orientation.		$L = \{\{1, 4\}, \{5, 2\}, (3, 6)\}$. $\{-1\}$
Calculate number of crossings = k	1 crossing.	$k = 1$.
Does $k = 0$?	$k = 1$	No.
Calculate components,	$3 \rightarrow 6$.	Components: $C_1 = \{3, 6\}$
Remove loops. Recalculate k .	$3 \rightarrow 6$ Remove (3,6)	$L = \{\{1, 4\}, \{5, 2\}, \{3, 6\}\}$ $k = 0$.
Does $k = 0$?	$k = 0$	Yes.
$P(L) = 1$		$P(L) = 1$.

We now have that the Homfly polynomial of the trefoil knot is:

$$P(T) = v^{-2} - zv^{-1}(v^{-2}P(L_+) - zv^{-1}(1)).$$

We now calculate the Homfly polynomial of this L_+ :

Step	Evaluation	Result
Read Dowker notation and crossing orientation.		$L = \{(4, 1), \{5, 2\}, (3, 6)\}$. $\{+1, -1\}$
Calculate number of crossings = k	2 crossings.	$k = 2$.
Does $k = 0$?	$k = 2$	No.
Calculate components.	$1 \rightarrow (5) \rightarrow 6$, $3 \rightarrow 4 \rightarrow (2)$.	Components: $C_1 = \{1, 6\}$ $C_2 = \{3, 4\}$
Remove loops.	No loops.	$k = 2$
Does $k = 0$?	$k = 2$	No.

Figure 24:

Step	Evaluation	Result
Recalculate components, let n = number of components.	$1 \rightarrow (5) \rightarrow 6,$ $3 \rightarrow 4 \rightarrow (2).$	$n = 2$, components: $C_1 = \{1, 6\}$ $C_2 = \{3, 4\}$
Does $n = 1$?	$n = 2$	No.
Let $i = 1$		$i = 1$
Is $i > n$?	$i = 1, n = 2$	No.
Look only at crossings involving elements from both C_1 and some other component.	$1 \in C_1$, and $4 \in C_2$, so look at $(4, 1).$ $3 \in C_2$ and $6 \in C_1$, so look at $(3, 6).$	Look at crossings: $\{(4, 1), (3, 6)\}.$
Of these, are all elements of C_1 under, or all over?	1 is over, 6 is over.	Yes.
$P(L) = \delta P(L - C_1)P(C_1)$	$L - C_1 = \{\{5, 2\}\},$ $C_1 = \emptyset$	$P(L) = \delta P(L - C_1)P(C_1)$

The Homfly polynomial of the trefoil knot is now:

$$P(T) = v^{-2} - zv^{-1}(v^{-2}(\delta P(L - C_1)P(C_1)) - zv^{-1}).$$

We now need to calculate the Homfly polynomial of these $(L - C_1)$ and C_1 . We start with C_1 :

Step	Evaluation	Result
Read Dowker notation and crossing orientation.		$L = \emptyset$
Calculate number of crossings = k .	No crossings.	$k = 0$
Does $k = 0$?	$k = 0$	Yes.
$P(L) = 1$		$P(L) = 1$

The Homfly polynomial of the trefoil knot is now:

$$P(T) = v^{-2} - zv^{-1}(v^{-2}(\delta P(L - C_1)(1)) - zv^{-1}).$$

We now calculate the Homfly polynomial of $L - C_1$:

Step	Evaluation	Result
Read Dowker notation and crossing orientation.		$L = \{\{5, 2\}\}$
Calculate number of crossings = k	No crossings.	$k = 0$
Does $k = 0$?	$k = 0$	Yes.
$P(L) = 1$		$P(L) = 1$

