A plane curve is a knot diagram in which each crossing is replaced by a 4-valent vertex, and so are dual to a subset of planar quadrangulations. The aim of this article is to introduce a new tool for sampling diagrams via sampling of plane curves. At present the most efficient method for sampling diagrams is rejection sampling, however that method is inefficient at even modest sizes. We introduce Markov chains that sample from the space of plane curves using local moves based on Reidemeister moves. By then mapping vertices on those curves to crossings we produce random knot diagrams. Combining this chain with flat histogram methods we achieve an efficient sampler of plane curves and knot diagrams. By analyzing data from this chain we are able to estimate the number of knot diagrams of a given size and also compute knotting probabilities and so investigate their asymptotic behavior.

1. Introduction

1.1. Background

A beautiful aspect of knot theory is that it brings together many different aspects of mathematics and leverages their tools so efficiently. An apt example of this phenomenon is knot diagrams, wherein the entanglement of a smooth string in space is studied as a combinatorial cartoon. From this view, any of the infinite manipulations of a loop of string are simply sequences of a finite number of diagram operations called Reidemeister moves [Alexander and Briggs 26, Reidemeister 48]. This combinatorial regime also serves an essential role in knot identification; many knot polynomials are calculated more naturally for diagrams than for space curves [Ewing and Millett 97]. Other invariants, like the important crossing number of a knot, are defined in terms of diagrams.

Knot theory is an important tool in many applied disciplines. Ring polymers exhibit knotting [Frisch and Wasserman 61, Trigueros et al. 01], which affects their function [Buck and Zechiedrich 04] and their chemical properties [Vanderzande 95]. Knotted configurations of polymers are studied through random knot models, where knots are sampled from some probability distribution with the aim of modeling physical behavior; for a good overview see [Orlandini and Whittington 07]. A canonical model of random knotting is that of self-avoiding polygons on the cubic lattice $Z^3$ [Sumners and Whittington 88]. A self-avoiding polygon is constructed by embedding a simple closed curve into $Z^3$ and by sampling these objects uniformly at random, one obtains a distribution over the space of knot embeddings. A surprising amount is still unknown for all but the most simple of such models. For example, it is still unproven (despite overwhelming evidence) that the exponential growth rates of knotted polygons of fixed knot type are independent of knot type [Rensburg and Rechnitzer 11].

As knot diagrams are more naturally suited for the study of invariants, in [Cantarella et al. 16], the first author together with Cantarella and Mastin proposed the random diagram model. In this model, one samples a random knot by, for a fixed number of crossings $n$, picking one of the finite number of knot diagrams with $n$-crossings uniformly. The diagram model behaves like many other physically motivated models in that unkotted diagrams are exponentially rare [Frisch and Wasserman 61, Delbrück 62, Sumners and Whittington 88, Diao 95, Chapman 17]. At the same time, this diagram model has advantages over other models of knotting. It is possible, for
example, to show, via a pattern theorem, that unknot diagrams almost certainly contain slipknots [Chapman 18], a result which remains a conjecture for unknotted self-avoiding polygons and Gaussian polygons [Millett 10].

Another major problem of combinatorial models of knots, is that the underlying objects are difficult to enumerate. The diagram model is no different—the best algorithms for enumerating knot diagrams require time that grows exponentially with the number of crossings [Zinn-Justin and Zuber 09]. If an efficient enumeration method were to exist, then this could be readily adapted to give a random sampling method (see, e.g. [Flajolet and Sedgewick 09]). In the absence of such a method, the most obvious approach has been to generate 4-valent maps uniformly at random, then assign crossings at random (see Figure 1). The result is accepted if it is a knot and rejected otherwise. However, the exponential growth rate of the subset of 4-valent maps corresponding to knot diagrams are strictly smaller than that of all 4-valent maps. Consequently, the probability that a random n-crossing 4-valent map will result in a knot diagram decays exponentially with n. For example, experiments in [Chapman 17] suggest that roughly 1% of samples are accepted at 60-crossings and 0.01% of samples are accepted at 150-crossing diagrams. The exponential decay in acceptance probability means that the expected time for this rejection sampling approach to produce a knot diagram will grow exponentially with the number of crossings. One way to overcome this is to manipulate a sampled 4-valent map until a knot diagram is obtained [Diao et al. 2012, Dunfield et al. 14], however the resulting space of knots is not sampled uniformly.

The absence of an efficient random knot diagram sampler is a major impediment to the study of random knots. The aim of this article is thus two-fold: First, we describe a new efficient method to sample knot diagrams directly with uniform probability using Metropolis style Markov chain Monte Carlo (MCMC) sampling [Metropolis et al. 53]. Second, we explore the new data gathered using the MCMC sampling method. Such Markov chains have been used to study other models of random knotting, particularly on the simple cubic lattice. Foremost among these are the pivot algorithm [Lal 69] and the BFACF algorithm [Berg and Foerster 81, Aragão de Carvalho et al. 83, Aragão de Carvalho and Caracciolo 83]. The former is extremely efficient [Madras and Sokal 88], while the latter has the advantage of conserving topology [Rensburg and Whittington 91]. [Guitter and Orlandini 99] augmented the BFACF algorithm with Reidemeister moves to study a model of flat-knots on the square-diagonal lattice.

This article focuses on sampling plane curves, which can be thought of as knot diagrams without crossing sign information (see Figure 1 and Section 2). Each plane curve of n-vertices maps to a unique set of 2n knot diagrams. Consequently if we can sample plane curves uniformly, then we can also sample knot diagrams uniformly. To avoid complications caused by symmetries, we sample from the space of rooted diagrams (explained below).

The main result of the article is a Markov Chain over the space of plane curves. By selecting transition probabilities we can sample from this chain with a Boltzmann distribution.

**Theorem 1.** Let D be a plane curve with 1 ≤ n vertices and let μ be the exponential growth rate of plane curves. The Markov chain described in Section 3.1 has stationary distribution given by

\[ \pi(D) \propto z^n, \]

provided 0 ≤ z < μ−1. Consequently, plane curves of a fixed size are sampled uniformly.

When running this Markov chain, we found that it was very difficult to obtain a good number of samples at large range of lengths. To overcome this problem we modified our transition probabilities based on Wang-Landau density of states estimation [Wang and Landau 01] — see Section 3. This method allows us to sample diagrams nearly uniformly in length (while

![Figure 1](image_url). By replacing crossings with vertices, knot diagrams (A) are mapped onto plane curves (B). However, not all 4-valent plane graphs correspond to knots. For example, the Hopf-link (C) maps to a 4-valent graph. To avoid complications caused by symmetries, we study rooted plane curves, in which one edge is selected and assigned an orientation (D).
still sampling uniformly within any given length) and additionally provides estimates of the number of plane diagrams. Let \( k_n \) be the number of rooted plane curves with \( n \) vertices, and let \( g_n \) be the estimate of \( k_n \) from the Wang-Landau algorithm. Then we have the following result.

**Theorem 2.** Let \( L \in \mathbb{N} \) and \( D \) be a plane curve with \( 1 \leq n \leq L \) vertices. The Markov chain described in Section 3.2 has stationary distribution given by

\[
p(\mathcal{D}) \propto \frac{1}{g_n}.
\]

While curves of different sizes are sampled with different probabilities, curves of a given size are sampled uniformly.

Notice that if we use this Markov chain to sample plane curves, then the probability of sampling any curve of size \( n \) is proportional to \( \frac{g_n}{s_n} \). So when \( g_n \) closely approximates \( k_n \), the resulting sample histogram will be approximately flat. To be more precise, if \( s_n \) denotes the number of samples of \( n \)-crossing curves, then we have \( s_n \frac{g_n}{k_n} \approx s_1 \frac{g_1}{k_1} \).

The efficiency of the Wang-Landau sampler then enables us to run a variety of plane curve and knot diagram sampling experiments and collect a number of statistics — see Section 4. We find that all of these data are within error bounds of that of the uniform rejection sampler, reaffirming that we are sampling from the appropriate distribution. We also examine the asymptotic behavior of these statistics, finding similarities with other classes of planar maps and knot models. In particular, we have the following conjectures:

**Conjecture 1.** The expected fraction \( p_{k,n} \) of degree-\( k \) faces in plane curves with \( n \)-vertices tends towards a non-zero constant for every \( k \).

**Conjecture 2.** The expected maximum face degree \( \mathbb{E}(\Delta^+_n) \) in plane curves with \( n \)-vertices grows as \( O(\log n) \).

In fact, it is reasonable based on the asymptotic behavior of this statistic for general maps [Gao and Wormald 00], to conjecture that \( \mathbb{E}(\Delta^+_n) \) grows as \( \log n \) with \( \log \log n \) corrections. Unfortunately we have not been able to confirm this correction as such subtle subdominant terms are very difficult to determine numerically.

**Conjecture 3.** The expected Casson invariant \( v_2 \) of an \( n \)-crossing knot diagram grows linearly in \( n \).

Finally, by assigning crossings at random we transform our random plane curves into random knot diagrams. We compute the HOMFLY-PT polynomial of the diagrams to classify their knot types. This allows us to collect data on knotting probabilities and examine their asymptotics. Based on our data, we have the following conjecture.

**Conjecture 4.** The probability, \( p_n(K) \), that a random knot of size \( n \) exhibits knot type \( K \) scales as

\[
p_n(K) \sim D_K p^n n^{N_K}
\]

where \( 0 < p < 1 \) is a constant independent of knot type, \( N_K \) is the number of prime components in \( K \), and \( D_K \) is a positive constant that depends on \( K \).

This conjecture is consistent with results for other families of random knots [Rensburg and Whittington 91, Deguchi and Tsurusaki 97, Orlandini et al. 98, Rensburg and Rechnitzer 11].

Section 2.1 defines key knot theory concepts and provides some additional context on the problem of enumerating plane curves. Section 2.2 describes the transitions used by our Markov chain. In Section 3, we describe the actual algorithms and prove the main theorem. Section 4 presents the results of experiments which verify the validity of the main theorem as well as explore the structure of large random plane curves and knot diagrams. Finally, in the concluding Section 5 we discuss progress on additional "diagram Markov chains" for different types of diagram objects, and some obstructions.

## 2. Preliminaries and definitions

### 2.1. Definitions

A knot is an embedding \( K : S^1, \rightarrow \mathbb{R}^3 \) of a loop into Euclidean 3-space. Typically, knots are considered up to ambient isotopy, wherein two knots are equivalent if one can be manipulated as a closed loop into the other, without self-intersection. For clarity, we call a specific loop embedding a knot and an equivalence class of knots a knot type. Reidemeister’s theorem [Alexander and Briggs 26, Reidemeister 48] transfers this topological theory into a combinatorial one as follows: A knot diagram of a knot \( K \) is a generic projection of the loop in space to the sphere, together with extra information at each double point indicating where one piece of the loop passes over the other (called crossings), as in Figure 1(a), up to oriented homeomorphisms of the sphere. Then two knots \( K_1 \) and \( K_2 \) are equivalent if and only if their diagrams are related by a sequence of Reidemeister moves, depicted...
in Figure 2. A significant advantage of the diagram view is that most knot invariants, properties of knots which only depend on their knot type, are naturally computed from their diagram representation [Kauffman 87, Freyd et al. 85].

There is a natural projection from knot diagrams to a strict subset of 4-valent planar maps called plane curves; simply replace each crossing with a vertex. A planar map is a (multi-)graph $G$, together with an embedding $i$ into the sphere $S^2$ so that each component of $S^2 \setminus i(G)$ is a topological disk. Necessarily, this means all planar maps are connected. A map is 4-valent if each vertex has degree 4.

Unfortunately, knot diagrams and plane curves are cumbersome to deal with as a result of potential symmetries. To avoid these complications can asymmetricize by marking one edge with a direction. Such objects are called rooted. In particular, each rooted $n$-vertex plane curve corresponds to a unique set of exactly $2^n$ rooted knot diagrams. For a discussion of the techniques and difficulties involved with considering plane curves and knot diagrams with symmetry see [Coquereaux and Zuber 16, Cantarella et al. 16, Valette 16].

