Knot Theory and DNA Topology

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Knot and Link Theory

Knot theory is a branch of mathematics, usually considered as a branch of low dimensional topology, which studies embeddings of the unit circle into the 3-space. Thus, a classical ***knot* is a smooth embedding**

$$k\colon S^1 \to \mathbb{R}^3.$$

There are various generalizations of this concept: wild knots: non-smooth embeddings, high dimensional knots: embedding an n-manifold to $\mathbb{R}^{n+2}$ etc.. We concentrate on classical knots. **A *link* is a (smooth) embedding of a disjoint union of circles:**

$$l\colon S^1 \times \{0\} \cup \dots \cup S^1 \times \{n\} \to \mathbb{R}^3.$$

A connected component of the image of the link is a *component* of the link and is itself a knot. In that way a knot is actually a special case of a link ($n = 1$). **Two knots k, k' (or links) are considered *equal* (denoted $k \sim k'$) if there is an orientation preserving homeomorphism $h\colon \mathbb{R}^3 \to \mathbb{R}^3$ which takes the other knot to the other: $k' = h \circ k$.**

MAIN QUESTION OF KNOT THEORY: Given two knots k and k', are they equal or not?

Examples of knots:

Note that these pictures are a good way to represent knots: they define a unique equivalence class of the embeddings, since you can easily reconstruct the knot from the picture. On the other hand any knot can be projected in a *nice* way [5] thus to obtain a picture like that.

Are any two of these knots equal? How could one prove that the first knot (the trivial knot or *unknot*) differs from all the others? On the other hand it seems easy to verify that there are two pictures of the same knot in the picture above (which ones?). To answer those questions one has to find a *knot invariant*.

A knot invariant is a function

$$F\colon \{\textbf{all embeddings } S^1 \to \mathbb{R}^3\} \to A,$$

where A is an arbitrary set such that $k \sim k' \Rightarrow F(k) = F(k')$. The important property of a knot invariant is that one can prove two knots to be not equal:

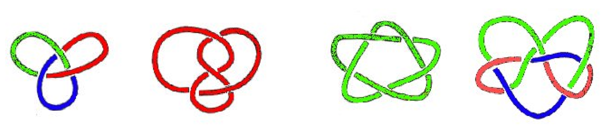
$$F(k) \neq F(k') \Rightarrow k \not\sim k'.$$

There exist a great deal of different knot invariants. One would require the following things for a knot invariant to be good:

1. given a knot, the invariant is easy to calculate
2. it distinguishes as many knots as possible
3. it is easy to find out whether two elements of A are the same or not.

EXAMPLES OF KNOT INVARIANTS:

- The fundamental group of the knot complement $\pi_1(\mathbb{R}^3 \setminus kS^1)$. It is an easy exercise to verify, that this is indeed an invariant. This invariant distinguishes knots quite well, but the condition (3) above is not satisfied: it is difficult to compare these groups. A great deal on the subject can be found in [5].
- How many ways is to colour a knot with three colours such that at each crossing *either one or three different colours meet*? This number is an invariant [1]. It is easy to check now that the trefoil knot with three crossings below is non-trivial.



Biological Question

There are plenty of topological questions arizing from DNA. We will discuss one aspect of them. Consider DNA double strand:

In reality it is never so straight as in this picture, on contrary, it is very tangled and supercoiled. Sometimes it has to be manipulated in one way or another: at replication (creating 2 copies from one double strand of DNA), invertion (inverting a subsequence of DNA), integration, deletion, when reading genes, when packing the DNA to fit in the cell nucleus.

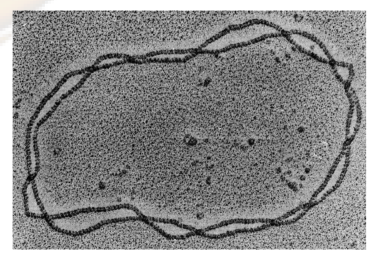
These topological changes are performed in particular **by** the so called ***site-specific recombinases*** which are certain proteins. For modern DNA-technology, scientific and other reasons

IT IS INTERESTING HOW SITE SPECIFIC RECOMBINASES WORK,

in particular, what kind of local changes do they do. Examples of possible local changes include:

QUESTION: HOW TO DETERMINE WHAT KIND OF A LOCAL CHANGE DOES A GIVEN RECOMBINASE DO?

