Knot Probabilities in Random Diagrams

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Suppose that one is given an n-crossing knot diagram chosen at random from the (finite) set of such diagrams. What is the probability that it is a diagram of the unknot? In this paper, we report on a computer experiment which gives precise answers to this and similar questions for $n \leq 12$ by direct enumeration and classification of knot diagrams. From the point of view of classical knot theory, this is a particularly simple model of random knotting. Part of our interest is to provide data which can be compared to results about more complicated distributions, such as the distribution of knots provided by selecting random closed equilateral n-gons, closed lattice walks, or in combinatorial models such as Even-Zohar et. al.ś *Petaluma* model.

1. DEFINITIONS

We begin with some definitions

Definition 1. We define a *link shadow* with n vertices to be an equivalence class of connected 4-regular embedded planar multigraphs with n vertices up to *shadow isomorphism* which is a graph isomorphism which preserves the counterclockwise order of edges around each vertex.

Examples of link shadows are shown below
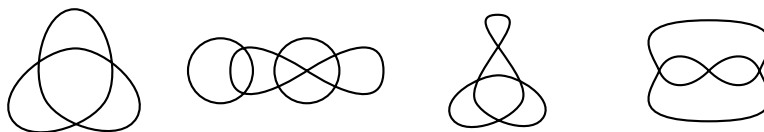
It is well-understood that the equivalence relation preserves the (spherical) embedding of the planar graph; in fact, the left and right-most shadows are actually equivalent under embedded isomorphism– we have just changed the "exterior" face of the projection from the sphere to the plane.

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We can partition the edges of a link diagram into *components* by defining two edges to be equivalent if they meet at a vertex at positions which are not cyclicly adjacent. We will call shadows with a single component *knot shadows*. They will be the focus of this paper.

It's standard in knot theory that

Proposition 2. *The finite set of knot shadows with n vertices is bijective to the finite set of generic immersions of S^1 into S^2 up to orientation-preserving diffeomorphism of the sphere.*

We can define a link diagram by

Definition 3. A *link diagram* is a link shadow where each component is oriented and each vertex is decorated with over-under information for the edges meeting at the vertex. We call these vertices *crossings*. The equivalence relation for these diagrams is the *diagram automorphism*: a shadow isomorphism which also preserves orientation and over-under information.

It is clear that there are at most $2^{\#\text{ components}}2^{\#\text{ crossings}}$ link diagrams associated to a given link shadow, but that this number may be reduced if there are nontrivial diagram automorphisms.

Various models of random knots have been proposed in the literature. In this paper, we will examine a quite natural one:

Definition 4. In the *random diagram model*, a random n-crossing knot is selected uniformly from the counting measure on the finite set of one-component n-crossing link diagrams.

We intend to compute knot probabilities directly in the random diagram model for (relatively) small n by direct enumeration of the collection of n-crossing random knots. Having the entire collection of diagrams will in addition allow us to study transitions between diagrams, but we will discuss this in future work.

2. PDCODES AND SOFTWARE ARCHITECTURE

One of us (Mastin) has given a detailed construction of a combinatorial object, called a PD-code, bijective to the knot diagrams. A PD-code is a set comprised of quadruples, where each entry in a quadruple may be viewed as an edge in a link diagram and each quadruple corresponds to a crossing. PD-codes seem to have been first used by the KnotTheory Mathematica package **cite Knot Atlas** developed by Dror Bar-Natan and his students.

Definition 5. Given a link diagram with labeled edges we generate the set of quadruples of the **PD-code** representing this diagram by the following procedure. For each crossing we include the quadruple of edge labels involved beginning with the incoming under-edge and proceeding around the crossings in the positively oriented direction of S (see Figure 1). We give a positive sign to incoming edges and a negative sign to outgoing edges.

$$\{[+4, -2, -5, +1], [+2, -6, -3, +5],$$
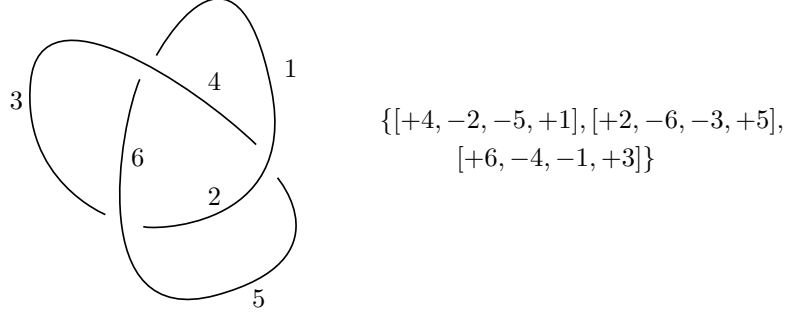$$[+6, -4, -1, +3]\}$$

FIG. 1: A diagram for 3_1 and its PD-code. The labels are only single integers here as there is only one component. Note that we may omit directional arrows as the orientation can be inferred from the ordering of the edge labels.

The details of the bijection between the PD-codes and link diagrams can be found in **cite PD-code Paper**. We will presently include the construction of a cell decomposition of S^2 associated with a PD-code as it will play a central roll in our algorithm for enumerating diagrams. The vertices of the cell decomposition will correspond to the quadruples appearing in the PD-code and the edges will be the edges of the diagram. In order to defined the faces we will introduce the **successor map** which essentially gives the next edge to appear if one were to walk along an edge and turn right a vertex.

Definition 6. If we represent the quadruples in the a PD-code as $[e_i^0, e_i^1, e_i^2, e_i^3]$, then we define the successor map by $s(e_i^j) = -e_i^{j+1 \mod (4)}$.