It will be useful for computations to consider the following equivalent view of maps. A 4-valent planar map $D$ with $n$-vertices can be viewed as a combinatorial map [Coquereaux and Zuber 16, Chapman 17], i.e. a pair $D = (\sigma, \tau)$ of permutations of $4n$ flags (sometimes called half-edges or arcs). In this view, $\sigma$ is a product of $n$ disjoint cycles of length 4 and $\tau$ is a product of $2n$ disjoint cycles of length 2. Additionally, it is required that the action of the permutation subgroup generated by $\sigma$ and $\tau$ is transitive on the $4n$ flags so the map is connected. Each cycle in $\sigma$ represents a vertex (it permutes the flags attached at each vertex counterclockwise) and each cycle in $\tau$ represents an edge (it involves the two flags that form an edge). The cycles of $\sigma \tau$ correspond to the faces of the map (each permutes the flags of a face clockwise). For 4-valent maps we also have $\sigma^2 \tau$, whose cycles correspond to orientations of link components or Gauss components. Each flag is contained in exactly one vertex, edge, and component.

Given flag $a$, let $e(a)$ be its edge (i.e. cycle in $\tau$), $v(a)$ be its vertex (i.e. cycle in $\sigma$), and $f(a)$ be its face (i.e. cycle in $\sigma \tau$).

Then the condition that $D$ is a planar map is precisely that product $\sigma \tau$ consists of $n+2$ cycles by Euler’s formula. Relaxing this condition and allowing $\sigma \tau$ to consist of $k$ cycles makes $D$ a map on a surface of genus $g = 1 - \frac{k-2}{2n}$. We forbid this for our objects, although in general it is interesting to consider maps on an arbitrary fixed surface $\Sigma$. If $\sigma^2 \tau$ consists of precisely two cycles, each necessarily of length $n$, then $D$ is a plane curve and each cycle in $\sigma^2 \tau$ corresponds to following the single immersed circle in one of its two possible orientations. Notice that a map is guaranteed connected if $\sigma^2 \tau$ consists of only two cycles. Figure 3 shows an example plane curve. Figure 4 shows a random decorated plane curve (knot diagram) and a random decorated 4-valent map (link diagram). The curve condition (that $\sigma^2 \tau$ has precisely 2 cycles) makes plane curves exponentially rare within the class of all 4-valent maps.

We note that if we relax either the planarity or the curve condition, the problem greatly simplifies. 4-valent planar maps themselves are well-understood, owing in part to Schaeffer’s bijection with blossom trees [Schaeffer 97]. This has been used to prove a stunning closed formula for the growth rate of alternating link types [Sundberg and Thistlethwaite 98, Thistlethwaite 98, Zinn-Justin and Zuber 02] as well as precise statistics for hyperbolic volumes of random alternating link diagrams [Obeidin 16]. On the other hand, relaxing planarity and considering curves on arbitrary surfaces leads one to the study of Gauss codes (usually depicted as signed chord or Gauss diagrams), which themselves are counted and well-understood [Nowik 09].

Denote by $\mathcal{K}$ the class of all rooted plane curves indexed by number of vertices, and let $K(t) = \sum_{n=1}^{\infty} k_n t^n$ be its generating function. For a plane curve $D$, let $|D|$ be the number of vertices in $D$ (equivalently, the size of $D$). Then the generating
function can also be written as
\[ K(t) = P(D_2 K_t | D) \]. The asymptotic behavior of the coefficients \( k_n \) is expected [Schaeffer and Zinn-Justin 04, Zinn-Justin and Zuber 09] to be
\[ k_n \sim C_2 n^{\beta - 2}(1 + O(1/\log n)). \] (2–1)

Neither a closed formula for \( k_n \) nor exact values of \( \mu, \gamma \) are known. Conformal field theory arguments suggest [Schaeffer and Zinn-Justin 04, Zinn-Justin and Zuber 09] that
\[ \gamma = -\frac{1 + \sqrt{13}}{6}. \]

Additionally, it is known that \( \mu \) exists [Chapman 17], with the best numerical estimate [Zinn-Justin and Zuber 09] \( \mu \approx 11.416 \pm 0.005 \). This sort of asymptotic growth is similar to that of self-avoiding walks and polygons in the cubic lattice \( \mathbb{Z}^3 \) [Hammersley 61, Madras and Slade 13] (with different constants). Indeed a great many combinatorial objects are known to be counted by sequences which have similar exponential growth with power-law correction; see Flajolet and Sedgewick [09] for many examples with \( n^{-1} \) corrections, and also [Conway and Guttmann 1996] for evidence of a \( n^{-3/2} \) correction in self-avoiding walks).

### 2.2. Shadow Reidemeister moves

In the subsection above, we have defined the set of rooted plane curves that we wish to sample. Unfortunately, as noted above, it is difficult to construct a rooted plane curve. Instead, we will describe a Markov chain that produces new plane curves by performing small local changes. The set of plane curves is closed under these manipulations. Further, any two plane curves are related by a sequence of flat Reidemeister moves, as;

**Theorem 3** (Hass and Scott 94, Graaf and Schrijver 97). Any plane curve can be brought to the trivial figure-eight twist curve seen in Figure 6 by a sequence of

\begin{align*}
\textbf{RI} & \quad \rightarrow \quad \textbf{RII} \\
\textbf{RII} & \quad \rightarrow \quad \textbf{RIII} \\
\textbf{RIII} & \quad \rightarrow \quad \textbf{RI}
\end{align*}


\begin{figure}
\centering
\begin{subfigure}{0.4\textwidth}
\centering
\includegraphics[width=\textwidth]{figure4}
\caption{Random knot diagram}
\end{subfigure}
\begin{subfigure}{0.4\textwidth}
\centering
\includegraphics[width=\textwidth]{figure5}
\caption{Random link diagram}
\end{subfigure}
\caption{A random knot diagram and a random link diagram, each of 100 vertices. Different link components are given different colors. These diagrams were sampled uniformly (using a rejection sampler in the case of the knot diagram) using an interface in pCurve [Ashton et al. 17] to PlanarMap [Schaeffer 99a], and graphics were generated using an orthogonal projection algorithm in pLink, part of SnapPy [Culler et al. 17]. Knot diagrams become exponentially rare as the number of vertices increases [Schaeffer and Zinn-Justin 04, Chapman 17], so are difficult to sample through rejection.}
\end{figure}

\begin{figure}
\centering
\begin{subfigure}{0.2\textwidth}
\centering
\includegraphics[width=\textwidth]{figure5a}
\caption{RI}
\end{subfigure}
\begin{subfigure}{0.2\textwidth}
\centering
\includegraphics[width=\textwidth]{figure5b}
\caption{RII}
\end{subfigure}
\begin{subfigure}{0.2\textwidth}
\centering
\includegraphics[width=\textwidth]{figure5c}
\caption{RIII}
\end{subfigure}
\caption{The three flat Reidemeister moves, RI, RII, RIII which act on plane curves. These are the natural analogs of Reidemeister moves on knot diagrams.}
\end{figure}
flat Reidemeister moves that never increase the size of the plane curve.

This result implies that there exists a sequence of moves between any two plane curves $D$, $N$. Furthermore, it implies that at each intermediate state between $D$ and $N$ the curve has no more vertices than the larger of $D$ and $N$. Chang and Erickson have proven in the arbitrary case that the maximum number of moves required is a small polynomial:

**Theorem 4** (Chang and Erickson 17). The maximum number of non-increasing flat Reidemeister moves required to trivialize a plane curve with $n$-vertices grows as $\Theta(n^{3/2})$. Consequently, it takes no more than $\Theta(n^{3/2})$ moves to transform a curve of $m \leq n$ vertices into a curve of $n$-vertices.

A similar pair of results, if flat Reidemeister I moves are forbidden, was proven by Nowik [Nowik 09]. In this case, the path of curves between a curve with $n$-vertices and its trivialization takes no more than $\Theta(n^2)$ moves and involves no intermediate curves with more than $n+2$ vertices.

These flat Reidemeister moves form the transitions for our Markov chain on $\mathcal{K}$. A key property is that they are all reversible. We define each transition in detail, noting their unique inverses, since such details are necessary for efficient implementation. Let $D$ be a rooted plane curve with root flag $a$.

### 2.2.1. Shadow Reidemeister I loop addition, $RI^+$

See Figure 7 (left) and consider the edge to be oriented from right to left. This defines two flags, $a_1$ and $a_2$, and we take $a_1$ to be the root flag. The addition of a loop on $a_1$ is always possible through the move $RI^+$.

Let $(a_1a_2) = e(a_1)$, and let $a_3, a_4, a_5, a_6$ be four new flags. Then $RI^+(D, a_1)$ is the rooted map produced by deleting edge $e(a_1)$ from $D$, then adding the vertex $(a_3a_4a_5a_6)$ and edges $(a_1a_4), (a_5a_6), (a_3a_2)$. The new root is the flag $a_6$. One can verify that this process is invertible, in particular that:

$$D = RI^-(RI^+(D, a_1), a_6).$$

### 2.2.2. Shadow reidemeister I loop deletion, $RI^-$

See Figure 7 (right). Loop deletion $RI^-$ is possible whenever, given the root flag $a = a_6$, the face $f(a_6)$ is a singleton (i.e. the corresponding face is a monogon).

If this is true, then $RI^-(D, a_6)$ is the rooted map produced from deleting the vertex $v(a_6) = (a_3a_4a_5a_6)$ and the edges $e(a_6) = (a_6a_5), e(a_3) = (a_3a_4), e(a_4) = (a_4a_1)$ from $D$, and adding the edge $(a_1a_2)$. The flags $a_3, a_4, a_5, a_6$ are discarded. The new root is the flag $a_1$. This process is invertible:

$$D = RI^+(RI^-(D, a_6), a_1).$$

### 2.2.3. Shadow Reidemeister II bigon addition, $RII^+$

See Figure 8 (left). Bigon addition $RII^+$ requires a second flag $b \in f(a)$. To simplify our implementation and forthcoming detailed balance arguments we furthermore require that $b$ be different from the root flag.
a, as we could obtain the same result of \( b = a \) by two sequential RI\(^+\) loop additions. Let \( a = a_1 \) and \( b = a_3 \).

The rooted map \( \text{RII}^+(D, a_1, a_3) \) is constructed from \( D \) as follows. Delete the edges \( e(a_1) = (a_1a_2) \) and \( e(a_3) = (a_3a_4) \) from \( D \). Add eight new flags \( a_5, a_6, a_7, a_8, a_9, a_{10}, a_{11}, a_{12} \). Add the vertices \( (a_6a_9a_2a_7) \) and \( (a_5a_9a_{12}a_{11}) \). Insert the edges \( (a_5a_9), (a_3a_{10}), (a_7a_8), (a_5a_6), (a_{11}a_{12}), \) and \( (a_9a_{11}) \). The new root is the flag \( a_6 \). This process is invertible:

\[
D = \text{RII}^-(\text{RII}^+(D, a_1, a_3), a_6).
\]

### 2.2.4. Shadow Reidemeister II bigon deletion, RI\(^-\)

See Figure 8 (right). Bigon deletion \( \text{RII}^- \) is possible provided the root flag \( a = a_6 \) is on a face \( f(a_6) \) which consists of precisely two flags (i.e., a bigon).

Additionally, it is required that the two exterior faces which are merged by the transition be distinct; this is required to preserve connectedness and genus. Indeed, Suppose that \( D \) is a curve embedded on an orientable surface of genus \( g \), so that \( v(D) - e(D) - f(D) = 2g - 1 \), but that the faces to be merged are not distinct. The number of vertices and edges decrease by 2 and 4 respectively by a RI\(^-\) operation, as usual, but the number of faces now remains fixed. This implies that the produced curve lives in either a surface of one fewer genus, or if the original map was embedded on the sphere, two disjoint spheres. Furthermore, it is required that neither of the two faces to be merged are monogons, as we forbid the inverse of this in the RI\(^+\) operation.

The rooted map \( \text{RII}^-(D, a_6) \) is constructed from \( D \) as follows. Delete the vertex \( v(a_6) = (a_6a_{10}a_9a_7) \) and the edges \( e(a_9) = (a_7a_9), e(a_{10}) = (a_{10}a_{11}), e(a_7) = (a_7a_8) \) and \( e(a_9) = (a_9a_5) \). Delete the vertex \( v(a_5) = (a_5a_{12}a_{11}) \) and the edges \( e(a_{12}) = (a_1a_{12}) \) and \( e(a_{11}) = (a_1a_{11}) \). Add the edges \( (a_1a_2) \) and \( (a_3a_4) \). The flags \( a_5, a_6, a_7, a_8, a_9, a_{10}, a_{11}, a_{12} \) are discarded. The new root is the flag \( a_1 \). This process is invertible:

\[
D = \text{RII}^+(\text{RII}^-(D, a_6), a_1, a_3).
\]

### 2.2.5. Shadow Reidemeister III triangle flip, RIII

See Figure 9. Triangle flipping RIII is possible provided the root flag \( a = a_8 \) lies on a face \( f(a_8) \) with precisely three flags, all of whom are contained in different vertices (i.e., a nondegenerate triangle).

