Self-Avoiding Random Loops

L. E. Dubins* A. Orlitsky† J. A. Reeds‡ L. A. Shepp‡

March 30, 1993

Steve Rice was truly admirable. He was so gentle that he disdained to use the word "no" in conversation, especially if you were wrong. Among his many mathematical skills were a deep knowledge of special functions, a prehistoric insight into Gaussianity, and a magical ability for numerical analysis.

Abstract

A random loop, or polygon, is a simple random walk whose trajectory is a simple, closed Jordan Curve. This article contributes to the study of random loops in two ways.

First, it initiates the study of the probability $P_n(x,y)$ that a random n-step loop contains a point (x,y) in the interior of the loop and shows that $p_n(\frac{1}{2},\frac{1}{2})$ is $\frac{1}{2}-\frac{1}{n}$. It is plausible that $P_n(x,y) \nearrow \frac{1}{2}$ for all (x,y), but we do not know this even for $(x,y)=(\frac{3}{2},\frac{1}{2})$.

Second, this note offers a way to simulate random n-step self-avoiding loops. Numerical evidence obtained with this simulation procedure suggests that $P_n(\frac{3}{2},\frac{1}{2}) \approx \frac{1}{2}-\frac{c}{n}$. Here is where Steve Rice's particular magic would have been especially useful.

*Department of Mathematics, University of California, Berkeley.

Research partially supported by NSF Grant DMS 86-01634

†AT&T Bell Laboratories, 600 Mountain Av., Murray Hill, NJ 07974

1 Introduction

Walks on the 2-dimensional rectangular grid correspond in an obvious way to walks on the Gaussian integers in the complex plane: the complex numbers $a + ib$ where a and b are integers and i is the square root of -1. For notational convenience, we describe the walks in the latter setting.

A *step* is an element of $\{1, -1, i, -i\}$ thought of as a unit step right, left, up, or down the complex plane. A *walk* is a sequence of steps. The *length of a walk* is the number of steps in the sequence. A walk of length n is an *n-walk*. Let $s_0, \ldots, s_{n-1}$ be an n-walk. Its *trajectory* is the sequence $t_0(s), \ldots, t_n(s)$ defined by: $t_0(s) = 0$ and, for $1 \le j \le n$, $t_j(s) = s_0 + \cdots + s_{j-1}$. It is the sequence of points in the complex plane visited by a walker who starts at 0, and follows the steps $s_0, \ldots, s_{n-1}$. For brevity, we write t_j for $t_j(s)$ and use s and t interchangeably to describe the same walk.

An n-walk s (or t) is *self-avoiding* if $t_j \ne t_k$ for all $0 \le j < k \le n$. A *random* self-avoiding n-walk is a uniformly distributed random element of the set of self-avoiding n-walks. Equivalently, it is a sequence of independent random variables $S_0, \ldots, S_{n-1}$, where $S_j = \pm 1, \pm i$, each with probability $\frac{1}{4}$, conditioned so that $T_j \ne T_k$ for all $0 \le j < k \le n$, where $T_0 = 0$ and $T_j = S_0 + \cdots + S_{j-1}$.

An n-walk s (or t) is a *self-avoiding n-loop* if $t_j \ne t_k$ for all $0 \le j < k < n$ *and* $t_0 = t_n$. Necessarily, n is even. A *random* self-avoiding n-loop is a uniformly distributed random element of the set of self-avoiding n-loops. Equivalently, it is a sequence of independent random variables $S_0, \ldots, S_{n-1}$, where $S_j = \pm 1, \pm i$, each with probability $\frac{1}{4}$, conditioned so that $T_j \ne T_k$ for all $0 \le j < k < n$, and $T_n = 0$, where $T_0 = 0$ and $T_j = S_0 + \cdots + S_{j-1}$.

As the list of references of this paper suggests, there are many papers that treat self-avoiding random walks and loops. Additional references, undoubtedly hundreds of them, can be obtained by key-wording on "self-avoiding" in the "Math. Reviews" or "Science

Abstracts" databases. Many of these papers arise in the study of polymer chemistry and statistical mechanical models e.g., Helfand and Pearson [1], Simon [2], and Chayes [3].

For papers of mathematical interest, see Hammersley [4], Kesten [5], Guttmann [6], Le Gall [7], Pippenger [8], and the references therein. Among other results, Hammersley [4] has shown that the number W_n of self-avoiding n-walks satisfies $\frac{1}{n}\log W_n \to \log\beta$ and that the number L_n of self-avoiding n-loops also satisfies $\frac{1}{n}\log L_n \to \log\beta$ (amazingly, the same β). He proved these facts by clever subadditivity arguments. Kesten [5] gave a functional-type equation for β and Guttmann [6] showed that $\beta = 2.6381 \pm .0002$.