We can now define a cell complex associated to a PD-code which recovers the link diagram on S^2.

Definition 7. For each orbit of the successor map s we construct an oriented polygon in the plane with sides given by the labels in each orbit where the labels are assigned clockwise around the polygon. The orientation of an edge agrees with the orientation inherited from the standard orientation of the plane for *negative* labels and disagrees with this orientation for *positive* labels. The orientations of the 2-cells is inherited from the standard orientation on the plane. The orientations of the edges is induced by the orientation of the 2-cells. This construction gives the **associated cell complex** to a given PD-code.

This construction gives a collection of oriented polygons in the plane whose edges are labeled by the edge labels of the given link diagram. If these polygons are glued according to the edge labels and orientations then the link diagram is reconstructed as the 1-skeleton of the resulting cell complex. The details of this construction can be found in **cite PD-code Paper**.

Definition 8. Given two PD-codes we say that a bijection between the edge labels is a **PD-code isomorphism** if it induces an isomorphism on the associated cell complexes.

It is clear that a lot of data about a pdcode is preserved by isomorphism: for instance, the number of crossings, edges, faces, and the numbers of edges around faces. We can use this information to rule out isomorphisms using a hashing scheme.

Definition 9. Suppose the pdcode P has V crossings, E edges, F faces, and C components. We assume that the faces are denoted $f_1, \ldots, f_F$ and the components are denoted $c_1, \ldots, c_C$. Further, let $\text{edges}(x)$ give the number of edges on a face or component. Then the *hash* of P is given by the tuple

$$\mathcal{H}(P) = (V, E, F, C, \{\text{edges}(f_1), \ldots, \text{edges}(f_F)\}, \{\text{edges}(c_1), \ldots, \text{edges}(c_C)\}).$$

The last two are unordered sets of integers.

It is clear that

Lemma 10. *If two pdcodes P_1 and P_2 are isomorphic, then $\mathcal{H}(P_1) = \mathcal{H}(P_2)$.*

Proof. The numbers V, E, F, and C are clearly preserved by isomorphism. The indices of edges and faces may be permuted by an isomorphism, but the number of edges on each can't change. Thus the *unordered sets* of edge counts for faces and component remain the same as well. $\square$

We can now build up an isomorphism between pdcodes by a series of definitions:

Definition 11. Suppose we have two pdcodes P and P' with the same hash.

- A bijection $\gamma : \{c_1, \ldots, c_C\} \to \{c'_1, \ldots, c'_C\}$ between the components of P and the components of P' is called *component-length preserving* if $\# \text{edges}(c_i) = \# \text{edges}(\gamma(c_i))$ for all i.

- Given such a component-length preserving bijection γ, a bijection $\epsilon : \{e_1, \ldots, e_E\} \to \{e'_1, \ldots, e'_E\}$ between the edges of P and the edges of P' is called *component-preserving* and *compatible with γ* if ϵ maps the edges of each c_i to the edges of $\gamma(c_i)$ by an element of the dihedral group $D_{\text{edges}(c_i)}$. That is, the edges of c_i are mapped in cyclic (or reverse-cyclic) order to the corresponding edges of $\gamma(c_i)$.

- Given a component-preserving bijection $\epsilon : \{e_1, \ldots, e_E\} \to \{e'_1, \ldots, e'_E\}$ between the edges of P and the edges of P', we say that a bijection $\nu : \{v_1, \ldots, v_V\} \to \{v'_1, \ldots, v'_V\}$ between the vertices of P and the vertices of P' is *compatible with ϵ* if

$$\nu(\text{head}(e_i)) = \text{head}(\epsilon(e_i)) \quad \text{and} \quad \nu(\text{tail}(e_i)) = \text{tail}(\epsilon(e_i)$$

when e_i is part of a component mapped by an orientation-preserving element of the dihedral group, and

$$\nu(\text{head}(e_i)) = \text{tail}(\epsilon(e_i)) \quad \text{and} \quad \nu(\text{tail}(e_i)) = \text{head}(\epsilon(e_i))$$

when e_i is part of a component mapped by an orientation-reversing element of the dihedral group.

- Given γ, ϵ, and ν that obey all the above conditions, we say that they are:

  - *globally orientation-preserving* if the set of edges e_i, e_j, e_k, e_l incident to each vertex v of P (in counterclockwise cyclic order) is mapped to the set of edges $\epsilon(e_i), \epsilon(e_j), \epsilon(e_k), \epsilon(e_l)$ incident to $\nu(v)$ in counterclockwise cyclic order.

  - *globally orientation reversing* if the $\epsilon(e_i), \epsilon(e_j), \epsilon(e_k), \epsilon(e_l)$ are incident to $\nu(v)$ but in clockwise cyclic order (for each v),

  - otherwise, the triple is *inconsistent*.

We then have

Proposition 12. *Given a pair of pdcodes P and P' with the same hash, each isomorphism of P to P' is given by a set of bijections γ between their components, ϵ between their edges, and ν between their vertices where*

- *γ is component-length preserving,*

- *ϵ is component-preserving and compatible with γ,*

- *ν is compatible with ϵ*

and the triple is globally orientation preserving or reversing (not inconsistent).