The rooted map \( \text{RIII}(D, a_8) \) is constructed from \( D \) as follows. Say that \( v(a_8) = (a_1a_2a_7a_8), e(a_8) = (a_9a_5), e(a_7) = (a_7a_8), \), \( v(a_6) = (a_5a_{11}a_{12}a_6), \) and \( v(a_9) = (a_3a_9a_{10}a_4) \). Delete vertices \( v(a_7), v(a_9), v(a_6) \) and edges \( e(a_7), e(a_9), \) and \( e(a_{10}) \). Insert vertices \( (a_6a_9a_{11}a_1), (a_2a_{10}a_7a_3), (a_4a_{12}a_9a_5) \) and edges \( (a_6a_9), (a_7a_{12}), \) and \( (a_{10}a_{11}) \). The new root is the flag \( a_{11} \). This process is invertible:

\[
D = \text{RIII}^+(\text{RIII}(D, a_8), a_{11}).
\]

### 3. Markov chain

The five flat Reidemeister moves described in the previous section allow us to define a Markov chain on the space plane curves. That the chain can move between any two given plane curves follows immediately from Theorem 3.

#### 3.1. A Boltzmann Markov chain on plane curves

Our Markov chain sampler for plane curves will have a stationary Boltzmann distribution; one which samples curves of different sizes with different probabilities but is uniform on curves of fixed size. In other words, for \( 0 \leq z \leq \mu^{-1} \) an arbitrary parameter, it has stationary distribution such that a curve \( D \) has probability

\[
\pi(D) \propto z^{|D|}.
\]

The parameter \( z \) is then used to control the mean size of sampled curves, and smaller values of \( z \) will concentrate the sampler on diagrams of fewer crossings.

Let \( p_1, p_2, p_3 > 0 \). These numbers correspond to the probabilities of performing, respectively, a Reidemeister I, II, or III move. Consequently, we must have \( p_i > 0 \).
Further, we must also have \(1-(p_1+p_2+p_3)>0\), as this quantity will correspond to the probability of selecting a new root flag. Let \(D_i\) be the input rooted plane curve with \(n\)-vertices and root flag \(a\) and perform one of the following six subprocedures with different probabilities. If a move fails then set \(D_{i+1} := D_i\).

[0] Re-rooting, with probability \(1-(p_1+p_2+p_3)\). Given the rooted diagram \(D_n\), forget the root and select a new root \(b\) for \(D_{i+1}\) from the \((4|D|)/(\aut D_i)\) choices. The probability that this transition succeeds is \(1-(p_1+p_2+p_3)\). Note that \(\aut D_i\) need not be calculated for this operation, as it is equivalent to choose one flag from the old rooted curve.

[1+] Loop addition, with probability \(p_1/2\). Sample \(0 \leq \alpha < 1\) and fail immediately if \(\alpha > z\). Return \(D_{i+1} := \text{RI}^+(D_i,a)\). The probability that this transition succeeds on any \(n\)-crossing plane curve \(D\) is \(zp_1/2\).

[1−] Loop deletion, with probability \(p_1/2\). Provided \(f(a)\) is a loop, return \(D_{i+1} := \text{RI}^-(D_i,a)\). The probability that this transition succeeds if root flag \(a\) has \(f(a)\) a loop in \(D\) is \(p_1/2\).

[2+] Bigon addition, with probability \(p_2/2\). Sample \(0 \leq \alpha < 1\) and fail immediately if \(\alpha > z^2\). The flag \(a\) lies along a face of \(d\) edges; provided \(d \neq 1\) (otherwise fail), uniformly sample the integer \(k\) between 1 and \(d-1\). The flag \(a' = (\sigma^k)(a)\) is a distinct flag along the same face as \(a\). Then return \(D_{i+1} := \text{RII}^+(D_i,a,a')\). The probability that this transition succeeds on any given additional flag \(a'\) along the root \(d\)-face is

\[
\frac{z^2p_2}{2(d-1)}.
\]

[2−] Bigon deletion, with probability \(p_2/2\). Fail if the flag \(a\) does not lie along a bigon, either of the faces to be merged are monogons, or if the faces to be merged are not distinct. The size \(d\) of the face which would be produced by bigon deletion is the sum \(|f(\tau\sigma(a))| + |f(\sigma^2\tau(a))| = d\). Sample \(0 \leq \beta < 1\) uniformly and fail if \(\beta > (d-1)^{-1}\). Otherwise, return \(D_{i+1} := \text{RII}^-(D_i,a)\). The probability that this transition succeeds provided a valid site for this move is

\[
\frac{p_2}{2(d-1)}.
\]

[3] Triangle flipping, with probability \(p_3\). Fail if the flag \(a\) does not lie along a nondegenerate triangle. Otherwise, return \(D_{i+1} := \text{RIII}(D_i,a)\). The probability that this transition succeeds assuming the root lies along a nondegenerate triangle is \(p_3\).

We will prove that in the limiting distribution the probability that any given \(n\)-crossing rooted plane curve \(D\) is chosen is

\[
\pi(D) = \frac{z^n}{K(z)},
\]

(3-2)

where \(K(z)\) is the value of the generating function \(K(t)\) at \(z\) so if \(K(z)\) converges to a number, \(\pi(D) \propto z^n\) (this happens provided \(z < \mu^{-1}\)). It follows that if we ignore the roots of the sampled diagrams in order to sample \textit{unrooted} diagrams, the probability of an unrooted diagram \(\tilde{D}\) being sampled is

\[
\pi(\tilde{D}) = \frac{4n}{K(z)\aut \tilde{D}} z^n.
\]

(3-3)

We note that as the probability that the automorphism group of a plane curve is trivial tends exponentially quickly to 1 [Chapman 17], the typical probability of an unrooted diagram \(\tilde{D}\) will be \(\pi(\tilde{D}) \propto 4nz^n\).

This Markov chain is ergodic as it satisfies the following three properties;

1. It is connected: It is possible to get from any one plane curve to another in a finite number of transitions. Provided \(p_1, p_2, p_3 > 0\) it is possible to get between any two pairs of unrooted curves (by Theorem 3); provided \(p_1 + p_2 + p_3 < 1\) it is guaranteed that any flag may be chosen as the root.
2. It is aperiodic: Since at each step there is a non-zero probability that the transition fails, there is no periodicity in the Markov chain.
3. The chain satisfies detailed balance: For any two curves \(D\) and \(N\), the transition probabilities \(P\) and curve probabilities \(\pi\) satisfy

\[
P(D \rightarrow N)\pi(D) = P(N \rightarrow D)\pi(N).
\]

This last point requires the most care and we discuss it below, with more details in Appendix A.

The fundamental theorem of Markov chains then yields the following result.

**Theorem 1** (Slightly restated). This Markov chain satisfies detailed balance. Furthermore, if \(p_1, p_2, p_3 \neq 0, (p_1 + p_2 + p_3) \neq 1,\) and \(z < \mu^{-1}\) the chain is ergodic with stationary distribution,

\[
\pi(D) = \frac{z^{|D|}}{\sum_k k!z^k} \propto z^{|D|}.
\]

The proof of this result is primarily routine. We have omitted some details which can be found in Appendix A.

**Proof.** We will begin by assuming that

\[
\pi(D) = \frac{z^{|D|}}{\sum_k k!z^k} \propto z^{|D|},
\]

(3-4)
and proving that detailed balance holds with this hypothesis. Notice that $z$ has been chosen sufficiently small so that the denominator converges [Chapman 17]. In all cases the denominator is the same and a common factor in the calculations that follow, so we omit it.

Let $D$ be a rooted plane curve of $n$-vertices and $a$ be the root flag in $D$. Observe first that the three pairs of reversing transitions $(RI^+,RI^-),(RII^+,RII^-),$ and $(RIII, RIII)$ all change the number of vertices by distinct complementary amounts; hence any two diagrams can be related by at most one pair of these transitions. Notice that if the vertex counts agree, then a pair of diagrams may be related by re-rooting. The main concern now is to prove the detailed balance holds with this hypothesis. Notice that in practice, there is no need between consecutive transitions to re-root more than once. In our experiments, we choose the five flat Reidemeister moves each with equal probability by taking $p_1 = 2/5, p_2 = 2/5$ and $p_3 = 1/5$.

### 3.2. Flat histogram sampling by Wang-Landau state density estimation

Our simulations in Section 4.1.1 show that the output curve sizes have high variance and change rather drastically with the parameter $z$. There are several different approaches that one might use to overcome this—such as multiple Markov chain Monte Carlo [Geyer 91, Orlandini 98]. We have, instead, chosen the flat histogram method invented by Wang and Landau [01]. The transition probabilities are chosen so that the number of objects sampled at size $n$ is approximately equal to the number of objects of $n$ and is ergodic. Furthermore, the probability of sampling any plane curve $D$ with $m \leq L$ crossings is,

$$
\pi(D) = \frac{z^m}{\sum_{z=1}^{L} k_z z^m} \propto z^m.
$$

**Proof.** This follows from Theorem 3 and the proof of the previous theorem.

At this stage we are free to choose $p_1, p_2, p_3$. It is not obvious, how they should be chosen to produce the most efficient sampling method. In practice, we simplified the problem by choosing $p_1 + p_2 + p_3 = 1$ and then applying a re-rooting move after each step. The ergodicity of this chain follows by very similar arguments.

**Corollary 6.** For $p = (p_1, p_2, p_3)$ with $p_1 + p_2 + p_3 = 1$, consider the Markov chain which differs from the prior by, before and after each transition step, uniformly randomly re-rooting the state curve. Setting $p_1 + p_2 + p_3 = 1$ eliminates the re-rooting transition. Then this Markov chain is ergodic.

The proof is quite standard, we give it in Appendix A. Notice that in practice, there is no need between consecutive transitions to re-root more than once. In our experiments, we choose the five flat Reidemeister moves each with equal probability by taking $p_1 = 2/5, p_2 = 2/5$ and $p_3 = 1/5$.
the Markov chain adjusting transition properties until the above condition approximately holds. These final transition properties are then used for a MCMC sampler.

We note that one could eschew the tuning phase and instead use either exact or asymptotically approximate values of $k_n$ when available. Setting $g_n = k_n$ when $k_n$ is known will likely improve the flatness of the sampling histogram, but depends on the existence of known values $k_n$; we ultimately take advantage of this in our later experiments. Determining $g_n$ by expected asymptotic values of $k_n$ also depends on the existence of known (or conjectural) asymptotic counts. We hope to generalize the sampler in future work to classes where these counts are not known, and so providing the framework here simplifies this. Additionally, this comes with the additional caveat that asymptotic growth rates are only reliable in the large $n$ limit. Indeed, in our case the slow decay of the conjectured $O(1/\log n)$ error term suggests that $n$ may need to be larger than the objects we can yet sample before the error grows sufficiently small. However, it is not unreasonable to use the conjectured asymptotic form to bootstrap the tuning phase: Initializing $g_n$ to their asymptotic estimates rather than 0 should speed up convergence provided the estimates are close.

There are three advantages to this strategy over Boltzmann MCMC sampling:

1. Mixing of the Markov chain is more efficient: Rather than get caught up in one small range of sizes (in part due to the local minimum bottleneck; see Section 4.1.1), with Wang-Landau tuning the Markov chain moves frequently between all sizes, see for instance the size-series in Figure 10. This improves the independence of two samples of the same size as all of the structure is “erased” when the Markov Chain moves down to the smaller states.

2. Guarantee of sampling objects of given size: The Markov chain produces objects of sizes up to $L$ with non-zero probability, so given enough tuning and enough random samples, a sufficient number of objects of a desired size will be sampled.

3. Approximate enumeration: Transition probabilities found during the tuning step are directly related to the counts of objects of each size. We use these data to estimate the number $k_n$ in Section 4.1.2.

Rather than depending on a single parameter $z$, sampling via a Wang-Landau implementation requires a data structure $(\ell, L, G)$, where:

- $\ell$ is the minimum size of plane curves. To ensure ergodicity, we always have $\ell = 1$, although further results on plane curves may allow $\ell$ to vary (possibly in terms of $L$) while still guaranteeing ergodicity.
- $L$ is the maximum size of plane curves.
- $G = \{G_{\ell}\}_{\ell = \ell}^L$ is a vector approximate enumeration data in the following sense: If $g_n = e^{\delta_n}$, then $g_n/g_{n-1} \approx k_n/k_{n-1}$. Since we do not know $k_n$ for $n \geq 28$, these data are gathered via a tuning phase (described in Section 3.3 below).

