The Combinatorial Revolution in Knot Theory

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not theory is usually understood to be the study of embeddings of topological spaces in other topological spaces. Classical knot theory, in particular, is concerned with the ways in which a circle or a disjoint union of circles can be embedded in \mathbb{R}^3 . Knots are usually described via *knot diaarams*, projections of the knot onto a plane with breaks at crossing points to indicate which strand passes over and which passes under, as in Figure 1. However, much as the concept of "numbers" has evolved over time from its original meaning of cardinalities of finite sets to include ratios. equivalence classes of rational Cauchy sequences, roots of polynomials, and more, the classical concept of "knots" has recently undergone its own evolutionary generalization. Instead of thinking of knots topologically as ambient isotopy classes of embedded circles or geometrically as simple closed curves in \mathbb{R}^3 , a new approach defines knots combinatorially as equivalence classes of knot diagrams under an equivalence relation determined by certain diagrammatic moves. No longer merely symbols standing in for topological or geometric objects, the knot diagrams themselves have become mathematical objects of interest.

Doing knot theory in terms of knot diagrams, of course, is nothing new; the Reidemeister moves date back to the 1920s [21], and identifying knot invariants (functions used to distinguish different knot types) by checking invariance under the moves has been common ever since. A recent shift toward taking the combinatorial approach more



Figure 1. Knot diagrams.

seriously, however, has led to the discovery of new types of generalized knots and links that do not correspond to simple closed curves in \mathbb{R}^3 . Like the complex numbers arising from missing roots of real polynomials, the new generalized knot types appear as abstract solutions in knot equations that have no solutions among the classical geometric knots. Although they seem esoteric at first, these generalized knots turn out to have interpretations such as knotted circles or graphs in three-manifolds other than \mathbb{R}^3 , circuit diagrams, and operators in exotic algebras. Moreover, classical knot theory emerges as a special case of the new generalized knot theory.

This diagram-based combinatorial approach to knot theory has revived interest in a related approach to algebraic knot invariants, applying techniques from universal algebra to turn the combinatorial structures into algebraic ones. The resulting algebraic objects, with names such as *kei*, *quandles*, *racks*, and *biquandles*, yield new invariants of both classical and generalized knots and provide new insights into old invariants. Much like groups arising from symmetries of geometric objects, these knot-inspired algebraic structures have connections to vector spaces, groups, Lie groups, Hopf algebras, and other mathematical structures.

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Consequentially, they have potential applications in disciplines from statistical mechanics to biochemistry to other areas of mathematics, with many promising open questions.

Virtual Knots

A *geometric knot* is a simple closed curve in \mathbb{R}^3 ; a *geometric link* is a union of knots that may be linked together. A *diagram* D of a knot or link K is a projection of K onto a plane such that no point in D comes from more than two points in K. Every point in the projection with two preimages is then a *crossing point*; if the knot were a physical rope laid on the plane of the paper, the crossing points would be the places where the rope touches itself. We indicate which strand of the knot goes over and which goes under at a crossing point by drawing the undercrossing strand with gaps.

Combinatorially, then, a knot or link diagram is a four-valent graph embedded in a plane with vertices decorated to indicate crossing information. We can describe such a diagram by giving a list of crossings and specifying how the ends are to be connected; for example, a *Gauss code* is a cyclically ordered list of over- and undercrossing points with connections determined by the ordering. See Figure 2.



Figure 2. A knot and its Gauss code.

Intuitively, moving a knot or link around in space without cutting or retying it shouldn't change the kind of knot or link we have. Thus we really want topological knots and links, where two geometric knots are topologically equivalent if one can be continuously deformed into the other. Formally, topological knots are *ambient isotopy* classes of geometric knots and links. In the 1920s Kurt Reidemeister showed that ambient isotopy of simple closed curves in \mathbb{R}^3 corresponds to equivalence of knot diagrams under sequences of the moves in Figure 3 [21]. In these moves, the portion of the diagram outside the pictured neighborhood remains fixed. The proof that a function defined on knot diagrams is a topological knot invariant is then reduced to a check that the function value is unchanged by the three moves.