Proof. Basically, this is the definition of pd isomorphic. $\qquad\square$

A few other observations are helpful:

Lemma 13. *If $\mathcal{H}(P) = \mathcal{H}(P')$ for pdcodes P and P', there is at least one component-length preserving $\gamma : \{c_1, \ldots, c_C\} \to \{c'_1, \ldots, c'_C\}$. All component-length preserving γ can be generated by iterating over a product of permutation groups.*

Proof. We can partition the components of P (and P') into subsets by component length. Since the hashes $\mathcal{H}(P)$ and $\mathcal{H}(P')$ match, these partitions correspond for P and P'. The component-length preserving γ are exactly those bijections which respect this partition: we can construct all such γ by taking a product of permutation groups whose orders are the size of the subsets. At worst, all subsets have size 1 and there is a single such γ. $\qquad\square$

Lemma 14. *Given a component-length preserving γ and component-preserving and compatible ϵ, and a set of orientations for the components of P, there is at most one $\nu : \{v_1, \ldots, v_V\} \to \{v'_1, \ldots, v'_V\}$ which is compatible with ϵ and consistently oriented on components and we can construct ν as below.*

Proof. Each vertex v of P is incident to four edges e_i, e_j, e_k, e_l. Without loss of generality, let's assume that $v = \text{tail}(e_i), \text{tail}(e_j), \text{head}(e_k)$ and $\text{head}(e_l)$. Then if ν is compatible with ϵ, we must have

$$\nu(v) = \text{tail}(\epsilon(e_i)) = \text{tail}(\epsilon(e_j)) = \text{head}(\epsilon(e_k)) = \text{head}(\epsilon(e_l)).$$

If the four terms on the right are equal, this uniquely defines $\nu(v)$. If not, there is no compatible ν. $\qquad\square$

We can now find all isomorphisms between two pdcodes computationally by a simple brute-force strategy:

1: **procedure** BUILDISOMORPHISMS(P,P')   ▷ Build isomorphisms between pdcodes P and P'
2:   **if** the hashes $\mathcal{H}(P)$ and $\mathcal{H}(P')$ are different **then**
3:    P and P' are not isomorphic. Return $\emptyset$.
4:   **end if**
5:   **for all** component-length preserving $\gamma : \{c_1, \ldots, c_C\} \to \{c'_1, \ldots, c'_C\}$ **do**
6:    **for all** compatible and component-preserving ϵ **do**
7:     **if** a compatible ν exists **then**
8:      **if** ν is globally orientation preserving or reversing **then**
9:       ϵ, ν define an isomorphism $P \to P'$
10:      **end if**
11:     **end if**
12:    **end for**
13:   **end for**
14: **end procedure**

It should be immediately clear that there are smarter ways to organize this computation: for instance, we could build only part of γ and ϵ before we start checking the consistency conditions for the existence of a compatible ν. Or we could map faces to faces by elements of the dihedral group on the grounds that faces are smaller than components. Or we could try for a more complicated hashing scheme which took into account the adjacency relations between faces. These sorts of ideas are implemented with great insight and care in graph isomorphism packages like *nauty* and *saucy*. However, making these types of changes makes the code more intricate and difficult to debug: in this project, our overall strategy is to use simple, straightforward algorithms in the hopes of minimizing the chance of errors.

3.   CONSTRUCTING THE DATABASE OF DIAGRAMS

Our first goal is to enumerate the link shadows– that is, the connected 4-regular embedded planar (multi)graphs– computationally. Since this is the heart of our work, we describe two independent algorithms for the enumeration. One is quite simple while the other is much more complex. We implemented, tested, and ran both of them independently to generate the database of diagrams, verifying that the results of the computations were the same.

3.1.   Dual quadrangulations and connect sums

Brinkmann et. al. [3] provided an algorithm to enumerate all of the simple embedded planar quadrangulations of S^2, up to embedded isomorphism. A quadrangulation is a planar graph where each face has four edges, as in the pictures below.
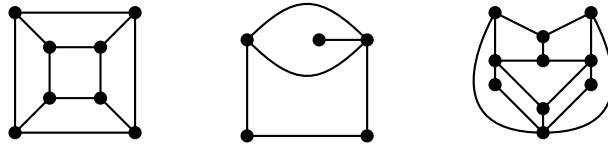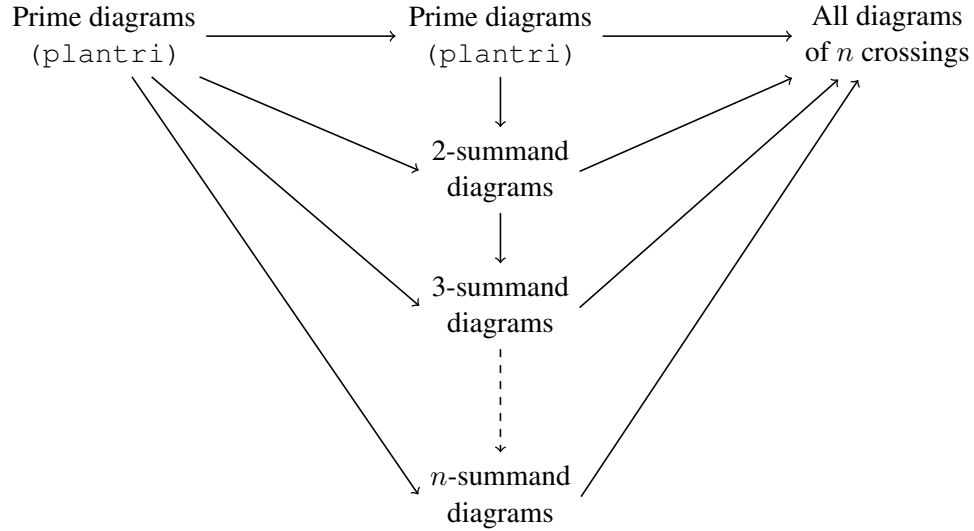

