Know your Knots

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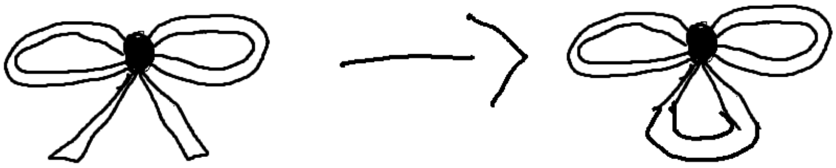
What is a knot?

To a non-mathematician, their first answer might be earphones, but in knot theory, a knot is something much stricter: a closed loop in three-dimensional space that cannot be untied into a plain circle. When earphones get tangled, untangling them is usually easy, which makes them useless for mathematics because once they come apart, there is nothing left to study. To avoid that problem, mathematicians join the two ends together and study the resulting closed curve. The simplest example is the unknot - the trivial knot. It is just a simple loop, or, as I call it, the not-knot.

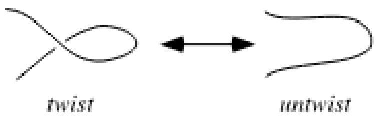


How mathematicians tell knots apart:

Two different diagrams can still represent the same knot, so mathematicians use Reidemeister moves to decide when two knots are equivalent. These moves are local changes that alter the diagram without changing the properties of the knot itself.

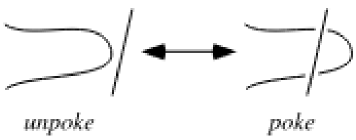
The three moves are twist, poke, and slide.

I.



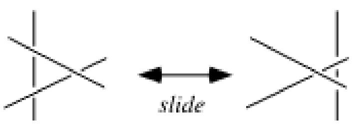
Reidemeister Move 1(RI) adds or removes a twist in the strand.

II.



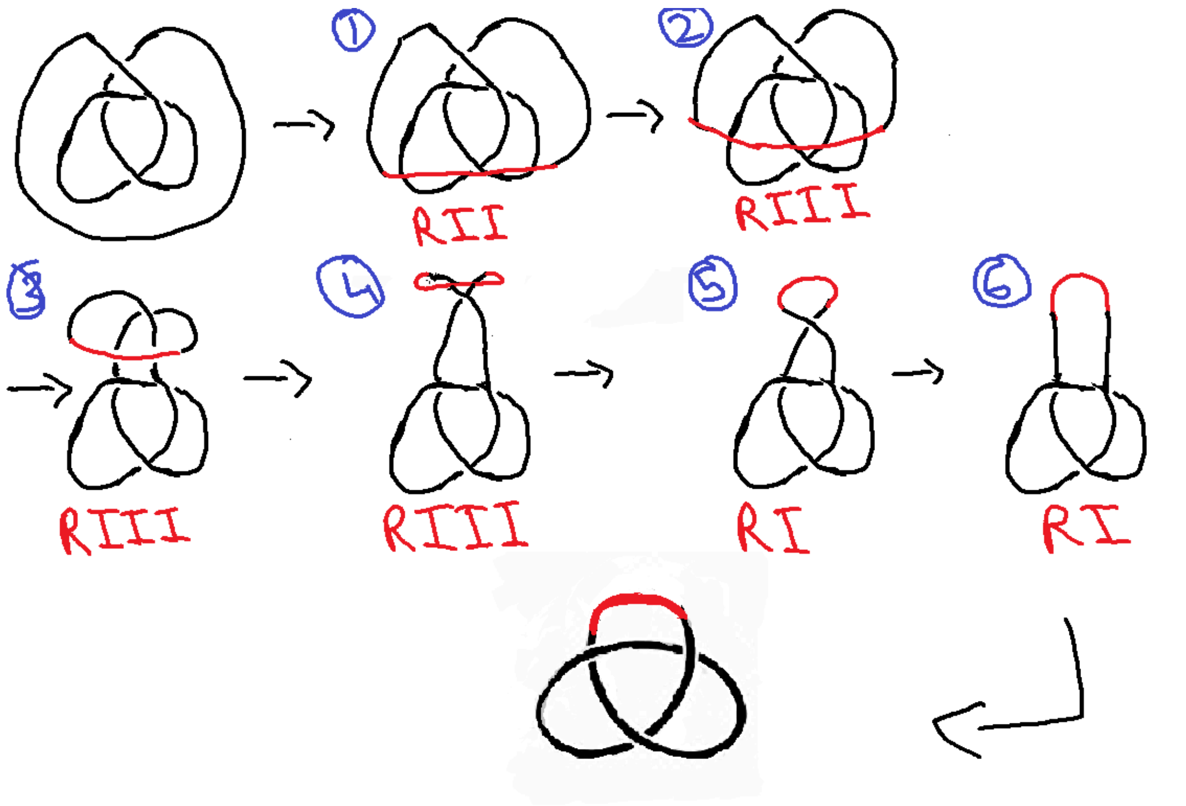
Reidemeister Move 2(RII) adds or removes two crossings between 2 strands.

