Asymptotic laws for random knot diagrams

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Abstract
We study random knotting by considering knot and link diagrams as decorated, (rooted) topological maps on spheres and pulling them uniformly from among sets of a given number of vertices \(n\), as first established in recent work with Cantarella and Mastin. The knot diagram model is an exciting new model which captures both the random geometry of space curve models of knotting as well as the ease of computing invariants from diagrams.

We prove that unknot diagrams are asymptotically exponentially rare, an analogue of Sumners and Whittington’s landmark result for self-avoiding polygons. Our proof uses the same key idea: we first show that knot diagrams obey a pattern theorem, which describes their fractal structure. We examine how quickly this behavior occurs in practice. As a consequence, almost all diagrams are asymmetric, simplifying sampling from this model. We conclude with experimental data on knotting in this model. This model of random knotting is similar to those studied by Diao et al, and Dunfield et al.

Keywords: random knot, knot probability, knot frequency, knot diagram, plane curve, random map

(Some figures may appear in colour only in the online journal)

1. Introduction

1.1. Random knotting

There are many models for sampling random knots, including those of self-avoiding lattice polygons [55], random Grassmannian space polygons [8, 7], random Chebychev polynomials [10], random braid words [39], and Petaluma [17]. In this paper we will discuss the random diagram model introduced in [6] under which knot diagrams are drawn uniformly from the set of all diagrams with a given number of crossings. Diagrams capture the geometry of space curves as every generic space curve can project to a knot diagram (which is not the case for braid diagrams and other similar models). The random diagram model is exciting as it...
combines both the geometry of space curve models of knotting with combinatorial ease of computing knot invariants from diagrams. There has been some work on sampling random knot diagrams [15, 16], but without regard to any specific distribution. As well, alternating knot and link diagrams have been studied [28, 40, 52] but alternating knot and link diagrams are a significantly restricted subclass of diagrams in general.

Classically, random knot models are of import to those studying polymer chains: random polymer chains at thermodynamic equilibrium are expected to behave like knots sampled with some appropriate distribution. Examples of models studied for this connection to polymers include self-avoiding lattice polygons, random Grassmannian polygons [8, 7, 27], Gaussian random polygons [30], and random equilateral polygons [14]. The technique of studying polymers through random knots is powerful and flexible; by using the appropriate model, different types of polymer chains and ambient environment can be studied. Appropriate curve models can account for thickness of the polymer strand [43], interactions of a polymer with a surface [25], self-interactions of the polymer [56], confinement of the polymer [22, 26, 48], polymers built from multiple types of monomer [53], and many other properties.

Many models of random knots, specifically those which are used for the simulation of polymer strands, obey the conjecture of Frisch, Wasserman, and Delbrück that almost all such objects are knotted or non-trivial. Indeed, it is a landmark result of Sumners and Whittington [55] (also discovered independently by Pippenger [42]) that this is true for self-avoiding polygon models of knotting. Their proof was adapted to numerous other models of random knotting, but it was as-of-yet unknown whether this behavior is exhibited in the random diagram model. That the random diagram model obeys this conjecture is the result which motivates this paper.

It is not yet known how the random diagram model ‘fits’ into the current vast jungle of random knot models and applications to polymers. It is not known either precisely how the random diagram model compares with 2d models of knots such as those described in [23, 38, 41]. Rather than argue a connection directly, this paper argues that the random diagram model is relevant in that it satisfies several universal properties satisfied by many models of random knots. The most important such property it shares is that it obeys the Frisch–Wasserman–Delbrück conjecture. After establishing a method to run experiments on the random diagram model, we examine data on the model and examine other universal properties numerically.

1.2. Overview

In [6], together with Cantarella and Mastin we provided a tabulation of all knot diagrams with crossing number up to 10. In this paper we begin by considering a slightly different object, rooted diagrams, for which the automorphism group is always trivial. We are then able to prove that in the large crossing number limit, knot diagrams behave similarly to rooted diagrams, so that our results carry over from the simpler rooted model to the unrooted model discussed in the prequel.

After introducing the key topological and combinatorial objects of interest, we discuss the motivating parallels that this model of knotting shares with those in the literature: Pattern theorems [33, 34], a key component of Sumners and Whittington’s proof, which assure that desired substructure appears often in fixed classes of objects. We show that a pattern theorem result holds for many different classes of diagrams, and provide constructions. We show then how this result implies the key theorems of the paper—that knot diagrams (rooted or unrooted) are both knotted and asymmetric.
We conclude with some experimental results. Experimentally, symmetries disappear rapidly (i.e. there are very few even in 10-crossing diagrams) so the rooted and unrooted numerics are close in the majority of our data set. We then examine the probabilities of different knot types and compare the behavior to different models of knotting. We finish with evidence that our numerics are somehow different than those of lattice polygon models of knotting in the sense that we obtain different limiting ratios of knot type appearances (see [47]).

2. Definitions

2.1. Knots, links, and tangles

A link is an isotopy class of embeddings of one or more circles into \( S^3 \). A knot is an isotopy class of embeddings of exactly one circle into \( S^3 \). Both of the prior are considered up to ambient isotopy of the embedded circles; roughly, this means that during the isotopy between two knots, the knot ‘cannot pass through itself’. A knot diagram (resp. link diagram) is an immersion of a circle (resp. any number of circles) into the oriented sphere \( S^2 \) which is generic in the sense that all intersection points are transverse double points, together with over-under (i.e. sign) information at each double point. The study of links and knots is well known to be equivalent to the study of link diagrams and knot diagrams up to the Reidemeister moves, shown in figure 1, by a theorem of Reidemeister [45].

To distinguish between space curves and their equivalence classes, we will use the term knot type to refer to a class of space curves, knots. The unknot is the ambient isotopy class of knots represented by the unit circle in \( S^3 \). A knot (or knot diagram) which represents the unknot is trivial. Knots and knot diagrams representing another class are knotted.

A k-tangle is a generic embedding of \( k \) closed intervals and any number of closed circles into \( B^3 \) so that precisely the \( 2k \) interval ends all lie in the boundary. A \( k \)-tangle diagram \( T \) is a generic immersion (generic in the same way as knot diagrams above) of \( k \) intervals and any number of circles into \( S^2 \) together with over-under information at each double point. In this paper, we will only discuss tangle diagrams in which all \( 2k \) ends of the intervals are all adjacent across some connected component of \( S^2 \setminus T \), so that the \( k \)-tangle diagram may be viewed as being an immersion into the disk \( D^2 \) with exactly the \( 2k \) interval ends lying in the boundary circle. An open strand of a tangle is any one interval; a closed strand of a tangle is any one circle.

2.2. Topological maps

Diagrams are actually considered up to ‘embedded graph isomorphism’. This precisely means that the viewpoint we should have is that of topological maps on surfaces [5, 35, 58].

1 Knot diagrams are immersions into the sphere rather than the plane both to draw parallels with how knots are embeddings into \( S^3 \) as well as to fit with the planar map framework in which this paper operates. The only difference between a knot diagram on the sphere and the plane is a choice of face (in the embedded graph sense), so the results herein could be easily adapted.
Definition. A map with $n$ vertices $M$ is a graph $\Gamma(M)$ embedded on a surface $\Sigma$ so that every connected component of $\Sigma \setminus M$ is a topological disk. The connected components of $\Sigma \setminus M$ are called the faces of $M$. If $\Sigma$ is the oriented sphere, then the map $M$ is planar. As each face must be a disk, maps’ underlying graphs are necessarily connected.

A map $M$ is 4-regular, 4-valent, or quartic if every vertex in the underlying graph $\Gamma(M)$ has degree 4.

It will be handy to view the data of maps as follows. A map with $n$ vertices decomposes as a triple $M = (A, E, V)$ called an arc-decomposition into arcs, edges, and vertices, where $A$ consists of $4n$ arcs (sometimes called half-edges or flags), $2n$ unordered pairs of arcs (the edges), and $n$ cyclic quadruples of arcs (the vertices), up to re-naming of arcs, so that each arc appears in exactly one edge and one vertex. These data define the embedding of a graph into a surface; the map is planar if this surface is the sphere. If $a$ is an arc in $M$, define $e(a)$ to be the unique edge containing $a$ and $v(a)$ to be the unique vertex which contains $a$. Maps are the same if they differ only by changing the set $A$ (re-indexing).

In this paper we will only consider planar maps, although by considering maps on any oriented surface of arbitrary genus and applying the ideas of this work one arrives at the study of virtual diagrams [61, 32].

Symmetry complicates the study of maps. A strategy to avoid this issue is to root the map by picking and directing a single edge:

Definition. A rooted map is a map together with a single edge marked with a direction, called a root edge.

An automorphism of a rooted map $M$ would be required to fix the root edge, its direction, and the orientation of the surface near the root; hence $\text{aut}(M)$ is the trivial group.