In the mid-1990s various knot theorists (e.g., [11, 14, 17]), studying combinatorial methods of computing knot invariants using Gauss codes and similar schemes for encoding knot diagrams, noticed that even the Gauss codes whose associated



Figure 3. Reidemeister moves.

graphs could not be embedded in the plane still behaved like knots in certain ways—for instance, knot invariants defined via combinatorial pairings of Gauss codes still gave valid invariants when ordinary knots were paired with nonplanar Gauss codes. A planar Gauss code always describes a simple closed curve in three-space; what kind of thing could a nonplanar Gauss code be describing?

Resolving the vertices in a planar four-valent graph as crossings yields a simple closed curve in three-dimensional space.¹ To draw nonplanar graphs, we normally turn edge-intersections into crossings, but here all the crossings are already supposed to be present as vertices in the graph. Thus we need a new kind of crossing, a *virtual crossing* which isn't really there, to resolve the nonvertex edge-intersections in a nonplanar Gauss code graph. To keep the crossing types distinct, we draw a virtual crossing as a circled self-intersection with no over-or-under information. See Figure 4.



Figure 4. Virtual moves.

It turned out that Reidemeister equivalence of these nonplanar "knot diagrams" was important in defining and calculating the invariants.

¹Actually, we only need $\mathbb{R}^2 \times (-\epsilon, \epsilon)$ —knots are almost two-dimensional!

Since Reidemeister equivalence classes of planar knot diagrams coincide with classical knots, it seemed natural to refer to the generalized equivalence classes as "knots" despite their inclusion of nonplanar diagrams. The computations were suggesting that familiar topological knots are a special case of a more general kind of thing, namely Reidemeister equivalence classes of "knot diagrams" which may or may not be planar. The resulting "combinatorial revolution" was a shift from thinking of the diagrams as symbols representing topological objects (ambient isotopy classes of simple closed curves in \mathbb{R}^3) to thinking of the objects themselves as equivalence classes of diagrams. To reject these *virtual knots* on the grounds that they do not represent simple closed curves in \mathbb{R}^3 would mean throwing away infinite classes of knot invariants, akin to ignoring complex roots of polynomials on the grounds that they are not "real" numbers.

Virtual crossings and their rules of interaction were introduced in 1996 by Louis Kauffman [17]. Since the virtual crossings are not really there, any strand with only virtual crossings should be replaceable with any other strand with the same endpoints and only virtual crossings. This is known as the *detour move*; it breaks down into the four *virtual moves* in Figure 4.

Despite their abstract origin, virtual knots do have a concrete geometric interpretation. Virtual crossings can be avoided by drawing nonplanar knot diagrams on compact surfaces Σ which may have nonzero genus,² providing "bridges" or "wormholes" that can be used to avoid edgecrossings. A virtual knot is then a simple closed curve in an ambient space of the form $\Sigma \times (-\epsilon, \epsilon)$ (called a thickened surface or trivial I-bundle). Virtual crossings are not crossings in the classical sense of two strands close together-the strands meeting in a virtual crossing are on opposite sides of the ambient space or "universe in which the knot lives"-but are instead artifacts of forcing a knot in a nonplanar ambient space into the plane. This diagrams-on-surfaces approach was introduced by Naoko and Seiichi Kamada, who dubbed the results abstract knots in [14]. Other ideas related to virtual knots conceived independently include Vladimir Turaev's virtual strings [24] and Roger Fenn, Richárd Rimányi, and Colin Rourke's welded braids [8].

Figure 5 shows the smallest nonclassical virtual knot interpreted as a list of labeled crossings which cannot be realized in the plane, a virtual knot diagram and a knot diagram drawn on a surface with nonzero genus.



Figure 5. A nonclassical virtual knot.

Generalized Knots

Once we have one new type of crossing, it is natural to consider others, spawning a zoo of new species of generalized knot types. Introducing a new kind of crossing requires new Reidemeister-style rules of interaction. These rules or *moves* are determined by the desired combinatorial, topological, or geometric interpretation. For example, Figure 6 illustrates how the geometric understanding of virtual knots as knot diagrams drawn on surfaces with genus permits some moves while forbidding others.



Figure 6. Geometric motivation for moves.