Figure 25:

```

1  def homfly_polynomial(dowker_code):
2      # Initialize variables
3      crossings = 0
4      components = 0
5      is_crossing_positive = True
6      u, v, z = 1, 1, 1
7
8      # Iterate through the Dowker code
9      for i in range(len(dowker_code)):
10         if dowker_code[i] == 0:
11             # Remove crossings with consecutive numbers
12             while i + 1 < len(dowker_code) and dowker_code[i + 1] == dowker_code[i] - 1:
13                 i += 1
14         else:
15             # Calculate the number of crossings
16             crossings += 1
17
18             # Determine the crossing type (positive or negative)
19             is_crossing_positive = dowker_code[i] > 0

```

Figure 26: Implementation of the Algorithm in Python

curve can be knotted but self-intersections are not permitted. This is called a $(1,1)$ -tangle. Similarly, fixing 4 points on the sphere (preferably evenly spread on a great circle) and connecting them with two curves embedded in B^3 gives a $(2,2)$ -tangle. So, $2n$ fixed points connected by n curves is called a (n,n) -tangle. A tangle is the set (B^3, T) , where T is the collection of curves joining the points in pairs. This notation will be shortened and we let T denote the tangle.

There are several different types of tangles but all tangles henceforth will be $(2,2)$ -tangles, and for simplicity referred to as tangles. Some terminology for the fixed points on S^2 : denote these NW, NE, SW and SE (for northwest, etc.). A tangle diagram is a projection formed according to the rules of knot diagrams with the extra restriction that the points $\{NW, NE, SW, SE\}$ should end up as shown in Figure 27. If you connect NW with NE, and SW with SE, outside of B^3 , as shown in Figure 28, you have formed the numerator of T , denoted

$N(T)$. Connecting NW with SW, and NE with SE instead, give the denominator of T , $D(T)$. The numerator and the denominator gives us a natural connection between knots (or links) and tangles. This make it possible to view a tangle as a part of a knot. article amsmath

Definition:

If an orientation-preserving homeomorphism $f : B^3 \rightarrow B^3$ satisfies the following conditions, then the tangles T_1 and T_2 are said to be equivalent:

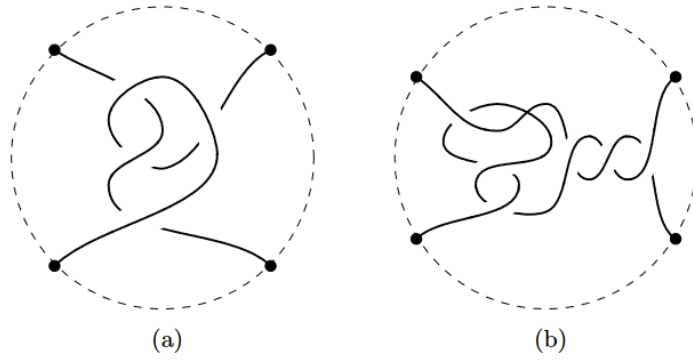


Figure 27: wo examples of tangles.

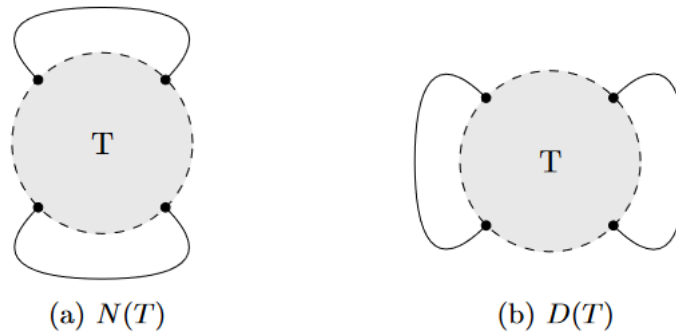


Figure 28: Numerator and denominator of a tangle.

