



A Combinatorial approach to Knot theory and its applications

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Overview and Basic Definitions

We are looking at knots and links using the combinatorial structure of various invariants. The current focus is the Jones polynomial, fraction invariant and the Alexander Polynomial. The aim is not just to classify the knots but to understand various other aspects of these knots and links which could be derived from their combinatorial structure. Further, we also look at a few applications of these combinatorial structures in Biology.

First of all, what is a knot?

A subset K of a space X is a **Knot** if K is homeomorphic to a sphere \mathbb{S}^p . More generally K is a **link** if K is homeomorphic to a disjoint union $\mathbb{S}^{p1} \cup \mathbb{S}^{p2} \dots \cup \mathbb{S}^{pr}$ of one or more spheres.

For our purposes we consider $X = \mathbb{R}^3$ and $p_i = 1, \forall i = 1, 2, \dots, r$.

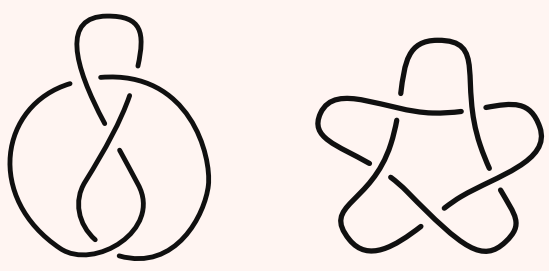


Figure 1. Figure 8 - 4₁, Cinquefoil- 5₁ Knots respectively

Equivalence of knots

Two knots or links K, K' are *equivalent* if there exists a homeomorphism $h : X \Rightarrow X$ such that $h(K) = K'$, or $(X, K) \cong (X, K')$. This is to say the two knots are ambient isotopic.

This notion is very well captured by the Reidemeister Moves:

Two **Knots** K, K' with diagrams D, D' are **equivalent if and only** if their diagrams are related by a finite sequence $D = D_0, D_1, \dots, D_n = D'$ of intermediate diagrams which are related by one of the following Reidemeister moves:

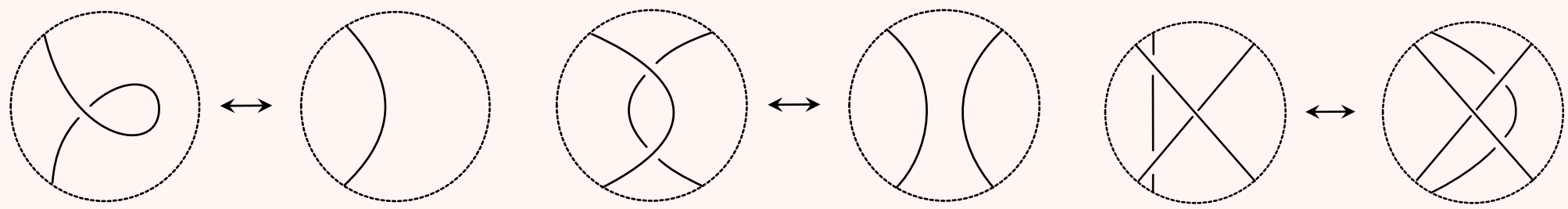


Figure 2. Type 1, Type 2 and Type 3 Reidemeister Moves respectively

Skein Relations Given a diagram D , skein relations are defined as follows:

- If D is a simple closed curve then $\langle D \rangle = 1$
- If D' is disjoint union of D and a simple closed curve, then $\langle D' \rangle = \delta \langle D \rangle$
- For any given D , we choose a crossing and obtain: $\langle D \rangle = A \langle \text{=} \rangle + B \langle \text{||} \rangle$, two types of smoothings of the crossing, where we derive values B and δ in terms of A using the invariance under Reidemeister moves. We get $B = A^{-1}$, while $\delta = -A^2 - A^{-2}$. For type 1 Reidemeister move, we need to correct for a factor, which we do using the Writhe.

Writhe is the sum of signs of the crossings of D according to the following convention(shortest distance under-crossing needs to cover to align with over-crossing).