Let $t_0, \ldots, t_n$ be a self-avoiding n-loop. The polygon formed by the points $t_0, \ldots, t_n$ along with the unit segments connecting t_j to t_{j+1} for $j = 0, \ldots, n-1$ form a simple closed, or Jordan, curve in the plane. Such a curve divides the plane into an inside region and an outside region. For any point (x, y) in the plane, we define

$$P_n(x, y) = P(\ (x, y) \in \text{inside region of a random } n\text{-loop}\ )\ .$$

In Section 2, we prove that

$$P_n\left(\frac{1}{2}, \frac{1}{2}\right) = \frac{1}{2} - \frac{1}{n}$$

hence $P_n(\frac{1}{2}, \frac{1}{2}) \nearrow \frac{1}{2}$ as $n \to \infty$. We conjecture that whenever x and y are both non-integers $P_n(x, y) \nearrow \frac{1}{2}$ as $n \to \infty$. However, we cannot prove it even for $(x, y) = (\frac{3}{2}, \frac{1}{2})$. It even seems difficult to prove $P_n(\frac{3}{2}, \frac{1}{2}) \leq P_n(\frac{1}{2}, \frac{1}{2})$ so, in Section 4, we resort to simulations.

The straightforward simulation technique for random self-avoiding n-loops that simply walks to a random nearest-neighbor not previously visited then returns to the origin, encounters two problems. First, one may reach a position that has no such nearest neighbors. According to Hemmer and Hemmer [9] and Hemmer [10], this happens after an average of about 71 steps. Thus, especially for large n, this simulation and others, for instance Aragao de Carvalho and Caracciolo [11], Bredner, Ben Avraham, and Havlin [12], Myers, Enrick, Edmond, and Lindgren [13], Berretti and Sokal [14], and Sariban, Binder, and Heermann [15], would not seem very useful. A second problem is ensuring that the walk returns to the origin after exactly n steps.

Instead, this note proposes a loop-generation algorithm that performs a random walk on a graph of all self-avoiding n-loops with a certain edge structure. The resulting process is a Markov chain, whose states are the self-avoiding n-loops. The edge structure of the graph and transition probabilities are chosen so that the equilibrium distribution of the Markov chain, hence of the derived loop, is uniform.

This technique is similar to, and draws heavily from, the pivot algorithm used to generate random walks (rather than loops). The pivot algorithm, invented by Lal [16], performs a random walk on a graph of all self avoiding n-walks. It has been used by Olaj and Pelinka [17], MacDonald, Jan, Hunter, and Steinitz [18], Hunter, Jan, and MacDonald [19], Stellman and Gans [20] and [21], and Freire and Horta [22]. A neat analysis of its performance is given in a recent paper by Madras and Sokal [23]. For completeness and clarity, their description of the pivot algorithm is duplicated in Section 3, and the loop algorithm is given in Section 4.

The number of iterations required to reach equilibrium in both the loop and the pivot algorithm seems to be small (perhaps linear or quadratic in n). However, there is no known proof that a polynomial number of iterations suffice for either the pivot or the loop algorithm.

2 Encircling (x, y)

Let T_0, $T_1, T_2, \ldots, T_n$ with $T_0 = T_n = 0$ be a random self-avoiding n-loop defined as in the previous section. Necessarily, n is even. The points $T_0, T_1, \ldots, T_n$ along with the unit segments connecting T_j to T_{j+1} for $j = 0, \ldots, n-1$ form a simple closed, or Jordan, curve J in the plane with vertices $T_0, \ldots, T_{n-1}$. Since a Jordan curve has an inside and an outside, one may ask whether or not a point (x, y) is inside, outside, or on the curve. If x and y are both non-integers, then the last possibility cannot happen and so (x, y) is either inside or on the curve.

Theorem 1 $P\left(\left(\frac{1}{2}, \frac{1}{2}\right) \text{ is inside } J\right) = \frac{1}{2} - \frac{1}{n}$.

Proof: Suppose that S (or T) is a random self-avoiding n-loop corresponding to the random Jordan curve J as above. Each T_k is a vertex of J. It is called *convex, concave*, or *straight*, according to whether the inside angle of J at T_k is 90°, 270°, or 180°. Let v, c, s be the number of convex, concave, and straight vertices of J, respectively, so that

$$n = v + c + s \; . \tag{1}$$

Consider the n Jordan curves $J_0, J_1, \ldots, J_{n-1}$ obtained by cyclically permuting the vertices to $T_j - T_j, T_{j+1} - T_j, \ldots, T_{j+n} - T_j$ for $j = 0, 1, \ldots, n-1$, where $T_{n+i} = T_i$ for $0 \le i < n$. Consider also the $4n$ Jordan curves obtained by rotating each of these n Jordan curves by 0°, 90°, 180°, 270° around the point 0. Some of these may be identical, but J may be any of these with equal probability. Once it is shown that the fraction f of these which contain $(\frac{1}{2}, \frac{1}{2})$ as an inside point is $\frac{1}{2} - \frac{1}{n}$, it will follow that

$$P\left(\left(\frac{1}{2}, \frac{1}{2}\right) \text{ is inside } J\right) = f = \frac{1}{2} - \frac{1}{n} \; . \tag{2}$$