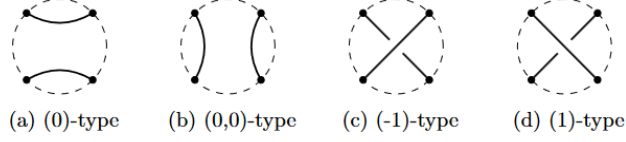


Figure 29: Exceptional tangles

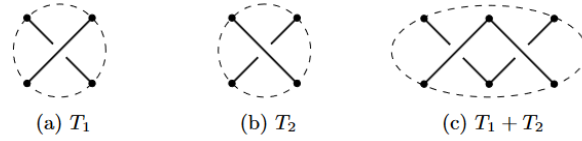


Figure 30: sum of tangles

1. f is the identity map for S^2 , i.e., the map keeps S^2 fixed,
2. $f(T_1) = T_2$.

As for knots, Reidemeister moves can be used to manipulate the tangle diagrams. It is, however, important to remember that the strings can never be drawn outside the circle. This would represent a part of the tangle leaving B^3 and in doing so creating more intersections in S^2 . The formal sum of tangles, $T_1 + T_2$, is formed by gluing the east hemisphere of B_1^3 (containing T_1) to the west hemisphere of B_2^3 (containing T_2), identifying NE and SE of T_1 to NW and SW of T_2 respectively. Lastly, remove the gluing face to make one ball B^3 containing $T_1 + T_2$. This is illustrated diagrammatically in Figure 30. A vital observation is that even if $N(T_1)$ and $N(T_2)$ are non-trivial knots, $N(T_1 + T_2)$ could still yield the unknot (or a trivial link).

Look at the tangles shown in Figure 29. These are four different types of tangles, the (0)-type, (0,0)-type also called the (1)-type, (-1)-type and (1)-type respectively. Collectively we call these tangles the exceptional tangles. With knots we restricted ourselves to tame knots, similarly we shall now restrict our study to what is called rational tangles.

Definition:

Suppose f is a homeomorphism that maps the ball B^3 to itself and maps the set of points $\{NW, NE, SW, SE\}$ to itself, but not necessarily as the identity map (i.e., f need not map NW to NW, etc.). A rational tangle is a tangle that is the image of the (0, 0)-type tangle under this homeomorphism. Rational tangles are in some literature referred to as trivial tangles. All exceptional tangles are rational, by rotating (0, 0) by $\pi/2$ we can obtain (0).

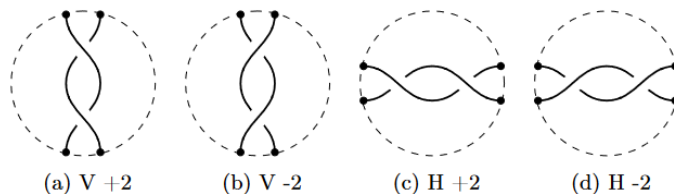


Figure 31: Orientations of vertical and horizontal twists

Imagine holding the ball with $(0, 0)$ in it, induce a half twist by taking the points SW and SE and rotating them around each other so they change places, this will give you either (1) or (-1) depending on which direction you rotate. There are many rational tangles and one way to form them is by doing twists, just as the one just described. A vertical twist is a twist around a vertical Axis that keeps NW and NE fixed but interchanges SW and SE. A horizontal twist is a twist around a horizontal axis performed by keeping NW and SW fixed and rotating so that NE and SE interchange. Each twist has a natural orientation, we call them positive twists and negative twists (denoted by $+$ and $-$ respectively), see Figure 31. Look at the exceptional tangles: (1) is obtained either by a negative vertical twist of (0) or a negative horizontal twist. Similarly, the (-1) -type comes from a positive twist. Description of vertical and horizontal twists. All trivial tangles can be made from (0) or $(0,0)$ using only vertical and horizontal twists. If we alternate between horizontal and vertical twists we get more complex looking tangles. A tangle constructed from twists will be denoted $T(a_1 \dots a_n)$ where $(a_1 \dots a_n)$ describes the sequence of twists in the following way:

- If n is even, start with the $(0, 0)$ -type, make a_1 vertical twists followed by a_2 horizontal, and so on alternating the twists, until you finally perform an horizontal twist.
- If n is odd, start with the (0) -type, make a_1 horizontal, a_2 vertical, ..., a_n horizontal.