We've seen that virtual crossings represent genus in the surface on which the knot diagram is drawn. *Flat crossings* are classical crossings where we forget which strand goes over and which goes under; these are convenient for studying the virtual structure separately from the classical structure and can be understood as "shadows" of classical crossings. *Singular crossings* are places where the knot is glued to itself with the strands meeting in a fixed cyclic order, that is, *rigid vertices*. Knots in *I*-bundles over nonorientable surfaces are known as *twisted virtual knots*; we indicate when a strand

²*Technically, we need to allow stabilization moves on the surface containing the knot diagram.*

has gone through a crosscap with a *twist bar* [2]. Figure 7 shows generalized crossing types with their geometric interpretations, Figure 8 lists some of their interaction laws, and Figure 9 shows some *forbidden moves* that look plausible but are not allowed based on the topological motivations for the new crossing types.



Figure 7. Generalized crossing types.

The combinatorial revolution also applies to higher-dimensional knots. Knotted surfaces in \mathbb{R}^4 have "diagrams" consisting of immersed surfaces in \mathbb{R}^3 with sheets broken to indicate crossing information. Combinatorially, such a knotted surface diagram consists of boxes containing triple points, boxes containing cone points, boxes containing pairs of crossed sheets, and boxes containing single sheets, each with information about how the boxes are to be connected. An abstract knotted surface diagram allows joining boxes in arbitrary ways, including ways that require virtual selfintersections to fit into \mathbb{R}^3 . An *abstract knotted* surface is then an equivalence class of such diagrams under the Roseman moves, the knotted surface version of the Reidemeister moves [4].

Introducing new types of crossings is not the only way to combinatorially generalize knots; much as altering the rules of arithmetic can change \mathbb{Z} into \mathbb{Z}_n , changing the list of allowed moves by replacing a move or adding or deleting moves also results in new types of "knots",

in which we now understand the term "knot" to mean "equivalence class of diagrams". As with the generalized crossing types, such alternative move-sets usually have a geometric or topological motivation. One example is *framed knots*, in which the geometric notion of fixing the linking number of the knot with its blackboard framing curve corresponds combinatorially to replacing the type I move with a writhe-preserving doubled I move, illustrated in Figure 10. Another example is *welded knots*, in which a strand may move over but not under a virtual crossing; welded virtual crossings are pictured as "welded to the paper".

Generalized knots have unusual properties not found in the classical knot world. Flipping a virtual knot over, that is, viewing it from the other side of the paper, generally results in a different virtual knot,³ unlike the classical case in which flipping over is just a rotation in space. Similarly, we can tie two virtual unknots sequentially in a string and get a nontrivial knot as a result! Figure 11 shows the Kishino knot, the result of joining two trivial virtual knots to obtain a nontrivial virtual knot [19]. The reader is invited to verify that the two knots on the left are trivial and to try to unknot the virtual knot on the right using only the legal moves from Figures 3 and 4 and not the forbidden moves in Figure 9. Proving that the Kishino knot is nontrivial turned out to be quite difficult, requiring algebraic invariants such as those in the next section.

Despite their apparent strangeness, generalized knots are increasingly finding applications both inside and outside of knot theory. Every invariant of virtual knots is automatically an invariant of ordinary classical knots. Virtual knot diagrams arise in computations in physics involving nonplanar Feynman diagrams [27]. Thinking of degree-*n* vertices as a type of crossing extends the combinatorial revolution to *spatial graph theory*, that is, embeddings of graphs in \mathbb{R}^3 , with applications in modeling of molecules in biochemistry, as well as areas of theoretical physics, such as spin networks.

Algebraic Knottiness

Turning knots into algebraic structures is an old idea, relatively speaking; the Artin braid groups were introduced in the 1920s [1], and many useful knot invariants (especially the "quantum invariants", which have connections to *quantum groups*, i.e., noncommutative noncocommutative Hopf algebras) have been derived from matrix representations of tangle algebras [15]. Including generalized crossings in our braids and tangles naturally yields corresponding new algebraic structures such as virtual braid groups and flat virtual tangle algebras, from which generalized quantum invariants can be derived. However, algebraification of knots via group theory or linear

³*Curiously reminiscent of complex conjugation...*



Figure 8. Rules of interaction for generalized crossings.



Figure 9. Forbidden moves.

algebra imposes certain *a priori* constraints on the resulting algebraic structures, for example, associativity of multiplication, which seem somehow artificial. More importantly, by insisting on forcing the algebraic structure into a predefined framework, we risk sacrificing useful information.

