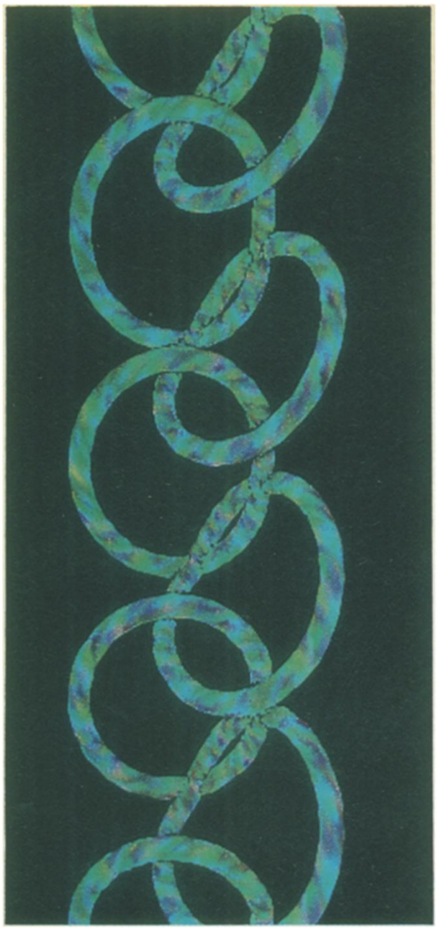


Dobkin/Princeton

Unknotting a Tangled Tale

The mathematics of telling knots apart unravels some of the twists and turns of molecular biology and hints at links with theoretical physics

By IVARS PETERSON

The mathematician's idea of a knot differs somewhat from that of a sailor or a boy scout. Unlike a knotted piece of rope, a mathematical knot has no free ends. Instead, it snakes through space, finally catching its tail to form a closed loop.

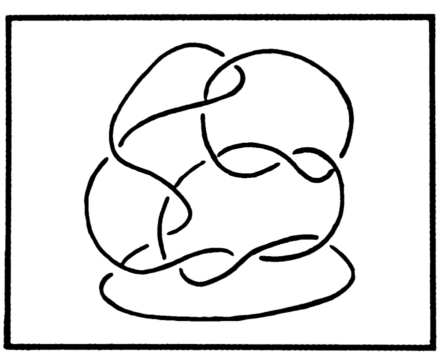
Yet mathematicians can ask the same questions about a knotted curve that a sailor might ask about a knotted rope. What kind of knot is it? Is the curve (or rope) really knotted? Can a second knot undo the first? And the fundamental problem of knot theory: How can different knots be distinguished?

The last few years have seen a resurgence of interest in knot theory, precipitated by the unexpected discovery of several new ways of mathematically distinguishing knots (SN: 10/26/85, p.266). Mathematicians are beginning to catch glimpses of what these methods mean geometrically. Molecular biologists are using them to understand how DNA strands can be broken, then recombined into knotted forms. And a few investigators are exploring tantalizing, mysterious hints of possible links between knot theory and theoretical physics.

"Right now this is a very exciting area," says mathematician Kenneth C. Millett of the University of California at Santa Barbara. "These are profoundly complicated problems. They represent a very big mystery. But there is a sense that the solution to this mystery will contain some revolutionary new concepts."

One way to tell whether a certain knot is really the same as a seemingly different knot, tied in another closed loop, is to try twisting and pulling one knot until it matches the other. If that can be done without cutting the loop, the two knots must be equivalent. However, failure to turn up a match, even after hours of fruitless labor, doesn't prove the two knots are different. Perhaps the right combination of moves was somehow overlooked.

Mathematically, the answer is to find a simple way to pin a label on a given knot so either two knots with the same label are equivalent or two knots with different labels are truly different. In the latter case, the label would be enough to indicate that no amount of twisting, pulling or pushing would ever transform one knot into the other. An easily calculated label would allow knot theorists to tell knots apart without having to go through the messy task of tangling with the knots themselves.



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Is this loop truly a knot or can it be deformed into an unknot, or circle?

To tackle the problem of classifying and distinguishing knots, mathematicians have adopted a set of rules that make knots more convenient to work with. Instead of analyzing three-dimensional knots, they examine two-dimensional shadows cast by these knots.