We allow $a_i = 0$, so we can have $T(3, 0)$ for example. It is beneficial, or rather it will give us a shorter notation, if we require that $a_i \neq 0$, for $i \neq n$. The following example illustrates why this restriction works.

Example: The tangles in Figure 27 are $T_a(2, 1, 1, 0)$ and $T_b(2, 2, 3)$.

7 From Knots to Genes: The real Meaning of the Beauty in studying DNA Topology!

One of the most significant applications of knot theory to biology is as it pertains to DNA, the molecule that contains the genetic code for all living organisms. DNA can be visualized as a complicated knot that must be unknotted

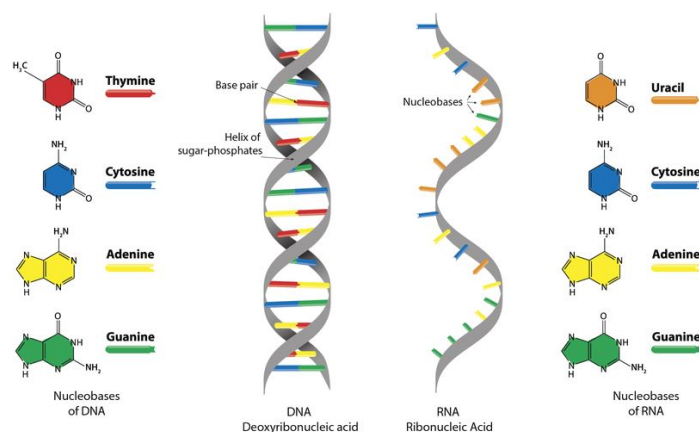


Figure 32: DNA and RNA Structure

by enzymes in order for replication or transcription to occur. It is perhaps not surprising then that connections between mathematical knot theory and biology have been discovered. By thinking of DNA as a knot, we can use knot theory to estimate how hard DNA is to unknot. This can help us estimate properties of the enzymes that unknot DNA.

7.1 A Background of DNA

DNA has a very particular structure illustrated in Figure 32: a DNA molecule is composed of two molecular strands twisted together in a double helix held together by pairs of nitrogenous bases bonded together in between them. There are four possible bases: adenine (A), thymine (T), guanine (G), or cytosine (C). However, there are only four specific pairings - AT, TA, CG, and GC - as adenine only bonds with thymine and guanine only with cytosine. Because of the small number of possible pairings, each DNA molecule must contain millions of pairs to hold all the genetic information necessary for life. To make matters worse, this genetic material is usually very tangled, which makes it very difficult to replicate, copy, or modify the DNA when the cell's biological mechanisms require it.

7.2 Topoisomerases and DNA Manipulation

In order to make these disorganized tangles of DNA easier to work with, cells use enzymes called topoisomerases to manipulate the DNA topologically. Specific enzymes can perform very sophisticated manipulations on DNA, but

topoisomerases can also perform several more general actions, as pictured in figure 33. Scientists use circular (cyclic) DNA, or DNA molecules whose ends are joined, to examine the effects of these enzymes. On linear DNA, any knots

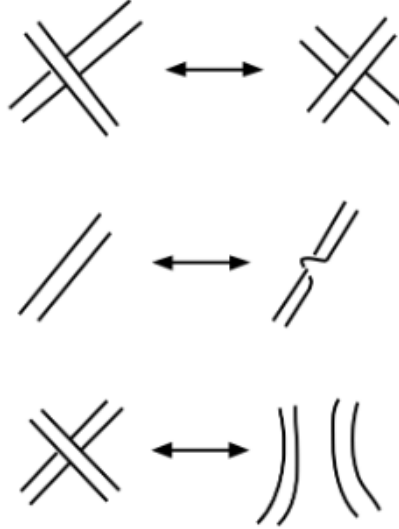


Figure 33: Three actions that topoisomerases can perform on DNA.