In the $M = (A, E, V)$ arc-decomposition, a rooting of $M$ is a pair $(M, a)$ of $M$ with an arc $a$. Maps have a well defined notion of dual map $M^*$, where there is an edge $\langle f_1, f_2 \rangle \in M^*$ if the face $f_1$ is adjacent to the face $f_2$ in $M$ (faces are adjacent if they share an edge along their boundaries). This definition guarantees a bijection between the vertices of $M$ and the faces of $M^*$. The dual map of a 4-regular map is a quadrangulation, i.e. a map for which the boundary of every face is a cycle of four edges. A quadrangulation is simple if it contains no parallel edges or loop edges (its underlying graph is simple).

Maps have a notion of substructure, which our pattern theorems will dictate:

Definition. A map $P$ with a marked face of $k$-edges is a submap of a map $M$ if there exists a cycle of $k$ edges (the cycle may repeat edges) in $M$ so that one of the two halves of $M$ separated by the cycle is identical to $P$.

2.3. Diagrams and shadows

Definition. A map decorated by a set $S$, $(M, s)$ is a map $M = (A, E, V)$ together with a mapping $s : V \to S$ which associates to each vertex of $M$ an element of $S$.

We can now rephrase the definitions of diagrams using the vocabulary of maps.

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2 This view is similar to that of combinatorial maps [11] or pdcodes [37], although knowing the connection is not necessary.

3 The notation of flag indicates that arcs belong not only to a unique crossing and edge, but also to a unique face, although this observation is not necessary here.
A link shadow with \( n \) crossings is a 4-regular planar map of \( n \) vertices. We will denote by \( L_n \) the set of all \( n \)-crossing link shadows and \( L = \bigcup_n L_n \) the class of all link shadows. Figure 2 shows a general planar map, and a link shadow.

A link diagram with \( n \) crossings is a 4-regular planar map decorated with \( S = \{+,-\} \). This is equivalent to making a choice of over-under strand information at each vertex, as demonstrated in figure 3. We will denote the set of \( n \)-crossing link diagrams by \( L_n \) and the class of all link diagrams by \( L = \bigcup_n L_n \).

Similar to maps, we can view link diagrams through an arc-decomposition \( D = (A,E,C) \), where \( A \) and \( E \) are the same, but \( C \) is the set of sign-decorated vertices called crossings.

Shadows and diagrams may be rooted by taking additionally an edge together with a choice of direction, as in figure 4. From here on, maps, shadows, and diagrams will be assumed rooted unless otherwise noted.

Remark. In order to be consistent with knot theory terminology, we use the word crossings to refer to the vertices of shadows and diagrams.

Remark. This definition has then that unrooted link shadows and link diagrams are nearly the same objects as in the prequel [6]. There are two differences:

1. As planar maps are defined on the oriented sphere, so too are our unrooted shadows (and diagrams) in this paper, as opposed to the unoriented sphere.
2. Our unrooted shadows (and diagrams) in this paper do not come with any ‘consistent’ choice of edge direction (i.e. an orientation of link components).
Notice that as there are at most $4n$ and at least 1 ‘oriented shadows with $n$ crossings on the oriented sphere’ to each ‘unoriented shadow with $n$ crossings on the unoriented sphere’, we get that asymptotically any results for our objects discussed herein hold for those examined in the prequel.

Indeed, $\mathcal{L}$ is just another name for the class of 4-regular planar maps counted by vertices; furthermore, the class of rooted planar quadrangulations is dual to $\mathcal{L}$. Hence, the class $\mathcal{L}'$ of link shadows has been counted exactly [58, 5]: if $\ell_n = |\mathcal{L}'_n|$, then:

$$\ell_n = \frac{2(3^n)}{(n+2)(n+1)} \binom{2n}{n} \sim \frac{2}{\sqrt{\pi}} 12^n n^{-5/2}.$$  

From this the exact counts of link diagrams can be determined as well. If $\lambda_n = |\mathcal{L}_n|$, then

$$\lambda_n = 2^n \ell_n = \frac{2^{n+1}(3^n)}{(n+2)(n+1)} \binom{2n}{n} \sim \frac{2}{\sqrt{\pi}} 24^n n^{-5/2}.$$  

Knot diagrams are the subset of link diagrams that have precisely one ‘link component’.

**Definition.** Define an equivalence relation on edges so that two edges are equivalent if they meet at opposite sides of a vertex. E.g. if the edges meeting at a vertex are indexed counter-clockwise as 0, 1, 2, 3, then the edges labeled 0 and 2 are equivalent, as are those labeled 1 and 3. A link component of a link shadow or diagram $D$ is an equivalence class of edges under this equivalence relation.

A knot shadow$^{4}$ is a link shadow which consists of precisely one link component. The set of knot shadows with $n$ crossings is denoted by $\mathcal{K}_n$ and the class of all knot shadows is denoted $\mathcal{K} = \bigcup_n \mathcal{K}_n$.

A knot diagram is a link diagram which consists of precisely one link component. The set of knot diagrams with $n$ crossings is denoted by $\mathcal{K}_n$ and the class of all knot diagrams is denoted $\mathcal{K} = \bigcup_n \mathcal{K}_n$.

**Remark.** Rooted knot diagrams have their unique link component oriented (there is a sense of direction around the circle), so we may translate raw sign information into over-under crossing information by using the usual definition as the sign of the cross product from the over trajectory to the under trajectory as in figure 5.

In the case of rooted link diagrams, not all link components are inherently oriented. However, after making any fixed a priori choice of deterministic algorithm to orient all of the link

$^4$ Kauffman calls these knot universes [31].
components in a rooted diagram, we can view signs as over-under information as in the case of knot diagrams.

Knot shadows $\mathcal{K}$ represent a curious, small subclass of $\mathcal{L}$. Indeed, exact counts for $k_n = |\mathcal{K}_n|$ and $\kappa_n = |\mathcal{K}'_n|$ are not known except by experiments and conjectures [28, 52]:

**Conjecture (Schaeffer-Zinn Justin 2004).** There exist constants $\mu$ and $c$ such that

$$\frac{\kappa_n}{2^n} = k_n \sim_{n \to \infty} c\mu^n \cdot n^{\gamma-2},$$

where

$$\gamma = -\frac{1 + \sqrt{13}}{6},$$

and $\mu \approx 11.415 \pm 0.005$.

This conjecture is of similar flavor to conjectures of the counts of both self-avoiding lattice walks and self-avoiding lattice polygons [24], which are also of the form [47, 36]

$$a_n \sim_{n \to \infty} c\lambda^n n^\alpha.$$

Indeed, a large number of different combinatorial models exhibit this type of growth; see Flajolet and Sedgewick [19] for examples.

Tangle diagrams may also be viewed in the language of maps:

**Definition.** A $k$-tangle shadow is a map embedded on a sphere which is 4-valent except for one distinguished ‘external’ vertex of degree 2$k$. A $yk$-tangle diagram is an unrooted $k$-tangle shadow decorated (at non-exterior vertices) with signs $\{+, -\}$.

A tangle shadow (resp. diagram) $T$ is contained as a subtangle, or simply contained, in a link shadow (diagram) $D$ if the dual of $T$, $T^*$ (with exterior face the dual of the exterior vertex), is a submap of $D^*$; for diagrams it is furthermore required that the signs of the crossings agree.

**Remark.** As in the case of rooted link diagrams above, after picking a deterministic scheme to orient all components (open and closed) from a tangle diagram together with choice of exterior arc, one can reconcile the view of crossing signs as over-under information.

We will view the exterior vertex of tangle shadows and diagrams as being ‘at infinity’ so that tangle shadows and diagrams appear to be 4-valent decorated maps with ‘loose’ edges in a common exterior face called arcs or legs, as shown in figure 6. This view matches up with the previous definition of tangle diagrams in $D^5$. 

![Figure 5](image-url)
Rooted diagrams (and shadows) may be viewed as directed long curves or two-leg diagrams (resp. shadows) by cutting the root edge into two directed half edges with one pointing towards its vertex (the hind leg) and one away (the front leg) as in figure 7. Two-leg diagrams are rooted 1-tangle diagrams.

We may view tangle diagrams from the arc-decomposition view; tangle diagrams are triples \((A, E, C)\) where some ‘exterior’ arcs do not belong to any edge and live in the same face.

Notation. When it is clear, we will henceforth use the term diagram to refer both to shadow and diagram objects (as shadows are diagrams with crossings decorated by a set of one element).

A key strength of the framework proposed in this paper is the simplicity with which the tools presented can be applied to other interesting classes of diagram objects. To demonstrate this, we will provide constructions for ‘prime’ and ‘reduced’ classes of diagrams as well;

Definition. A diagram \(D\) is prime if it has more than 1 vertex and is not 2-edge-connected, i.e. there is no way to disconnect the underlying graph of \(D\), \(\Gamma(D)\), by removing 2 edges. A diagram which is not prime is composite. A rooted diagram is two-leg-prime if it cannot be disconnected by removing two edges, one being the root edge. This property is dependent on the choice of root; figure 8 gives a diagram for which one rooting is two-leg prime, but the other is not.

A shadow or diagram \(D\) is reduced if it has no disconnecting vertices (i.e. isthmi).

It is important to note that prime knot diagrams can represent knot types which are composite. The condition of being a prime knot diagram is purely graph-theoretic.