To prove that, suppose that vertex T_j of J is convex. Then exactly 1 of the 4 rotations of J_j contains $(\frac{1}{2}, \frac{1}{2})$. If T_j of J is concave then exactly 3 of the 4 rotations of J_j contain $(\frac{1}{2}, \frac{1}{2})$ and if S_j is straight then exactly 2 of the 4 rotations of J_j contain $(\frac{1}{2}, \frac{1}{2})$. Therefore,

$$f = \frac{v + 3c + 2s}{4n} \; .$$

Since the total signed curvature of a simple closed planar polygon is $\pm 2\pi$ it follows that

$$v - c = 4$$

and so, by (1) and (2),

$$f = \frac{2v + 2c + 2s + c - 4}{4n} = \frac{1}{2} - \frac{1}{n}\,. \quad \Box$$

The above proof shows that the fraction of rotations and cyclic permutations of any n-loop which contain $(\frac{1}{2}, \frac{1}{2})$ is $\frac{1}{2} - \frac{1}{n}$. It is worth noting that one can prove somewhat more, that the rotations can be ignored.

The *translation-shape* of an n-loop, J, with nodes $T_1, \ldots, T_n$ is the set S of n n-loops $J - T_j$, $1 \leq j \leq n$, obtained by translating J by the negatives of the vectors T_j.

Theorem 2 The probability that a simple, nearest-neighbor, symmetric random walk on the planar integral lattice generates an n-loop that contains the point $(\frac{1}{2}, \frac{1}{2})$ in its interior, given that the random walk generates an n-loop of any specified translation shape is $\frac{1}{2} - \frac{1}{n}$.

This theorem is easily seen to follow from, and indeed to be equivalent to, the following more elementary proposition. But first a tiny bit of notation is useful.

For an n-loop J with nodes t_j, $1 \leq j \leq n$, let $W = W(J)$ be the set of j such that $t_j + (\frac{1}{2}, \frac{1}{2})$ is in the interior of J.

Proposition 1 For every n-loop J, W(J) has cardinality $\frac{n}{2} - 1$.

Proof: Plainly, the proposition holds when J is a one by one square, that is, when $n = 4$. For $n \geq 6$, write $n = 2k$, and suppose that the proposition holds for all $n' < n$, that is, for all $k' < k$. To establish the induction step, namely, that the proposition then necessarily holds for k, consider first those n-loops that have a special structure. A self-avoiding random walk all of whose steps are identical is a *straight walk*. A U-*turn* is a self avoiding walk t with these properties: the first and second steps are distinct, the last and next to last steps are distinct, the first step s is followed by a straight walk which in turn is followed by $-s$, which is the last step of t.

A pair of nodes on an n-loop J is *special* for J if: (a) the pair of nodes partitions J into two (self-avoiding) walks at least one of which is a U-turn, and (b) no proper convex combination of the pair of nodes is on J. The induction will be established in two stages. Stage 1 uses the induction hypothesis to show that, for n-loops J that have a pair of special nodes, $W(J)$ does have cardinality $\frac{n}{2}-1$, and Stage 2 will be a proof that every n loop has a pair of special nodes.

Proof of Stage 1. Let J' be the loop obtained from J by substituting for the U-turn the straight line segment joining the special pair of nodes of J. Plainly, the length of the U-turn exceeds by 2 the length of the line segment joining its end points. Therefore, the length of J exceeds by 2 the length of J'. So J' is an $(n-2)$-loop. By the inductive assumption

$$W(J') \text{ has cardinality } \frac{n-2}{2} - 1 = \frac{2k-2}{2} - 1 = k-2\ ,$$

so, for Stage 1 it plainly suffices to see that the cardinality of $W(J)$ exceeds by 1 the cardinality of $W(J')$. To this end, the set of nodes of J will be partitioned into two sets V and S, and the set of nodes J' into two sets S' and V' in such a manner that $S \bigcap W(J)$ has the same cardinality as $S' \bigcap W(J')$, and the cardinality of $V \bigcap W(J)$ exceeds by 1 the cardinality of $V' \bigcap W(J')$, which, once established, will complete the proof. For V, choose the set of four (geometric) vertices of the U-turn, that is, its first two and last two nodes, and for S the set of all other nodes of J. Let V' be the pair of special nodes which is, of course, a subset of V, and let S' be the set of all other nodes of J'. To see that $S \bigcap W(J)$ has the same cardinality as $S' \bigcap W(J')$, it is sufficient to exhibit a bijective map Ψ of S onto S' that carries $S \bigcap W(J)$ onto $S' \bigcap W(J')$.

To define Ψ, first partition S into the two sets, $S \bigcap S'$ and α, its complement relative to S, and partition S' into $S \bigcap S'$ and α', its complement relative to S'. On $S \bigcap S'$, let Ψ be the identity. If $S \bigcap S' = S$, that is, if α is void, the definition of Ψ is complete. Otherwise, notice that there is a unique translation of α onto α', and let Ψ agree with this translation on α.