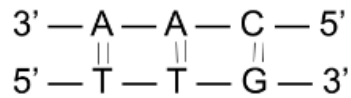


Figure 34: Linear duplex DNA is antiparallel.

caused by the enzyme would slip off the end, while they would be captured in a circular molecule. Both single-stranded and duplex (double-stranded) forms of cyclic DNA are common not only in bacteria and viruses but also in human mitochondria. However, although they appear naturally, scientists often apply enzymes to artificially created, synthetic cyclic DNA to determine their effects. To create this cyclic DNA, scientists attach the tail ends of a strand of linear duplex DNA to the head ends. However, a wrinkle appears when we consider that DNA has a set orientation. Each strand contains sugar molecules, and depending on the orientation of the sugar molecules at either end, one end is defined as 3' and the other as 5'. Further, the structure of linear duplex DNA is antiparallel, so one strand's 3' end will correspond to the other's 5' end, and vice versa.

When attaching the heads to the tails, we must attach a 3' end to a 5'

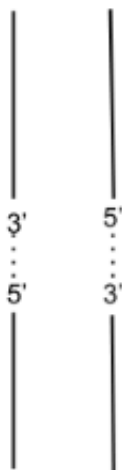


Figure 35: Because the 3' end of DNA must be attached to a 5' end, each strand's head gets attached to its own tail

end, as illustrated in figure 35. Therefore, each strand's head gets attached to its own tail, and the strands form a link rather than a knot. We keep the fundamental structure of cyclic DNA in mind when we examine the effects of enzymes on these molecules. One particular action an enzyme may take is site-specific recombination, where the enzyme attaches to two specific sites on two strands of DNA (recombination sites), cuts the strands connecting these sites, and reconnects the ends in a new order.

To study these site-specific recombinations more closely, scientists create single-stranded circular DNA molecules that contain copies of the recombination sites. They can then examine the DNA after introducing the enzyme to see how the molecule's structure has changed. When creating these circular molecules, scientists also choose an orientation for each recombination site. This is possible because each recombination site is defined as a nonpalindromic sequence of base pairs that can be read differently either forwards or backwards. There are two possibilities for this circular DNA: either we have direct repeats, where both recombination sites face the same direction, or inverted repeats, where they face opposite directions (Figure 37). The goal is to choose orientations that will match when the enzyme pulls the sites together. When the sites are pulled together, the resulting molecule, called a product, can take on several forms, as shown in figure 38. In this setting, we can examine the effects of enzymes by using tangles. The substrate molecule (the molecule before the enzyme acts): the site tangle T , where the enzyme acts, and the substrate tangle S , the rest

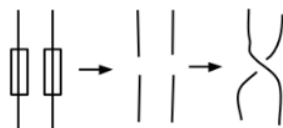


Figure 36: An example of a site-specific recombination. Here, the enzymes recombine the two strands such that they form a new crossing

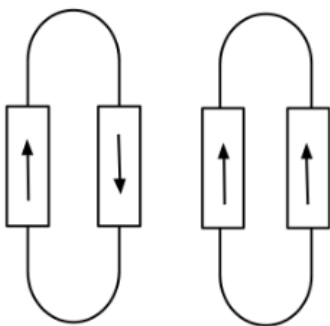


Figure 37: Direct repeats (left) and inverted repeats (right) on a piece of cyclic DNA.

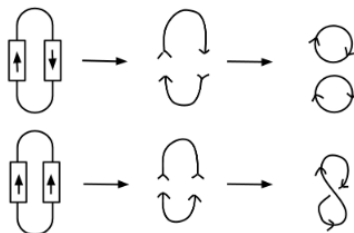


Figure 38: Direct repeats (top) produce a two-component link, while inverted repeats (bottom) produce a projection of the unknot.