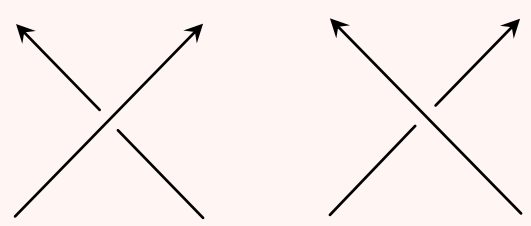


Figure 3. The first type of crossing assigns a sign +1(Undercrossing moves clockwise), while the second assigns -1 (Undercrossing moves anti-clockwise).

A **Quandle** is a set X with an operation $\triangleright : X \times X \rightarrow X$ such that the following three conditions are satisfied:

- For all $x \in X, x \triangleright x = x$.
- Given \triangleright there exists an inverse function \triangleright^{-1} such that $\forall x, y \in X$:
 $(x \triangleright y) \triangleright^{-1} y = x = (x \triangleright^{-1} y) \triangleright y$
- $\forall x, y, z \in X, (x \triangleright y) \triangleright z = (x \triangleright z) \triangleright (y \triangleright z)$.

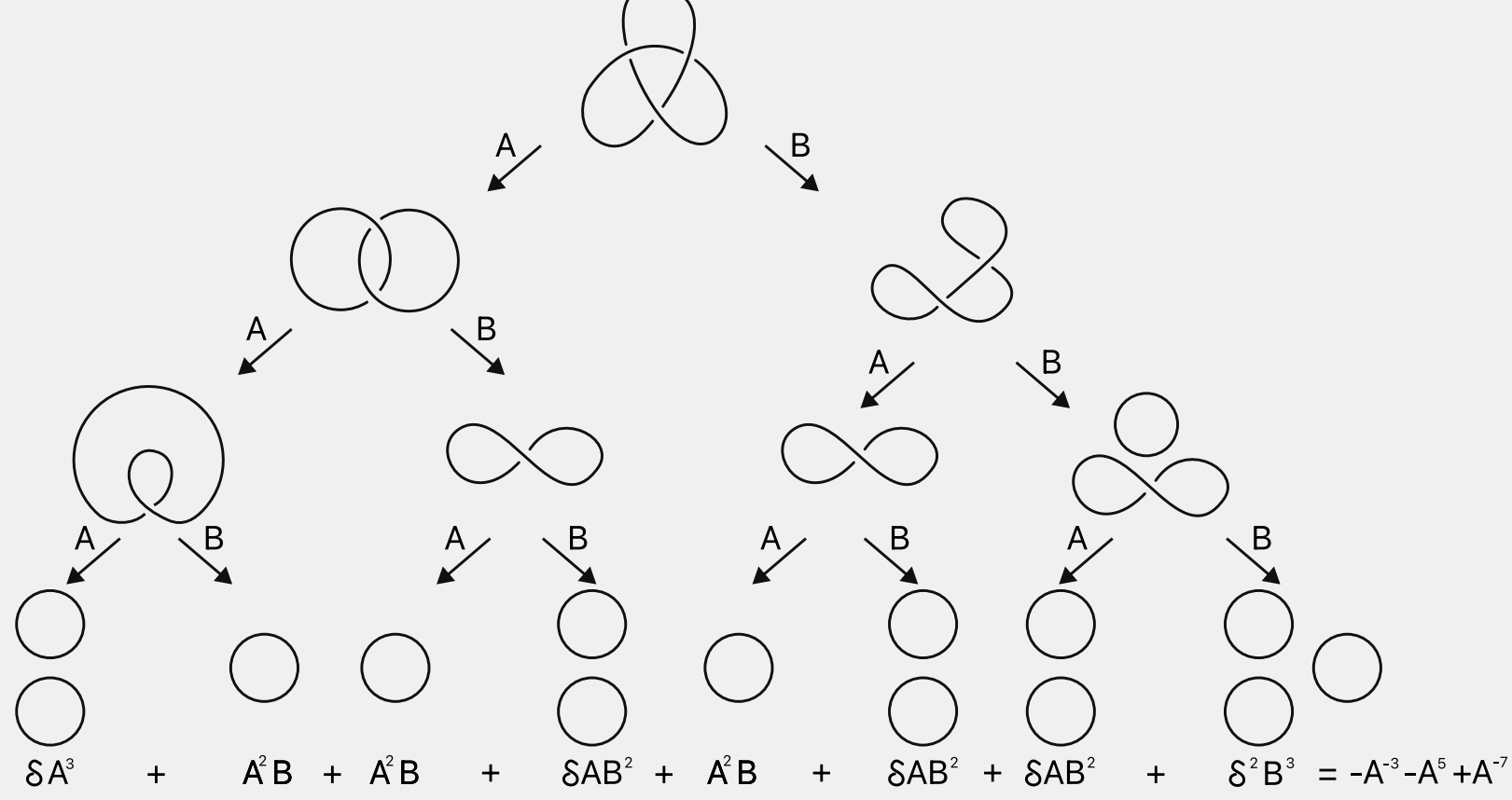
Span of the Jones Polynomial

Jones Polynomial ($V_L(t)$) for an oriented link L is given by substituting A^{-4} by t in $f_D(A) = (-A^3)^{-w(D)} \langle D \rangle$ for any diagram D of L , where $\langle D \rangle$ is as obtained from the skein relations with $B = A^{-1}$ and $\delta = -A^2 - A^{-2}$ and $w(D)$ is the writhe of the diagram D . Here we look at two different combinatorial formulations of the Jones polynomial and on the way we discover two important results regarding knots.

The state-sum formula Given D a link diagram, then we can obtain the bracket polynomial from the following formula:

$$\langle D \rangle = \sum (-A^2 - A^{-2})^{|sD|} A^{|s|}$$

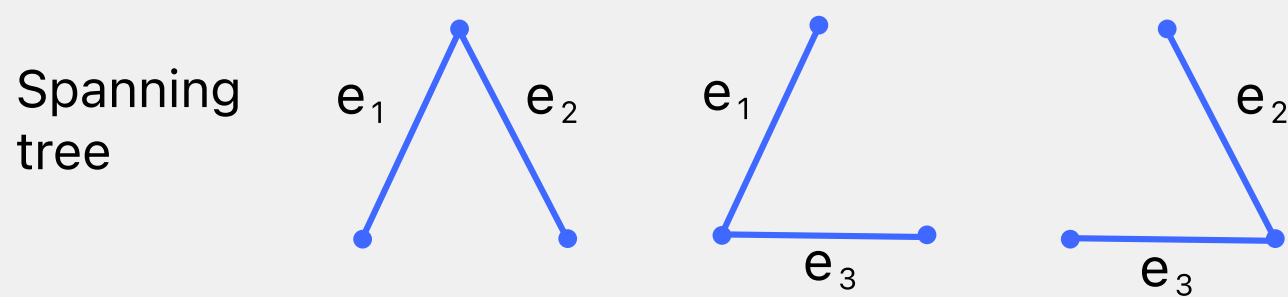
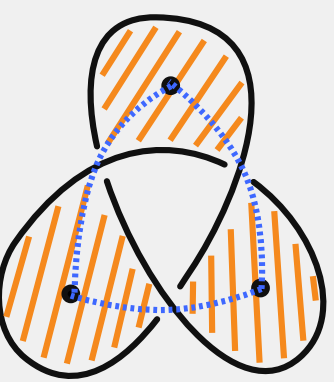
where sum is taken over all the states of the diagram D .



Let L be an oriented link with a connected diagram D of n crossings. Then, $\text{span}(V_L(t)) \leq n$. If further D is alternating and reduced, then $\text{span}(V_L(t)) = n$, and the alternating diagram has the least number of crossings.

Spanning tree expansion of Jones polynomial using the Tutte polynomial and further Γ polynomial.