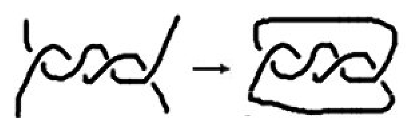
It is almost impossible to detect the change while it is happening: molecules move fast, the change happens fast and is very local. On the other hand one can detect how does the recombinase change the knot type. It is much easier to detect (using gel electrophoresis and electron microscopy) the knot or link type of a big circular DNA-molecule (see the picture on the right).



Tangle Model

Let k be a knot and $B = B(x, r)$ a ball with radius r, which intersects the knot exactly in four points. The part of the knot inside B is called a *tangle*. Equivalently **a tangle is two arcs embedded in** $B(0, 1)$ with end points lying on the boundary ∂B. One can add tangles to each other:

and turn them into knots or links:



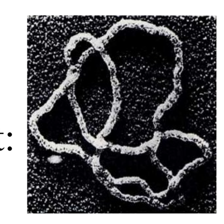
The above operation is denoted by N (coming from the word *numerator* for reasons unexplained here), i.e. given a tangle T, $N(T)$ is the knot or link obtained by gluing upper edges together and lower edges together.

EXAMPLE OF A PROBLEM: Suppose we know the tangles T, T_1, T_2, T_3, T_4 and the tangles O and R are unknown. Given the information that $N(O+T) = T_1$, $N(O+R) = T_2$, $N(O+R+R) = T_3$ and $N(O+R+R+R) = T_4$, find O, R and $N(O+R+R+R+R)$.

Biologically this means that we put in a test tube DNA molecules which look like T_1 and then let an enzyme affect on them once, twice and three times. As products we get T_2 T_3 and T_4 respectively. Then we try to predict future action of the enzyme and reconstruct the local change resulting in R.

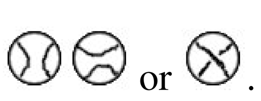
One such particular equation was solved already in 1990 by D. W. Sumners and C. Ernst [7] who developed the first aims of the tangle model and tangle calculus. In their work the enzyme in question was Tn3 resolvase and T_1, T_2, T_3 and T_3 were respectively

Further, they predicted (proved mathematically under some reasonable biological and mathematical assumptions) that the product after the next step of affection would be

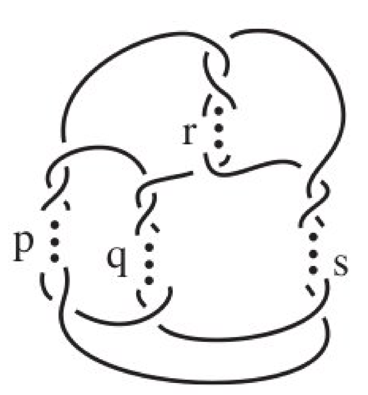
 and were correct: 

Recent Developement

A lot can be understood classifying all possible knots that can be obtained from the trivial knot by applying to one fixed local change. In 2007 Dorothy Buck and Erica Flapan [4] showed that if the recombinase satisfies three (biologically good) assumptions

1. The enzyme makes its change to a spot, which looks like .
2. The ball, which contains the spot to be changed does not pierce through a supercoil or a branch point in a nontrivial way and no persistent knots are trapped in the branches outside of that ball. (For an explanation ask the author.)
3. The product after recombining has one of the following forms: .

then the products will be knots of the following form:



This is of course a neat poster example of what is going on. There are a lot of more similar classifiacation results and many more developement is being done in this field. See the list of references on the right for some interesting articles.

References

The references denoted with ⋆ are refered somewhere in this poster. Those with ⋆⋆ are a suggested reading for someone interested in, but unfamiliar with knot theory.

References

[1] ⋆⋆ Colin C. **Adams** *The Knot Book: An Elementary Introduction to the Mathematical Theory of Knots.* AMS 2004.

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[3] D. **Buck**, C. **Verjovsky Marcotte**, *Tangle solutions for a family of DNA-rearranging proteins*, Mathematical Proceedings of the Cambridge Philosophical Society 139 no. 1, 2005, pp. 59–80.

[4] ⋆ D. **Buck**, E. **Flapan** *A Topological Caracterization Of Knots And Links Arising From Site-Specific Recombination*, arXiv:0707.3896v1, [math.GT] 26 July 2007.

[5] ⋆ **Burde**, **Zieschang**, *Knots*. de Gruyter Studies in Mathematics 5, Berlin, New York 1985.

[6] ⋆⋆ Louis **Kauffman**, *On Knots* Princeton University Press, New Jersey, 1987.

[7] C. **Ernst**, D. W. **Sumners**, *A calculus for rational tangles: applications to DNA recombination.*