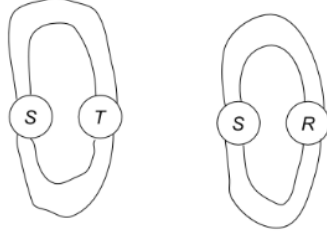


Figure 39: Enter Caption



Figure 40: The Whitehead link. For an image of the figure-eight knot,

of the molecule that the enzyme does not affect. After the enzyme acts, the site tangle is replaced by the recombination tangle, denoted by R (Figure 39), in the product molecule. To represent the molecules formed by these tangles, we use the notation $N(Q)$, which denotes the knot or link formed when we connect the top two and bottom two strands of a knot Q to each other. We also let $Q + V$ denote the tangle we get when we add the tangles Q and V . Therefore, we can write the substrate molecule as $N(S + T)$ and the product molecule as $N(S + R)$. Studies of this type have been done on many enzymes, including Tn3 re- solvase, which acts on cyclic DNA with direct repeats. Usually, this enzyme acts in the same way that we describe above - by replacing the T tangle with an R tangle - but occasionally, it will add in extra R tangles. Adding these extra tangles produces more complicated product molecules: adding two R tangles instead of one produces the figure-eight knot, while adding three produces the Whitehead link (Figure 40).

7.3 Writhe and Supercoiling

As we have seen, enzymes usually act on DNA molecules by adding and subtracting tangles at the recombination sites. However, the term "site" is a little



Figure 41: A ribbon modeling cyclic duplex DNA.

misleading - in fact, though the enzyme attaches to a particular location on the DNA, its actions affect the shape of the entire molecule. In order to describe these broader-reaching effects, we must define some new terminology relating to cyclic duplex DNA. Because duplex DNA is made of two antiparallel strands (Figure 34), we can model it as a flat ribbon, with the strands on each edge of the flat side, as seen in Figure 41. Because it is cyclic, we can make this ribbon a continuous loop. We now define several characteristics of this ribbon that will allow us to examine it in greater detail.

Definitions

Definition : Twist: The twist of a ribbon R is given as $Tw(R)$. It is, as the name suggests, a measure of how twisted around its own axis a ribbon is. We calculate twist by taking half of the sum of the $+1$ s and -1 s occurring at crossings of the ribbon's axis and one of its two edges. The $+1$ s and -1 s are determined in the same manner as linking number (see Figure 12).

Definition: Writhe: The writhe of a ribbon R is given as $Wr(R)$. It measures how contorted the axis of the ribbon is. The writhe of a ribbon is the average signed crossover number over all possible projections of the ribbon in space.

Definition : Signed crossover number: The signed crossover number is the sum of $+1$ s and -1 s occurring at crossings of the axis with itself. The signs of these crossings are determined in the same manner as linking number (see Figure 12).

Our final term is, in fact, an old term being applied to a new situation: linking number.

Definition : Linking number (of a ribbon): To calculate the linking number of a ribbon R , denoted as $Lk(R)$, we first treat the two edges of the ribbon as components of a link. The linking number of the ribbon is equal to the linking number of this link.

To summarize, we now have three new measures: twist, writhe, and linking number. Twist measures how twisted an axis and an edge are, writhe measures how twisted the axis is about itself, and linking number measures how twisted the two edges are with each other.

Individually, each of these values gives us an interesting piece of information about a ribbon. Together, however, they have an even more interesting relation

discovered independently by James White of UCLA, Brock Fuller of Caltech, and Czech mathematician G. Calugareanu:

$$Lk(R) = Tw(R) + Wr(R).$$

In words, this equation tells us that changes in twist and changes in writhe must balance each other exactly regardless of how we change the position of a ribbon, since the linking number stays constant.

In the context of a physical piece of cyclic duplex DNA, we also take into account the number of base pairs in the molecule. DNA naturally twists at a rate of 10.5 base pairs per twist, and twisting any more frequently than this will overwind the DNA.