Again, the counts of prime link shadows and prime link diagrams are known precisely. Exact counts are known from their bijection with simple quadrangulations [1];
\[ \frac{p\lambda_n}{2^n} = p\ell_n = \frac{4(3n)!}{n!(2n+2)!}. \]

The counts for prime knot diagrams are again unknown.

2.4. Composition of tangle diagrams

Key arguments that we discuss in this paper involve the ability to compose two diagrams in order to produce new diagrams with certain properties. We will describe this by first discussing methods of composition for tangle diagrams and then providing equivalences between diagrams and tangle diagrams.

Given two tangle diagrams \( T = (A_T, E_T, C_T) \) and \( S = (A_S, E_S, C_S) \) with respective exterior arcs \( \{t_1, t_2, \ldots, t_{2k}\} \) and \( \{s_1, s_2, \ldots, s_{2\ell}\} \) and a collection of unordered pairings
\[
\mu = \{(t_i, s_{j_1}), (t_i, s_{j_2}), \ldots, (t_i, s_{j_r})\}
\]
where each \( t_i \) and \( s_j \) appears at most once, define the \((k + \ell - r)\)-tangle diagram \( T\#_{\mu} S \) to be the tangle diagram
\[
T\#_{\mu} S = (A_T \cup A_S, E_T \cup E_S \cup \mu, C_T \cup C_S).
\]

Given an arbitrary choice of \( \mu \), it is possible that \( T\#_{\mu} S \) is non-planar or that not all exterior arcs of \( T\#_{\mu} S \) lie on the same face. We will define and use some specific tangle diagram compositions which avoid these pitfalls.

2.4.1. Connect summation. Analogous to the connect sum operation on knots in space, there is a notion of **diagram connect sum** on diagrams.

**Definition.** Given 1-tangle diagrams \( T, S \) with exterior arcs \( \{t_1, t_2\} \) and \( \{s_1, s_2\} \) and a pair of arcs \( (t_i, s_j) \) with \( i, j \in \{1, 2\} \), there is a complementary pair of arcs \( (t_{i'}, s_{j'}) \) with \( i \neq i' \) and \( j \neq j' \). So define the connect sum of the head \( t_i \) of \( T \) to the tail \( s_j \) of \( S \):
\[
T\#_{(t_i, s_j)} S = T\#_{(t_i, s_j)} (A_T \setminus \{e\}, E_T \setminus \{e\}, C_T) S.
\]

An example of this process is given in figure 9.

Given a diagram \( D = (A, E, C) \) and an edge \( e = (ab) \) in \( D \), define the 1-tangle diagram \( D \setminus e \) to be the 1-tangle diagram \((A, E \setminus \{e\}, C)\) with exterior arcs \( a \) and \( b \).

A diagram and a choice of arc \((D, a)\) is equivalently a 1-tangle diagram \((D \setminus \{e(a)\}, a)\). So given a 1-tangle diagram and a choice of 'tail' exterior arc \((T, b)\), define the connect sum of \( T \) to \( D \) by \( a, b \) to be
\[
D\#_{(a,b)} T = (D \setminus e(a))\#_{(a,b)} T.
\]

An example of connect summation of a tangle diagram into a diagram is given in figure 10.
Link components behave predictably under connect summation: if the tangle diagrams \( T, S \) have \( \tau, \sigma \) closed circle components respectively, then \( T \# S \) has exactly \( \tau + \sigma + 1 \) closed circle components (independent of choice of head and tail for the connect summation). It follows then that if \( D \) is a knot diagram and \( T \) is a tangle diagram with no closed circle components that \( D \# T \) is always itself a knot diagram. This can be seen as the tangle diagram \( D \setminus \{ e \} \) itself has no closed circle components independent of choice of \( e \) as \( D \) was a knot diagram.

2.4.2. Cyclic composition. We can extend this definition to tangle diagrams with additional exterior arcs, but we will then focus on tangle diagrams with precisely four.

**Definition.** Given \( k \)-tangle diagrams \( T, S \) with external arcs
\[
\{ t_1, \ldots, t_{2k} \}, \{ s_1, \ldots, s_{2k} \},
\]
choices \( t_i \) and \( s_j \) of arcs induce ordered tuples \( t_i, \ldots, t_{2k}, s_j, \ldots, s_{2k} \) by enumerating the external arcs of \( T \) counterclockwise and \( S \) clockwise, starting with the chosen arcs. Then with \( \mu = \{(t_i, s_j), \ldots, (t_{2k}, s_{2k})\} \), define the composition to be the link diagram
\[
T \#_{\mu} S = T \#_{\mu} S.
\]

By this choice of \( \mu \), as \( T \) and \( S \) are both planar, so too is the composition \( T \#_{\mu} S \).

The number of components in the resulting diagram will depend (in addition to the count of closed loop components) on the ordering of the external arcs of \( T, S \) as well as the precise matching. If however we are dealing with tangle diagrams of four exterior arcs, we can be assured the existence of a choice for \( \mu \) which can guarantee some control over the number of link components of the resultant diagram.

Consider the case where \( T, S \) are 2-tangle diagrams with \( \tau, \sigma \) closed components respectively. Let the exterior arcs of \( T \) be indexed counterclockwise as \( \{ t_i \}_{i=1}^{4} \) and the exterior arcs of \( S \) be indexed counterclockwise as \( \{ s_i \}_{i=1}^{4} \). For each tangle diagram, color one open strand blue and the other open strand red. Up to changing colors or switching \( T \) with \( S \) there are four possibilities for cyclic composition.

1. The exterior arcs of both \( T \) and \( S \) are colored counterclockwise blue-red-blue-red. In this case, the two open components always close into two distinct link components, and the resulting number of components is \( \tau + \sigma + 2 \). This situation is shown in figure 11(A).

2. The exterior arcs of \( T \) are colored counterclockwise blue-blue-red-red and those of \( S \) are colored counterclockwise blue-red-red-blue. In this case, the two open components always close into two distinct link components, and the resulting number of components is \( \tau + \sigma + 2 \). This situation is shown in figure 11(B).
(3) The exterior arcs of $T$ are colored counterclockwise blue-blue-red-red and those of $S$ are colored counterclockwise blue-red-blue-red. In this case, the two open components always close into one link component, and so the resulting number of components is $\tau + \sigma + 1$. This situation is shown in figure 12(A).

(4) Finally, if the exterior arcs of $T$ and $S$ are both colored counterclockwise blue-blue-red-red, the two open components always close into one link component, and so the resulting number of components is $\tau + \sigma + 1$. This situation is shown in figure 12(B).

Notice then that given a knot diagram $D$, taking a crossing $x$, ignoring its sign, and designating it as the boundary vertex of a tangle diagram produces the 2-tangle diagram denoted $D \setminus x$ (there is some abuse of notation here; we are actually removing both the crossing $x$, the four arcs in $x$, and the edges in which those arcs resided from $D$). Furthermore, as $D$ is a planar knot diagram, $D \setminus x$ must have its exterior arcs colored blue-blue-red-red as in the case of $T$ in case (3) above (as the crossing $x$ is necessarily colored blue-red-blue-red). Hence given any 2-tangle diagram $S$ there exists at least one way to compose $(D \setminus x) \# S$ so that it is a planar knot diagram.
3. Asymptotic structure theorems for diagrams

3.1. The Frisch–Wasserman–Delbrück conjecture

The study of random knotting arises in numerous areas, principal among which is polymer physics: polymers (such as DNA or proteins) are considered to be strings in space and in many cases their function (or lack thereof) depends on any ‘knots’ that appear within [54, 44]. The random diagram model of random knotting is then: given a number \( n \) of crossings, sample uniformly an unlabeled knot diagram with \( n \) crossings and return its knot type. It is similar to models of [15] and [16], but these models do not sample from any well-understood measure on spaces of knot diagrams.

In the context of DNA topology, Frisch and Wasserman [21] and Delbrück [13] independently conjectured:

**Conjecture (Frisch–Wasserman 1962, Delbrück 1961).** As the size \( n \) of a randomly sampled knot grows large, the probability that it is knotted tends to 1.

The first proof of the conjecture was for \( n \)-step self-avoiding lattice polygons, a landmark result by Sumners and Whittington [55]:

**Theorem (Sumners–Whittington 1988).** As the number of steps \( n \) of a self-avoiding lattice polygon grows large, the probability that the polygon is knotted tends to 1 exponentially quickly.

Shortly thereafter the conjecture was proved in view of other models of space curves: gaussian random polygons [30], and equilateral random polygons [14].

As mentioned, the primary purpose of this work is to ascertain that the Frisch–Wasserman–Delbrück (FWD) conjecture holds in our model;

**Theorem 1.** As the number of crossings \( n \) of a randomly sampled knot diagram grows large, the probability that the diagram is knotted tends to 1 exponentially quickly.