Plainly, Ψ is a bijection of S onto S'. For the nontrivial property of Ψ, verify that for each $v \in S$, there is an infinite ray ρ' emanating from $v + (\frac{1}{2}, \frac{1}{2})$ that is parallel to one of the coordinate axes, and a parallel infinite ray ρ' emanating from $\Psi(v) + (\frac{1}{2}, \frac{1}{2})$, such that the intersection of ρ with J is identical with the intersection of ρ' with J'. Certainly, therefore, $\rho \bigcap J$ has odd cardinality if, and only if, $\rho' \bigcap J'$ does. Therefore, $v + (\frac{1}{2}, \frac{1}{2})$ is in the interior of J if, and only if, $\Psi(v)$ is in the interior of J'. That is, $v \in W(J)$ if, and only if, $\Psi(v) \in W(J')$. As so Ψ maps $S \bigcap W(J)$ onto $S' \bigcap W(J')$.

So, to complete the argument for Stage 1, it is plainly necessary, and sufficient, to verify that the number of elements of the four element set V that are in $W(J)$ exceeds by one the number of elements of the two element set V' that are in $W(J')$. This is perhaps most easily done by considering separately the two cases according as the proper convex combinations of the two special nodes are interior or exterior to J, and for each of these two cases the four subcases according to the four possible orientations of the U-turn. Though it is unfortunate to have eight cases, it is fortunate that for each of them, the assertion about V and V' is easily verified.

Proof of Stage 2. Let J be any n-loop with $n \geq 6$. This stage shows that J possesses a special pair of nodes. First verify that J includes a U-turn. Indeed, let L be, for instance, a horizontal line of support of J, say from below. Then $L \bigcap J$ is a non-empty disjoint union of nonempty closed intervals each of which is a subwalk of J, obviously straight. Each of these intervals, I, determines a unique U-turn included in J obtained by supplementing I with the step of J emanating from each end point of I. So, included in J is a U-turn of minimal length. Let U be one such, and let v and w be the first and last nodes of U. Then v and w constitute a special pair of nodes of J. For, were they not, then U would not be of minimal length, as can be seen, thus.

Suppose first that some proper convex combinations of v and w were in J and some were not. **Case 1** Suppose the intersection of J with the set of proper convex combinations of v and w is closed. Then it would be a non-empty union of a finite number of non-empty closed intervals. Each of these closed intervals together with the two steps of J emanating from the end points of the interval would constitute a U-turn whose length is less than the length of U. **Case 2** The intersection is not closed. Then U is of length at least 4, but there exists a U-turn of length 3, as is easily seen. Consider next the case that every proper convex combination of v and w were in J. Then the union of this set with U is a rectangle included in the loop J. So J must be this rectangle. Since this rectangle has width 1, and $n \geq 6$, its length, in the usual elementary sense, exceeds its width. Obviously, this rectangle would then include a U-turn of length less than that of U. The only remaining case is that no proper convex combination of v and w is in J. So v and w constitute a special pair of nodes of J. This completes the proof.

We are indebted to John Tillinghast for stimulating, and to G. D. Chakerian for providing, another argument for Proposition 1. This second argument is based on the observation that the area, A, of the interior of J is the number of open lattice squares included in the interior of A. (Here, a lattice square is simply a one by one square whose vertices are lattice points.) Some of these lattice squares have their lower left-hand corners in the interior of J, the rest have their lower left-hand corners in $W(J)$. So A is simply $I + |W(J)|$ where I is the number of lattice points in the interior of J and $|W(J)|$ is the cardinality of $W(J)$. But there is also, another beautiful formula for A, known as Pick's Formula, namely A is $I + \frac{1}{2}B - 1$ where B is the number of lattice points on J. Consequently, $|W(J)| = \frac{1}{2}B - 1 = \frac{n}{2} - 1$. For a reference to Pick's formula, which is valid for a larger class of polygons than loops, see, for example Coxeter [24].

Let $P_n(x,y)$ denote the probability that J encircles (x,y). The argument of Theorem 2 shows that $P_n(x,y) = \frac{1}{2} - \frac{1}{n}$ for all (x,y) inside the unit square: $|x|,|y| < 1$. However, we do not know the corresponding $P_n(x,y)$ for any other point in the plane. The difficulty with obtaining a corresponding simple formula for say $P_n(\frac{3}{2},\frac{1}{2})$, is that the fraction of translations of an n-loop which contains $(\frac{3}{2},\frac{1}{2})$ is not constant but depends on the shape of the n-loop.

For that reason, we resort to simulations. The algorithm devised for generating random n-loops is described in Section 4. This algorithm draws heavily from the so called pivot algorithm[1] for generating random n-walks which is described in the next section.