Now suppose an enzyme doubles the number of tangles in a cyclic duplex DNA molecule. This will double the twist, because each edge crosses over the axis twice as many times, and the linking number, because the edges cross over each other twice as many times. However, doubling the number of twists means there are fewer base pairs per twist - half as many, to be exact. To return to its natural twist rate, the DNA will decrease its twist - but according to Equation (1), the decrease in twist must be accompanied by an increase in writhe to keep the linking number constant. In the context of a physical piece of cyclic duplex DNA, we also take into account the number of base pairs in the molecule. DNA naturally twists at a rate of 10.5 base pairs per twist, and twisting any more frequently than this will overwind the DNA. Now suppose an enzyme doubles the number of tangles in a cyclic duplex DNA molecule. This will double the twist, because each edge crosses over the axis twice as many times, and the linking number, because the edges cross over each other twice as many times. However, doubling the number of twists means there are fewer base pairs per twist - half as many, to be exact. To return to its natural twist rate, the DNA will decrease its twist - but according to Equation mentioned above a decrease in twist means an increase in writhe. As writhe increases, the axis of the ribbon will become more twisted around itself and will become contorted in space in an effect known as supercoiling. Thus when an enzyme adds too many more tangles to a cyclic duplex DNA molecule, though it performs this action at a specific site, it can change the shape and position of the entire molecule. Biochemists today use electrophoresis in gels to detect these changes and further study the effects of enzymes on DNA. Scientists use electron microscopes to take pictures of DNA. Underlying and overlying segments are distinguished by using a protein coating. The flattened DNA is then visualized as a knot. The unknotting number and ideal crossing number can then be estimated. For several DNA fragments with the same knot number, Cu , there may be a variety of different forms as the DNA is twisted and distorted. However, the average writhe and crossing number can be estimated for a particular ideal knot number.

A more convenient procedure for determining the crossing number of DNA knots involves using gel electrophoresis. The distance DNA fragments move on an electrophoretic gel is highly correlated with the average crossing number (see graph). The ideal knot number is given on the graph (reproduced from Stasiak et al 1996).

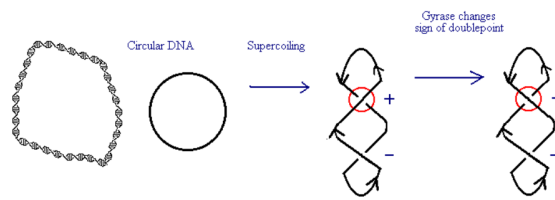


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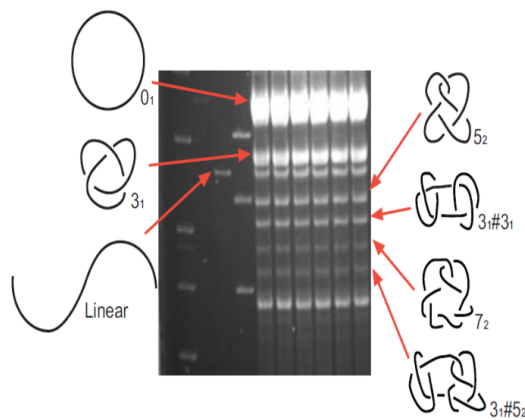


Figure 43: Gel electrophoretic separation of DNA knots (By Sergei Mirkin).

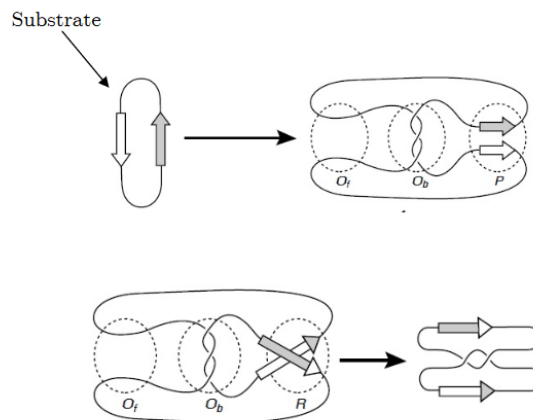


Figure 44: Site specific recombination based on tangle model (De witt Sumner, American Mathematical Society, 1995).

