An Introduction to Knot Theory

Rishi Nair

This is one of the three winning articles of the 2021 MathemAttic Article Contest. The other winning pieces will appear in later issues of this Volume.

We provide a brief introduction to some fundamentals of knot theory and its applications. The topics covered include knot notations and an overview of proving knot equivalence by Reidemeister moves and knot invariants. We conclude with a discussion on some practical applications of knot theory and review some of the recent advances in this field.

1 What is Knot Theory?

Knot theory is a branch of topology concerned with the properties of mathematical knots. When we think of knots, shoelaces, sailing knots, and neckties often come to our minds. Mathematical knots are very similar to the listed examples but have their two loose ends fused together. Formally, a mathematical knot is a simple closed polygonal curve in three-dimensional Euclidean space $\mathbb{R}^3$. You can also think of a mathematical knot as a twisted circle; if you trace your fingers along the knot from a starting point on the knot, you should be able to find your way back to the starting point.

The most basic example of a knot is a circle. It meets the criteria of a knot we have set above since it is essentially a line with no tangles whose ends have been fused. In knot theory, we classify the circle as an unknot or a trivial knot – this is because certain knots can be untangled or unknotted into a circle. The trefoil knot is the simplest non-trivial knot, which can be created by forming an overhand knot and joining its two loose ends as shown in Figure 1b. There are a plethora of knots, of which many are equivalent, meaning they can be manipulated by a sequence of carefully designed operations to have the same appearance.

The first steps in the study of mathematical knots were taken by Carl Friedrich Gauss in the 1830s; however, the origins of knot theory as we know it today can be traced back to theoretical research on the atomic structure of matter later in the same century. During that period, some scientists theorized that vacuum was made up of a special matter called the "aether." In an attempt to classify and organize atoms, mathematician/physicist William Thomson proposed that an atom can be modeled as a knotted vortex of aether [1]. This idea increasingly grew in popularity among the scientific community. Mathematician/physicist Peter Guthrie Tait was inspired by Thomson's idea and attempted to create a system to classify knots,

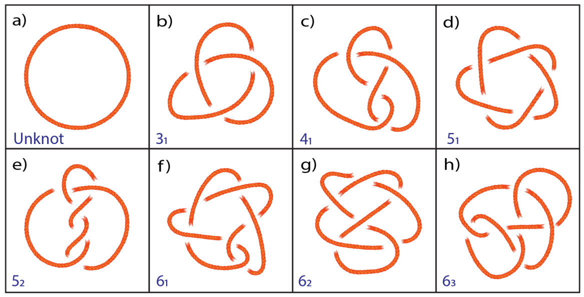

Figure 1: A visual representation of some elementary knots along with their Alexander-Briggs notation.

which could then be used to find order amongst atoms [1]. Eventually new theories came along that disproved the "aether" hypothesis. Nevertheless, these innovative ideas developed in the context of atomic theory laid the foundations of modern knot theory.

A graphical representation of eight basic knots that are distinct from one another is shown in Figure 1. Although physical knots exist in a three-dimensional space, we can represent them in two dimensions by splitting the line strand that goes underneath another line strand at each intersection point (notice the small gaps between the strands at the intersection points in Figure 1). Such graphical visualizations of knots are known as knot diagrams.

Mathematicians often use the so-called Alexander-Briggs notation to numerically represent and classify knots. In the Alexander-Briggs notation, any knot is represented as X_Y, where X denotes the crossing number and Y denotes the order of the knot. The crossing number equals the minimum number of intersection points in any projection of the knot, while the order of a knot is a number assigned to each knot such that no two distinct knots have the same Alexander-Briggs notation. Figure 1 shows the Alexander-Briggs notation for some basic knots. It can be noted that knots d) and e) have the same crossing number; however, since these two knots are distinct, we assign them different orders so that they can be differentiated by their Alexander-Briggs notation.

Mathematicians have devised different ways of representing and analyzing knots which enable us to discover unique patterns and properties. We will cover some of these ideas in the next section.