State of e_j	L	D	l	d	\bar{L}	\bar{D}	\bar{l}	\bar{d}
μ_{ij}	$-A^{-3}$	A	$-A^3$	A^{-1}	$-A^3$	A^{-1}	$-A^{-3}$	A



State	LLd	LdD	IDD	
Weight	A^{-7}	$-A^{-3}$	$-A^5$	$= A^{-7} - A^{-3} - A^5$

Rational Tangles and their fraction

A tangle is an analogue of a link except that it has free ends. The number of strands entering and exiting the tangle box are always even and there exists no free ends inside the tangle box. A **Rational Tangle** in a vague sense is just a tangle which can be unwound by simply allowing the fixed ends to move along the boundary. The result we looked at is that the rational tangles can be fully described by an associated fraction. This is called the Conway's Theorem.

Conway's Theorem: Two rational tangles are ambient isotopic if and only if their fractions are equal.

Rational tangles can be thought of as sums of series of **Horizontal** and **Vertical** twists on the fixed ends on the boundary. Let t_a denote a tangle with a horizontal twists and $\frac{1}{t_a}$ denotes the tangle with a number of horizontal twists after rotating it 90° in anticlockwise direction and taking a mirror image.

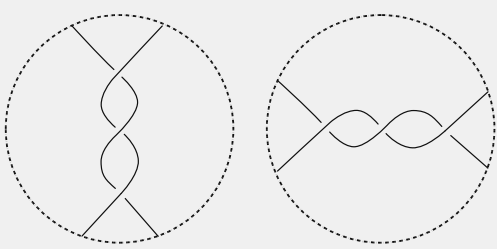


Figure 4. $\frac{1}{t_3}$ integer tangle and t_3 integer tangle

This gave us the following formulation for the Rational tangles:

$$t_{a_n} + \frac{1}{t_{a_{n-1} + \frac{1}{\dots + \frac{1}{t_{a_1}}}}} \text{ and } \frac{1}{t_{a_n} + \frac{1}{\dots + \frac{1}{t_{a_1}}}}$$

Where, t_{a_i} denote the tangles with a_i horizontal twists. Further replacing t_{a_i} with a_i gives us a continued fraction. Using this **continued fraction form** we obtain one side of the Conway's theorem.

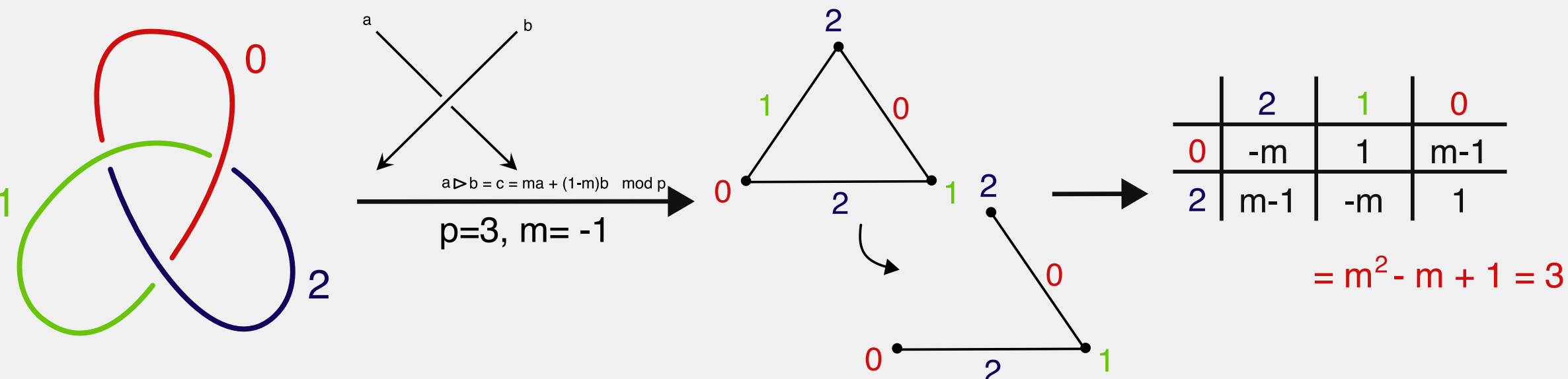
Coloring the knots

First we define p -colorability and Linear Alexander Quandle. Then we extract a palette graph and further a spanning forest from the given knot and coloring. Using this spanning forest we define an adjacency matrix. The determinant of the matrix obtained from deleting a column of adjacency matrix gives us the Alexander Polynomial for the knot. In this process we also obtain the lower bound for the minimum number of distinct colors required by a knot to satisfy the coloring conditions.