3 Generating a random self-avoiding n-walk

The pivot algorithm for generating a random self-avoiding n-walk was invented by Lal [16]. A description and neat analysis of it appeared in Madras and Sokal [23]. That description is slightly modified here so as to set the background for the loop algorithm offered in Section 4.

The pivot algorithm simulates a Markov chain whose states are all self avoiding n-walks and whose unique equilibrium distribution is uniform over the states. The algorithm does so by performing a random walk on a directed graph whose vertices are the self-avoiding random walks in the plane and whose edges, possibly multiple, are defined via the following transformations on the set of n-walks.

Each k in $\{0,\ldots,n-1\}$ determines 4 transformations on the set of n-walks. Each of these transformations, applied to a walk t, preserves the initial trajectory $t_0,\ldots,t_k$ determined by t and k, and transforms the terminal trajectory $t_{k+1},\ldots,t_n$ by one of four rigid motions: the reflection in the horizontal or vertical line that contains t_k; the rotation of $\pm\frac{\pi}{2}$ radians that has t_k for its fixed point. Let T_k^v, T_k^h, T_k^+, and T_k^- designate the four transformations.

[1] Not to be confused with the pivot algorithm in linear programming.

Figure 1: T_k^v and T_k^- operating on a simple walk

Figure 1 depicts the effect of T_k^v and T_k^- on a simple walk. Letting $\overline{z}$ denote the complex conjugate of z, one has:

$$\begin{aligned}
T_k^v(s_0, \ldots, s_{n-1}) &\stackrel{\text{def}}{=} (s_0, \ldots, s_{k-1}, \overline{s_k}, \ldots, \overline{s_{n-1}}) \\
T_k^h(s_0, \ldots, s_{n-1}) &\stackrel{\text{def}}{=} (s_0, \ldots, s_{k-1}, -\overline{s_k}, \ldots, -\overline{s_{n-1}}) \\
T_k^+(s_0, \ldots, s_{n-1}) &\stackrel{\text{def}}{=} (s_0, \ldots, s_{k-1}, is_k, \ldots, is_{n-1}) \\
T_k^-(s_0, \ldots, s_{n-1}) &\stackrel{\text{def}}{=} (s_0, \ldots, s_{k-1}, -is_k, \ldots, -is_{n-1}).
\end{aligned}$$

Remarks:

1. Each T_k^h and T_k^v is its own inverse, and T_k^+ is the inverse of T_k^-.

2. Some of the $4n$ transformations, performed on a self-avoiding n-walk, yield a self-intersecting n-walk. Indeed, for each n-walk t with $n \geq 2$ and each $k \in \{1, \ldots, n-1\}$, at least one of the above four transformations transforms t into a self-intersecting walk.

The graph $G_n \stackrel{\text{def}}{=} \langle V_n, E_n \rangle$ on which the random walk is performed can now be defined. V_n is the set of self-avoiding n-walks. For each $v \in V_n$, consider all of the above $4n$ transformations. If a transformation takes v to another self-avoiding n-walk, $v' \in V_n$, add the edge (v, v') to E_n. If a transformation takes v to a walk that is not self-avoiding, add the self edge (v, v) to E_n.

For any two distinct n-walks v and v' in V_n, there is at most one transformation that takes v to v', hence at most one edge (v, v'). However, there might be multiple edges (v, v), corresponding to several transformations taking v to a walk that is not self-avoiding.

The construction implies that the outdegree of each node (the number of edges emanating from it) is exactly $4n$. From Remark 1 above, the edge (v, v') exists if and only if the reverse edge, (v', v) exists too. In addition, every self edge contributes one to both the in and out degree of a vertex. Therefore the indegree of each vertex is also $4n$.

Recall that a *path of length l* from a vertex v to a vertex v' in a directed graph $G = \langle V, E \rangle$ is a sequence $v_0, \ldots, v_l$ of vertices such that $v_0 = v$, $v_l = v'$, and $(v_j, v_{j+1}) \in E$ for $0 \leq j < l$. The *distance* from v to v' in G is the smallest length of all paths from v to v'. G is called *strongly connected* if for all pairs v, v' of vertices, there is a path from v to v' and a path from v' to v. The *diameter* of a strongly connected graph is the maximum, over all pairs v, v' of vertices, of the distance from v to v'.

Theorem 3 (Madras and Sokal [23]) The graph G_n:

1. has indegree and outdegree $4n$ for each vertex,

2. is strongly connected,

3. has diameter at most $4n$.

Proof: Assertion 1 follows from the discussion above. For a proof of 2 and 3, let t be a walk and define $d(t) = |\mathrm{re}(t_n)| + |\mathrm{im}(t_n)|$ to be the L_1 distance between t_0 and t_n. An index $k \in \{1, \ldots, n-1\}$ is a *turn of t* if $s_k \neq s_{k-1}$. Denote the number of turns of t by $c(t)$. A walk without turns is *straight*.