---

![Figure 10. A time-series plot of the size sampled planar curves. This shows that the chain regularly visits curves of very different sizes.](image-url)
Given the approximate enumeration data $G_n = \log (g_n)$, define probabilities
\[
\text{tp}(n,m) = \min\{1, \exp \{G_n - G_m\}\} = \min\{1,g_n/g_m\} \approx k_n/k_m,
\] (3-8)
unless $m < \ell$ or $m > L$ in which case $\text{tp}(n,m) = 0$.

Wang-Landau flattened MCMC sampling then works as follows. The implementation which follows is largely the same as the Boltzmann implementation, with each transition instead required to pass a check of probability $\min\{1,g_n/g_{n+k}\}$, where $n$ is the size of the input curve and $k$ is the change in size of the transition operation. Let $p_1, p_2, p_3 > 0$ and $(p_1 + p_2 + p_3) < 1$ and let $D_i$ be the input rooted plane curve with $n_i$ vertices and root flag $a$ and perform one of the following six moves with different probabilities. If a move fails then set $D_{i+1} := D_i$.

[0] Re-rooting, with probability $1-(p_1 + p_2 + p_3)$. Given the rooted diagram $D_i$, forget the root and select a new root $b$ for $D_{i+1}$ from the $(\text{aut}D_i)/(4|D_i|)$ choices. The probability that this transition is chosen and succeeds is $1-(p_1 + p_2 + p_3)$.

[1'] Loop addition, with probability $p_1/2$. Sample $0 \leq \alpha < 1$ and fail immediately if $\alpha > \text{tp}(n_i,n_{i+1})$. Return $D_{i+1} := \text{RI}^+(D_i,a)$. The probability that this transition is chosen and succeeds on an $n$-crossing rooted plane curve is
\[
\text{tp}(n,n+1) \frac{p_1}{2} = \min\left\{1, \frac{g_n}{g_{n+1}} \right\} \frac{p_1}{2}. \tag{3-9a}
\]

[1] Loop deletion, with probability $p_1/2$. Sample $0 \leq \alpha < 1$ and fail immediately if $\alpha > \text{tp}(n_i,n_{i-1})$. Provided $f(a)$ is a loop, return $D_{i+1} := \text{RI}^-(D_i,a)$. The probability that this transition is chosen and succeeds is $f(a)$ is a loop is
\[
\text{tp}(n,n-1) \frac{p_1}{2} = \min\left\{1, \frac{g_n}{g_{n-1}} \right\} \frac{p_1}{2}. \tag{3-9b}
\]

[2'] Bigon addition, with probability $p_2/2$. Sample $0 \leq \alpha < 1$ and fail immediately if $\alpha > \text{tp}(n_i,n_{i+2})$. The flag $a$ lies along a face of $d$ edges; provided $d \neq 1$ (otherwise fail), uniformly sample the integer $k$ between 1 and $d - 1$. The flag $a' = (\sigma^k,\tau^j)$ is a distinct flag along the same face as $a$. Then return $D_{i+1} := \text{RI}^+(D_i,a,a')$. The probability that this transition is chosen and succeeds on an $n$-crossing plane curve with an given cofacial flag $a'$ is
\[
\text{tp}(n,n+2) \frac{p_2}{2(d-1)} = \min\left\{1, \frac{g_n}{g_{n+2}} \right\} \frac{p_2}{2(d-1)}. \tag{3-9c}
\]

[2] Bigon deletion, with probability $p_2/2$. Sample $0 \leq \alpha < 1$ and fail immediately if $\alpha > \text{tp}(n_i,n_{i-2})$. Fail if the flag $a$ does not lie along a bigon or either of the faces to be merged is a monogon. The size $d$ of the face which would be produced by bigon deletion is the sum $|f((\tau^j\sigma^k))| + |f((\sigma^j\tau^k))| = d$. Sample $0 \leq \beta < 1$ uniformly and fail if $\beta > (d-1)^{-1}$. Otherwise, return $D_{i+1} := \text{RI}^-(D_i,a)$. The probability that this transition is chosen and succeeds provides a valid site for this move is,
\[
\text{tp}(n,n-2) \frac{p_2}{2} = \min\left\{1, \frac{g_n}{g_{n-2}} \right\} \frac{p_2}{2(d-1)}. \tag{3-9d}
\]

[3] Triangle flipping, with probability $p_3$. Fail if the flag $a$ does not lie along a nondegenerate triangle. Otherwise, return $D_{i+1} := \text{RIII}(D_i, a)$. The probability that this transition is chosen and succeeds if a lies along a nondegenerate triangle is $p_3$.

### 3.3. Wang-Landau tuning

Before sampling, we have to gather data for $e^{\theta G_n} = g_n$ (the approximate enumeration) via a tuning algorithm with parameters $\ell$, the smallest size diagram to allow in the sample space (always in this article $\ell = 1$, as otherwise it is not necessarily clear if the Markov chain is ergodic), $L$, the largest size diagram in the sample space, $\epsilon$, which describes the desired flatness of the sampling histogram, and $\Delta$, a threshold for flatness of a histogram of occurrences.

A starting point $D_0$ in the sample space of diagrams is chosen; our algorithm starts with the figure-eight diagram in Figure 6. The values $G_n$ are initialized to 0. Finally, a scaling factor $F$ is initialized; we start it at $F = 1$.

The algorithm then proceeds as follows.

1. If $F < \epsilon$, terminate.
2. A histogram $H = (H_n)_{n=\ell}^L$ of bins $\ell$ to $L$ inclusive is initialized empty. This histogram will track the occurrences of diagrams of size $n$ at each step of the Markov chain.
3. Step, via the Wang-Landau weighted algorithm described above, producing $D_{i+1}$ from the current $D_i$.
4. Every $S_0$ steps, increment $H_{|D_{i+1}|}$ by 1, and increment $G_{|D_{i+1}|}$ by $F$.
5. Every $S_1$ steps, check if the histogram is $\Delta$-flat, i.e., check if
\[
\min H \frac{\sum_{i=\ell}^L H_i}{L - \ell} > \max H \frac{1}{1 + \Delta}. \tag{3-10}
\]

If so, let $F := F/2$ and proceed with step (1). Otherwise repeat step (3).
The numbers $S_0$, $S_1$ are somewhat arbitrary, however $S_1$ should be chosen to allow sufficient time for the chain to diffuse over all sizes. We note that, especially for large spreads of $\ell$ and $L$, the tuning phase may be time-consuming. As the algorithm is tuning and $G$ is being updated, the chain is not ergodic as it does not satisfy the detailed balance condition. However, during the tuning phase the quantities $g_m$ approach $k_m$ (up to a multiplicative constant), so that $g_m/g_l$ approaches $k_m/k_l$. At any given point, one may cease updating $G$ and use the resulting fixed probabilities. This chain will satisfy detailed balance and so be ergodic. This tuned $G$ data may then be reused for a number of further simulations without recalculation.

**Theorem 2.** Let $L \in \mathbb{N}$ and $D$ be a plane curve with $1 \leq n \leq L$ vertices and let $g_n$ be fixed. The Markov chain described in Section 3.2 has stationary distribution given by

$$\pi(D) \propto \frac{1}{g_n}.$$  

While curves of different sizes are sampled with different probabilities, curves of a given size are sampled uniformly.

As was noted in the introduction, the probability of sampling any curve of $n$-crossings is then proportional to $\frac{k_n}{g_n}$. Hence when $g_n$ closely approximates $k_n$, this ratio is approximately constant, and if we use this chain to generate samples, the resulting histogram is approximately flat. To be more precise, if $s_n$ denotes the number of samples of size $n$, then $s_n \frac{k_n}{g_n} \approx s_l \frac{k_l}{g_l}$. This is illustrated by our sample histogram in Figure 11.

**Proof.** We will begin by assuming that

$$p_1, p_2, p_3 > 0, (p_1 + p_2 + p_3) < 1,$$

and $\ell = 1$, the Markov chain can reach all plane curves (as all plane curves can be changed through a crossing-non-increasing pathway to the curve with one crossing). Hence in this case, the Markov chain is ergodic.

By Corollary 6, we are able to simplify the Markov chain by re-rooting between steps, and only using the five Reidemeister transition operations as we did in the Boltzmann case. Again, in our simulations

![Figure 11](https://example.com/figure11.png)

**Figure 11.** (Left) Distribution of plane curve sizes from a run of the Wang-Landau sampler. The sample histogram flatness is $\max\{0.97945, 1 - (1.024075 - 1)\} = 97.94\%$. (Right) Distribution of plane curve sizes from two independent halves of the Wang-Landau sampler data, before aggregation.
(detailed in the next section) we chose \((p_1, p_2, p_3) = (2/5, 2/5, 1/5)\).

4. Simulations and data

We implemented both MCMC samplers in C++. Plane curves are stored as combinatorial maps; a collection of vertices, edges, and flags with bidirectional references between flags and their vertices, as well as flags and their edges. At each step, an edge is selected from the diagram at random; this takes \(O(1)\) time, and the parameter \(0 < \alpha < 1\) is sampled uniformly at random. Both of the RI moves, as well as the RIII move take constant time. The RII⁺ move requires an extra random number \(0 \leq \gamma < 1\) which determines the second flag for the transition and is performed in constant time. The RII⁻ move requires both the sampling of the additional number \(0 \leq \beta < 1\) as well as a count of the face sizes diagonal to the bigon. A plane curve has average face degree strictly increasing and limiting on 4, so counting a face size requires a constant number of operations on average.

For low numbers \(n\) of crossings, it is also possible to sample plane curves uniformly through rejection sampling. A single sample is produced by sampling 4-valent maps uniformly until a plane curve is obtained. The maps are sampled via Gilles Schaeffer’s bijection with blossom trees [Schaeffer 97] using his PlanarMap software [Schaeffer 99a, 99b]. The rejection step is simple, but plane curves are exponentially rare [Schaeffer and Zinn-Justin 04], making this approach ineffective even for relatively small sizes: On a quad core 3.4Ghz Intel i5-75000 machine, sampling \(10^5\) 10-crossing curves takes 4.9 seconds, but sampling the same number of 100-crossing curves takes 712.6 seconds. For comparison, it only takes 21.9 seconds to sample \(10^5\) 100-vertex 4-valent maps.

In this section, we examine data from our simulations. First, we examine the distributions of plane curve sizes that our implementations produce. Then, we check how well our Wang-Landau implementation converges to the uniform distribution across fixed sizes by comparing statistics to the rejection sampler. The data of these sections are based on the following sampler runs:

1. **Wang-Landau (WL)**. We tuned Wang-Landau Markov chain to \(f < 10^{-8}\) with histogram flatness threshold \(\Delta = 0.01\), which took approximately 500 minutes. After verifying that our tuning scheme provides approximate enumerations close to known enumerations \(k_n\) of small plane curves (c.f. Section 4.1.2), we updated our tuning data so that \(g_n = k_n\) where \(k_n\) is known.

We gathered 10 independent, equally sized sets of data for diagrams of size \(1 \leq n \leq 500\) with \(10^5\) steps between each sample using the same tuning data. In total, we drew a total of \(2 \times 10^7\) samples. Afterwards, we aggregated all of the data from these independent runs. Each independent sampling run took 17.8 hours. The sampled size probability distribution for this run is presented in Figure 11. The minimum number of samples for any size is \(3.9178 \times 10^4\).

2. **Rejection**. Using a rejection sampler for plane curves, we gathered \(10^4\) samples of plane curves with \(n\)-vertices, for each \(n = 5m\) from 5 to 100. This took approximately 40 minutes.

3. **All 4-valent maps**. Using a uniform sampler for all 4-valent maps, we gathered precisely \(10^4\) samples of 4-valent maps with \(n\)-vertices, for each \(n = 5m\) from 5 to 100. This took approximately 30 seconds.

Finally, we examine how our Wang-Landau sampler augmented to sample knot diagrams compares to the rejection sampler, as another check on the theoretical limiting distribution and our implementation.

4.1. Size distributions

We first examine the sample histograms of the Boltzmann and Wang-Landau samplers. This serves several purposes: First, as we are unable to sample diagrams of given fixed size, we would like to know how frequently we will sample a particular size using these methods. Second, in order to avoid correlated samples we would like our Markov chain to explore the full range of lengths frequently. Last, we can use comparisons of the sampled size distribution to better understand the counting sequence of plane curves.