This approach is possible because even the most tangled configuration can be shown as a continuous loop whose shadow winds across a flat surface, sometimes crossing over and sometimes crossing under itself. In drawings of mathematical knots, tiny breaks in the lines signify underpasses or overpasses, while arrows indicate the direction of travel around a loop.

A loop without any twists or crossings – in its simplest form, a circle – is called an unknot. The simplest possible knot is the overhand or trefoil knot, which is really just a circle that winds through itself. In its plainest form, this knot has three crossings. It also comes in two forms: left-handed and right-handed configurations, which are mirror images of each other.

Only one knot has four crossings, and two distinct knots have five crossings. Mathematicians have proven the club expands rapidly from there to a total of 12,965 identifiable knots with 13 or fewer crossings, excluding mirror images. Thirteen is the highest number of crossings for which a complete catalog of knots now exists. Because knots may also be intertwined, like links in a chain, the complexities multiply rapidly.

One approach to distinguishing knots is to use the arrangement of crossings in a knot diagram to produce an algebraic formula that serves as a label for the knot. Such a label, which stays the same no matter how much a given knot may be deformed or twisted, is known as an invariant.

In 1928, John W. Alexander discovered a systematic procedure for generating such a formula. Expressed as positive or negative powers of some variable with integer coefficients, his simple polynomials for characterizing and labeling knots — such as the expression $t^2 - 3t + 1$ — turn out to be remarkably useful, though not foolproof.

If two knots have different Alexander polynomials, then the knots are definitely not equivalent. For instance, the trefoil knot carries the label $t^2 - t + 1$, whereas a figure-8 knot is $t^2 - 3t + 1$. But two knots that have the same polynomial aren't necessarily equivalent. The procedure doesn't distinguish, for example, between a knot's left-handed and right-handed forms.

It took mathematicians several decades to understand why the Alexander polynomials work and which knot properties the polynomials capture. In Alexander's method, only the crossing type — over or under — and the crossing arrangement make a difference. His formula is the mathematical equivalent of systematically snipping the knot's two strands at each crossing and refastening the ends into a simpler arrangement.

In the 1960s, mathematician John H. Conway, exploiting this new understanding, developed an easier method for computing any Alexander polynomial. Conway's method recognizes that a knot can be progressively unknotted by changing selected over and under crossings. Step by step, his unknotting game leads to an Alexander polynomial.

In 1984, Vaughan F. R. Jones of the University of California at Berkeley unexpectedly discovered a connection between von Neumann algebras — mathematical techniques that play a role in quantum mechanics — and braid theory. A mathematical braid can be thought of as a set of hanging strings that have been twisted together in some pattern. The top and bottom ends of such a braid pattern can be tied together to form a knot.

This chain of reasoning — from physics to braids to knots — led Jones to the formulation of a new type of polynomial invariant. Later, Louis H. Kauffman of the University of Illinois at Chicago redefined the Jones polynomial, cutting it loose from its origins in von Neumann algebras and expressing it in terms of altered crossings in knot diagrams. Kauffman explains his scheme in the March issue of THE AMERICAN MATHEMATICAL MONTHLY.

Jones' discovery prompted a great deal of excitement in the mathematical community because his polynomial invariants detect the difference between a knot and its mirror image. Furthermore, it stimulated the discovery of many more such invariants. Now, says Joan S. Birman, presently at Princeton (N.J.) University, "there are more polynomials than anybody knows what to do with."

"It's like a zoo," adds Millett. Just as animals can be put into families that fall into a kind of evolutionary hierarchy, the newly discovered invariants reveal similar relationships. "They appear to have certain properties that tie them closely together," he says. But some mathematicians fear the simple cases so far investigated may be exceptions to the rule. Millett and W.B.R. Lickorish of the University of Cambridge in England describe the most important of the new invariants in the February MATHEMATICS MAGAZINE.

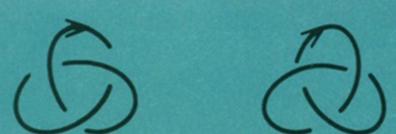
It seems clear all these invariants are part of a still larger picture that mathematicians barely glimpse. They know none of the first 12,965 knots has a polynomial that equals 1: the polynomial of the unknot. But they also know present theories can't distinguish certain classes of distinct knots.