The combinatorial diagrammatic viewpoint suggests a method for deriving the minimal algebraic structure determined by Reidemeister equivalence of knot diagrams: start by labeling sections of a knot diagram with generators of an algebraic structure and defining operations where the pieces meet at crossings. The Reidemeister moves then determine axioms for our new algebraic structure.

We can divide the resulting algebraic structures into *arc algebras* where the labels are attached to *arcs*, that is, portions of the knot diagram from one undercrossing point to the next (which can be traced without lifting your pencil), and *semiarc algebras* where the generators are *semiarcs*, that is, portions of the knot diagram obtained by dividing at both over- and undercrossing points.

For example, if we label arcs in a knot diagram with generators and define an operation $x \triangleright y$ to mean "the result of x going under y", then the Reidemeister moves tell us the minimal axioms the algebraic structure must satisfy in order to respect the knot structure. The resulting algebraic object, called a *kei* (圭) or *involutory quandle*, was defined in the 1940s by Mituhisa Takasaki [23]. See Figure 12.

Definition. A *kei* is a set *X* with a map \triangleright : $X \times X \rightarrow$ *X* satisfying for all $x, y, z \in X$,

- (i) $x \triangleright x = x$,
- (ii) $(x \triangleright y) \triangleright y = x$, and
- (iii) $(x \triangleright y) \triangleright z = (x \triangleright z) \triangleright (y \triangleright z)$.

The first axiom says every element is idempotent; the second says that the operation is its own right-inverse, and the third says that in place of associativity, we have self-distributivity. Note the parallel with the group axioms. Examples of kei structures include Abelian groups with $x \triangleright y =$ 2y - x and $\mathbb{Z}[t]/(t^2)$ -modules with $x \triangleright y = tx + t$ (1 - t)y.

Giving a knot diagram an *orientation* (preferred direction of travel) lets us relax the requirement that the \triangleright operation is its own right-inverse, instead requiring only that \triangleright has a right-inverse operation \triangleright^{-1} . We then think of $x \triangleright y$ as x crossing under *y* from right to left and $x \triangleright^{-1} y$ as *x* crossing under *y* from left to right. The resulting algebraic object is called a *quandle*.

Definition. A *quandle* is a set *X* with maps \triangleright , \triangleright^{-1} : $X \times X \rightarrow X$ satisfying for all $x, y, z \in X$,

- (i) $x \triangleright x = x$, (ii) $(x \triangleright y) \triangleright^{-1} y = (x \triangleright^{-1} y) \triangleright y = x$, and (iii) $(x \triangleright y) \triangleright z = (x \triangleright z) \triangleright (y \triangleright z)$.

It is not hard to show that in a quandle we have $x \triangleright^{-1} x = x$ for all x, that the inverse operation \triangleright^{-1} is also self-distributive, and that the two operations are mutually distributive. Indeed, these facts can be proved algebraically from the axioms or graphically using Reidemeister moves. Examples of quandle structures include kei, which form a subcategory of the category of quandles, as well as groups, which are quandles under *n*-fold conjugation $x \triangleright y = y^{-n}xy^n$ for $n \in \mathbb{Z}$, $\mathbb{Z}[t^{\pm 1}]$ -modules



Figure 10. Framed version of Reidemeister I move.



Figure 11. The Kishino virtual knot.

with $x \triangleright v = tx + (1 - t)v$ (called *Alexander auandles*), and symplectic vector spaces with $\mathbf{x} \triangleright \mathbf{y} =$ $\mathbf{x} + \langle \mathbf{x}, \mathbf{y} \rangle \mathbf{y}.$

The arc algebra arising from framed oriented moves is called a rack.

Definition. A *rack* is a set with operations satisfying quandle axioms (ii) and (iii) but not necessarily (i).

The rack axioms are equivalent to the seemingly circular requirement that the functions f_{γ} : $X \rightarrow X$ defined by $f_{y}(x) = x \triangleright y$ are rack automorphisms. Racks blur the distinction between elements and operators, as every element of a rack is both an element and an automorphism of the algebraic structure. Examples of rack structures include quandles, modules over $\mathbb{Z}[t^{\pm 1}, s]/s(t + s - s)$ 1) with $x \triangleright y = tx + sy$ (known as (t, s)-racks), and *Coxeter racks*, inner product spaces with $\mathbf{x} \triangleright \mathbf{y}$ given by reflecting \mathbf{x} across \mathbf{y} [9].