This result will follow from the fractal structure of knot diagrams. We will prove results for rooted knot diagrams which extend (asymptotically) to the unrooted case as there are always at least 1 and at most \( 4n \) rooted diagrams to every unrooted diagram. Asymptotically, any numerical results on rooted diagrams apply up to a factor of \( 4n \) for the unrooted diagrams as;

**Theorem 2.** As the number of crossings \( n \) of an (unrooted) knot diagram grows large, the probability that the diagram has a nontrivial automorphism group tends to 0 exponentially quickly.

These two results answer two experimentally motivated questions posed in [6] in the affirmative. Indeed, theorem 2 suggests that, for large \( n \), experiments (see section 6) for unrooted knot diagrams can be run instead on rooted knot diagrams and results will differ only in that the rooted diagrams \( 4n \)-to-1 cover unrooted diagrams. While sampling rooted knot diagrams uniformly is still nontrivial, it is reasonably quick to generate rooted knot diagrams of 70 crossings using rejection sampling (but it as of yet computationally infeasible to tabulate even all 12-crossing unrooted diagrams).

3.2. The pattern theorem

Sumners and Whittington’s proof of the FWD conjecture for self-avoiding lattice polygons makes use of Kesten’s pattern theorem [33, 34, 36] which states that patterns—short walk configurations—appear linearly often in long self-avoiding walks.
3.2.1. Attachment. We make use of a similar strategy: theorem 2 of Bender et al [4] provides a pattern theorem for maps, provided a strategy of attaching a desired pattern. However, we must be careful in the case of knot or link diagrams, our decorated maps with extra structure. We thus retrace the proof while keeping this in mind. Say that if $D$ is a link diagram, then $e(D)$ is the number of edges in the diagram $D$. The proof depends on the existence of an ‘attachment’ scheme:

**Definition.** Let $Q$ be a tangle diagram, $\mathcal{M}$ some class of diagrams, and $\mathcal{H}$ a subclass of $\mathcal{M}$. A viable attachment of the tangle diagram $Q$ into $\mathcal{H}$ is a method of taking a diagram $D \in \mathcal{H}$ and producing new diagrams $D'$ that contain $Q$ as a subtangle diagram satisfying:

1. For some fixed positive integer $k$, at least $\lfloor e(D)/k \rfloor$ possible non-conflicting places of attachment exist. This means that at least $\lfloor e(D)/k \rfloor$ attachment operations (of $Q$) to a single diagram can be ‘parallelized’ and all performed at once to a diagram to produce a new diagram with at least $\lfloor e(D)/k \rfloor$ copies of $Q$ contained as subtangle diagrams.

2. Only diagrams in $\mathcal{M}$ are produced.

3. For any diagram produced as such we can identify the copies of $Q$ that have been added and they are all pairwise vertex disjoint. Identifying tangle diagrams in diagrams is simple since a diagram contains a tangle diagram if there is some dual cycle whose interior is the tangle diagram itself. We will consider only $Q$ which are always pairwise disjoint, and hence any attachment would satisfy the latter half of this condition.

4. Given the copies of $Q$ that have been added, the original diagram and associated places of attachment are uniquely determined. For our attachments, we will provide suitable ‘inverse’ operations which are themselves parallelizable (since instances of $Q$ are disjoint). This condition then follows.

Our tangle diagram compositions yield then the two attachment schemes which are relevant to the examples that follow.

**Definition.** Consider the 1-tangle diagram of one strand $Q$ which is two-leg-prime and asymmetric with tail arc $b$. Let $\mathcal{M}$ be one of:

1. all (rooted) link diagrams,
2. all (rooted) knot diagrams, or
3. provided $Q$ is reduced, all (rooted) reduced knot or link diagrams.

Then define the attachment edge replacement by, given a diagram $D$ and any arc $a$ in $D$, defining $D'$ to be the new diagram $D' = D \#(b,a)Q$.

**Proposition 3.** Edge replacement is a viable attachment for choices of $\mathcal{M}$ enumerated above.

**Proof.** We consider each required property.

1. There are at least $n - 1 \geq \lfloor n/2 \rfloor$ places of attachment to a rooted diagram $D$ with $n$ edges; non-conflicting ways to connect sum $Q$ into $D$ are precisely the number of non-root edges of $D$. Given a collection $\{a_i\}_{i=1}^r$ of different arcs, none of whom share an edge, in $D$, edge replacements performed in any order will produce the same diagram (since edge replacement does not alter any arcs or edges in $D$ besides the arc chosen and its edge).

2. Depending on the choice of tangle diagram $Q$ and class of diagrams $\mathcal{M}$, diagram connect sum can be shown to keep diagrams in $\mathcal{M}$. Namely, provided a tangle diagram $Q$ of one strand, this attachment does not change the number of link components of diagrams.
Furthermore, if $Q$ is reduced, then the introduction of $Q$ into a diagram by connect summation introduces no new disconnecting vertices.

(3) We can identify the copies of $Q$ inside the resultant diagram by our definition of what it means for a tangle diagram to be included in a diagram. Provided $Q$ is two-leg-prime, occurrences of $Q$ must be pairwise disjoint:

Suppose to the contrary that $Q_1$ and $Q_2$ are instances of $Q$ contained as subtangle diagrams in a diagram $D$, which are not disjoint. The definition of being a subtangle diagram means there exists some dual cycle of edges $(e_1, e_2)$ which isolates the tangle diagram $Q_1$ from the rest of $D$; the cycle is necessarily of length 2 as $Q$ is a 1-tangle diagram.

Now, the condition that $Q_1$ and $Q_2$ are not disjoint means that, without loss of generality, the edge $e_2$ appears in the interior of $Q_2$. However, $Q_2 \setminus e_2$ is necessarily disconnected, which contradicts that $Q$ was two-leg prime. So instances of $Q$ must be pairwise disjoint.

(4) Edge replacement is an invertible operation. Given an instance of $Q$ in $D$ which is identified by the dual edge cycle $(e_1, e_2)$, we can recover the diagram $D'$: without loss of generality, as $Q$ is asymmetric, we can assume that $e_1 = (ab)$ is the edge which connects the tail arc $b$ of $Q$ to the arc $a$ of $D$. Removing $e_1$ and $e_2$ from $D$ yields the pair of 1-tangle diagrams $D'$ and $Q$. Denote by $c$ the arc of $D'$ which is not $a$. Then $D'$ is the tangle diagram $D'$ together with additional closing edge $e_3 = (ac)$ and we have that $D = D' \#(a, b)Q$. We made no choices in this procedure beyond choice of instance of $Q$ inside $D$ and each step was entirely local.

Hence, edge replacement is a viable attachment.

If instead we have a $k$-tangle diagram $Q$ (for $k > 1$) we can still define an attachment into diagrams by first joining together pairs of all but two exterior edges to produce a 1-tangle diagram $Q'$ (some choice is involved here—there are infinitely many ways to close any given tangle). This 1-tangle diagram $Q'$ can then be attached by edge replacement.

For classes of prime diagrams which are not closed under connect summation, we have an alternate attachment;

**Definition.** Consider the nontrivial 2-tangle diagram $Q$ that is asymmetric and at least 4-edge-connected with designated arc $b$. Let $\mathcal{M}$ be either the class of prime link diagrams or, if $Q$ consists of precisely two open strands and no closed components, the class of prime knot diagrams. Then define the **crossing replacement** of a given diagram $D$ and an arc $a$ in $D$ to be the diagram $D' = D \#(a, b)P_{\sigma}$, where $\sigma$ is the sign of the crossing $c(a)$ in $D$ and $P_{\sigma}$ is the tangle diagram containing $Q$ as defined in figure 13.

**Proposition 4.** Crossing replacement is a viable attachment for choices of $\mathcal{M}$ enumerated above.
Proof. We consider each required property.

(1) For the class of all prime link diagrams, any choice of an arc in a diagram provides a crossing attachment of $Q$ which is a link diagram. For the class of all prime knot diagrams on the other hand, each crossing has at least one choice of arc for which the insertion of $P_\sigma$ produces a knot diagram. So for any diagram and for each crossing inside the diagram, there exists at least one viable location for crossing replacement, and provided crossing replacements happen at different crossings, they are independent. So there exist at least $n/2\geq\lceil n/2 \rceil$ non-conflicting places of attachment of $Q$ into a diagram with $n$ edges.

(2) Provided an appropriate $Q$, the attachment is closed in $\mathcal{M}$ as we only choose appropriate arcs.

(3) We can identify the copies of $P_\sigma$ inside the resultant diagram by our definition of what it means for a tangle diagram to be included in a diagram. Suppose that $P_1$ and $P_2$ are instances of $P_\sigma$ which are not disjoint in $D$ ($\sigma$ does not matter and can be different for each $P_\sigma$).

That $P_1$ and $P_2$ are not disjoint means that the boundary cycle $(e_1, e_2, e_3, e_4)$ of $P_1$ must in some part enter the interior of the instance $P_2$. Notice that as $Q$ is nontrivial, there is no dual path of length 1 through $P_2$; this implies that the subpath which is inside $P_2$ cannot be length 1. Conversely, it cannot be length 3 (switch the roles of $P_1$ and $P_2$). So the subpath would have to be of length 2; as the dual map is a quadrangulation, a dual path of length two would have to be trivial (which cannot happen by the structure of $P_1$) to begin at one face and end at the face opposite. However, by the structure of $P_1$ and by the fact that $Q$ is nontrivial this is impossible.