Claim: Every self-avoiding n-walk t that is not straight can be transformed by one of the $4n$ mappings to a self-avoiding n-walk t' such that either:

1. $d(t') \geq d(t)$ and $c(t') = c(t) - 1$, or
2. $d(t') \geq d(t) + 1$ and $c(t') = c(t)$.

The theorem follows from this claim because at most $c(t) + n - d(t)$ such transformations need be applied to an n-walk t before it becomes straight and, plainly, $d(t) > 0$ and $c(t) \leq n - 1$. Hence for any self-avoiding walk t, there is a sequence $t^1, \ldots, t^m$ of self-avoiding n-walks such that: $t^1 = t$, t^m is straight, $m \leq 2n - 1$, and for $k = 1, \ldots, m-1$, the edge (t^k, t^{k+1}) is in E_n. Since any straight n-walk is adjacent in G_n to any of the other 3 straight n-walks, and since the inverse of each transformation is also an allowed transformation, it follows G_n is strongly connected and has diameter of at most $4n - 1$.

Proof of Claim: Let R be the smallest rectangle with sides parallel to the axes that includes (circumscribes) t. Since t is not straight, no two sides of R coincide.

If t_n is a corner of R, let k be the largest turn index of t. Plainly, t_k is on one of the two sides of R that contain t_n. Of the two transformations T_k^+ and T_k^- let T be the one for which s'_k is s_{k-1} and let $t' = T(t)$. It is easy to see that t' satisfies part 1.

If t_n is not a corner of R, then, without loss of generality:

a) t_n is neither on the top side, nor on the bottom side of R, and

b) t_0 is not on the top side of R.

Let k be such that t_k is on the top side of R, and $t' = T_k^v(t)$. Then t' satisfies part 2. $\square$

To generate a pseudo-random n-walk, perform a random walk on G_n as follows. Starting at any vertex of G_n, sequentially visit the vertices of G_n according to the following rule. While at vertex v, uniformly pick one of the $4n$ edges (v, v') emanating from v and move to v' (the edge (v, v') can be a self edge). By the following well known theorem, the equilibrium distribution of the vertices visited is uniform on V_n.

Theorem 4 Let G be a directed, strongly-connected, multigraph with in and out degree d for all vertices and at least one self-edge. Then the Markov chain γ which moves from a vertex v along an edge emanating from v to the destination vertex of the edge, uniformly over all edges emanating from v, has the uniform distribution on G as its unique equilibrium distribution.

Proof: Let $P(v \rightarrow v')$ be the probability of moving from v to v' in one step. The stationary distribution π obeys the equilibrium equation:

$$\pi(v') = \sum_{v \in V} \pi(v) P(v \rightarrow v')$$

for all $v' \in V$. For the random process γ, $P(v \rightarrow v')$ is $m(v, v')/d$ where $m(v, v')$ is the multiplicity of the edge (v, v'). Hence, $\sum_{v \in V} P(v \rightarrow v') = \sum_{v \in V} m(v, v')/d = d/d = 1$ and the uniform distribution satisfies the equilibrium equation. Since there is at least one self edge, the graph is aperiodic. Since G is strongly connected, the states communicate and and π is unique. $\square$

Remarks:

1. If all vertices have k or more self-edges attached to them, then k self-edges can be removed from each vertex. A random walk performed on the resulting graph would reach equilibrium faster than the original walk. However, computing the largest such k seems time consuming.

2. The graph G_n is *symmetric*: the number of (v, v') edges equals the number of (v', v) edges for all v and v'. Suppose G_n is amended to a symmetric graph G'_n by adding non-self edges. It is clear that parts 2 and 3 of the theorem remain valid. An easy application of the Weyl or Rayleigh-Ritz Lemma (e.g. Lawler and Sokal [25]) shows that each eigenvalue of the incidence matrix A'_n of G'_n is smaller than the corresponding eigenvalue of the incidence matrix A_n of G_n. Hence a random walk on G_n would approach equilibrium more rapidly. On the other hand, additional edges increase the amount of computation performed at each step of the algorithm. The trade-off seems hard to determine.

3. The construction given in this section generalizes to d-dimensions (see Madras and Sokal [23]); the description here was restricted to $d = 2$ for clarity.

4 Generating a random self-avoiding n-loop

This section describes an algorithm for generating self-avoiding, uniformly-distributed, random n-loops. The ideas and definitions are similar to those of the Pivot Algorithm described in the previous section. However here the transformations are somewhat more complex, depend on a pair of vertices, and operate on arbitrary segments of the loop rather than terminal segments only.

An *n-loop* is a sequence $s_0, \ldots, s_{n-1}$ of steps (elements of $\{1, -1, i, -i\}$) such that $s_0 + \cdots + s_{n-1} = 0$. An n-loop $s_0, \ldots, s_{n-1}$ is *self-avoiding* if the sequence $t_0, \ldots, t_n$ defined by $t_0 = 0$, and $t_j = s_0 + \cdots + s_{j-1}$ for $1 \leq j \leq n$, satisfies $t_j \neq t_k$ for $0 \leq j < k < n$.