"For any of the polynomials we have around at the moment, there are knots that are definitely different — proved to be so by some other method — but that have the same polynomial," Kauffman says. On the other hand, no one has yet found a knot with a Jones polynomial equal to 1 that can't be deformed into a circle.

In other words, the Jones polynomial may turn out to be a detector of knotting. Computing the Jones polynomial for a given tangle and finding that the polynomial equals 1 would be a guarantee that the loop is merely a cleverly disguised circle and contains no knot. However, mathematicians aren't yet ready to bet on this possibility.

In attempting to unlock the secrets of the new polynomial invariants, mathematicians experiment by drawing lots of pictures and using hours and hours of computer time. They audition knots, looking for qualities that would focus attention on what the new invariants reveal and what they hide.

Computing a particular invariant for a given knot is often quite complicated and time-consuming. The difficulty is that the time needed to compute the invariant goes up exponentially with the number of crossings. This makes a knot with, say, 40 crossings almost impossible to check, even by computer. Millett and his colleagues have been developing improved



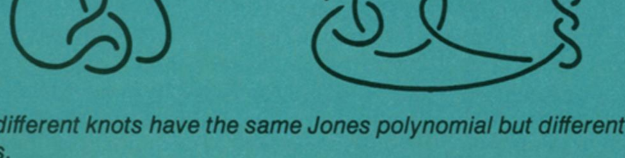
Left-handed and right-handed trefoil knots.

$(-2\ell^2 - \ell^4) + \ell^2 m^2$

$(-\ell^{-2} - 1 - \ell^2) + m^2$

$(3\ell^4 + 2\ell^6) + (-4\ell^4 - \ell^6)m^2 + \ell^4 m^4$

The first three entries in a table of knots. The two-variable, polynomial expression associated with each knot is known as a Laurent polynomial, one of the recently discovered types of knot invariants and a descendant of the Jones polynomial.



These two different knots have the same Jones polynomial but different Laurent polynomials.

Millett et al./MATHEMATICS MAGAZINE

methods, or algorithms, for computing the polynomials on both supercomputers and special-purpose computers.

Like physicists who are trying to make sense of the particles and forces that make up the physical world, knot theorists are looking for something akin to a grand unified theory that would explain all invariants and all knots. They hope eventually to find a complete invariant that distinguishes any two knots.

Also missing is the "bus stop" invariant – a formula so simple that a mathematician waiting at a bus stop could pick any knot that springs to mind and quickly compute whether that particular tangled mess is really an unknot or a disguised version of some other familiar knot.

Moreover, no one really understands what the new invariants mean geometrically. The Jones polynomial apparently encodes many kinds of data about knots, but in very strange ways. Jones is now trying to formulate a three-dimensional version of the new invariants that can be applied directly to a knot in three-dimensional space rather than to the two-dimensional diagram produced by the knot's shadow.

"It turns out that this can be done," says Jones, "but I haven't quite nailed down the three-dimensional formula yet." Such a formula, from which any of the two-dimensional invariants could be derived, would be a significant step toward understanding what the invariants mean.

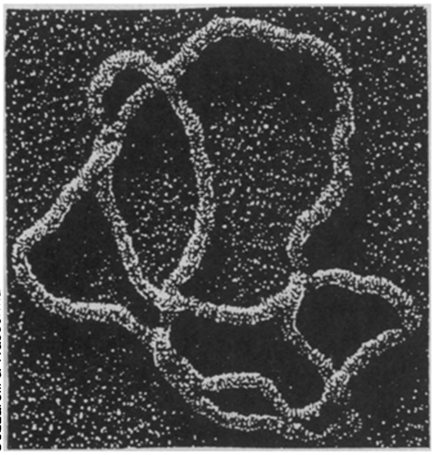
"All these things are in the air," says Birman. "Somebody's going to put it together, but it hasn't been done yet."

The procedure for computing invariants – cutting crossings, then forming new links – bears an uncanny resemblance to biological processes in which enzymes break apart protein strands or DNA molecules, then recombine them. "If you're asking, as a knot theorist, the question of what kind of knots can you get by these recombination moves, then, in fact, you may well be asking questions that are relevant to molecular biology," Kauffman says.