III.

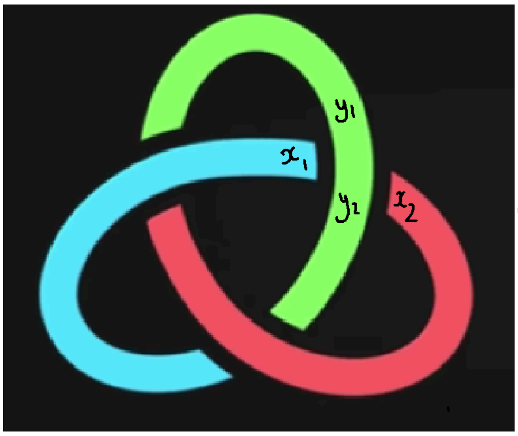


Reidemeister Move 3(RIII) slides a strand under or over a crossing.

Using Reidemeister moves, the knot below can be simplified to the reduced trefoil.



Only 6 Reidemeister moves reduced the knot above and proved it was the same knot; for more complex knots, achieving this with these moves alone is difficult. Mathematicians introduced knot invariants, which are properties or quantities that remain unchanged even with Reidemeister moves. An example of a knot invariant is *p*-colourability, where *p* is a prime number greater than two. *p*-colourability has two rules: use at least two colours and assign each colour a value from 0 to *p*-1.



blue = 0
red = 1
green = 2

To be p-colourable:

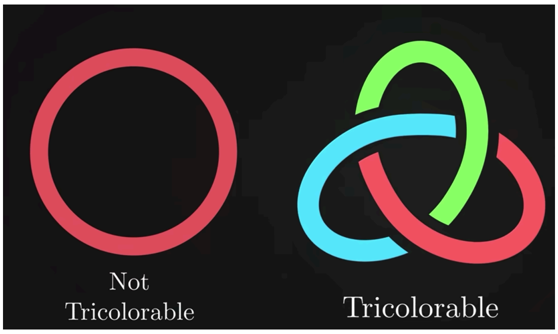
$(y_1+y_2)\%3 = (x_1+x_2)\%3$

$(2+2)\text{Mod } 3 = 1$

$(0+1)\text{Mod } 3 = 1$

Using the assigned colour values with modulo-*p* arithmetic yields a constant value at every intersection.

Summing the horizontal values on the intersection and dividing it by *p* will give you the same remainder as when you sum the vertical values on the intersection and divide it by *p*.



The Unknot is not *p*-colourable as there is no way to colour the diagram whilst using 2 or more colours.

For the trefoil, it passes the *p*-colourability test, since 3 is a prime number, there are 3 different colours at each intersection, and modulo 3 arithmetic works.