A *random* self-avoiding n-loop is a random element of the set of self-avoiding n-loops, each picked with equal probability. Equivalently, it is a sequence of independent random variables $S_0, \ldots, S_{n-1}$, where $S_j = \pm 1, \pm i$, each with probability $\frac{1}{4}$, conditioned so that $T_j \neq T_k$ for all $0 \leq j < k < n$, and $T_n = 0$, where $T_0 = 0$ and $T_j = S_0 + \cdots + S_{j-1}$.

The random self-avoiding n-loops are generated by randomly walking on a graph of self-avoiding n-loops whose edges are defined via the set of transformations described below.

In an n-loop, step j follows step $j-1$ for $1 \leq j \leq n-1$ and step 0 follows step $n-1$. It is therefore useful to view the step-indices as integers modulo n. Step s_n, for example, is identified with s_0. Accordingly, the *interval* $\{k, \ldots, l\}$ for $k > l$ is defined as the set $\{k, \ldots, n-1\} \bigcup \{0, \ldots, l\}$. For $k \leq l$, the *interval* $\{k, \ldots, l\}$ is plainly defined as the set $\{k, \ldots, l\}$. Similarly, the sequence $s_k, \ldots, s_l$ for $k > l$ denotes the sequence $s_k, \ldots, s_{n-1}, s_0, \ldots, s_l$.

For each ordered pair of distinct indices $k, l \in \{0, \ldots, n-1\}$, define two transformations:

1. Rotation between k and l:

$$T_{k,l}^{rot}(s_0, \ldots, s_{n-1}) \stackrel{\text{def}}{=} (s'_0, \ldots, s'_{n-1})$$

   where

$$s'_j \stackrel{\text{def}}{=} \begin{cases} s_{l+k-j} & \text{if} \quad j \in \{k, \ldots, l\}; \\ s_j & \text{otherwise.} \end{cases}$$

2. Reflection between k and l:

$$T_{k,l}^{ref}(s_0, \ldots, s_{n-1}) \stackrel{\text{def}}{=} (s'_0, \ldots, s'_{n-1})$$

   where

$$s'_j \stackrel{\text{def}}{=} \begin{cases} \overline{i s_{l+k-j}} & \text{if} \quad j \in \{k, \ldots, l\}; \\ s_j & \text{otherwise.} \end{cases}$$

Figure 2: Rotation and reflection transformations of n-loops

Both transformations preserve all steps in $\{s_{l+1}, \ldots, s_{k-1}\}$ but modify the steps $s_k, \ldots, s_l$. A rotation rotates the set $\{t_k, \ldots, t_l\}$ around the midpoint $(t_k + t_l)/2$ in the complex plane. A reflection reflects the set $\{t_k, \ldots, t_l\}$ in the perpendicular bisector of t_k and t_l. Figure 2 depicts the affect of these transformations on a simple loop. A rotation always transforms an n-loop into another n-loop, not necessarily self-avoiding, while a reflection transforms a loop into another loop if and only if $\mathrm{re}(t_k) - \mathrm{re}(t_l) = \mathrm{im}(t_k) - \mathrm{im}(t_l)$. That is, the line connecting t_k and t_l in the complex plane has slope 1. Even then, the resulting loop is not necessarily self-avoiding.

The graph $H_n = \langle V_n, E_n \rangle$ is then defined analogously to G_n. V_n is the set of self-avoiding n-loops. Each loop $v \in V_n$ and each of the above $4\binom{n}{2}$ transformations contribute an edge to E_n. If the transformation takes v to another self-avoiding n-loop $v \in V_n$, the edge is (v, v'), if the transformation does not take v to another self-avoiding n-loop, the edge is the self-edge (v, v).

Theorem 5 The graph H_n:

1. has in and out degree $4\binom{n}{2}$ for each vertex,

2. is strongly connected,

Figure 3: A loop with 22 turns and three of its support lines

3. has diameter at most $2n-6$.

Proof: Part (1) follows from the definition; parts (2) and (3) are proved next. The points $t_0, t_1, \ldots, t_n$ along with the unit segments connecting t_j to t_{j+1}, $j = 0, \ldots, n-1$ form a simple closed curve J in the plane which therefore has an inside and an outside.

A straight line in the plane is called a *support line for J* if it goes through at least two points of J but does not intersect the inside of J. A support line is called *external* if it contains three points a, b, c, in that order, such that $a, c \in J$ but b is outside J. It is called *horizontal* or *vertical* if it is horizontal or vertical as a line, otherwise it is called *diagonal.*

As with walks, an index $k \in \{0, \ldots, n-1\}$ is called a *turn of t* if $s_k \neq s_{k-1}$. The number of turns of t is denoted by $c(t)$. For $n > 2$, every n-loop has at least 4 turns. An n-loop with 4 turns ($c(t) = 4$) is called a rectangle. Figure 3 illustrates some of these concepts.