(4) Crossing replacement is an invertible operation. Given an instance of $P_\sigma$ in $D$ which is identified by the dual edge cycle $(e_1, e_2, e_3, e_4)$, we can recover the diagram $D'$: without loss of generality, as $P_\sigma$ is asymmetric, we can assume that $e_1 = (ab)$ is the edge which connects the tail arc $b'$ of $P_\sigma$ to the arc $a$ of $D$. Removing $e_1, e_2, e_3$, and $e_4$ from $D$ yields the pair of 2-tangle diagrams $D'$ and $P_\sigma$. Denote by $x,y,z$ the arcs counterclockwise around $D'$ after $a$. Then $D'$ is the tangle diagram $D''$ together with the four arcs brought together into a crossing $x$ with sign $\sigma$ identified from $P_\sigma$. We have that $D = D' \#_{(a,b)} P_\sigma$.

We made no choices in this procedure beyond choice of instance of $P_\sigma$ inside $D$ and each step was entirely local.

Hence, crossing replacement is a viable attachment. \hfill $\square$

3.2.2. Pattern theorems for diagrams. Given a generating function $F$, let $r(F)$ be its radius of convergence. Being able to attach desired subtangle diagrams as above yields:

**Theorem 5.** Let $\mathcal{H}$ be some class of link diagrams on any surface and let $Q$ be a tangle diagram that can be contained in diagrams in $\mathcal{H}$. Let $M(x)$ be the generating function by the number of edges for $\mathcal{H}$. Let $H(x)$ be the generating function by the number of edges for those link diagrams $M$ in $\mathcal{H}$ that contain less than $c_\mathcal{H}$ pairwise disjoint copies of $Q$: call this class $\mathcal{H}'$. Suppose there is a viable attachment for $Q$ into $\mathcal{H}$. If $0 < c < 1$ is sufficiently small, then $r(M) < r(H)$. The diagrams may be rooted or not.

The proof of the theorem makes use of a lemma of Bender et al:

**Lemma (4, lemma 3).** If

(1) $F(z) \neq 0$ is a polynomial with non-negative coefficients and $F(0) = 0$,
(2) $H(w)$ has a power series expansion with non-negative coefficients and $0 < r(H) < \infty$, 

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\( (3) \) for some positive integer \( k \) the linear operator \( \mathcal{L} \) is given by \( \mathcal{L}(w^n) = z^k(F(z)/z)^{[n/k]} \), and 
\( (4) \) \( G(z) = \mathcal{L}(H(w)) \).

then \( r(H)^k = r(G)^{k-1}F(r(G)) \).

The proof of the theorem then remains almost unchanged from the original theorem. The class \( \mathcal{M} \) of diagrams and tangle diagrams \( P \) considered determine the attachment scheme.

**Proof of theorem 5.** Let \( G(z) \) be the generating function which counts the ways by edges of attaching some number between 0 and \([n/k]\) copies of \( Q \) to diagrams in \( \mathcal{M} \) counted by \( H(x) = \sum h_n x^n \). The method of attachment leads to the relation \( G(z) = \mathcal{L}(H(w)) \), with \( \mathcal{L} \) as defined in the lemma, where \( F(z) = z + z^k \) and \( q \) is the number of edges added when a copy of \( Q \) is attached, as 
\[
G(z) = \sum_{Y \in \mathcal{M}} z^{q(Y)} \left( 1 + z^{q-1} \right)^{[q(Y)/k]} = \mathcal{L}(H(w)).
\]

Let \( g_n \) be the coefficients of \( G(z) \).

Suppose \( M \in \mathcal{M} \) contains \( m \) copies of \( Q \). By property (3) of our attachment, \( m \leq n = e(M) \).

If \( M \) had been produced from some diagram \( K \in \mathcal{M} \) by our attachment process, we can find all possible \( K \) by removing at least \( m - cn \) copies of \( Q \) from \( M \). It is possible to bound from above the number of ways to do this by
\[
\sum_{j \geq m-cn} \binom{m}{j} = \sum_{k \leq cn} \binom{n}{k} < \sum_{k \leq cn} \binom{n}{cn} \leq n^{(e/c)n} = n^{\left( \frac{e}{c} \right)^n} =: t_n.
\]

If \( M(x) = \sum m_n x^n \), then this means that \( t_n m_n \geq g_n \), so \( m_n \geq g_n / t_n \). Hence,
\[
1/r(M) \geq \limsup_{n \to \infty} \left( g_n / t_n \right)^{1/n} = \lim_{n \to \infty} (t_n)^{-1/n} \limsup_{n \to \infty} \left( g_n \right)^{1/n} \geq (c/e)^r / r(G).
\]

By the prior lemma, \( r(H)^k = r(G)^{k-1} \) so that
\[
r(H) / r(M) \geq (1 + r(G)^{q-1})^{1/k} (c/e)^r.
\]

As there are fewer than \( 12^n \) planar maps with \( n \) edges [3], a trivial bound on the coefficients \( h_n \) of \( H(x) = h_n \leq (12^n)^{(\kappa n/2)} \) where \( \kappa \geq 1 \) is the size of the set of decorations on the vertices of the diagram (in the scope of this paper, \( \kappa = 2 \) or 1). This provides the bound \( r(H)^k \geq 1/(12\sqrt{\kappa})^k \).

Then, as \( \lim_{x \to q+} (c/e)^r = 1 \) and \( r(G)^k (1 + r(G)^{q-1}) = r(H)^k \geq 1/(12\sqrt{\kappa})^k \) so that
\[
r(G) \geq 1/(12\sqrt{\kappa}(1 + r(G)^{q-1})^{1/k}) \geq 1/(24\sqrt{\kappa}),
\]
it follows that \( r(H)/r(M) > 1 \) for sufficiently small \( c \), completing the proof of the theorem.  \( \square \)

\[5\] The power of \( 1/n \) on \( \limsup_{n \to \infty} (g_n) \) is missing in the original proof of Bender et al.
The conclusion is about radii of convergence of two power series; application of the Cauchy-Hadamard theorem, together with one additional hypothesis, gives the stronger result:

**Theorem 6 (Pattern theorem; [4]).** Suppose that for the class $\mathcal{M}$ and the tangle $Q$ all of the hypotheses of theorem 5 apply. Additionally suppose that $\mathcal{M}$ grows smoothly, i.e. that, with $m_n = |\mathcal{M}_n|$, the limit $\lim_{n \to \infty} m_n^{1/n}$ exists.

Then there exists constants $c > 0$ and $d < 1$ and $N > 0$ so that for all $n \geq N$, we have that the number of diagrams $m_n$ and the number $h_n$ of such diagrams which contain fewer than $cn$ copies of the tangle $Q$ obey:

$$\frac{h_n}{m_n} < d^n,$$

i.e. the tangle $Q$ is ubiquitous.

Because of Euler’s formula, the number of vertices, edges, or faces in a link shadow or planar quadrangulation is entirely determined by choosing any one cardinality. Hence, we can size shadows and diagrams by the number of vertices and still keep the above results.

### 3.3. Smooth growth

In order for the (stronger) corollary to hold, we require that the class of diagrams grow smoothly, i.e. that (for $m_n = |\mathcal{M}_n|$) the limit $\lim_{n \to \infty} m_n^{1/n}$ exists.

The key in proving this behavior is the strengthening of Fekete’s lemma [46, 60] reproduced below:

**Theorem. (Wilker–Whittington 1979 [60]).** Let $f(m)$ be a function with $\lim_{m \to \infty} m^{-1}f(m) = 1$ and $\{a_n\}$ be a sequence. Suppose that $a_n a_m \leq a_{n+f(m)}$ for all $n, m$ sufficiently large and that $a_n^{1/n}$ is bounded above (for all of our cases we have the trivial bound for all planar maps of 144). Then

$$\lim_{n \to \infty} a_n^{1/n} = \limsup_{n \to \infty} a_n^{1/n} = 1/r < \infty$$

where $r$ is the radius of convergence of the series $\sum_{n=1}^{\infty} a_n z^n$ and furthermore $a_n \leq (1/r)^{f(n)}$.

For $f(m) = m$ we recover the usual result. Observe as well that functions $f(m) = m + k$ satisfy the hypothesis for fixed $k$.

### 4. Applications to classes of rooted diagrams

#### 4.1. The pattern theorem for rooted link diagrams

As noted, the classes $\mathcal{L}$ of rooted link shadows and $\mathcal{P}\mathcal{L}$ of rooted prime link shadows have been counted exactly; they both hence grow smoothly. Pattern theorems for these two classes hence follow given satisfactory tangle diagrams $P$ and attachment operations.
4.1.1. Rooted link diagrams. For the class of all rooted link shadows and any two-leg-prime 1-tangle diagram $P$, the connect summation with $P$ is a viable attachment, see proposition 3. Hence we conclude that asymptotically almost surely any two-leg-prime tangle diagram $P$ is contained linearly often in an arbitrary link diagram $D$.