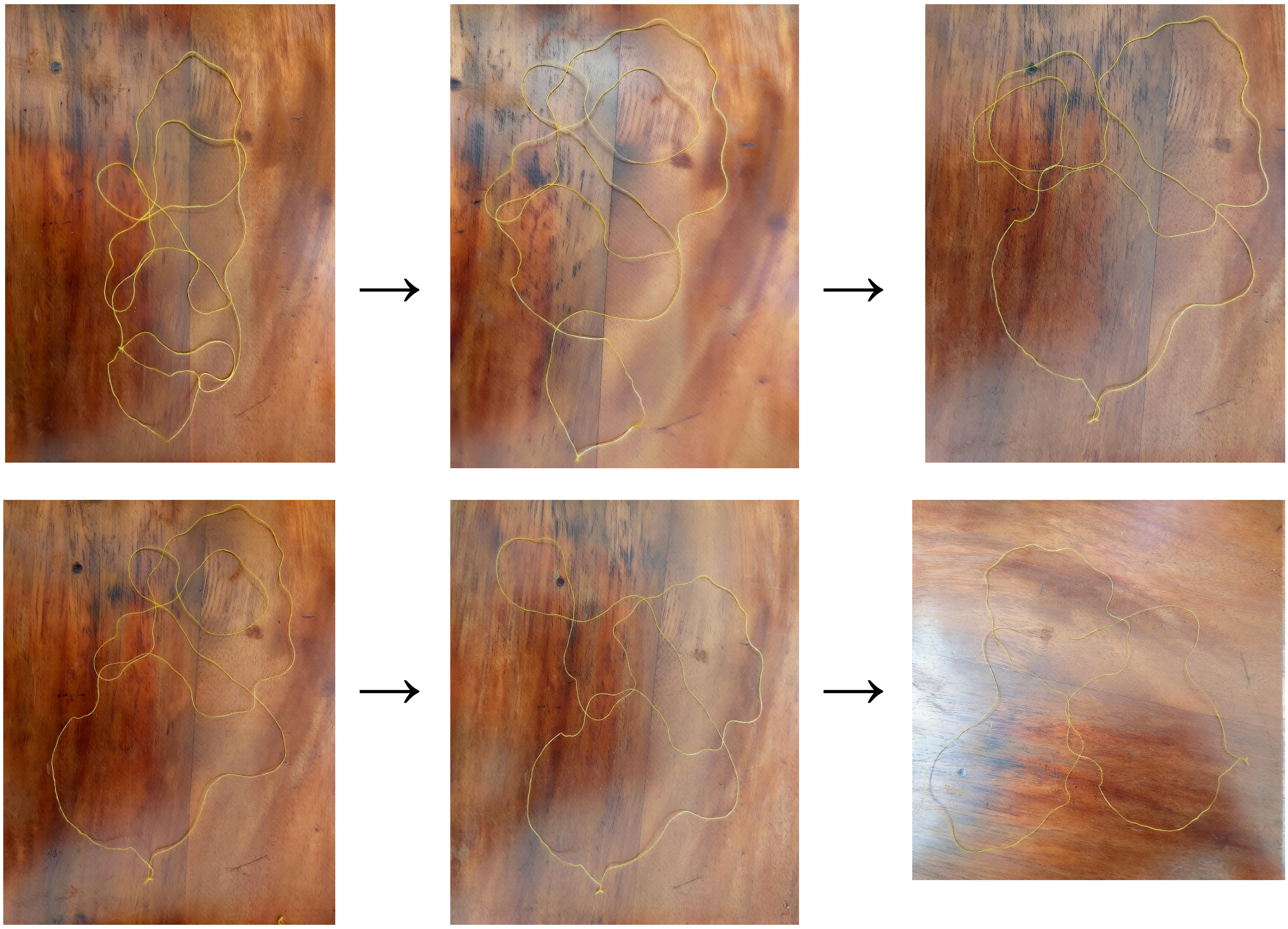
The figure-of-eight knot is not tricolourable, as there is always one intersection with 2 colours rather than 3, but it is 5-colourable.

p-colourability is not a perfect invariant, as different knots can have the same *p*-colourability. That is why mathematicians also use other invariants, such as the Alexander and HOMFLY-PT polynomials, to compare knots. If two knots do not share an invariant, they cannot be the same knot; however, sharing one invariant does not prove that two knots are the same.

Test Time!

Now it is time to put these ideas to the test. The two diagrams below may look different, but do they represent the same knot?

Are the two knots the same? If you are unsure, create a model and try to perform Reidemeister moves. If you can't create a model yourself, the diagram below shows what Reidemeister moves you need to complete to get from the knot on the left to the knot equivalence.



The 5 moves shown above are RI, RI, RIII, RI, RI, which proves the 2 knots are equivalent; however, there may be other combinations of moves that also prove the 2 knots are equivalent. As seen above, there are so many different projections/diagrams of the figure-of-eight knot, let alone other, more complex knots, that we need a way to represent them in 3D space.

Geometric Representation

So far, we have thought of knots as diagrams that can be compared and classified, but knot theory can go further by describing knots as precise geometric objects. Parametric equations trace the knot as a curve in three-dimensional space. These equations describe the exact (x, y, z) coordinates of that laser at any given time.

A parametric knot is written as three equations, one for each axis/ dimension :

$$x = x(t)$$
$$y = y(t)$$
$$z = z(t)$$
$$\text{where } t \in [0, 2\pi]$$

When t runs through a full interval, the point $(x(t), y(t), z(t))$ traces out the entire knot. By using suitable sine and cosine functions, mathematicians can make these equations form knots. To build a knot from scratch, there are 4 steps:

Step 1) Pick the knot you want to draw.

Step 2) Start from a simple closed circle with coordinates ($\cos(t)$, $\sin(t)$)

Step 3) Add extra frequencies to create crossings. Similar to adding waves to a calm pool, manipulating frequencies turns a simple circle into a knot. By making the point move up and down (z-axis) while it circles the centre (x and y axes), we create the "over-under" crossings necessary for a knot.

$$x(t) = \cos(t) + \cos(mt)$$
$$y(t) = \sin(t) + \sin(nt)$$
$$z(t) = \sin(kt)$$

Step 4) Check that it is the correct knot type and does not self-intersect

Step 5) Confirm the knot type is correct by inspecting the diagram against knot invariants.