The dual graph to a quadrangulation is a connected 4-regular embedded planar multigraph, as shown below left. However, if the quadrangulation is simple, the dual graph is what we will call a *prime* diagram: it cannot be decomposed by embedded circles which intersect the diagram in only two edges. We will call diagrams with such a system of decomposing circles *composite*; an example of a non-simple quadrangulation and its (composite) dual graph is shown below right.
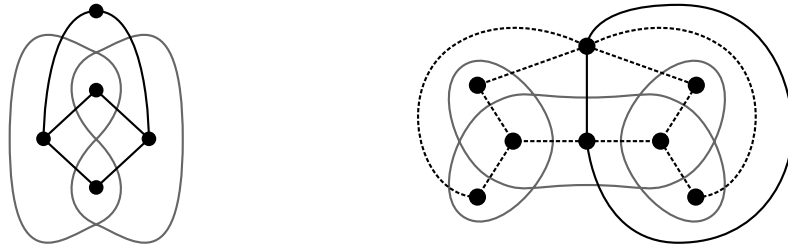
The *plantri* software of Brinkmann and McKay [3 **?**] can be used to generate the dual graphs of the planar simple quadrangulations of given number of vertices. Since an easy Euler characteristic

argument shows that the number of vertices in the dual graph of a quadrangulation is 2 less than the number of vertices in the quadrangulation, we can use this to enumerate the connected 4-regular embedded planar multigraphs which are prime.

To enumerate all diagrams, we recall (as is standard in knot theory) that every composite diagram is uniquely expressed as a collection of prime diagrams joined along pairs of edges by the connect sum operation. Of course, this regularly generates isomorphic diagrams when the prime diagrams have a nontrivial automorphism group. It would be interesting and fun to predict when this happens and arrange to avoid generating duplicate diagrams by tracking edge orbits under the automorphism group of each diagram. However, in keeping with our strategy of simple, robust code, we simply construct all connect sums iteratively and check for isomorphisms with existing pdcodes using the hashing/brute force strategy for isomorphism checking detailed above. The process is shown below

Prime diagrams $\longrightarrow$ Prime diagrams $\longrightarrow$ All diagrams
(plantri)   (plantri)   of n crossings

2-summand diagrams

3-summand diagrams

n-summand diagrams

where the arrows indicate "all possible connect sums (and entry into the database with isomorphic copies of an existing diagram rejected)" or simply "entry into the database with isomorphic copies rejected".

3.2. Expansions of embedded planar simple graphs

Our next strategy will be much more complicated (and somewhat slower to run), but it serves as crucial check on the previous computation. The basic idea is to define a smaller class of graphs so that the graphs we are interested in can be obtained from the base class of graphs by various expansion moves. Lehel [?] gave a strategy for generating all 4-regular graphs in this way

from the octahedral graph. Instead of using Lehel's strategy directly, we build on the method of Brinkmann and McKay [3?] for enumerating isomorph-free embedded planar graphs; we extend their work here to generate the class of graphs that we're interested in.

We now define four expansion moves of embedded planar graphs with vertex degree ≤ 4 which generate new embedded planar graphs of vertex degree ≤ 4 with the same number of vertices, but additional edges:

Definition 15. The four expansion operations that we will use are the following:

- E_1 Loop insertion adds a loop edge to a vertex of degree 1 or 2, as below. (Note: Loop insertion can be performed on each side of a vertex of degree 2).

- E_2 reversing edge doubling duplicates an existing edge joining vertices of degree < 4 so as to create a new bigon face. Note that the (counterclockwise) order of the two vertices is reversed on the two vertices.
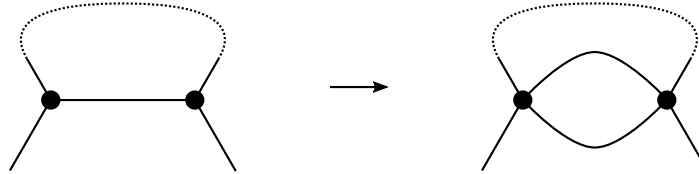
- E_3 preserving doubling also duplicates an existing edge joining vertices of degree < 4, but keeps the counterclockwise order of the edges the same on each at each of the two vertices. This sort of doubling is only available if the original edge is a cut edge of the graph.
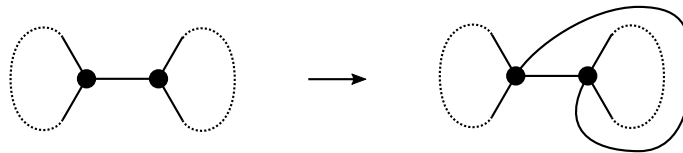
- E_4 pair insertion adds a pair of edges simultaneously, joining two vertices of degree 2 which are both on two faces of the embedding, as below.
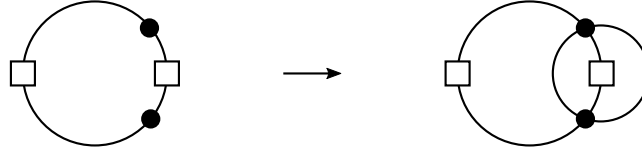
We can now show

Proposition 16. *Every connected 4-regular embedded planar (multi)graph G can be obtained from a connected, embedded planar simple graph of vertex degree ≤ 4 G_0 by a series of E_1, E_2, E_3, and E_4 expansions.*

Equivalently, any connected 4-regular embedded planar (multi)graph G can be reduced to a connected embedded planar simple graph G_0 of vertex degree ≤ 4 by a series of E_1, E_2, E_3, and E_4 reductions. The embedded isomorphism type of G_0 is determined by the embedded isomorphism type of G (the order in which the reductions are performed doesn't matter).