From this we see that:

**Proposition 7.** Almost every rooted link diagram has more than one component. Additionally, almost every rooted link diagram is neither the unknot nor a split link of unknots. In other words there exists $d < 1$ and $N > 0$ so that for $n \geq N$,

\[ P(\text{a rooted link diagram } L \text{ with } n \text{ crossings has one component}) < d^n, \]

\[ P(\text{a rooted link diagram } L \text{ with } n \text{ crossings represents the unknot}) < d^n, \]

and

\[ P\left( \text{a rooted link diagram } L \text{ with } n \text{ crossings represents a split link of unknots} \right) < d^n. \]

**Proof.** Consider the attachment of tangle diagram $\Phi$ in figure 14(A). This attachment satisfies the hypotheses of theorem 6 and the class of rooted link diagrams grows smoothly, so there exists $c > 0, d < 1,$ and $N > 0$ so that for all $n \geq N$,

\[ P(\text{a rooted link diagram } L \text{ with } n \text{ crossings contains } \leq cn \text{ copies of } \Phi) < d^n. \]

Now, any of the conditions enumerated in the proposition would imply that the rooted link diagram with $n$ crossings contains precisely no copies of the tangle diagram $\Phi$; but this condition happens with probability less than $d^n$, providing the result.

4.1.2. Rooted prime link diagrams. In the case of rooted prime link diagrams, however, connect summation with any nontrivial 1-tangle diagram $P$ immediately removes the prime condition. Hence in this case we must use crossing replacement with 2-tangle diagrams that are prime, which is viable by proposition 4. We can see then that:

**Proposition 8.** Almost all rooted prime link diagrams consist of more than one component. Additionally, almost all rooted prime link diagrams are neither unknots nor split links of unknots.
Proof. Consider the tangle diagram $X$ in figure 14(B). For a rooted prime link diagram to satisfy any of the claims above, it would have to not contain a copy of $X$. However, $X$ can be attached by crossing replacement into the class of rooted prime link diagrams in a way satisfying the hypotheses of theorem 6. Furthermore, the class of rooted prime link diagrams grows smoothly, leaving the result.

\[\square\]

4.2. The pattern theorem for rooted knot diagrams

Unlike classes of rooted link diagrams, $\mathcal{K}$ and its subclasses often do not have exact counting formulas. Hence in these cases we not only must provide satisfactory attachment schemes for tangle diagrams, we must additionally prove smooth growth of the counting sequences.

4.2.1. Rooted knot diagrams. Provided that the tangle diagram $P$ consists of precisely one component, proposition 3 has that the class $\mathcal{K}$ of all rooted knot diagrams is closed under connect sum with $P$.

So it only remains to prove that the class of knot diagrams grows smoothly for pattern theorem results to follow. It suffices to prove that the class of rooted knot shadows grow smoothly as there exist precisely $2^n$ rooted knot diagrams for each rooted knot shadow of $n$ crossings.

\[\text{Theorem 9. The class } \mathcal{K} \text{ of rooted knot shadows grows smoothly. That is, the limit } \lim_{n \to \infty} k_1^n/n \text{ exists and is equal to } 1/\tau(K).\]

Additionally, the class of reduced rooted knot shadows grows smoothly.

\[\text{Proof. Observe that } k_nk_m \leq k_{n+m} \text{ for any pair } n,m \text{ as given any two knot shadows of size } n,m, \text{ say } K_1 \text{ and } K_2 \text{ respectively, we have the injection defined as in figure 15 where the shadows are joined end-to-end. As } n \text{ and } m \text{ are known quantities, the separating edge between } K_1 \text{ and } K_2 \text{ in the product is determined, and the inverse is well defined on the image. The result then follows by the above result on super-multiplicative sequences, with } f(m) = m. \text{ This proof works for both the case of general knot diagrams, as well as the case of reduced rooted diagrams, as connect summation does not introduce any new isthmi.} \square\]

\[\text{Proposition 10. Almost every rooted (general or reduced) knot diagram is knotted. Furthermore, almost every rooted (general or reduced) knot diagram contains any 1-component, prime 1-tangle diagram } P \text{ 'linearly often': For any such prime 1-tangle diagram } P, \text{ there exists } N \geq 0 \text{ and constants } d < 1, c > 0 \text{ so that for } n \geq N,\]

\[P(\text{a knot diagram } K \text{ contains } \leq cn \text{ copies of } P \text{ as connect summands}) < d^n.\]

\[\text{Proof. The first statement will follow immediately from the second, given a prime 1-tangle diagram corresponding to a prime knot diagram which is not an unknot such as the prime trefoil tangle diagram } T \text{ in figure 10(B). The second is a corollary of theorems 6 and 9: let } P \text{ be a prime 1-tangle diagram which can be found as a connect summand of a knot diagram (i.e. it has one link component). If } m_n \text{ is the number of knot diagrams, then there exists } c > 0, d < 1,\]
and $N > 0$ so that for all $n \geq N$, $\frac{h_n}{m_n} < d^n$, where $h_n$ is the number of knot diagrams which contain at most $cn$ copies of $P$ as connect summands. This ratio is precisely the probability in the second statement.

The proof follows for reduced rooted knot diagrams precisely the same. □

### 4.2.2. Rooted prime knot diagrams.

We can also show that, given a prime 2-tangle diagram $P$ with reasonable assumptions, we can obtain a pattern theorem for $P$ inside of the class $\mathcal{PK}$ of prime knot diagrams. The viable attachment here is crossing replacement discussed earlier.

It does however remain to be shown that the class $\mathcal{PK}$ grows appropriately smoothly. We only need apply a slight modification to the prior argument.

**Theorem 11.** The class $\mathcal{PK}$ of prime knot shadows grows smoothly.

**Proof.** For any $n > 3$ a prime shadow will have no monogons, and we can define a composition on prime shadows as in figure 16.

This operation adds precisely two vertices and is invertible on its image. We will define the inverse of a diagram $D$ to be the diagram obtained by performing a ‘flat Reidemeister II move’ to delete the bigon containing the arc labeled $g_1$ and then by deleting the edge $(bc)$ between vertices indexed $m$ and $m + 1$ by traversal order starting at the tail $d$, if such a diagram exists and is valid. This process is depicted in figure 17. This inverse proves that

$$p_np_m \leq p_{n+f(m)},$$

where $f(m) = m + 2$. This, together with the above theorem on super-multiplicativity completes the proof. □
Hence,

**Proposition 12.** Almost every rooted prime knot diagram is knotted. Furthermore, almost every rooted prime knot diagram contains any 2-component, prime 2-tangle diagram \( P \) ‘linearly often’: For any such prime 2-tangle diagram \( P \), there exists \( N \geq 0 \) and constants \( d < 1 \), \( c > 0 \) so that for \( n \geq N \),

\[
P(\text{a prime knot diagram } K \text{ contains } \leq cn \text{ copies of } P) < dn.
\]

**Proof.** The proof of the latter statement is nearly identical to that of proposition 10, except with crossing replacement instead of connect summation. A 2-tangle diagram whose insertion guarantees that a diagram be knotted is depicted in figure 18, from which the former statement follows.

\[
\square
\]

5. Asymmetry of diagrams

It is a theorem of Richmond and Wormald [49] that ‘almost all maps are asymmetric’, in classes of maps which have a pattern theorem. Indeed, this theorem applies to classes of shadows considered in this paper. Notice then that classes of diagrams then too must be asymmetric as the decoration imposes additional constraints on symmetry.

Say a tangle shadow \( P \) is *free* in a class of rooted knot shadows \( \mathcal{C} \) if any knot shadow obtained by removing a copy \( P_1 \) of \( P \) from a shadow \( K \) and re-attaching \( P \) in any fashion such that the exterior legs of \( P \) match up with the loose strands of \( K \setminus P_1 \) is in \( \mathcal{C} \).

We then restate the theorem as it pertains to shadows:

**Theorem (Richmond–Wormald 1995).** Let \( \mathcal{C} \) be a class of rooted shadows. Suppose that there is a tangle shadow \( P \) such that for all shadows in \( \mathcal{C} \), all copies of \( P \) are pairwise disjoint and such that \( P \)

- (1) has no reflective symmetry in the plane,
- (2) satisfies the hypotheses for the pattern theorem 6 for \( \mathcal{C} \), and
- (3) is free in \( \mathcal{C} \)

then the proportion of \( n \)-crossing shadows in \( \mathcal{C} \) with nontrivial automorphisms (that need not preserve neither root nor orientation of the underlying surface) is exponentially small.

It has been suggested without proof in [52, 11] that classes of knot shadows are almost surely asymmetric. We can now prove these results for \( \mathcal{K} \) and \( \mathcal{PK} \) by providing appropriate tangle shadows \( P \).
Proposition 13. The proportion of knot shadows in $\mathcal{K}$ with nontrivial automorphisms is exponentially small. Additionally, the proportion of knot diagrams in $\mathcal{K}$ with nontrivial automorphisms is exponentially small.