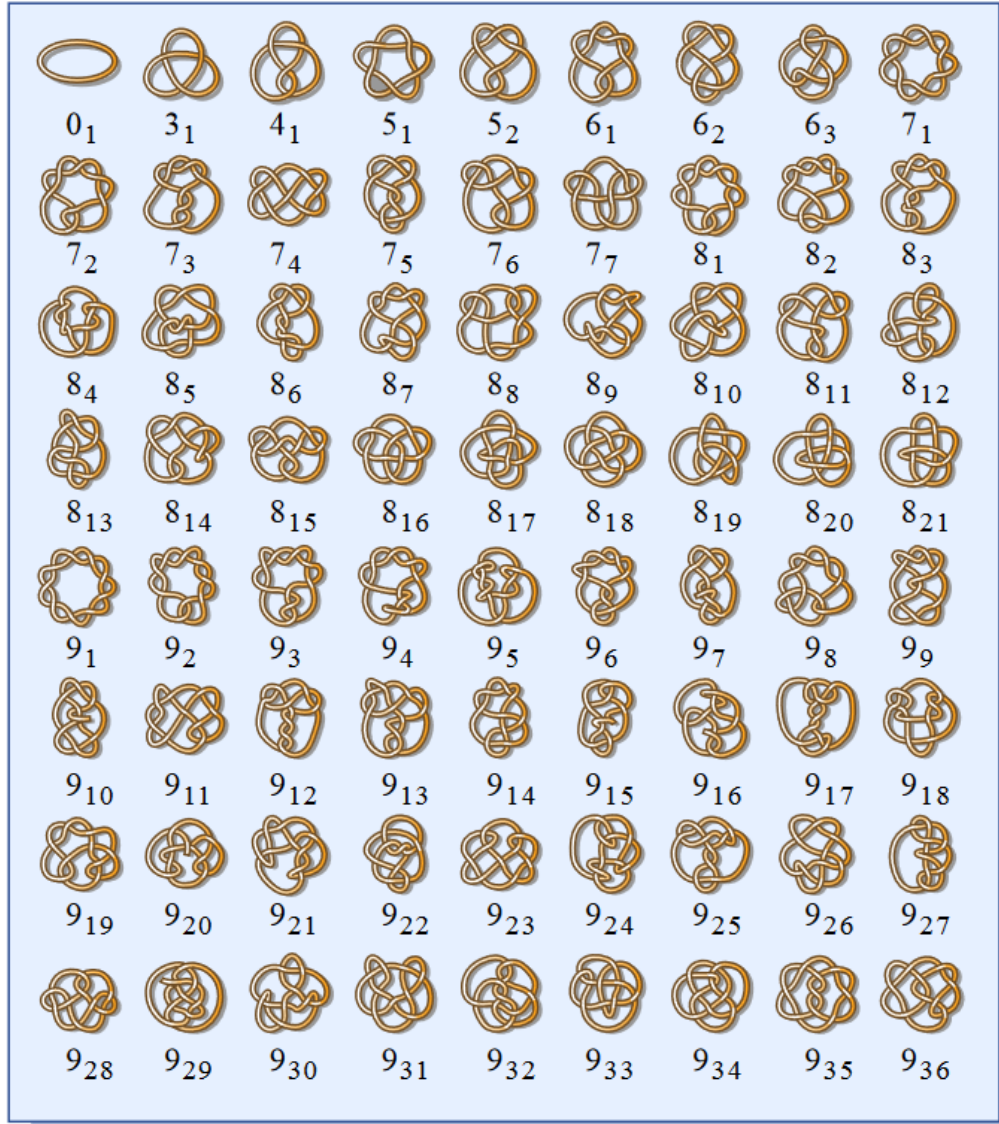


Figure 45: Knot classification by minimal crossing number. Note that there are 13 more possible knots than shown here with minimal crossing number nine.

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