4.1.1. Boltzmann sampler implementation and the Boltzmann parameter \(z\)

The MCMC sampler approximating the Boltzmann distribution on plane curves (described in Section 3.1) samples from a distribution,

\[
\pi(D) \propto z^{|D|},
\]

where the parameter \(z\) affects the size of plane curves produced. Hence the probability of sampling any plane curve of size \(n\) is proportional to \(k_n z^n\). As noted above, we choose \(z < 1/\mu\) and so by Equation 2-1 this probability is asymptotic to \((\mu z)^n n^{-2}\). Note that \(\gamma\) is...
expected to be negative so any choice of 
$z < \mu^{-1} \approx 0.0876$ will not, a priori produce a finite local maximum.

To observe this we ran a number of experiments sampling $10^6$ plane curves of a maximum size of 200 crossings with varying $z$. These data produce the approximate size distributions of Figure 12. This figure implies that it is difficult to pick $z$ to obtain samples at large size while still sampling many objects of small size.

We note that we want our algorithm to return to small sizes on a regular basis. First, returning to small sizes “erases” the entire object before producing a new sample. Second, the best known result on ergodicity relies on paths through small plane curves. Not enough is known about the connectivity of the space of plane curves to alleviate these concerns, providing strong justification for using the Wang-Landau sampler variant instead.

4.1.2. Wang-Landau implementation

In comparison with the MCMC Boltzmann sampler, the tuning phase of the Wang-Landau sampler ensures that the size distribution sampled is actually approximately flat. Figure 13 demonstrates how values of $g_n$ approach the exact numbers of rooted plane curves,

Figure 12. Histogram of samples from various MCMC runs, with different $z$-values. The maximum size plane curve was 200 vertices. The mixing time was $10^3$ steps, and a total of $10^6$ samples were drawn. The run for $z = 0.05$ took 65 seconds to complete, the run for $z = 0.1$ took 93 seconds, and run time generally increased with $z$.

Figure 13. As the tuning phase proceeds, the values $G_n = \log g_n$ converge to $G_{\text{final}}$. We also observe that $G_{\text{final}} \approx \log k_n$ for available exact enumeration data, $n \leq 27$. 

Convergence of $G$
As mentioned, the Wang-Landau algorithm tuning step provides an estimation of ratios in the counting sequence for plane curves. We can use these data to provide approximations to the numbers of curves of given sizes. Using the tuning data for the run above ($\ell = 1, L = 500, f < 10^{-8}, \Delta = 0.01$) we obtained approximate counts for $n = 1$ to $n = 27$ and can compare the approximations to the precise counts from [Zinn-Justin and Zuber 09] in Table 1. All approximate counts are within 0.004 of their exact value.

We are able to obtain estimates for the unknowns $\mu$ and $\gamma$ in the predicted asymptotic growth formula $k_n \sim C \mu^n n^{-2}$ from Wang-Landau $g_n$ data. We attempted to use simple ratio estimates $r_n = g_{n+1}/g_n \sim \mu \left( 1 + \frac{\gamma - 2}{n} \right)$, however the results are extremely noisy. Instead we used linear regression to fit to the model

$$\log g_n = \log C + n \log \mu + (\gamma - 2) \log n$$

Since we expect the $g_n$ data to be noisier for larger $n$ we fitted the above linear form to a subset of the data $\{g_n | 10 \leq n \leq n_{\text{max}}\}$. We then varied $n_{\text{max}}$ to get a rough estimate of corrections to the above asymptotic form. The resulting estimates (as functions of $n_{\text{max}}$) are shown in Figure 14. These results are consistent with earlier estimates [Zinn-Justin and Zuber 09] of $\mu \approx 11.416$ and $\gamma = -\frac{1 + \sqrt{13}}{6} \approx -0.768$.

### 4.2. Face degrees in plane curves

In this section we seek statistics which distinguish plane curves from all 4-valent maps. A simple class of statistics to gather from random maps are vertex and

| n | WL estimated $k_n$ | Exact $k_n$ | % Error |
|---|---------------------|-------------|---------|
| 1 | 2                   | 2           | 0       |
| 2 | 8                   | 8           | -4.07 \times 10^{-2} |
| 3 | 42.01               | 42          | 3.49 \times 10^{-2} |
| 4 | 260.15              | 260         | 5.61 \times 10^{-2} |
| 5 | 1,796.5             | 1,796       | 2.79 \times 10^{-2} |
| 6 | 13,404.48           | 13,396      | 6.33 \times 10^{-2} |
| 7 | 1.06 \times 10^3    | 1.06 \times 10^3 | 5.25 \times 10^{-2} |
| 8 | 8.71 \times 10^3    | 8.71 \times 10^3 | 6.43 \times 10^{-2} |
| 9 | 7.42 \times 10^3    | 7.42 \times 10^3 | 3.99 \times 10^{-2} |
| 10 | 6.5 \times 10^3    | 6.5 \times 10^3 | 6.25 \times 10^{-2} |
| 11 | 5.82 \times 10^3    | 5.83 \times 10^3 | -4.2 \times 10^{-2} |
| 12 | 5.32 \times 10^3    | 5.32 \times 10^3 | 7.57 \times 10^{-2} |
| 13 | 4.95 \times 10^3    | 4.94 \times 10^3 | 0.12 |
| 14 | 4.66 \times 10^3    | 4.65 \times 10^3 | 0.16 |
| 15 | 4.44 \times 10^3    | 4.43 \times 10^3 | 0.16 |
| 16 | 4.28 \times 10^3    | 4.27 \times 10^3 | 0.12 |
| 17 | 4.16 \times 10^3    | 4.16 \times 10^3 | 8.45 \times 10^{-2} |
| 18 | 4.08 \times 10^3    | 4.08 \times 10^3 | 0.1 |
| 19 | 4.04 \times 10^3    | 4.03 \times 10^3 | 0.19 |
| 20 | 4.02 \times 10^3    | 4.02 \times 10^3 | 0.18 |
| 21 | 4.04 \times 10^3    | 4.02 \times 10^3 | 0.3 |
| 22 | 4.07 \times 10^3    | 4.06 \times 10^3 | 0.25 |
| 23 | 4.12 \times 10^3    | 4.11 \times 10^3 | 0.24 |
| 24 | 4.19 \times 10^3    | 4.18 \times 10^3 | 0.19 |
| 25 | 4.29 \times 10^3    | 4.28 \times 10^3 | 0.3 |
| 26 | 4.41 \times 10^3    | 4.39 \times 10^3 | 0.38 |
| 27 | 4.54 \times 10^3    | 4.53 \times 10^3 | 0.25 |
face degrees. Plane curves, as a subclass of 4-valent planar maps, only ever have vertex degree 4, so only face statistics are nontrivial. Euler’s formula implies that the average face degree for any 4-valent map of \( n \)-crossings is \( 4n/(n + 2) \), so this also cannot distinguish plane curves from its superclass. However, we will see that the distribution of face degrees differs.

### 4.2.1. Face degree probabilities

We check the counts of faces of fixed degree which appear (for a curve of \( n \)-crossings, this takes \( O(n) \) time to compute as all plane curves have 4\( n \) flags, each of which needs only be visited once). These quantities are expected to exhibit linear growth, in agreement with the results for a large number of map classes [Liskovets 99]. In fact, it is known:

**Theorem 7.** Let \( k \geq 1 \), and let \( p_{k,n} \) denote the probability that an arbitrary face of a random plane curve of \( n \)-crossings has degree-\( k \). Namely, notice that \((n + 2)p_{k,n}\) is the expected number of degree-\( k \) faces in a random plane curve of \( n \)-crossings. Then

\[
1 > \limsup_{n \to \infty} p_{k,n} \geq \liminf_{n \to \infty} p_{k,n} > 0. \tag{4–3}
\]

**Proof.** Certainly, \( 0 \leq p_{k,n} \leq 1 \) for all \( n, k \) as they denote probabilities; furthermore, \( \sum_{k=1}^{n} p_{k,n} = 1 \). The pattern theorem for plane curves [Chapman 17] says that, for any prime substructures \( T_k \) containing a \( k \)-gon, there are constants \( c_k > 0, 1 > d_k > 0 \) and \( N \geq 0 \) so that for all \( n \geq N \) the probability that an arbitrary plane curve of size \( n \) contains more than \( c_k n \) copies of \( T_k \) is at least \( 1 - d_k^n \).

So for \( n \geq N \), \((n + 2)p_{k,n} > (1 - d^n)c_k n\). Solving for \( p_{k,n} \) and passing to \( \liminf \) yields,

\[
\liminf_{n \to \infty} p_{k,n} \geq \liminf_{n \to \infty} (1 - d^n)c_k \frac{n}{n + 2} = c_k. \tag{4–4}
\]

That \( 1 > \limsup_{n \to \infty} p_{k,n} \) for any \( k \) follows from that for \( \ell \neq k \) the existence of a \( \ell \)-gon lowers the number of faces which may be \( k \)-gons. That all \( \liminf_{n \to \infty} p_{k,n} > 0 \) yields the result. \( \square \)

The following proposition summarizes the results we will use for planar 4-valent maps.

**Theorem 8** (Follows from [Gao and Richmond 94, Liskovets 99]). As the number of vertices tends to infinity, the expected fraction of faces of degree-\( k \) in a random 4-valent map is,

\[
\frac{1}{k} [y^k] \left( (1/3)(1 + y/2)^{-\frac{1}{2}}(1 - 5y/6)^{-\frac{1}{2}} \right). \tag{4–5}
\]

**Proof.** This is a rephrasing of selected results in [Gao and Richmond 94, Liskovets 99] in the language of 4-valent maps. Let \( q_{k,m} \) be the probability that the root vertex of an arbitrary planar map of \( m \) vertices has degree-\( k \), and let \( q_k = \lim_{m \to \infty} q_{k,m} \). These limits exist and Theorem 1 of [Gao and Richmond 94] says that their generating series is,

\[
\sum_{k \geq 0} q_k y^k = (1/12)(1 + y/2)^{-\frac{1}{2}}(1 - 5y/6)^{-\frac{1}{2}}. \tag{4–6}
\]

Duality of the class of rooted planar maps says the same result holds for faces. The bijection between \( m \)-edged rooted planar maps and \( m \)-faced rooted planar quadrangulations then says the same result holds for vertices in quadrangulations (see for instance the proof of Proposition 12 in [Benjamini and Curien 13]). Whence \( q_{k,m} \) can be viewed as the probability that the root vertex of a \( m \)-vertex quadrangulation has degree-\( k \) and similarly \( q_k \) can be interpreted in this light.

Now let \( p_{k,m} \) be the probability that an arbitrary vertex of a \( m \)-vertex quadrangulation has degree-\( k \) and let \( p_k = \lim_{m \to \infty} p_{k,m} \). Section 2.5 in [Liskovets 99] relates, for a quadrangulation of \( m \) vertices, the probabilities \( q_{k,m} \) and \( p_{k,m} \) by,
Table 2. Limiting face degree densities. Theoretical fits for 4-valent $p_k$ come from Taylor series expansion of the result in Theorem 8. Experimental columns are the slopes of linear functions fit to data using least squares; quoted errors are the errors in regression.

| $k$ | 4-valent $p_4$ theoretical | 4-valent $p_4$ | Rejection $p_4$ | Wang-Landau $p_4$ |
|-----|-----------------------------|---------------|-----------------|-----------------|
| 1   | $\frac{7}{3} = 0.3$        | 0.3328±2 · 10^{-4} | 0.3496±2 · 10^{-4} | 0.3503±1 · 10^{-5} |
| 2   | $\frac{6}{3} = 0.16$       | 0.1662±2 · 10^{-4} | 0.1407±1 · 10^{-4} | 0.1407±1 · 10^{-5} |
| 3   | $\frac{5}{2} = 0.12037$    | 0.1200±2 · 10^{-4} | 0.1222±1 · 10^{-4} | 0.1224±1 · 10^{-5} |
| 4   | $\frac{6}{2} = 0.08488$    | 0.0846±1 · 10^{-4} | 0.0831±1 · 10^{-4} | 0.08296±9 · 10^{-6} |
| 5   | $\frac{8}{3} \approx 0.06404$ | 0.0641±2 · 10^{-4} | 0.0662±2 · 10^{-4} | 0.06621±2 · 10^{-6} |
| 6   | $\frac{15}{7} \approx 0.048448$ | 0.0484±2 · 10^{-4} | 0.0500±1 · 10^{-4} | 0.04999±2 · 10^{-6} |
| 7   | $\frac{14}{6} \approx 0.03753$ | 0.03769±8 · 10^{-5} | 0.0395±1 · 10^{-4} | 0.03935±2 · 10^{-6} |
| 8   | $\frac{16}{7} \approx 0.02922$ | 0.0292±1 · 10^{-4} | 0.0305±1 · 10^{-4} | 0.03062±5 · 10^{-6} |
| 9   | $\frac{15}{6} \approx 0.02299$ | 0.0232±1 · 10^{-4} | 0.02419±8 · 10^{-5} | 0.024176±4 · 10^{-6} |

$$p_{k,m} = \frac{4(m-2)q_{k,m}}{m-k} \sim 4 \frac{q_{k,m}}{k}, \quad \text{as } m \text{ becomes large.} \quad (4–7)$$

So $p_k$ and $q_k$ are related by $p_k = 4q_k/k$. Noting that 4-valent maps with $n$-vertices are dual to quadrangulations with $n + 2$ vertices yields the result.