This is true for reduced knot shadows as well.

Proof. Let $P$ be the 1-tangle shadow in figure 19. $P$ is a viable candidate for the pattern theorem for knot shadows under connect sum attachment. Furthermore $P$ has no reflective symmetry by inspection, and any of the ways of attaching $P$ keep the object in the class of knot shadows (as $P$ is a 1-tangle shadow consisting of one component). This proves that knot shadows are asymmetric. The proof for reduced knot shadows is identical. □

Proposition 14. The proportion of prime knot shadows in $\mathcal{K}$ with nontrivial automorphisms is exponentially small. Additionally, the proportion of knot diagrams in $\mathcal{K}$ with nontrivial automorphisms is exponentially small.

Proof. Take $P$ as in figure 20. Then $P$ consists of exactly two link components and is of blue-red-blue-red type; any way of replacing a vertex in a knot shadow with a 2-tangle shadow of blue-red-blue-red type keeps the number of link components constant and hence is free. Furthermore, $P$ satisfies the hypotheses for theorem 10 together with crossing replacement. Finally, asymmetry of $P$ proves the claim. □

Application of the above theorems provides us with the following corollary which enables us to transfer any asymptotic numerical results or sampling results on rooted diagrams to unrooted diagrams.

Figure 19. The (prime, reduced) 1-tangle shadow $P$ which shows that knot shadows are asymmetric.

Figure 20. Choice of 2-tangle shadow $P$ for proving that prime knot shadows are asymmetric.
Corollary 15. Let $L$ be a uniform random variable taking values in the space $K_n$ or $L_n$. Then there exist constants $C, \alpha > 0$ so that $\Pr(\text{aut } L \neq 1) < Ce^{-\alpha n}$. Hence, rooted diagrams behave like unrooted diagrams and there are a.a.s. $4n$ rooted diagrams to each unrooted diagram.

Indeed, link diagrams with $n$ vertices are dual to quadrangulations with $n + 2$ faces; there are $n + 2$ ways of choosing the ’exterior’ root face and then 4 ways of rooting the edges around this chosen face. Hence if $\tilde{\ell}_n, \tilde{k}_n$ are the counts of unrooted link or knot diagrams we have that in the limit,

$$\tilde{\ell}_n \sim \frac{\ell_n}{4(n + 2)} \quad \text{and} \quad \tilde{k}_n \sim \frac{k_n}{4(n + 2)}.$$

6. Some numerical results

6.1. Methods

Gilles Schaeffer’s PlanarMap software [51] is able to uniformly sample in $O(n)$ time many different classes of maps including both rooted 4-valent planar maps (rooted link shadows) and rooted 4-connected 4-valent planar maps (rooted prime link shadows) by using a bijection between maps and objects called blossom trees [52, 50].

The class of blossom trees relevant to generating 4-valent planar maps is a class of rooted plane trees for which every interior node has one child called a bud, and two children which are either other nodes or leaves. PlanarMap generates these trees in linear time, changes the root node to a leaf, and then closes the tree in average linear time by joining adjacent buds to leaves in counterclockwise order (starting at the leaf which was previously the root).

We have incorporated PlanarMap as a library into the space curve and knot diagram toolkit plCurve [2]. This has enabled functionality in plCurve to uniformly sample rooted link diagrams (resp. rooted prime link diagrams) with $n$ crossings by:

1. Sample a rooted link shadow (resp. rooted prime link shadow) with the aid of PlanarMap uniformly in $O(n)$ time. (Additional details on how PlanarMap does this, especially in the context of plane curves, can be found in [52].)
2. Sample a sign vector in $\{+, -\}^n$ uniformly. This information, together with the link shadow sampled in the step prior, uniquely yields a rooted link diagram or rooted prime link diagram sampled uniformly from the set of $n$-crossing rooted link diagrams or $n$-crossing rooted prime link diagrams, respectively.

As the condition of being a knot diagram or shadow is independent of choice of sign, we can furthermore introduce after step 1 a rejection of all shadows with more than 1 link component. Rejection does not affect the probabilities which with valid diagrams are sampled, and hence this augmented procedure uniformly samples rooted knot diagrams (resp. rooted prime knot diagrams).

Culler and Dunfield’s PLink software [12] is able to produce images of knot and link diagrams using an orthogonal projection routine. This enables one to visualize individual diagram objects. There are two important caveats to this visualization:

1. Currently, PLink does not support rooting of edges.
2. PLink can produce a number of geometrically different embeddings for any given diagram object, all of which are combinatorially equivalent.
The plCurve software has an interface to PLink which enables viewing graphical representations of the diagrams sampled. An example of such a knot diagram with 150 crossings is presented in figure 21.

The data below was gathered from the following experiments:

(1) First, for each $10 \leq n \leq 64$, we attempted to gather $500,000$ uniform $n$-crossing rooted knot diagram samples, with 49 tries to sample a knot diagram per sample. This means that for each of the $500,000$ calls to sample a rooted knot diagram, we generated at most 49 rooted link shadows, rejecting shadows until either (a) a rooted knot shadow was sampled, or (b) 49 unsuccessful attempts were made. This data is exhibited in figures 22(A), 23 and 25(A).
We further sampled precisely 20,000 diagrams for all $65 \leq n \leq 100$ for the curve fitting data in figure 26, table 1, and figure 27.

(2) A similar experiment was run, for all $10 \leq n \leq 64$ with 49 attempts, except we sampled rooted prime knot diagrams by rejection sampling on rooted prime link diagrams as described above. This data is exhibited in figures 22(B), 24 and 25(A).

(3) To detect the ratios of knot diagrams to link diagrams, another experiment was run wherein for each $10 \leq n \leq 65$, we sampled uniformly 100,000 rooted link diagrams. The same was done for rooted prime link diagrams. This data is the basis for figure 25(B).

Knots were classified by their HOMFLY polynomial [20], which distinguishes knots of the types studied ($0_1, 3_1, 4_1, 5_1, 5_2, 3_1\#3_1$) for diagrams of low crossing number using software lmpoly of Ewing and Millett [18] implemented within plCurve. For larger diagrams, the HOMFLY polynomial is not necessarily a complete invariant. However, these clashes are

Figure 23. Probabilities of some typical knot types as the number of crossings varies from $n = 10$ to $n = 64$. 500,000 samples were attempted for each $n$, although samples were discarded if a knot diagram was not produced after 49 attempts. There were, e.g. 258,377 samples for $n = 64$.

Figure 24. Probabilities of some typical knot types in prime diagrams as the number of crossings varies from $n = 3$ to $n = 64$. 500,000 samples were attempted for each $n$, although samples were discarded if a knot diagram was not produced after 49 attempts. There were, e.g. 496,151 samples for $n = 64$. 
expected to be rare and hence immaterial for the analysis that follows. Furthermore, it is believed at least that the HOMFLY polynomial distinguishes the unknot; a counterexample would disprove the fabled ‘Jones Conjecture [31], and would be a monumental discovery by itself 6.

We note additionally that our data ignores chirality of knot types: the knot types $3_1, 5_1, 5_2$ admit both left- and right-handed chiralities (which are distinguished by the HOMFLY polynomial), but the chirality is ignored as the probability of the two mirror-images are identical in the diagram model. Finally, under the composite knot type $3_1 \# 3_1$ is data for both the granny knot, its mirror image, and the square knot, all of whom have equal probability as well.

6.2. Data and observations

A typical concern with results on asymptotic behavior is whether it only applies to knot diagrams with an absurd number of crossings. This is common when discussing physical knotting—most polymers are not infinitely long and hence exhibit only finite complexity! However, exact and numerical results show that the asymptotic behavior we have discussed is actually attained very quickly.

A critical example of this is that almost all 10-crossing knot diagrams have no nontrivial automorphisms. This is exhibited in figure 22, where knot diagrams with at least 8 crossings and prime knot diagrams with at least 13 crossings have nearly no symmetries. Hence while it is infeasible to sample unrooted knot diagrams by enumeration, by corollary 15 sampling rooted knot diagrams is greatly effective.

6.2.1. Knotting in diagrams. We will now consider relative appearances of various knot types among knot diagrams. This allows us to expand on our results in [6]. Although we no longer

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6 A recent paper of Tuzun and Sikora has verified the conjecture up to 22 crossings [59], so our data on the unknot is accurate at least up to and including $n = 22$. 

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Figure 25. The exponential decay of knot diagrams among link diagrams makes rejection sampling more difficult as the number of crossings increases. (A) Number of successful samples for diagrams in gathering the above data. For each of 500000 samples, a maximum of 49 attempts is made to generate a knot diagram, and if unsuccessful, the sample is discarded. (B) Ratio of knot diagrams to link diagrams in the generic and prime cases. Data was gathered by sampling 100000 link diagrams and counting the number of samples with precisely one link component.
have exact numerics, we can break past the 10-crossing barrier with relative ease and good precision. Compare the chart in figure 23 to table III in [6].