An illustration of the process we describe is
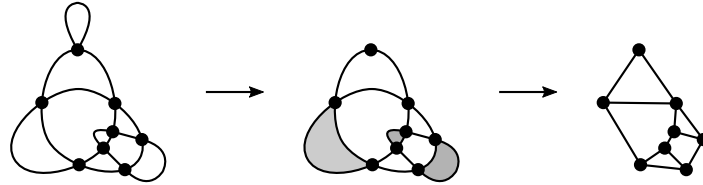
Proof. We will prove the second statement, reducing in stages from some $G_n = G$ to G_0 by performing one reduction at each step. The number of steps we can perform is clearly finite, since each reduces the number of edges by at least one. So suppose we are at stage G_i. If there are no loop or multiple edges, we're done, and this is the simple graph G_0.

If there is a loop edge, we can remove it with a E_1 move.

If there is a multiple edge, we must consider several cases. We can think of each vertex of G_i as retaining a list of 4 connection points, ordered counterclockwise, from the initial embedding of G. Since we have performed some reductions already, some of these may be empty, but at least two are filled at each end of the multiple edge. Pick one vertex of the multiple edge and call it v and the other vertex w.

If the edge multiplicity is four, G is ⊘⊘. This is obtained from the graph with one edge and two vertices by three E_2 moves.

If the edge multiplicity is three or two, there is at least one connection point on v which is not occupied by a copy of the multiple edge followed immediately by a connection point which is

occupied by a copy e of the multiple edge. Without loss of generality, we'll call e the *base copy* of the multiple edge, and its connection point to at v position 0 around v. The remaining connection points will be numbered 1, 2, and 3. By construction, the edge joined to v at position 3 (if any) is not connected to w. We can label the other end of the base copy e position a on the second vertex w, and label the other positions b, c, and d, again counterclockwise.
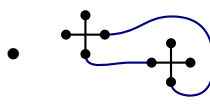
If the edge multiplicity is three, only one of these positions is unoccupied by a copy of the multiple edge. Looking at the three cases (below), we can see that by parity, it must be position b, and the pair of copies $0a$ and $2c$ of the multiple edge can be removed by a E_4 operation.
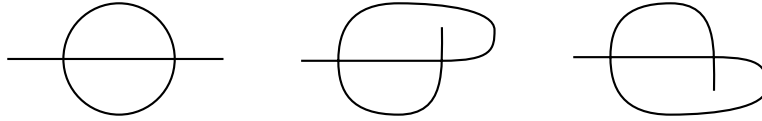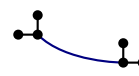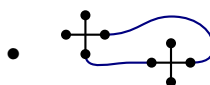

By parity, because we came from a 4-regular embedded planar graph only the leftmost case can occur at any stage in the reduction process.
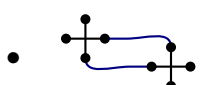
We have now disposed of the case where edge multiplicity is three.

If edge multiplicity is two, there is one edge unaccounted for, which joins either position 1 or 2 on vertex v to position b, c, or d on vertex w. Therefore, there are six cases to address. We consider them in order, starting with the $1x$ configurations.
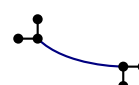

In the $1b$ configuration, the multiple edge forms a 2-cycle dividing the portion of the graph G connected to cd from the portion connected to 23. Deleting $1b$ requires a E_3 move, and the remaining base edge is a cut edge of all further-reduced G_i, as shown at right.
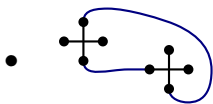

The $1c$ configuration is forbidden by parity.

In the $1d$ configuration, the multiple edge forms a bigon face. Deleting $1d$ uses an E_2 reduction, and yields the configuration at right. The remaining base edge may or may not be a cut edge of the further G_i.

One might think that the $2-$ configurations are simply rearrangements of those above, but this is not true. A genuinely new case arises for $2c$.

The $2b$ configuration is forbidden by parity.
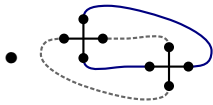
In the $2c$ configuration, by parity, the graph G must have connected 1 and d and also 3 and b. None of our moves change the connectivity of the graph (because we never delete all copies of a multiple edge), so the current graph G_i still joins these pairs of connection points. This means that we are in position for an E_4 pair reduction, resulting in the graph at right.
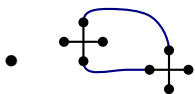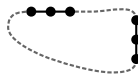
The $2d$ configuration is forbidden by parity.

Along the way, our analysis has been entirely local: we need only consider a single vertex to decide whether we can apply an E_1 reduction and a pair of vertices to decide on E_2, E_3, and E_4 operations. To show that order of operations doesn't matter, we need to show that whether or not we can apply these operations does not depend on which reductions have already been performed. First, we note that since we never remove all copies of multiple edge, we never change the connectivity of the graph during the reduction process.

The three copies of a multiplicity three edge must bound two bigons, and this does not change as we reduce other edges. Therefore, the E_4 move is always available for all multiplicity three edges.

Whether a multiplicity two edge is eligible for an E_2 move depends only on the positions of the ends of the multiple copies on their vertices, which doesn't change as we reduce. Therefore, this operation can always be performed (or is always forbidden), regardless of which reductions have already been performed.

Whether a multiplicity two edge is eligible for a E_3 or E_4 operation depends not only on the positions of ends of edges on their vertices, but also on the connectivity of the (reduced) graph. However, as we noted above, the connectivity of the graph doesn't change as we perform reductions.

It is clear that the isomorphism type of G_0 does not depend on the order of reduction– after all, in the end we are simply reducing the multiplicity of multiple edges of the edge.

It takes only a moment longer to realize that the embedding of G_0 is determined as well– this embedding is determined by the cyclic order of (surviving) edges around their vertices. We will have deleted some edges from many of these vertices by the time we reach G_0, potentially leaving

many empty connections. However, the cyclic order of the surviving edges won't be affected by the order in which these connections were emptied.