To form a more egalitarian algebraic structure, we can divide an oriented knot diagram at both over- and undercrossing points and let the semiarcs at a crossing act on each other as in Figure 13. The semiarc algebra of an oriented knot is called a *biquandle*; it is defined by a mapping of ordered pairs $B: X \times X \to X \times X$ satisfying certain invertibility conditions together with the set-theoretic Yang-Baxter equation

$$(B \times I)(I \times B)(B \times I) = (I \times B)(B \times I)(I \times B)$$

where $I: X \to X$ is the identity map. See [10] for more.

The category of biquandles includes quandles as a subcategory by defining $B(x, y) = (y \triangleright x, x)$. An example of a biquandle which is not a quandle is an *Alexander biguandle*, a module over $\mathbb{Z}[t^{\pm 1}, s^{\pm 1}]$ with B(x, y) = (ty + (1 - ts)x, sx) where $s \neq 1$.

Including new operations at virtual, flat, and singular crossings with axioms determined by the corresponding interaction rules yields a family of related algebraic structures such as virtual biquandles, singular quandles, semiquandles, and more.

Each generalized knot has an associated algebraic object determined by the types of crossings it contains and the equivalence relation defining it. Unoriented knots have fundamental kei; oriented knots have fundamental guandles and biguandles; framed oriented knots have fundamental racks,



Figure 12. Involutory quandle (kei) operation and axioms.

and so forth. As with generalized knots themselves, our new algebraic objects are equivalence classes of strings of symbols under Reidemeisterstyle equivalence relations, which we can also understand as algebraic axioms.

Much like groups, examples of kei, quandle, rack, and biquandle structures are found throughout mathematics, lurking just beneath the surface in vector spaces, modules over polynomial rings, Coxeter groups, Hopf algebras, Weyl algebras, permutations, and more. It is important to note that not every kei, quandle, and so forth comes from a specific knot or link; rather, labelings of knots by these algebraic objects are preserved by the Reidemeister moves.

New Knot Invariants

Theorem (Joyce, 1982). *There exists a homeomorphism* $f : S^3 \rightarrow S^3$ *taking an oriented knot* K *to another oriented knot* K' *if and only if the fundamental quandles* Q(K) *and* Q(K') *are isomorphic.*

When he introduced the term "quandle" in his 1982 dissertation, David Joyce showed that the fundamental quandle is a *complete* invariant of classical knots up to ambient homeomorphism. Roger Fenn and Colin Rourke later showed that the fundamental rack classifies irreducible framed oriented links in certain three-manifolds. Despite these powerful results, perhaps due to the impracticality of comparing algebraic structures described by generators and relations, most knot theorists shunned arc algebras in favor of other invariants. Indeed, kei, quandles, and racks have been independently rediscovered sufficiently often



Figure 13. Biquandle operations.

to have accumulated an impressive collection of alternative names, such as "crystals", "distributive groupoids", and "automorphic sets" [16, 20, 3].

As a complete invariant up to ambient homeomorphism, the knot quandle determines many other classical knot invariants. Indeed, many wellknown invariants can be easily derived from the knot quandle: the fundamental group of the knot complement and the Alexander invariants, for instance, can be computed from a presentation of the knot quandle. The hyperbolic volume of a knot has recently been shown to be a quandle cocycle invariant [12]. Even the celebrated Jones polynomial can be understood in terms of deformations of matrix representations of arc and semiarc algebras [7].

With the combinatorial revolution in knot theory, interest in arc and semiarc algebras and their knot invariants has been reinvigorated. One useful method for getting computable invariants from arc algebras is to compute the set of homomorphisms from the knot's fundamental arc algebra into a target arc algebra T. Such a homomorphism assigns an element of the target object to each arc in a diagram of the knot, and such an assignment determines a unique homomorphism provided the crossing relations are satisfied. These homomorphisms can be pictured as "colorings" of the knot diagram by elements of T.

If the target object T is finite, then the set of homomorphisms will likewise be finite, and we can simply count homomorphisms to get a computable integer-valued invariant known as a *counting invariant*. Figure 14 shows all colorings of the trefoil knot by the three-element kei R_3 with operation table given by

\triangleright	1	2	3
1	1	3	2
2	3	2	1
3	2	1	3.