2 Some Fundamental Concepts in Knot Theory

A fundamental question in knot theory is whether two knots are equivalent. In other words, it is possible that two knots can look different but fundamentally be the same. If two knots have a different appearance but are fundamentally the

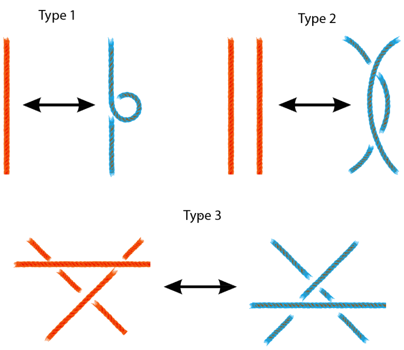

Figure 2: The three Reidemeister moves.

same, we call these two knots equivalent. In the 1920s, Kurt Reidemeister [7] proved that two knots are equivalent if one knot can be rearranged into the other knot using a sequence of certain moves that does not involve cutting or tearing the knot. There are three such types of moves which are now known as Reidemeister moves.

Figure 2 shows a graphical representation of the three Reidemeister moves. The type 1 Reidemeister move can be described as inserting or removing a twist in a knot. The type 2 move can be described as creating or eliminating two crossings within a knot. The type 3 move can be described as sliding a line strand from one side of a crossing to the other side.

Consider the seemingly complicated knot shown in Figure 3a. We will apply a sequence of Reidemeister moves to show that this knot is equivalent to the unknot (circle). We first apply a type 2 move to arrive at Figure 3b. Following this, we apply another type 2 move followed by a type 2 and a type 1 move to arrive at the unknot.

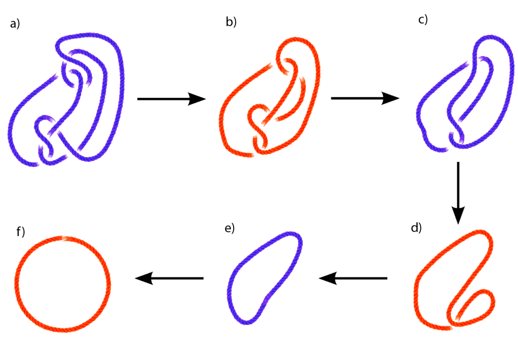

Figure 3: Reidemeister moves being used to simplify a knot into an unknot.

Mathematicians have studied if an upper bound can be established on the number of Reidemeister moves required to prove that two knots are equivalent. Haas and Lagarias proved an interesting result that the upper bound on the number of moves required to transform a complex knot with n crossings into an unknot is given by 2^{nc}, where $c = 10^{11}$ [8]. In other words, if we cannot transform a given complex knot into an unknot by 2^{nc} moves, then the given knot is not equivalent to an unknot. Note that the upper bound is significantly larger than the number of atoms in the known universe! Although this upper bound is incredibly large, the upper bound is computable. Having an upper bound therefore enables us to determine, in principle, if a knot is equivalent to an unknot in a finite amount of time.

A more elegant approach for finding if two knots are equivalent is to use the notion of knot invariants. A knot invariant can be thought of as a function that assigns a quantity for any given knot such that equivalent knots are assigned the same quantity. While these quantities are the same for equivalent knots, knot invariants by themselves aren't necessarily enough to tell if two knots are equivalent. If the invariants computed for two knots are not equal, then the knots are distinguishable from each other, and if the quantities are the same, they could potentially be equivalent. Two things to consider how effective an invariant is are how easy it is to compute that invariant for a given knot and how selective it is at differentiating nonequivalent knots.

One of the most basic knot invariants is tricolourability. A knot is considered to be tricolourable if each of its line strands can be assigned a colour such that: (1) all line strands are coloured, (2) a minimum of two colours are used and a maximum of three colours are used, and (3) at each intersection, the colours of the three line strands must all be the same colour or all be different colours. It can be shown that tricolourability is preserved by the three Reidemeister moves, and therefore is an invariant.

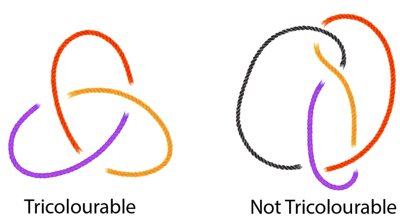

Figure 4: The tricolourability invariant idea applied to two knots.