One might worry that the choice of *which*[1] copy of an edge of multiplicity two to delete could affect the embedded isomorphism type after an E_2 or E_3 reduction, but it's easy to check that the two possible reduced configurations are (embedded) graph isomorphic by looking at the pictures above. Formally, the point is that the two copies of the edge are adjacent in the cyclic ordering of edges at each vertex, so the surviving copy is always in the same cyclic position relative to surviving edges incident to the vertex. □

We can use this theorem to come up with a strategy for generating diagrams. Basically, we will start by enumerating embedded planar simple graphs of vertex degree ≤ 4 using *plantri*, then expand them to 4-regular embedded planar graphs using the moves above. Afterwards, we will see that we can generate embedded isomorphic graphs with different expansion sequences, so we will have to filter the graphs into isomorphism classes. We start with two lemmas:

Lemma 17. *If the embedded planar graph of vertex degree ≤ 4 G_0 is obtained from a 4-regular embedded planar multigraph G by the reduction process of Proposition 16 then either every vertex of degree one in G_0 has exactly one loop edge in G and one multiedge of multiplicity two obtained by E_2 or E_3 or the graph is ⊗.*

Proof. If we expand G_0 to G using the four moves, three empty connections on the vertex must be filled during the process. If they are filled by redoubling the existing edge, then the degree of the vertex at the other end of the edge was also one, and we get ⊗. Otherwise, we must fill two by adding a loop edge, and the other by doubling the existing edge. □

Lemma 18. *Two pairs of vertices ab and cd on the unit circle may be joined by nonintersecting chords inside the circle if and only if the pairs are unlinked on the circle. That is, if ab and cd are adjacent in the cyclic ordering of the four vertices, as opposed to an order such as $acbd$ or $adbc$ where the pairs alternate.*

We can now design an algorithm to produce all possible expansions of G_0, a given connected embedded planar simple graph of vertex degree ≤ 4 as an integer constraint satisfaction problem. By Lemma 17, we must add a loop to each vertex of degree one in G_0 eventually. We can save time by doing so at the start of the computation. We will therefore assume that loops have been added to create a *prepared* graph G_1, and each vertex has degree 2, 3, or 4.

We will now define four classes of variables:

- l_i for every vertex v_i of degree 2

---

[1] Remember that the choice of "base edge" was arbitrary.

- $d_{i,j}$ for every non-cut edge e_{ij} in the graph joining vertices of degree < 4.

- $c_{i,j}$ for every cut edge e_{ij} joining vertices of degree < 4.

- $p_{i,j}$ for every pair of vertices v_i, v_j which both have degree 2 and are both on two different faces of the embedding

We take the subscripts to be unordered. That is, $d_{4,17}$ and $d_{17,4}$ are the same variable, since the edges $e_{4,17}$ and $e_{17,4}$ are the same edge.

These variables will all be valued in $0 - 1$, and represent the absence or presence of E_1 loop edges, E_2 or E_3 doubles of existing edges and E_4 insertions of new pairs of edges. We can now define two sets of equations relating these variables.

Definition 19. We define the *vertex degree equations* for a prepared graph G_1 to be the collection of equations indexed by the vertices of G_1 given below. For each vertex index i of degree $\delta(i)$ in G_1

$$\delta(i) + 2l_i + \sum_j d_{i,j} + \sum_j c_{i,j} + 2 \sum_j p_{i,j} = 4$$

where the sums are taken over all j for which the appropriate variables exist. These equations express the fact that in a complete expansion, the vertex degrees must all be four.

The pair variables $p_{i,j}$ satisfy an additional set of equations:

Definition 20. For each $p_{i,j}$ and $p_{k,l}$ so that the vertices v_i, v_j, v_k and v_l are on the same pairs of faces, and so that the vertices are in the (cyclic) order v_i, v_k, v_j, v_l or v_i, v_l, v_j, v_k we have an additional *linking equation*

$$p_{i,j} + p_{k,l} \leq 1$$

These equations express the fact that the edges corresponding to a linked pair of endpoints along a face must intersect inside the face. Therefore, if two pair variables are linked, at most one of them can take the value 1. For instance, in the situation below where there are four vertices of degree two along a pair of faces, we have six pair variables, two of which obey an additional linking equation.
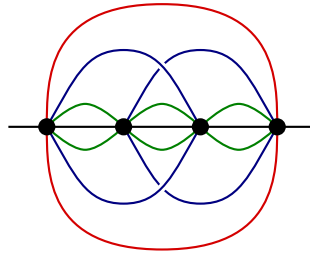
We note that in the end, at most two of the pair variables above can have value 1, but that a number of combinations are ruled out by vertex degree equations instead of linking equations.

We have defined everything so that

Proposition 21. *Every assignment of $\{0, 1\}$ to the variables l_i, $d_{i,j}$, $c_{i,j}$, and $p_{i,j}$ which obeys the vertex degree equations and linking equations corresponds to an expansion of the connected planar graph G_1 with vertex degrees 2, 3, and 4 and loop edges only to a collection of embeddings for the connected planar 4-regular multigraph G.*

Proof. Actually, there is only a little to check. By the arguments in the proof of Proposition 16, the order of expansion moves is irrelevant. So suppose there are n expansions, and we've chosen an order for them, and are trying to generate a family of graphs $G_1, G_2, \ldots, G_n = G$. If we can perform the indicated expansions at all, we will generate a unique connected 4-regular planar multigraph G (we will see that the embedding of G depends on choices we make along the way). So suppose we have generated a given (embedded) G_i, and are trying to expand to G_{i+1}.