For example, researchers are applying knot theory and knot invariants to the study of DNA configurations during enzyme-directed recombination processes. Photographs of protein-coated DNA molecules, taken through an electron microscope, clearly show that DNA strands can form into loops that are sometimes knotted. But it's often hard to tell from a photograph whether a given tangled loop of DNA is actually knotted or whether one knotted loop is really the same as another.

"What we used to do was to take a piece of string and try to make it in the same shape as we saw by electron microscopy," says molecular biologist Nicholas R. Cozzarelli of the University of California at Berkeley, "and then, by twisting or bending that string, see if we could deform it into a pattern we had seen in another case. That worked for simple cases, but the inability to go from one state to another didn't prove that the path doesn't exist. We had to get some help from the mathematicians."

By working with invariants such as the Jones polynomial, Cozzarelli and his team could mathematically label the knots they saw in their experiments and identify knots that were the same. From this evidence, they could work out the logical order in which DNA strands are cut and recombined to produce certain configurations – tracking the sequence of steps by which one structure is gradually transformed into another during the basic life-supporting processes that take place within cells. "Instead of manipulating DNA, you can manipulate equations," Cozzarelli says.


Cozzarelli & Wasserman

An electron micrograph of a protein-coated DNA strand clearly shows the crossings indicating the strand is knotted. Researchers, by tracing the logic of DNA recombinations, predicted the existence of this particular knotted form, which has six crossings, and subsequently found and photographed it.

Such information allows Cozzarelli to make predictions about the existence of DNA configurations not yet found. In one instance, his group predicted that a specific six-crossing knot must be the next step in a sequence of molecular reactions. When they went looking for it, they found the predicted knotted loop. An account summarizing the work done by Cozzarelli and his colleagues appears in the JOURNAL OF MOLECULAR BIOLOGY (1987, Vol. 197, pp. 585-603).

The problem of classification is now essentially solved for known DNA knots and chains, says James H. White of the University of California at Los Angeles. "And techniques are available to solve any additional problem that comes up."

Knot theory has potential applications not only in molecular biology but also in physics. In fact, the mathematical classification of knots started in the late 19th century when British scientist Lord Kelvin hypothesized that atoms were knotted vortices in the ether, an invisible fluid then thought to fill all space. By classifying knots, he hoped to organize the known chemical elements into a periodic table. Kelvin's atomic theory died, but the mathematical study of knots survived, and now researchers are seeing hints of new links between knot theory and physics.

"There seem to be fascinating relationships with physics, and the relationships are surprising at one level and perhaps not so surprising at another," Kauffman says. For example, knots are physical to begin with, and knot diagrams sometimes resemble diagrams physicists draw to represent interactions between elementary particles. "You can think of putting at the crossing of a knot the mathematics that's related to the interaction of two particles," he says. A knot diagram becomes a way of summing up all the different kinds of interactions that can take place.

A similar scenario could apply in statistical mechanics – to the behavior of molecules in a condensing vapor or the lining up of electron spins when a material becomes magnetized. "In a physical situation, you often have a summation over a lot of different interactions that can happen, and the [knot] invariants seem to be . . . averages over all these different possibilities," Kauffman says.

Some mathematicians have also been using a particular set of equations, sometimes used by physicists in statistical mechanics, to find new knot invariants. "There's something extremely mysterious going on," says Jones. "This purely mathematical device that physicists use to solve their models in statistical mechanics and field theory is precisely the thing that generates other [knot] invariants. It's very tempting to try to find out if this mathematical relationship has any physical meaning."

Any possible connections, if they exist at all beyond mere coincidence, are likely to be subtle. "The most intriguing aspect of the whole thing, is that there might be some kind of duality between field theories in physics and knot invariants in mathematics," Jones says. If that were the case, then a physicist – to evaluate whether two apparently different field theories describing, say, forces between certain particles, are truly different – could convert the problem into a question about knots and knot invariants.

Originally, Jones discovered the first new invariant by taking a route beginning in theoretical physics. "It took me a long time to really believe that there was some continuing connection with physics," he says. "The similar framework looked like an accident. Now I'm pretty convinced that there really is something going on." □