We have computed linear regressions using least squares for 4-valent maps sampled using the Schaeffer bijection, plane curves sampled using rejection, and plane curve sampled using our Wang-Landau sampler for face degrees from 1 to 9 and presented these data in Table 2 alongside precise densities obtained via Taylor series expansion on the result of Theorem 8.

We present these data for small face sizes in Figure 15. Since the sampled 4-valent maps and the plane curves sampled using rejection are statistically independent, we have computed error bars as a single standard error. To arrive at error bars for a given statistic for our Wang-Landau data we computed both a standard error from the data and away from the arbitrary 4-valent map data.

We note that: Random curve diagrams have fewer bigons and quadrangles than generic 4-valent maps. This phenomenon is specific to degrees 2 and 4 (at least for face degrees at most 9); every other degree face is more common in random plane curves.

It is furthermore expected of classes of random maps that, for fixed size, number of faces of fixed degree-$k$ is a normally distributed statistic [Drmota and Panagiotou 13]. In Figure 16 below, we compare distributions of different $k$-gon ratios for $n = 40$ and $n = 100$ crossings. As expected, the curves show a close similarity between the uniformly sampled curves and the Wang-Landau MCMC sampled curves. In the cases of 1- and 2-gons, it is easy to see a difference from the all 4-valent map sampler. In the case of larger faces, the differences in averages are on a much smaller order, and the curves are no longer possible to distinguish. In all cases, it seems that as the number of crossings $n$ grows large, the distributions are approximately normal. We also examined the variances in these distributions and found that they grow linearly with $n$—see Figure 17.

We note here that the face degree probabilities are closely related to the probability that a given Markov chain transition succeeds on a given diagram, although it is actually the quantity $q_{k,n} = \frac{k p_{k,n} (n+2)}{4n}$ discussed prior which is at play (transitions by definition occur at the root along the root face). Namely, the probability that an RII move can succeed is $q_{3,n+2} \approx 0.09182$ (not taking into account rejection of degenerate triangles), the probability that an RI- operation will succeed is $q_{1,n+2} \approx 0.08760$, and the probability that an RI- operation will succeed is $q_{2,n+2} \approx 0.07036$ (not taking into account the extra Metropolis-Hastings step required to create large faces or other invalid sites, see the description of move RI- in Section 3).

We reinterpret briefly the probabilities $p_{k,n+2}$ in the context of random knot diagrams. We note that in the case of prime alternating diagrams, face degrees are related to the hyperbolic volume of the resulting knot [Obeidin 16]. We further note that a random curve has $\approx 0.35(n+2) > (n+2)/3$ monogons says that a random knot diagram has, on average, at least $.35(n+2)$ vertices that have no impact on the knot type and could be immediately reduced by a Reidemeister I move. One half of all crossing assignments for bigon vertices can be reduced by Reidemeister II moves, so a random knot diagram will
have around $0.14(n + 2)/2$ bigons that can be removed by Reidemeister II moves.

### 4.2.2. Maximum face degree

Another quantity of interest in the study of planar maps is the maximum vertex degree $D_n$ and the maximum face degree $D_n/C_3$. As noted above, $D_n = 4$ because all vertices are 4-valent, so we examine expectation of $D_n/C_3$. It is expected that this quantity exhibits $\Theta(\log n + \log \log n)$ growth as it does for general maps. A result of [Gao and Wormald 00] has that for general maps the expected maximum face degree is:

$$E(D_n/C_3) = \frac{\ln(n) - \frac{1}{2} \ln(\ln(n))}{\ln(6/5)} + O(1). \quad (4-8)$$

We present the difference between expectations and that of general maps in Figure 18. From this, it does not appear that plane 4-valent maps exhibit the same behavior as the general map case: Indeed, as the bijection between arbitrary maps and 4-valent maps makes both faces and vertices into 4-valent map faces, the expected maximum vertex degree $D_n/C_3$ is in fact an
expectation of a maximum $\mathbb{E}(\max(\Delta_n, \Delta^*_n))$ over both vertex and face degrees of arbitrary maps. We have plotted histograms of the maximum face degree distribution in curves and 4-valent maps for fixed size in Figure 19. These distributions are clearly not Gaussian. We note that the histograms of all cases look similar even though they have differing means (see Figure 18), this can be explained by noting that
the difference between the means is small and growing very slowly in \( n \).

We present the data for \( E(D^{\Delta}_{\pi n}) \) of the Wang-Landau MCMC sampler up to 500 crossings—it is impractical to gather samples of this size from the rejection sampler—in Figure 20. The \( O(\log(n)) \) trend continues, as hypothesized. We also plot the variance of this statistic divided by \( \log(n) \)—this shows that our data is consistent with the \( O(\log(n)) \) variance computed for general rooted maps in [Gao and Wormald 00]. However the negative slope for large \( n \) indicates that it could be smaller than this.

We note that the quantity \( E(D^{\Delta}_{\pi n}) \) is related to the success rate of the RII transition, and suggests that the rejection rate for creating large faces through this transition is roughly bounded by \( 1/\Theta(\log n) \).

4.3. Average Casson invariant

Our results above suggest that objects we sample using our Wang-Landau algorithm are giving the same statistics as those generated using rejection sampling. To further test this idea, we can compare further plane curve statistics.

Plane curves are equivalent to Arnol’d’s spherical curves [Arnol’d 95]. Thus, we can check \( Z \)-valued spherical curve invariants for plane curves (these are not defined in the case of a general 4-valent map).

Figure 17. A plot of the variance in the distribution of \( k \)-gon counts for \( k = 1, 2, 3, 7 \) and for the maximal face degree against \( n \). These indicate that the variance in these statistics grows linearly with \( n \).

Figure 18. Average size of largest face \( \Delta_n \).
These are both simple to compute and interesting knot theoretically: By following the crossings in order around the plane curve and counting those which are “interlaced”, we are able to compute $\langle 2St + J^+ \rangle$ in $O(n^2)$ time (we direct the reader to [Arnol’d 95] for more details). This curve invariant is in fact related to a knot invariant, the finite type invariant $v_2$, also called the Casson invariant: $\langle 2St + J^+ \rangle$ is the expected value of $v_2$ over all possible over-under crossing sign assignments to the plane curve. A comparison of $\mathbb{E}(v_2)$ data for Wang-Landau MCMC and rejection samples are presented in Figure 21; the data are remarkably consistent.

We present the data for $\mathbb{E}(v_2)$ up to 500 vertices generated from the Wang-Landau algorithm in Figure 22. Our data suggest that the average $v_2$ invariant grows linearly with the number of crossings with a limiting slope of $0.0268 \pm 0.001$. As a comparison, Even-Zohar et al. [16] prove that for the Petaluma model of random knots, the expectation of $v_2$ grows quadratically with size with leading coefficient $1/24 \approx 0.0417$. As the petal diagrams of size $n$ of the Petaluma model can be viewed as “star diagrams” with $\frac{n^2-3n}{2}$ crossings, size in the Petaluma model is related quadratically to that of our model. Thus, it is reasonable that our average $v_2$ data should grow linearly. It is also expected that the distribution of $\mathbb{E}(v_2)$ over curves of a fixed size tends to be normal; we present histograms of this in Figure 23 that appears to agree with this hypothesis.

4.4. Knotting probabilities

The main aim of constructing these Markov chains was to provide an efficient mechanism to sample large random knot diagrams. We have used the Wang-Landau chain to sample random plane curves which we then use to construct random knot diagrams. This
The last step is done by mapping each vertex to an over or under crossing uniformly at random. We then use knot invariants to determine the topology of the resulting diagram and we compare the resulting knotting probabilities to those found using the rejection sampler.

In [Chapman 17] the first author gathered data for knotting probabilities in knot diagrams of size up to 100 crossings. We have used our Wang-Landau sampler to produce random knot diagrams and classify them by HOMFLY-PT polynomial using lmpoly [Ewing and Millett 91, 97] of size up to 230 crossings. There are two reasons that we have not investigated beyond this size. First, the version of lmpoly included with plCurve [Ashton et al. 17] will not compute HOMFLY-PT polynomials of diagrams of more than 255 crossings. Second, the difficulty of computing the HOMFLY-PT polynomial increases dramatically with the number of crossings; the algorithm employed by lmpoly has exponential run time [Ewing and Millett 91] and computation is known to be NP-hard. We gathered data using twenty independent runs (from the same tuning data for $1 \leq n \leq 230$ with $f < 10^{-8}$ and $\Delta = 0.01$). In each run we took $10^5$ steps between

![Figure 21](image1.png)

**Figure 21.** (Left) Average $-\frac{1}{8}(2St + J^*) = E(v_2)$. (Right) Same statistic with approximate leading linear behavior subtracted to amplify detail. As this statistic is not well-defined for an arbitrary 4-valent map, that data is not present.

![Figure 22](image2.png)

**Figure 22.** The average $v_2$ invariant appears to have linear dominant order growth. Here we present its ratio by number of crossings for finer resolution, where a naïve least squares linear regression suggests a slope of $(2.68 \pm 0.1) \times 10^{-2}$. 
samples, and a total of $1.15 \times 10^7$ diagrams were sampled. Each run took approximately 10 hours to compute, with HOMFLY-PT polynomial calculation being the primary bottleneck. Two independent groups of ten independent runs each were aggregated providing two independent sets of data. The histograms for sizes sampled are presented in Figure 24. We note some caveats for these experiments:

1. The HOMFLY-PT polynomial is not sufficient to distinguish all knot types, and indeed there are infinite families of knots demonstrating this [Kanenobu 86]. However, it is still unknown whether the unknot $0_1$ is the only knot with trivial HOMFLY-PT polynomial; this is related to the still open Jones Conjecture [Kauffman 87].

2. To facilitate a greater number of samples, we imposed a timeout on lmpoly’s HOMFLY-PT calculation of 10ms. See Figure 25. Knots whose HOMFLY-PT failed to be calculated before this cutoff are still counted and categorized as unclassified. Hence it is possible that probabilities presented in our data which follows are smaller than the actual. There is evidence that these failures are rare for simple knots such as the trefoil and the unknot—see Figure 26. We note that the uniform data presented alongside our MCMC sampled data were gathered at a larger timeout.

3. We ignore chirality in these data. A chiral knot is a knot which is different than its mirror, such as the trefoil $3_1$, while an achiral knot like the figure-eight knot $4_1$ is equivalent to its mirror image. By symmetry (i.e. by flipping all crossing signs simultaneously), it can be seen that the probability of drawing a chiral knot is equivalent to that for its mirror image. For the case of the chiral granny $3_1#3_1$ and achiral square $3_1#3_1^*$ composite knots, our data suggest that the square...
knot is as likely as either chiral image of the granny knot; we hence suppress data for the granny knot.

It is believed that for lattice models of random knots the number $\kappa_n(K)$ of knot diagrams with fixed knot type $K$ has asymptotic growth rate

$$\kappa_n(K) \sim C_K \tau_K^n n^{2x_K+N_K},$$

where $C_K$ depends on the knot type and $N_K$ is the number of prime components making up the knot type $K$. It is believed that the constant $\tau_K$ does not depend on the knot type [Rensburg and Whittington 91, Deguchi and Tsurusaki 97, Orlandini et al. 98]. It has been proved that $\tau_0$ exists for many lattice models (this follows from standard supermultiplicativity arguments) and also for random knot diagrams [Chapman 17], however it is still an open problem to prove the existence of $\tau_K$ for any other knot type. It is known, however, that $\tau_0$ is strictly smaller than $2\mu$ for random knot diagrams [Chapman 17]; which is comparable to a similar result for self-avoiding polygons [Sumners and Whittington 88, Pippenger 89]. There is strong numerical evidence for self-avoiding polygons that the exponent $x_K$ is independent of knot type [Orlandini et al. 98, Rensburg and Rechnitzer 11]. Consequently

Figure 25. The time taken to compute the HOMFLY-PT polynomial increases dramatically with the complexity of the knot diagram. Accordingly, we imposed a time-cutoff on these computations and if the invariant was not computed before the indicated time then it was left unclassified. In this figure we show the proportion of knot diagrams that failed to be classified as a function of the number of crossings and the cutoff time.