A standard trefoil parameterisation is

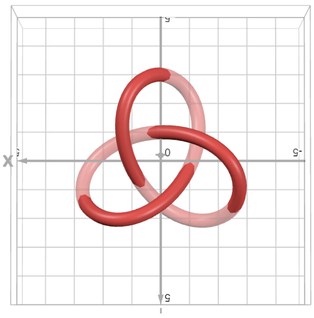
$$x(t) = \sin(t) + 2\sin(2t)$$

$$y(t) = \cos(t) - 2\cos(2t)$$

$$z(t) = -\sin(3t).$$

On Desmos 3D, the formula below plots the trefoil.

$$(\sin t + 2\sin 2t, \cos t - 2\cos 2t, -\sin 3t)$$
$$0 \le t \le 2\pi$$



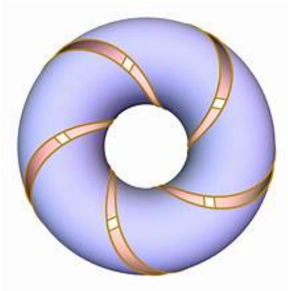
A more intuitive way to build a knot is to imagine a piece of string wrapped around the surface of a torus (a doughnut). A *(p,q)* torus knot can be parameterised by:

$$\gamma(t)=((R+r\cos(qt))\cos(pt),\ (R+r\cos(qt))\sin(pt),\ r\sin(qt))$$

R = distance of the centre of the doughnut to the centre of the tube

r = radius of the tube itself

$R > r > 0$, and p and q are coprime integers.



torus knot

To break down the equation:

- p represents how many times the string loops through the centre hole (the long way).
- q represents how many times it wraps around the "tube" itself (the short way).
- p and q are coprime, so the curve closes after one single component rather than multiple, giving a knot rather than a link

The simple trefoil can also be drawn as the (2,3) - torus knot.

$$x(t)=(2+\cos 3t)\cos 2t\ , y(t)=(2+\cos 3t)\sin 2t,\ z(t)=\sin 3t$$

- $\cos(2t)$ and $\sin(2t)$ make the curve go around the main axis twice
- $\cos(3t)$ and $\sin(3t)$ make it wobble 3 times
- 2 and 3 are coprime, so the curves close up as one knot instead of breaking into multiple loops

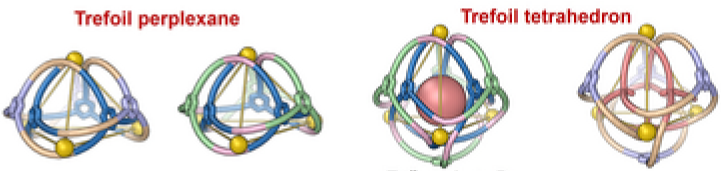
<u>Why classification matters</u>

There are many different ways to represent knots, from diagrams to parametric equations, but how do you organise the plethora of knots? In a periodic table, elements are organised by atomic number. Knot tables are the same, with knots being organised by crossing number - the number of intersections in the knot.

Knot tables typically list prime knots, since connected sums of prime knots form composite knots. As the number of crossings grows, distinguishing knots becomes much harder, which is why classification tools like invariants are so important. Classification is important because it gives mathematicians a way to sort knots into families, spot patterns, and decide when two very different-looking diagrams are really the same knot in disguise. This kind of classification helps us understand knots that appear in DNA and other real structures.

Real-world knotting

Trefoil cages are trefoil-shaped molecules that can contain other molecules. Trefoil cages can be more stable because their knotted structure makes them harder to break apart or rearrange. In this way, knot theory helps explain why some molecular cages are unusually robust.



DNA topoisomerases (biological mathematicians) are proteins that help untangle DNA during replication. DNA replication is essential to life and works by initially unwinding the double helix into 2 separate strands; however, during this process, the tension can become so high that the DNA 'supercoils' onto itself, making it impossible to separate the strands. Type 2 topoisomerases work by cutting, separating and reconnecting the strands carefully so that the DNA will not knot again. This process is key to understanding how knots are detected in nature.

Modern connection

Knot theory helps predict protein structure in AlphaFold. AlphaFold is an AI that predicts protein interactions; however, it is hard to assess whether these predictions are physically plausible because of the complexity of protein shapes. Studies of AlphaFold outputs have identified 7_1-knot highly knotted proteins, including composite knots and even a7_1-knot.

Knot theory is a topological check for the AI-generated molecular structure. Since knotting can significantly impact folding pathways and stability, it is also important to recognise it to understand how it affects the protein's properties.

Conclusion

Knot theory began as Lord Kelvin's theory of atomic structure and has developed into a powerful tool for understanding much more than abstract diagrams. From Reidemeister moves and polynomial invariants to parametric equations, knot theory gives mathematicians a way to describe, compare, and classify knots with precision. Its importance extends beyond mathematics into real-world structures such as DNA, molecular cages, and proteins, where knotting can affect stability and function. Knot theory shows how a simple question about loops can lead to deep insights in science, biology, and even AI prediction.

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