The finiteness condition for coloring objects is not required; if the target kei is infinite but has a topology, for instance, then the set of homomorphisms itself is a topological space whose topological properties then become knot invariants [22].

Counting invariants are only the beginning; any invariant of algebraically labeled knot diagrams



Figure 14. Kei colorings of the trefoil by R_3 .

defines an *enhancement* of the counting invariant by taking the multiset of invariant values over the set of colorings of the knot. One simple example uses the cardinality of the image subkei of a kei homomorphism; instead of counting "1" for each kei homomorphism $f : Q(K) \to T$, we record $t^{[\operatorname{Im}(f)]}$, obtaining a polynomial invariant

$$p(t) = \sum_{f:Q(K)\to T} t^{|\mathrm{Im}(f)|}$$

which has the original counting invariant as p(1). For example, the trefoil in Figure 14 has counting invariant 9 with respect to R_3 and enhanced invariant $p(t) = 3t + 6t^3$. A more sophisticated example of an enhancement is the family of CJKLS quandle cocycle invariants which associate a *Boltzmann weight* $\phi(f)$ with each quandle coloring f, determined by a cocycle in the second cohomology of T [5]. In true combinatorial-revolutionary spirit, such two-cocycles have a geometric interpretation as virtual link diagrams [4].

Enhancement of counting invariants in which we replace a cardinality with a set is a basic example of a more general phenomenon known as *categorification*, in which simpler structures are replaced with higher-powered algebraic structures. Pioneered by mathematical physicists such as Louis Crane and John Baez, categorification involves replacing sets with categories, operations with functors, and equalities with isomorphisms. A prime example is *Khovanov homology*, in which a combinatorial algorithm for computing the Jones polynomial from a knot diagram is turned into a graded chain complex whose Euler characteristic is the Jones polynomial, with the homology groups forming a new, stronger invariant [18]. Similar methods have been applied to the HOMFLYPT polynomial and various other quantum knot invariants, resulting in new, stronger categorified knot invariants. This remarkable idea has sparked a firestorm of new research too vast to adequately address in this space. Nonetheless, we once again see the combinatorial revolution in action, as what was previously merely notation has itself become a mathematical object of interest.

Not Just for Knot Theorists

While arc and semiarc algebras such as quandles and racks have obvious utility in defining knot invariants, fundamentally they are basic algebraic structures analogous to groups or vector spaces whose potential for applications elsewhere in mathematics is still largely unexplored. The fact that groups are first encountered as sets of symmetries does not limit their applications to geometric rotations and reflections; similarly, despite their knotty origin, quandles, racks, and biquandles are likely to have many applications not tied to knots and links.

Starting with a symmetry group, if we take the subset consisting of only rotations, we get a subgroup; taking the subset consisting of only reflections, however, yields not a subgroup but a subkei. Conjugation in a group is a quandle operation; the resulting *conjugation quandles* quantify the failure of commutativity by turning it into an algebraic structure, analogously to commutators turning associative algebras into Lie algebras. Indeed, kei, quandles, and racks can be found lurking wherever operations are noncommutative.

The applications of generalized knots and knotinspired algebraic structures are just starting to be explored, and many open questions remain. One rich source of project ideas comes from a simple question: anywhere groups are found, we can ask what results when we replace the group with a kei, quandle, or rack. Replacing the knot group with the knot quandle eliminates the need to worry about the peripheral structure, for example, and replacing groups with quandles simplifies monodromy computations analogously [3, 25]. Work is currently under way on the Dehn quandle of a surface (analogous to the mapping class group), as well as on quandle and rack homology, quandle Galois theory, and much more [26, 6]. What arc algebra structures might be lurking in elliptic curves, dynamical systems, or tensor categories?

Knot diagrams have now come full circle, from schematic representations of geometric curves in space to interesting mathematical objects in their own right. The shift from thinking of knots as topological to typographical objects gives us new flexibility and opens the door to new discoveries and applications. As was the case with complex numbers, there has been some resistance to virtual knot theory from the old guard, though this author's subjective impression is that the tide is turning as more knot theorists embrace the new generalized knot theory and its related algebraic structures. In addition to providing new technical tools for knot theorists and other mathematicians, generalized knots provide a novel perspective on what it means to be a knot.

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