Figure 26. The probability of a knot being classified as an unknot and a trefoil as a function of the number of crossings and the time-cutoff of the HOMFLY-PT computation. These data show that increasing the cutoff does not significantly affect this probability. This is consistent with the hypothesis that most HOMFLY-PT computation failures are for complicated knots.
we conjecture for random knot diagrams that
\[ \kappa_n(K) \sim C_K \tau_0^n n^2 + N_K, \]  
(4–10)
where \( \alpha = \gamma - 2 \), where \( \gamma \) is the same “universal” critical exponent [Schaeffer and Zinn-Justin 04] in the asymptotic formula for plane curves. This asymptotic form is consistent with the idea that the knotted portion of a random knot diagram is localized—see Figure 27.

Under this assumption, the probability that a random knot diagram of size \( n \) exhibits knot type \( K \) scales as
\[ p_n(K) = \kappa_n(K)/\kappa_n \sim D_K \rho^n n^{N_K}, \]  
(4–11)
where \( 0 < \rho < 1 \). We plot knot probability data from both our Wang-Landau sampler and rejection sampling in Figure 28. We see that both sampling methods agree and that the data is consistent with the scaling form in Equation 4–11. In particular, in Figure 29, we plot the logarithm of the knotting probabilities divided by \( n^{N_K} \) and see that the resulting slopes are extremely similar. A simple linear regression of these data shows that \( \rho \approx 0.95 \). This is evidence that the growth rate of random knot diagrams of fixed knot type \( K \) is independent of \( K \) and that
\[ \tau_K = \tau_0 \approx 2 \times 11.41 \times 0.95 = 21.7. \]  
(4–12)

The authors intend to test this hypothesis further in future work.

As a final comparison to the uniform sampler data, we compute ratios of knot probabilities as in [Rensburg and Rechnitzer 11]. Namely, the expected growth rates of knot probabilities has that, for two knot types \( K \) and \( L \), the ratio of probabilities should obey,
\[ \frac{p_n(K)}{p_n(L)} \sim \frac{D_K \rho^n n^{N_K}}{D_L \rho^n n^{N_L}} = \frac{D_K}{D_L} n^{N_K - N_L}. \]  
(4–13)

Hence we expect \( p_n(K)/p_n(L) \cdot n^{N_K - N_L} \) to tend to a constant as \( n \) increases. We plot these data for ratios of prime knots in Figure 30, and for ratios of unknots to prime knots Figure 31. We also show the ratios of square knots to trefoils and unknots in Figure 32. While these ratio data are noisy for larger \( n \) they are consistent with the above scaling form.

5. Conclusion

We have described a new Markov chain Monte Carlo method for sampling random plane curves efficiently. This then trivially extends to sample random knot diagrams by mapping vertices to crossings. This enables us to sample of large knot diagrams which are otherwise simply too rare to sample by rejection sampling methods. Due to the difficulty of tuning the Boltzmann MCMC to sample diagrams of a wide range of sizes, we modified our original Markov chain

Figure 27. A random trefoil knot diagram of 50 crossings; the knotted portion of the curve is highlighted. We see that the knotted portion is quite small and this is expected to be typical.

Figure 28. Plots for a WL sample against the data for a rejection sampler in [Chapman 17]. Plots for other knot types are similar, and rejection data are consistent with WL sampled data throughout.
to use the flat histogram methods of Wang and Landau. This results in a chain that samples approximately uniformly across a wide range of sizes, and additionally gives estimates of the numbers of plane curves and knot diagrams. These estimated counts are in agreement with previously conjectured asymptotic forms. Hence we conclude that our MCMC implementation can attain similar accuracy of the uniform rejection methods in far less time. We have then tested the data from the Wang-Landau chain against data from a rejection sampler and find strong agreement across a wide range of statistics.

Plane curves are a subset of 4-valent maps and it is not well understood how different these two sets of objects are. With this in mind, we computed the average maximum face degree and face degree degree distributions and find significant differences. One of the main aims of sampling random plane curves is to study random knotting. Our Wang-Landau sampler allows us to generate significant numbers of random knot diagrams of a range of sizes. We have then classified the knot types of those diagrams using HOMFLY-PT polynomials. These data allow us to conjecture that random knot diagrams have very similar asymptotic behavior to other models of random knotting, such as self-avoiding polygons. These asymptotic forms are consistent with the idea that the knotted portion of a random knot diagram is quite localized. We also give evidence that the HOMFLY-PT polynomial software [Ewing and Millett 97] that

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**Figure 29.** After normalizing by a factor of $n^{-N_K}$ (where $N_K$ is the number of prime components of the knot type $K$), knot probabilities are all approximately log-linear.

**Figure 30.** Ratios of probabilities of prime knot types in diagrams. Probabilities within each ratio are taken from independent runs of the MCMC sampler. Legend entries are sorted by their values at $1/n = 0.05$. 
we used struggles to compute invariants of complicated knots, but does succeed for simple knots, even when their embeddings might be very large.

5.1. Future work

The Markov transitions presented here are based on “shadows” of the Reidemeister moves on knot diagrams. It is thus natural to consider a Markov chain on knot diagrams generated by similar transitions corresponding to the proper Reidemeister moves, taking into account over-under signing of the diagram. This would produce a Markov process on the so-called Reidemeister graph [Barbensi and Celoria 18]. Indeed, we expect this Markov chain to be ergodic (with ergodicity classes being fixed knot types), and we expect transitions to be of similar computational complexity. It would also have the advantage of not requiring a knot-classification step. We note, however, that Corollary 5 fails in this case; it is known that there are diagrams who represent the same knot type, but whose transition paths all involve an increase in the number of crossings [Kauffman and Manturov 06].

To make matters worse, unlike the spaces of plane curves where the diameter has $n^{3/2}$ growth [Chang and Erickson 17], the upper bound on the diameters

![Figure 31. Ratios of probabilities of the unknot with prime knots, with correction factor $n$. Probabilities within each ratio are taken from independent runs of the MCMC sampler. Legend entries are sorted by their values at $1/n = 0.05$.](image1)

![Figure 32. Ratios of probabilities of the square knots to trefoils and unknots (with corrections of $n$ and $n^2$ respectively. Probabilities within each ratio are taken from independent runs of the MCMC sampler. Legend entries are sorted by their values at $1/n = 0.05$.](image2)
of the spaces of knot diagrams is far larger [Hass and Lagarias 01, Nowik 09, Lackenby 15]. Hence in the case of knot diagrams, care must be taken to ensure that there are satisfactory parameters for the Markov chain to converge to the uniform distribution in a reasonable amount of time. It should also be noted that rejection sampling becomes even less efficient for sampling fixed knot types, since not only are knot diagrams exponentially rare in the space of 4-valent maps, but knot diagrams of a specific type are exponentially rare in the space of knot diagrams.

Beyond sampling knot diagrams with fixed knot type, the flat Reidemeister moves discussed in this article also apply to planar immersions of any fixed number of circles. These diagrams are called link shadows; the smallest such object is the unique 2-crossing 4-valent planar map of 2 link components. In this case, the Markov chain is still ergodic (the proof of Theorem 1 is not affected by the immersion having a different number of link components). Hence this technique could be used to sample large immersions of any fixed number of link components. We could also restrict or alter the transitions; for instance we could remove the shadow Reidemeister I move, whence the ergodicity classes of the Markov chain would be spherical curves of fixed spherical Whitney number [Arnol’d 95, Nowik 09]. Further, by using Reidemeister moves instead of flat Reidemeister moves, one could also sample link diagrams of fixed link types.

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References

[Alexander and Briggs 26] J. W. Alexander and G. B. Briggs. “On Types of Knotted Curves.” Ann Math. 28:1/4 (1926), 562. doi:10.2307/1968399.

[Arnogão de Carvalho and Caracciolo 83] C. Arnogão de Carvalho and S. Caracciolo. “A New Monte Carlo Approach to the Critical Properties of Self-Avoiding Random Walks.” J Phys France. 44:3 (1983), 323–331. doi:10.1051/phys:01983004403032300.

[Arnogão de Carvalho et al. 83] C. Arnogão de Carvalho, S. Caracciolo, and J. Fröhlich. “Polymers and $g|\phi|^4$ Theory in Four Dimensions.” Nuclear Phys B. 215:2 (1983), 209–248. doi:10.1016/0550-3213(83)90213-4.

[Arnoł’d 95] V. I. Arnoł’d. “The Geometry of Spherical Curves and the Algebra of Quaternions.” Russ Math Surv. 50:1 (1995), 1. doi:10.1070/ RM1995v050n01ABEH001662.

[Ashton et al. 17] T. Ashton, J. Cantarella, and H. Chapman. plCurve: Fast polygon library. Available online (http://www.jasoncantarella.com/wordpress/software/plcurve/), 2017.

[Barbensi and Celoria 18] A. Barbensi and D. Celoria. “The Reidemeister Graph Is a Complete Knot Invariant.” ArXiv Preprints, Available online (http://arxiv.org/abs/1801.03313v1), 2018.

[Benjamini and Curien 13] I. Benjamini and N. Curien. “Simple Random Walk on the Uniform Infinite Planar Quadrangulation: Subdiffusivity via Pioneer Points.” Geom Funct Anal. 23:2 (2013), 501–531. doi:10.1007/s00039-013-0212-0.

[Berg and Foerster 81] B. Berg and D. Foerster. “Random Paths and Random Surfaces on a Digital Computer.” Phys Lett B. 106:4 (1981), 323–326. doi:10.1016/0370-2693(81)90545-1.

[Buck and Zechiedrich 04] G. R. Buck and E. L. Zechiedrich. “DNA Disentangling By Type-2 Topoisomerases.” J Mol Biol. 340:5 (2004), 933–939. doi:10.1016/j.jmb.2004.05.034.

[Cantarella et al. 16] J. Cantarella, H. Chapman, and M. Mastin. “Knot Probabilities in Random Diagrams.” J Phys A Math Theor. 49:40 (2016), 405001. doi:10.1088/1751-8113/49/40/405001.

[Chang and Erickson 17] H.-C. Chang and J. Erickson. “Untangling Planar Curves.” Discrete Comput Geom. 58:4 (2017), 889–920. doi:10.1007/s00454-017-9907-6.

[Chapman 17] H. Chapman. “Asymptotic Laws for Random Knot Diagrams.” J Phys A Math Theor. 50 (2017), 225001. doi:10.1088/1751-8121/aa6e45. arXiv: 1608.02638 [math.GT].

[Chapman 18] H. Chapman. “Slipknotting in the Knot Diagram Model.” arXiv.org. Available online (https://arxiv.org/pdf/1803.07114.pdf), 2018.

[Conway and Guttmann 96] A. Conway and A. J. Guttmann. “Square Lattice Self-Avoiding Walks and Corrections to Scaling.” Phys Rev Lett. 77:26 (1996), 5284.
[Coquereaux and Zuber 16] R. Coquereaux, and J.-B. Zuber. “Maps, Immersions and Permutations.” J Knot Theory Ramificat. 25:8 (2016), 1650047. doi:10.1142/s0218216516500474.

[Culler 17] M. Culler, N. M. Dunfield, and J. R. Weeks. SnapPy, a computer program for studying the geometry and topology of 3-manifolds. Available online (http://snappy.computop.org), 2017.

[Delbrück 62] M. Delbrück. “Knotting Problems in Biology.” Chap. 5. In Mathematical Problems in the Biological Sciences, edited by R. Bellman, pp. 55–63. Providence, RI: American Mathematical Society, 1962.

[Diao 95] Y. Diao. “The Knotting of Equilateral Polygons in \( \mathbb{R}^3 \).” J Knot Theory Ramificat. 4:2 (1995), 189–196. doi:10.1142/S0218216595000090.

[Diao et al. 12] Y. Diao, C. Ernst, and U. Ziegler. “Generating Large Random Knot Projections.” Chap. 23. In Physical and Numerical Models in Knot Theory, edited by J. A. Calvo, K. C. Millett, J. E. Rawdon, and A. Stasiak, pp. 473–494. Singapore: World Scientific, 2012.

[Drmota and Panagiotou 13] M. Drmota, and K. Panagiotou. “A Central Limit Theorem for the Number of Degree-k Vertices in Random Maps.” Algorithmica. 66:4 (2013), 741–761. doi:10.1007/s00453-013-9751-x.