If the next expansion is a E_1 expansions indicated by a positive l_i, it is possible as long as the vertex degree at v_i is small enough. This is true, because of the corresponding vertex degree equation. We must choose which side of the edge to insert the loop; each choice yields a different embedding of G_{i+1}, and following the various possibilities will lead to a family of embeddings for $G_n = G$.

If the next expansion is an E_2 indicated by a positive $d_{i,j}$, it is possible as long as the vertex degrees of v_i and v_j are small enough. This is true by their vertex degree equations. There is only one way to make this expansion, leading to a unique embedding for G_{i+1}.

If the next expansion is an E_2 or E_3 expansion indicated by a positive $c_{i,j}$ variable, it is (again) possible if the vertex degrees at v_i and v_j are small enough (which is again true by the vertex degree equations) *and* if $e_{i,j}$ is a cut edge of G_i. We never apply these expansions more than once to an edge, so $e_{i,j}$ is a cut edge of G_i since it was a cut edge of G_1. Choosing between E_2 and E_3 expansions will yield different embeddings of G_{i+1} and we must follow both possibilities to generate the final family of embeddings of G.

This much was easy. If the next expansion is of type E_4, there is more to check. First, we note that there is no ambiguity in embeddings here: if we can do the E_4 expansion, we can do it in only one way and we generate a unique embedding of the graph G_{i+1}. But can we do it at all? Each E_4 indicated by a positive $p_{i,j}$ requires several conditions. First, vertex degrees at v_i, v_j must be small enough, which is checked as before by vertex degree equations. But the v_i and v_j must still be on two faces in the expansion G_i, which is not obvious, because previous E_4 expansions have split faces of G_1 into smaller faces in G_i. Let us suppose that v_i and v_j were on the pair of faces F_1 and F_2 of the original graph.
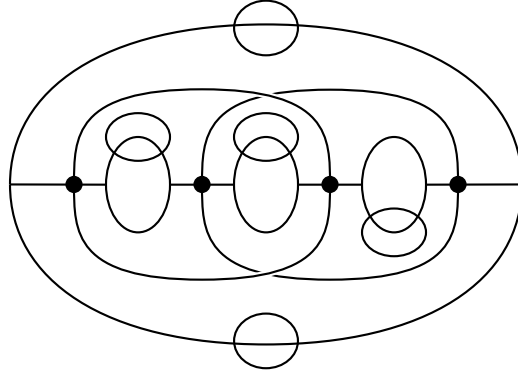
The pair of faces can make contact with each in several disconnected arcs, as shown above. Further, additional pair edges can share F_1 or F_2 with some other face. However, slicing F_1 can only separate v_i and v_j if the endpoints of the splitting arc link v_i and v_j on F_1. This can't happen if the splitting arc is part of a pair which share F_1 with some other face (as shown), as the interfaces of F_1 and other faces are all connected.

But if the splitting arc also shared F_1 and F_2, the corresponding pair variable $p_{k,l}$ is related to $p_{i,j}$ by a linking equation if and only if adding that arc would leave v_i and v_j on different faces. The linking equation implies that only one of the arcs indicated by $p_{i,j}$ and $p_{k,l}$ is present in the expansion; since we have assumed that $p_{i,j}$ is positive, no such $p_{k,l}$ can have already been inserted earlier in the expansion process. This concludes the case where the interface of F_1 and F_2 was disconnected.
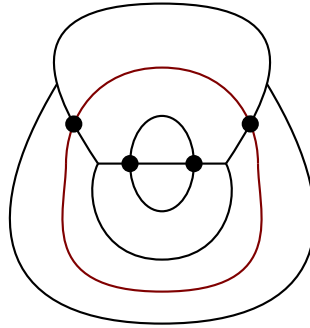

If the interface between F_1 and F_2 is connected, than either might have a disconnected interface with (at most one) other face, as shown above. This case is only cosmetically different– again the key point is that the pair v_i, v_j can link along the boundary of F_1 (or F_2) with a pair edge which also shares F_1 and F_2 while pairs involving a third face won't link the vertices we're interested in.

We last have only to observe that by the vertex degree equations, the final graph G is a 4-regular planar multigraph. Since we have only added edges along the way, G is connected because G_1 was. $\qquad\square$

We have reduced the problem to that of building and satisfying the vertex degree and linking equations. This problem is basically standard, and we use the usual branch-and-bound algorithm. We must define a canonical order on the variables (it doesn't matter how, but to be specific, in our implementation we sort the classes of variables in the order $l_i \prec d_{i,j} \prec c_{i,j} \prec p_{ij}$ and in dictionary order by the (sorted) pair $\{i, j\}$ within each class). Then we enumerate the possible assignments of $\{0, 1\}$ to variables recursively, pruning the tree whenever a vertex degree or linking equation is violated. As usual, this is in theory possibly exponentially slow, but in practice efficient enough for small n.

We now consider the problem of dividing the results into embedded isomorphism classes. We first observe that we have already shown in Proposition 16 two different reduced graphs G_0 and G_0' cannot expand to the same G since the embedded isomorphism type of the reduction G_0 is determined by the embedded isomorphism type of the expansion. However, it is possible for two different collections of expansion moves for the *same* graph G_0 to produce isomorphic G and G' as in the picture below:
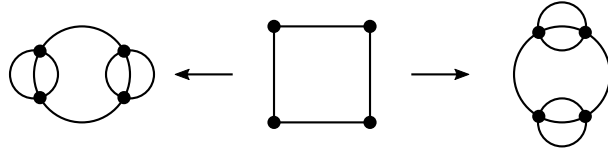
Therefore, we must insert each expansion we generate from a solution to the vertex degree and linking constraints into a container which rejects the solution if an embedded isomorphic graph already exists in the container. Though very fast graph isomorphism checkers such as *nauty* and *saucy* might speed things up, the number of vertices here is very small and we get entirely acceptable performance simply by using a hashing scheme and then attempting to build isomorphisms by pruned search.