Of note is the exponential decay of the proportion of unknots $0_1$ as the number of crossings grow large. In fact, data shows that the number of (both left- and right-) trefoils $3_1$ exceeds that of the unknot $0_1$ at around $n = 44$ crossings. Additionally, the trend for the square and granny knots, labeled $3_1 \# 3_1$, has it decaying at a far slower rate than any of the prime knot
types. This is in line with conjectures for models of random knots that the growth rates of knot types $K$ should accrue an additional polynomial growth factor of $n$ for each prime knot type in the decomposition of $K$ \cite{47}. Also of note is the so-called ‘51,52 inversion’, where the knot 52 is more likely than the torus knot 51. This was exhibited in the earlier exact data of \cite{6} and persists through the entire scope of the data gathered. We present a more thorough examination of this data with comparisons to other models in the following section 6.2.2.

Our rejection sampling methods additionally apply in the case of sampling knot diagrams with different graph-theoretic constraints. For instance, it extends to provide a sampler for prime knot diagrams, which have underlying map structure which is 4-edge connected. As dictated by proposition 14, the number of asymmetries of prime knot diagrams tends to zero exponentially quickly as in figure 22. We also present data for the proportions of knots in prime diagrams in figure 24. While the precise numerics differ, notice that prime diagrams exhibit the same interesting behavior as generic diagrams discussed prior. Namely, (1) unknots are exponentially rare and become less prevalent than trefoils (albeit sooner in the case of prime diagrams, occurring at around $n = 30$ crossings), (2) the composite square and granny knots show slower decay than knots of prime type, and (3) the $5_1,5_2$ inversion.

### Table 1. Parameters for the curve fits in figure 26. Compare, e.g. to table II in \cite{57} which presents similar data for the model of Gaussian random polygons.

| Knot type $K$ | $C_K$ | $\mu$ | $\alpha$ |
|---------------|-------|-------|----------|
| $0_1$         | 1.026 ± 0.009 | $(9.524 ± 0.002) \times 10^{-1}$ | 3.090 ± 0.004 |
| $3_1$         | $(1.32 ± 0.08) \times 10^{-2}$ | $(9.434 ± 0.008) \times 10^{-1}$ | 3.36 ± 0.03 |
| $4_1$         | $(1.1 ± 0.1) \times 10^{-3}$ | $(9.36 ± 0.02) \times 10^{-1}$ | 3.85 ± 0.06 |
| $5_1$         | $(1.4 ± 0.4) \times 10^{-5}$ | $(9.23 ± 0.03) \times 10^{-1}$ | 4.9 ± 0.1 |
| $5_1, n \geq 30$ | $(1.1 ± 0.3) \times 10^{-4}$ | $(9.38 ± 0.02) \times 10^{-1}$ | 4.15 ± 0.09 |
| $5_2$         | $(6 ± 1) \times 10^{-5}$ | $(9.24 ± 0.03) \times 10^{-1}$ | 4.7 ± 0.1 |
| $5_2, n \geq 30$ | $(4.7 ± 0.9) \times 10^{-4}$ | $(9.41 ± 0.01) \times 10^{-1}$ | 3.92 ± 0.07 |
| $3_1 \# 3_1$ | $(4 ± 1) \times 10^{-6}$ | $(9.27 ± 0.03) \times 10^{-1}$ | 4.4 ± 0.1 |
| $3_1 \# 3_1, n \geq 30$ | $(2.8 ± 0.4) \times 10^{-5}$ | $(9.406 ± 0.009) \times 10^{-1}$ | 3.74 ± 0.05 |

**Figure 27.** Fitting the curves $y = ae^{b/n}$ to the ratios of knotting probabilities provides estimates for the asymptotic value.
An observation from running the above experiments is that knot diagrams appear to be more prevalent in prime diagrams than generic knot diagrams! Indeed, nearly all rejection samples of prime knot diagrams are successful (see figure 25(A)) as opposed to the 50% success rate of sampling generic diagrams of 64 crossings. A more precise computation of the proportion of knot diagrams to link diagrams is exhibited in figure 25(B), where we can see that there is indeed a far greater proportion of knot diagrams in the prime diagram case to the generic, at least up to 65 crossings. Fitting the curve \( k_n/l_n = C \mu^n a^n \) to each of these data sets yields \( C = 1.26 \pm 0.01, \mu = 0.9503 \pm 0.0002, a = -0.287 \pm 0.005 \) in the generic case and \( C = 0.99 \pm 0.03, \mu = 0.9749 \pm 0.0006, a = -0.17 \pm 0.01 \) in the prime case. In the generic case, multiplying by the (known) number of link shadows yields that the exponential growth of knot shadows is approximately \( 12 \mu = 11.404 \pm 0.0024 \) close to that of prior work of Jacobsen and Zinn Justin [28] discussed in section 2.1 and that the power law growth term is \( a - 5/2 = -2.287 \pm 0.005 \). This differs from the conjectured value of \( -\frac{1+\sqrt{13}}{6} \approx -2.67 \), and suggests that further data is required for an adequate fit. Applying the same analysis to the prime case yields that the exponential growth rate of prime knot shadows should be \( 24 \mu = 23.40 \pm 0.0145 \) and the power law growth term to be \( a - 5/2 = -2.67 \pm 0.01 \), which agrees rather well with Schaeffer and Zinn Justin’s conjectured value of \( -\frac{1+\sqrt{13}}{6} \approx -2.67 \).

Hence it is worth summarizing these interesting properties of the prime knot diagram model. First, prime link diagrams admit exact enumeration like general link diagrams and are hence easy to sample. In addition, there is a higher success rate of sampling knot diagrams inside of prime diagrams as opposed to general diagrams. Second, the difficulty of inserting ‘boring’ structure into prime knot diagrams suggests that there is far more variety in the knot types which arise than in the general case. So, prime diagrams are a natural class to find diagrams representing exotic knot types with large minimum crossing number. Some evidence to this is the fact that alternating, prime knot diagrams are minimal in that they have the fewest number of crossings over all diagram representations of their knot type. Finally, the smaller size of the class of prime diagrams (as opposed to the general case) suggests that fewer samples may be required to have a better statistical understanding of the space.

6.2.2. Expected behavior and comparisons to other models. As noted by many prior authors [47, 57], it is expected that, for a fixed knot type \( K \) with a factorization into \( N_K \) components, the probability \( p_n(K) \) that a knot diagram of \( n \) crossings is of type \( K \) obeys asymptotically

\[
p_n(K) = C_K \mu^n a^{n-3+N_K}
\]

for a constant \( C_K \) depending on \( K \), and constants \( \mu \) and \( a \) which are expected to be independent of \( K \). For the various knot-type probability data gathered in figure 23 above, we used scipy’s [29] least-squares fitting algorithm to fit a curve of the form above. For latter types, we provide two fits; one using all available data and one only using points with \( n \geq 30 \). These fits are presented graphically in figure 26 and the parameter data is provided in table 1. Universality suggests that the parameters \( \mu \) and \( a \) for each fit should all be close, which they appear to be.

A stronger concept of universality for random knot models discussed by Rechnitzer and Rensburg in [47] posits that among models of random knotting that although the exponential growth rate \( \mu \) may change, for any knot types \( K_1 \) and \( K_2 \) which decompose into the same number of prime components the ratios \( p_n(K_1)/p_n(K_2) \) may be universal. While their results suggest that their conjecture holds for different lattice polygon models of knotting, our data is strong evidence that the conjecture does not extend to the knot diagram model.
Fits depicted in figure 27 suggest that the limiting ratios $p_n(3_1)/p_n(4_1) \approx 2.4632 \pm 0.0001$, $p_n(3_1)/p_n(5_1) \approx 4.651 \pm 0.002$, and $p_n(4_1)/p_n(5_1) \approx 1.8872 \pm 0.0004$, all of which are orders of magnitude different from the lattice model ratios of Rensburg and Rechnitzer [47].

7. Conclusion

We have shown a pattern theorem for knot diagrams, which is one of the most important results when working with models of random knots. As a consequence, we were able to show that like most other models of knotting used in studying physical polymers, large diagrams are asymptotically almost surely knotted. This suggests that the diagram model may describe certain types of polymer knotting, although the question of which remains open.

Another consequence of the pattern theorem—that almost all knot diagrams are asymmetric—greatly simplifies the sampling of knot diagrams uniformly. A result of this is a rejection sampler for rooted knot diagrams (of several different graph-theoretic types), which is implemented in plCurve [2] and publicly available. It remains open however whether it is possible to sample directly (i.e. without rejection) from the class of knot diagrams, eliminating the inefficiencies caused by the exponential decay of knot diagrams in link diagrams. As progress towards this, together with Rechnitzer we have constructed a Markov Chain Monte Carlo algorithm for sampling knot diagrams with a distribution limiting on the uniform distribution across diagrams with fixed crossing number [9].

Given the similarities to other models of random models, we mention a driving theme behind studying the diagram model: the ease of computing knot invariants such as the HOMFLY polynomial [20] together with the more topological definition of diagrams suggests that we can prove new theorems for the knot diagram model which remain conjectures in classical models of random knotting. Similarities with space curve models then suggest that there is a way to transfer these results backwards to their original models.

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