[Dunfield et al. 14] N. Dunfield, A. Hirani, M. Obeidin, A. Ehrenberg, S. Bhattacharyya, and D. Lei. Random Knots: A Preliminary Report. Available online (http://www.math.uiuc.edu/~nmd/preprints/slides/random_knots.pdf), 2014.

[Even-Zohar et al. 16] C. Even-Zohar, J. Hass, N. Linial, and T. Nowik. “Invariants of Random Knots and Links.” Discrete Comput Geom. 56:2 (2016), 274–314. doi:10.1007/s00454-016-9798-y.

[Ewing and Millett 91] B. Ewing and K. C. Millett. “A Load Balanced Algorithm for the Calculation of the Polynomial Knot and Link Invariants.” In The Mathematical Heritage of C. F. Gauss, pp. 225–266. River Edge, NJ: World Scientific Publishing, 1991.

[Ewing and Millett 97] B. Ewing and K. C. Millett. “Computational Algorithms and the Complexity of Link Polynomials.” In Progress in Knot Theory and Related Topics, vol. 56, pp. 51–68. Hermann, Paris: Travaux en Cours, 1997.

[Flajolet and Sedgewick 09] P. Flajolet and R. Sedgewick. Analytic Combinatorics. Cambridge, UK: Cambridge University Press, 2009.

[Freyd 85] P. Freyd, D. Yetter, J. Hoste, W. B. R. Lickorish, K. Millett, and A. Ocneanu. “A New Polynomial Invariant of Knots and Links.” Bull Am Math Soc. 12:2 (1985), 239–247. doi:10.1090/s0273-0979-1985-15361-3.

[Frisch and Wasserman 61] H. L. Frisch and E. Wasserman. “Chemical Topology I.” J Am Chem Soc. 83:18 (1961), 3789–3795. doi:10.1021/ja01479a010.

[Gao and Richmond 94] Z. Gao and L. Richmond. “Root Vertex Valency Distributions of Rooted Maps and Rooted Triangulations.” Eur J Combinator. 15:5 (1994), 483–490. doi:10.1016/eujc.1994.1050.

[Gao and Wormald 00] Z. Gao and N. C. Wormald. “The Distribution of the Maximum Vertex Degree in Random Planar Maps.” J Combinat Theory Ser A. 89:2 (2000), 201–230. doi:10.1006/jcta.1999.3006.

[Geyer 91] C. J. Geyer. “Markov Chain Monte Carlo Maximum Likelihood, Computing Science and Statistics.” In Proceedings of the 23rd Symposium Interface, pp. 156–163. Fairfax Station, VA: Interface Foundation of North America, 1991.

[Graaf and Schrijver 97] M. D. Graaf and A. Schrijver. “Universality of Random Knotting.” J Knot Theory Ramificat. 6245 (1997), 134–156. doi:10.1016/j.jctb.1997.1754.

[Guisard and Orlandini 99] E. Guissard and E. Orlandini. “Monte Carlo Results for Projected Self-Avoiding Polygons: a Two-Dimensional Model for Knotted Polymers.” J Phys A Math Gen. 32:8 (1999), 1359–1385. doi:10.1088/0305-4470/32/8/006.

[Hammersley 61] J. M. Hammersley. “The Number of Polygons on a Lattice.” Math Proc Camb Phil Soc. 57:3 (1961), 516. doi:10.1017/S030500410003557X.

[Hass and Lagarias 01] J. Hass and J. Lagarias. “The Number of Reidemeister Moves Needed for Unknotting.” J Amer Math Soc. 14:2 (2001), 399–428.

[Hass and Scott 94] J. Hass, and P. Scott. “Shortening Curves on Surfaces.” Topology 33:1 (1994), 25–43. doi:10.1016/0040-9383(94)90033-7.

[Henrich and Nelson 10] A. Henrich and S. Nelson. “Semiquandles and at Virtual Knots.” Pac J Math. 248:1 (2010), 155–170. doi:10.2140/pjm.2010.248.155.

[Kanenobu 86] T. Kanenobu. “Infinitely Many Knots with the Same Polynomial Invariant.” Proc Am Math Soc. 97:1 (1986), 158–158. doi:10.1090/s0002-9939-1986-0831406-7.

[Kauffman 87] L. H. Kauffman. “State Models and the Jones Polynomial.” Topology 26:3 (1987), 395–407. doi:10.1016/0040-9383(87)90009-7.

[Kauffman and Lambropoulou 06] L. Kauffman and H. S. Lambropoulou. “Hard Unknots and Collapsing Tangles.” Paper presented at the Introductory Lectures on Knot Theory: Selected Lectures presented at the Advanced School and Conference on Knot Theory and its Applications to Physics and Biology ICTP, Trieste, Italy, May 11–29, 2006.

[Kauffman and Manturov 06] L. H. Kauffman and V. O. Manturov. “Virtual Knots and Links.” Proc Steklov Inst Math. 252:1 (2006), 104–121. doi:10.1134/s0081543806010111.

[Lackenby 15] M. Lackenby. “A Polynomial Upper Bound on Reidemeister Moves.” Ann Math. 182:2 (2015), 491–564.

[Lal 69] M. Lal. “Monte Carlo Computer Simulation of Chain Molecules I.” Mol Phys. 17:1 (1969), 57–64.

[Liskovets 99] V. A. Liskovets. “A Pattern of Asymptotic Vertex Valency Distributions in Planar Maps.” J Combin Theory Ser B. 75:1 (1999), 116–133. doi:10.1006/jctb.1998.1870.

[Madras and Slade 13] N. Madras and G. Slade. The Self-Avoiding Walk. Probability and Its Applications. Boston: Birkhauser. Available online (https://books.google.com/books?id=soFCAAQBAJ), 2013.

[Madras and Sokal 88] N. Madras, and A. D. Sokal. “The Pivot Algorithm: A Highly Efficient Monte Carlo Method for the Self-Avoiding Walk.” J Stat Phys. 50:1–2 (1988), 109–186.
Appendix A: Complete detailed balance proofs

Detailed balance equations for Boltzmann Markov chain; Theorem 1. We check the detailed balance equations for each transition:

1. Suppose that $N = R_1^+(D, a)$ with root flag $b$. This means that $N$ is unique in that $D = R_1^-(N, b)$. Then

$$P(D \rightarrow N) \pi(D) = P(N \rightarrow D) \pi(N)$$

so the equation holds.

2. Suppose that $N = R_1^+(D, a, a')$ with root flag $b$. This means that $N$ is unique in that $D = R_1^-(N, b)$. The flags $a, a'$ lie along a face in $D$ of degree $d$. Then

$$P(D \rightarrow N) \pi(D) = P(N \rightarrow D) \pi(N)$$

so the equation holds.

3. Suppose that $N \neq R_1^+(D, a)$ and that $N$ is a re-rooting of $D$. Then

$$P(D \rightarrow N) \pi(D) = P(N \rightarrow D) \pi(N)$$

so the equation holds.
Because $D$ and $N$ differ only by a re-rooting, their underlying number of automorphisms are the same; \( \text{aut } D = \text{aut } N \). Hence equality follows.

4. Suppose that $N = RIII(D,a)$ has root $b$ and that $N$ is not a re-rooting of $D$. Then $N$ is unique in that $D = RIII(N,b)$, so

$$ P(D \rightarrow N)\pi(D) = P(N \rightarrow D)\pi(N) $$

$$ z^n p_3 = z^n p_3. $$

5. If $N = RIII(D,a)$ has root $b$ and $N$ is a re-rooting of $D$, then the transition probabilities of the previous two cases are summed (as the different transitions are independent), so that

$$ P(D \rightarrow N)\pi(D) = P(N \rightarrow D)\pi(N) $$

$$ \left( p_3 + (1 - (p_1 + p_2 + p_3)) \frac{\text{aut } D}{4n} \right) z^n $$

$$ \left( p_3 + (1 - (p_1 + p_2 + p_3)) \frac{\text{aut } N}{4n} \right) z^n. $$

Proof of Corollary 6. As this Markov chain can perform all flat Reidemeister transitions and achieve all curve rootings, this Markov chain explores the space of curves. It remains to show that detailed balance holds.

For a pair of diagrams $D, N$, let $P_p(D \rightarrow N)$ denote the probability of transitioning from $D$ to $N$ under this modified Markov chain. Let $P_p'(D \rightarrow N)$ be the probability of transitioning from $D$ to $N$ under the original Markov chain (no interstitial re-rooting). Finally, let $P_p(D \rightarrow B)$ be the probability of transitioning from $D$ to $N$ under the original Markov chain with all $p_i = 0$ (only re-roots are performed).

Notice that $P_p(D \rightarrow N) = \sum_B \sum_C P_p(C \rightarrow N)P_p'(B \rightarrow C) P_p(D \rightarrow B)$, where the sums are over all rooted curves. Then,

$$ P_p(D \rightarrow N)\pi(D) = \sum_B \sum_C P_p'(C \rightarrow N)P_p'(B \rightarrow C)P_p(D \rightarrow B)\pi(D) $$

$$ = \sum_B \sum_C P_p'(C \rightarrow N)P_p'(B \rightarrow C)P_p'(B \rightarrow D)\pi(B). $$

$$ = \sum_B \sum_C P_p'(N \rightarrow C)P_p'(C \rightarrow B)P_p'(B \rightarrow D)\pi(C). $$

$$ = \sum_B \sum_C P_p'(N \rightarrow C)P_p'(C \rightarrow B)P_p'(B \rightarrow D)\pi(N). $$

$$ = P_p(N \rightarrow D)\pi(N), $$

so detailed balance holds for the modified Markov chain, and hence it is ergodic. □

Detailed balance equations for Wang-Landau Markov chain; Theorem 2. The main concern now is that transitions must pass an additional Metropolis-Hastings check of \( \min \{1,g_m/g_n\} \). Note that for any $g_m > 0$,

$$ \min \{1,g_m/g_n\} = g_n. $$

We check the detailed balance equations for each transition:

1. Suppose that $N = RII^+(D,a)$ with root flag $b$. This means that $N$ is unique in that $D = RII^-(N,b)$. Then

$$ \min \left\{1, \frac{g_n}{g_{n+1}} \right\} \frac{p_1}{2 R_{g_n}} = \min \left\{1, \frac{g_{n+1}}{g_n} \right\} \frac{1}{2 R_{g_{n+1}}} $$

$$ \min \left\{1, \frac{g_{n+1}}{g_n} \right\} \frac{1}{2 R_{g_{n+1}}} = \min \left\{1, \frac{g_n}{g_{n+1}} \right\} \frac{p_1}{2 R_{g_n}}. $$

so the equation holds.

2. Suppose that $N = RII^+(D,a',a')$ with root flag $b$. This means that $N$ is unique in that $D = RII^-(N,b)$. The flags $a,a'$ lie along a face in $D$ of degree $d$. Then

$$ \max \left\{1, \frac{g_n \cdot p_2}{g_{n+2}} \right\} \frac{1}{2(d-1) R_{g_n}} = \max \left\{1, \frac{g_{n+2} \cdot p_2}{g_n \cdot p_2} \right\} \frac{1}{2(d-1) R_{g_{n+2}}} $$

Because $D$ and $N$ differ only by a re-rooting, their underlying number of automorphisms are the same; \( \text{aut } D = \text{aut } N \). Hence equality follows.

4. Suppose that $N = RIII(D,a)$ has root $b$ and that $N$ is not a re-rooting of $D$. Then $N$ is unique in that $D = RIII(N,b)$, so

$$ P(D \rightarrow N)\pi(D) = P(N \rightarrow D)\pi(N) $$

$$ \frac{P_3}{R_{g_n}} = \frac{P_3}{R_{g_n}}. $$

5. If $N = RIII(D,a)$ has root $b$ and $N$ is a re-rooting of $D$, then the transition probabilities of the previous two cases are summed (as the different transitions are independent), so that

$$ P(D \rightarrow N)\pi(D) = P(N \rightarrow D)\pi(N) $$

$$ \left( p_3 + (1 - (p_1 + p_2 + p_3)) \frac{\text{aut } D}{4n} \right) \frac{1}{R_{g_n}} $$

$$ = \left( p_3 + (1 - (p_1 + p_2 + p_3)) \frac{\text{aut } N}{4n} \right) \frac{1}{R_{g_n}}. $$

In all other cases, the transition probabilities are symmetrically zero. Hence we conclude that detailed balance holds with the hypothesized probability distribution. □