The unknot is not tricolourable since it consists of only a single strand and therefore we cannot use at least 2 colours. Figure 4 illustrates how the tricolourability invariant can be computed for two knots. The knot on the left (trefoil) is tricolourable since we can colour each strand (following rules 1 and 2) such that at each intersection, the colours of the three line strands are all different. Therefore the trefoil knot is not equivalent to the unknot. On the other hand, the knot on the right (4_1) of the Figure is not tricolourable. We have left one strand uncoloured because no matter which colour we assign to this strand, we cannot meet the third rule of tricolourability. This means that we cannot use the tricolourability invariant to prove that the 4_1 knot is not equivalent to the unknot. However, the tricolourability invariant can be used to tell that the two knots of Figure 4 are distinct from each other.

Knot polynomials (typically in one or two variables) are another type of knot invariants. The Alexander polynomial introduced in 1923 is considered to be the first knot polynomial and was the only polynomial invariant for nearly 50 years. This invariant was later refined by John Conway and is now known as the Alexander-Conway polynomial. In 1984, Vaughan Jones discovered a new polynomial invariant which inspired further work on this topic. A notable development was the Kauffman polynomial which can be considered to be a generalization of the Jones polynomial. Knot polynomials do not provide a definitive way of determining whether two knots are equivalent. In practice, certain knots that are not equivalent can have the same knot polynomials. Nevertheless, knot polynomials have proved to be powerful tools to compare complex knots using computational methods.

Interested readers can refer to the introductory text by Adams [10] for a detailed exposition on the fundamentals of knot theory. It is worth noting that even though knot theory is abstract in nature, many of the fundamental concepts are accessible to anyone with a basic understanding of mathematics.

3 Practical Applications and Recent Advances

While knot theory is generally thought of as a field of pure mathematics lying at the intersection between topology, algebra and combinatorics, it plays an important role in several other fields of study in the theoretical and applied sciences. Knot theory is used in biochemistry and chemistry to study and analyze knotted structures such as DNA, proteins, knotted polymer structures and certain enzymes. Due to the long structure of DNA strands, they typically form complex knots [2]. Certain biological processes such as mitosis (cell division) can alter and change these knots by tangling and untangling them. Knot theory can provide valuable insights into the structural changes that happen during these processes.

Knot theory has a diverse range of applications and can also be used in optics, cryptography and even in history, anthropology and archaeology. [3]. Broadly speaking, in a field of study where objects that resemble knots are present, we can apply knot theory to classify and find properties of the knots. This information can then provide us with useful insights. Let's take archaeology for example. We can examine knotted structures present in embroidery and in sculptures. If we take two different sculptures with knots in them and find that the knots are equivalent, we can hypothesize that these structures came from the same geographical location or are from regions with similar cultural influences.

Recently, Lisa Piccirillo, a former graduate student at the University of Texas (who is now an Assistant Professor at MIT) solved a famous knot theory problem related to the Conway knot. The Conway knot, as shown in Figure 5, is a fairly simple knot whose crossing number is only 11. For nearly 50 years, ever since John Horton Conway first proposed this knot, there has been a mystery about this knot that has baffled many mathematicians. This mystery was whether the Conway knot was a slice knot. Slice knots are knots that can be found when a knotted sphere in a four-dimensional space is sliced open; an example of a slice knot is 6_1 shown in figure 1f. In 2020, Lisa Piccirillo answered this long-standing question and proved that the Conway knot was not a slice knot [4].

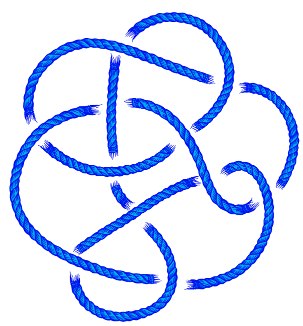

Figure 5: The Conway knot.