Let K be a knot, given an odd prime p , and a non-null integer m , s.t. K admits a non-trivial (p, m) -coloring, we have the following inequality:

$$2 + \lfloor \ln_M(p) \rfloor \leq \text{mincol}_{p,m}(K)$$

where $M = \max\{|m|, |m-1|\}$, and either $m \neq 2$ or $m = 2$ and $\Delta_K^0(m) \neq 0$.



The minimum number of colors are given by: $2 + \lfloor \log_2(3) \rfloor = 2 + 1 = 3 \leq \text{mincol}_{3,-1}(3_1)$

Applications in Biology

Quandles and Protiens Proteins are linear molecular chains which exhibit different levels of structure. The tertiary structure of proteins or simply the folding of the protein is believed to define various functions and properties, and here we apply knot theory to study the topology of the folding exhibited by proteins. To achieve this we develop a modified version of Knot theory which works for linear chains, instead of the usual mathematical knot which is homeomorphic to a closed loop. For this purpose, we take different structural components and determine their behaviour when a folded protein is embedded as a linear segment in three dimensions. Then we represent these using Gauss codes or color them using Quandles to help distinguish between proteins using an algebraic structure.

Given two projections of proteins and a choice of bundle, we can calculate the number of solutions possible for the coloring. If the number of solutions for the two proteins is different, then they are not topologically equivalent.

An example of protein structure colored using a bundle is:

Consider the following oriented bundle: $(\mathbb{Z}_{15}, \triangleright, R_1, R_2, R_3)$, s.t. $x \triangleright y = 8(x+y)$, $x \triangleright^{-1} y = 2x-y$, $R_1(x, y) = 2x-y$ and $R_2(x, y) = 7x-6y$

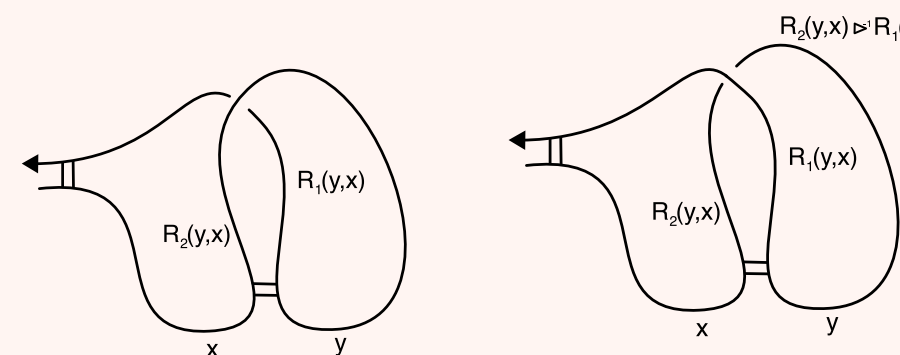


Figure 5. Two different structures and their corresponding possible colorings: P_1 , $6(y-x) = 0$, colorings= 45, P_2 , $11(y-x) = 0$, colorings= 15

Site-Specific Recombination and Rational Tangles Knots found in nature are generally considered to be rational knots. In biological phenomenon such as site-specific recombination, we can consider under various assumptions a specific case where the recombinase acts on the same site every time. In a general case, given a Substrate(S), Tangle site(T) and a Recombination site(R), we can generate the numerator closure, such that we have atleast two equations in these three unknowns: $N(S+T) = \text{Substrate}$ and $N(S+R) = \text{Product}$. We can obtain the projections of substrate and product under electron microscopy from which we can ascertain the structures of substrate and the recombination site which in turn can help explain mechanism for various recombination processes.

References and Acknowledgements

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