The overall workflow is then as follows:
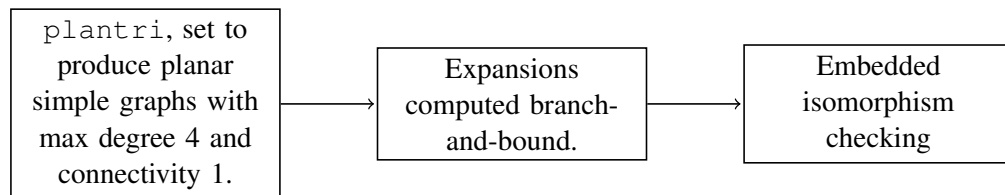
4. COMPUTING AND VERIFYING THE RESULTS

We implemented the above algorithms in C and used them to generate a database of knot diagrams up to 10 crossings. The longest run took several days on a desktop computer. The most important question, of course, is how the computation was checked. Of course, our implementation was careful and involved quite a bit of internal self-checks as well as testing against *valgrind* for memory problems, and writing a suite of unit tests for the codebase. However, good programming practices can only provide a limited measure of confidence in the results, so we continued to test our work. The first and most important test was to verify that the databases obtained by connect summing and by expansions were identical.

We were also able to check against some existing enumerations. Kápolnai et. al. classified spherical "multiquadrangulations"[4], which are the duals of our diagrams as explained in Section 3.1. Their table 2 of the count of multiquadrangulations matches our count of diagrams exactly through 8 crossings (note that the quadrangulation has two more vertices than the dual knot diagram has crossings, so their data is shifted by two). It's worth observing that these authors also use *plantri* , so their results are not completely independent from ours. Still, it provides some comfort to see that their implementation on top of *plantri* produces the same results as ours.

A less obvious and more theoretical check comes from the work of Bouttier et. al. , who provide an explicit generating function for the number of "tetravalent two-leg diagrams with geodesic distance 0 between the two legs"[2, (4.13)]:

$$\frac{24g - 1 + \sqrt{1 - 12g}}{9g(1 + \sqrt{1 - 12g})} = 1 + 2g + 9g^2 + 54g^3 + 378g^4 + 2916g^5 + \dots$$

Basically, these are isomorphism classes of oriented "long curves" in the plane. One of our spherical curves can generate as many as $4n$ of these curves by choosing an edge and orientation. However, the resulting planar long curves are not all distinct if the spherical curve has a nontrivial automorphism group. Thus, there is no simple way to translate from this count to ours. However, we do know the automorphism group of each diagram, so we can predict the number of marked-edge planar diagrams by the following procedure:

¡insert procedure¿

Our counts of spherical diagrams (of all numbers of components) then produce the data below, which matches the prediction from the generating function above.

For knot diagrams in particular, Arnol'd has given counts of the number of immersions of the unoriented circle into the unoriented sphere with n crossings for n from 0 to 5 [1, page 79]. This is sequence A008989 in the Online Encyclopedia of Integer Sequences, with an extension to $n = 7$ credited to Guy H. Valette. We could not find a published reference for Vallette's extension of the table, but our data for knots does match A008989 including the extension. These counts are given in the table below:

¡insert table of counts here¿

5. CLASSIFYING KNOT TYPES

Our database of diagrams contains all diagrams of knots and links with n crossings. Though very few of these are knot diagrams (the subject of this paper), there seems to be no obvious graph-theoretic way to avoid generating link diagrams. So our next move is to simply compute the number of components in each diagram and throw out the diagrams with more than one component. This gives us the following table of the number of diagrams we've found:

¡data¿

Matt and Harrison write something about assigning crossings and orientations, and give data on expansions

Matt and Harrison write something about their respective knot identification strategies and the verification that they match

6. RESULTS

giant pictures, compared with tait's classification our distributions monogon and bigon fractions degree of alternatingness universal properties? comparison with distribution from ERPs, lattice walks, and petaluma.

An experiment to do: make a histogram of the number of diagrams which are all unknots, those that are mostly unknots, those that are partially unknots, and so forth.

I think this should partially explain the unknot fraction; the idea is that we should be able to count diagrams which can't possibly be knots (that is, stuff with only R1's) and see that while they eventually become exponentially scarce, they are (in this data) quite prevalent. Of course, it would be better if we also knew an upper bound on the total number of diagrams (maybe from Thistlethwaite's paper?), so that we could get an asymptotic bound on the decay rate.

7. FUTURE DIRECTIONS

transitions, unknotting number and so forth.

[1] V I Arnol d. Plane curves, their invariants, perestroikas and classifications. In *Singularities and bifurcations*, pages 33–91. Amer. Math. Soc., Providence, RI, 1994.

[2] J Bouttier, P Di Francesco, and E Guitter. Geodesic distance in planar graphs. *Nuclear Physics. B*, 663(3):535–567, 2003.

[3] G Brinkmann, G Brinkmann, B D McKay, and B D McKay. Fast generation of planar graphs. *MATCH Commun. Math. Comput. Chem*, 58(2):323–357, 2007.

[4] Richárd Kápolnai, Gábor Domokos, and Tímea Szabó. Generating spherical multiquadrangulations by restricted vertex splittings and the reducibility of equilibrium classes. *Periodica Polytechnica Electrical Engineering*, 56(1):11–10, 2012.