In 2017, researchers at the University of Illinois Chicago wrote a research paper on analyzing RNA molecules and proteins using knot theory. Due to the long structure of RNA molecules, they knot themselves in order to fit into human cells. These researchers created a new system of knot polynomials designed specifically for the purpose of studying RNA. Using this new system of knot polynomials, they classified the topology of different RNA molecules and modeled certain effects and bonds in various knotted protein molecules [5].

Not only can knot theory be used to analyze knotted biological structures but it can also be used to design bullet proof vests. In 2017, a team of scientists led by Professor David Leigh at the University of Manchester created the world's tightest knot and were awarded a Guinness World Record for this breakthrough. They created a 20 nanometer long molecular knot that has 8 crossings and is composed of 192 atoms [6]. A computer generated molecular model of the 192-atom knot is shown in Figure 6. This knot was created using a "self-assembly" technique which involves knitting molecular strands around metal ions. These tight molecular knots can be used to create ultra-strong materials.

Bullet-proof vests are currently made up of a material called kevlar, a plastic made up of tightly packed rigid molecular rods. In the near future, kevlar may be replaced by tightly knotted polymer strands. Polymer strands tend to be much lighter and stronger when compared to materials such as kevlar. By tightly knot-

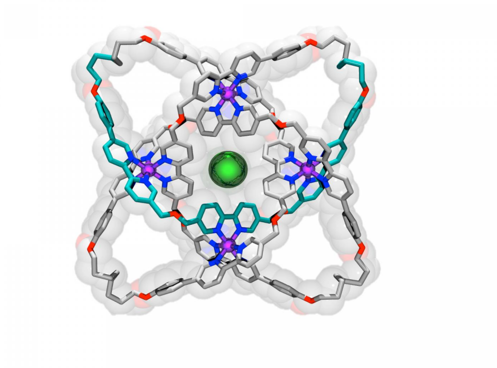

Figure 6: A model of the “worlds tightest” 192-atom knot [9].

ting these polymer strands, material scientists are able to create strong and durable construction materials [6]. The phenomena of polymer strands being stronger when knotted can be observed in spider webs. Spider web strands are very fragile and can be easily broken apart. However, once woven together, they are very strong and durable.

Although knot theory started off as the core ingredient in a now discredited theory of atomic matter based on aether, things have almost come back a full circle. Mathematicians and physicists have found interesting connections between knot theory and quantum field theory. When a classical particle moves from one point to another, it follows a smooth path that obeys Newton’s laws of motion. In contrast, a quantum particle follows an irregular path when travelling from one point to another. Due to the Heisenberg uncertainty principle, the exact location of a quantum particle at some point in time and its trajectory of motion are both unknown. This means that there are multiple possible paths that a quantum particle can take. When analyzing the trajectory of a quantum particle, we usually have to compute averages over all possible paths. For each possible path, there is a “probability amplitude” for the quantum particle to reach its destination. This amplitude is given by the Wilson operator. If we regard the space-time trajectory of a quantum particle as a knot, the value of its Jones polynomial (a polynomial invariant) is equal to the average value of the Wilson operator [11]. This means that the Jones polynomial of the trajectory of a quantum particle can be used to estimate its expected path. Edward Witten’s seminal work in this area led to him being awarded the Fields medal in 1990. He is the first physicist to win this prestigious award.

Researchers have investigated how the relationship between knot theory and quantum field theory can be leveraged to solve problems related to quantum computers. When building quantum computers, engineers face the problem of decoherence, which is when a quantum system loses its quantum properties due to interactions with the external environment. In principle, a topological quantum computer that effectively drags particles around each other in a knotted space-time orbit may be less vulnerable to decoherence and therefore fault-tolerant [12]. The quest to build a robust topological quantum computer that could potentially revolutionize fields from drug discovery to cryptography continues [13].

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Rishi Nair is a grade 11 student at the University of Toronto Schools. He is interested in various aspects of mathematics with a particular emphasis on the applications of mathematics to physics and computer science. His first exposure to topology was at the 2021 Math Academy summer program on knot theory organized by the Department of Mathematics at the University of Toronto. This experience inspired him to write an expository article on knot theory to introduce others to this fascinating topic. Rishi Nair is also an avid programmer, guitar player and music enthusiast.