The following facts are evident.

1. If t is not a rectangle, then t has an external support line.

2. If a horizontal or a vertical external support line of t intersects t at t_k and t_l, and the segment between t_k and t_l is not all on J, then, $t' \stackrel{\text{def}}{=} T^{rot}_{k,l}(t)$ is a self-avoiding n-loop, t and t' have the same number of turns, i.e., $c(t') = c(t)$, and t' has a diagonal external support line.

3. If a diagonal external support line of t intersects t at t_k and t_l, and the segment between t_k and t_l is not all on J, then $t' \stackrel{\text{def}}{=} T^{rot}_{k,l}(t)$ is a self-avoiding n-loop and $c(t') = c(t) - 2$.

Claim: Every self-avoiding n-loop with $k > 4$ turns can be transformed via at most two transformations to a self-avoiding n-loop with $k - 2$ turns.

Proof: Let t be a loop with $k > 4$ turns. By fact 1, it has external support lines. If at least one of them is diagonal, the claim holds by fact 3. If all are vertical or horizontal then, from fact 2, t can be transformed to a self-avoiding n-loop t' with k turns (hence, not a rectangle), which has a diagonal support line. From fact 3, t' can be transformed to a self-avoiding n-loop t'' with $c(t'') = c(t) - 2 = k - 2$.

This shows that any self-avoiding n-loop is connected to a rectangle via a path of length $\leq n - 4$ in H_n. If t' and t'' are two self-avoiding n-loops, there are paths of length $\leq n - 4$ connecting them to rectangles r' and r'' respectively. These rectangles need not be the same (in fact, the number of horizontal segments, that is, $|\{i : s_i \text{ is } 1 \text{ or } -1\}|$ is invariant under rotation transformations, and so r' and t' will have the same number of horizontal segments). However, it is possible to transform any rectangle to any other rectangle via one rotation and one reflection transformation, showing that the diameter is at most $2n - 6$. $\square$

The theorem can be used to generate a pseudo-random n-loop as in Section 3. Again, one can add non-self edges and delete self-edges to speed mixing. For example, one could reflect about 135° lines as well as about the 45° lines used in $T^{ref}_{k,l}$. Note also that rotations preserve the number of horizontal (and vertical) segments in a loop while reflections preserve its area. Thus both are required to connect the graph.

5 Some numerical evidence to support the conjecture

Figure 4 describes the exact values for $n \leq 26$ of:

$$P_n\left(\frac{3}{2}, \frac{1}{2}\right) = \frac{\text{number of self-avoiding } n\text{-loops enclosing } (\frac{3}{2}, \frac{1}{2})}{\text{number of self-avoiding } n\text{-loops}}$$

and of the function $c(n)$ satisfying:

$$P_n\left(\frac{3}{2}, \frac{1}{2}\right) = \frac{1}{2} - \frac{c(n)}{n}$$

n	number of self-avoiding n loops	number of loops encircling $(\frac{3}{2}, \frac{1}{2})$	$P_n(\frac{3}{2}, \frac{1}{2})$	$c(n)$
4	8	0	0	2
6	24	2	0.083	2.5
8	112	18	0.161	2.714
10	560	120	0.214	2.857
12	2976	756	0.254	2.952
14	16464	4674	0.284	3.026
16	94016	28892	0.308	3.083
18	549648	179272	0.326	3.129
20	3273040	1118244	0.342	3.167
22	19781168	7014638	0.355	3.199
24	121020960	44246384	0.366	3.225
26	748039552	280558888	0.375	3.248

Figure 4: Exact values of $P_n(\frac{3}{2}, \frac{1}{2})$ and $c(n)$ for $n \leq 26$

The last case was calculated in tens of hours. Using one of Steve's favorite graphical techniques, P_n was plotted versus $\frac{1}{n}$. The intercept was very close to $\frac{1}{2}$ which seems to imply that $P_n(\frac{3}{2},\frac{1}{2}) = \frac{1}{2} - \frac{c}{n} + o(\frac{1}{n})$ for some fixed c. Unfortunately, the numbers $c(n)$ in the table keep increasing and the last calculated value is only $P_{26}(\frac{3}{2},\frac{1}{2}) = .375$, so this is not enough evidence to support the conjecture. Using the generation algorithm of the previous section, we performed non-systematic simulations for larger values of n, up to 300. They seem to informally support the conjecture, but give us no real estimate for c. More careful use of the simulation method is required.

Acknowledgements

We thank G.D. Chakerian, Peter Doyle, John Tillinghast, and Allan R. Wilks for useful discussions.

References

[1] E. Helfand and D.S. Pearson, 'Statistics of the entanglement of polymers: Unentangled loops and primitive paths', *J. Chem. Phys.* 79, pp. 2054-2059, 1983.

[2] B. Simon, 'Fifteen Problems in Mathematical Physics, Perspectives in mathematics', Birkhauser, Boston, 1984.

[3] J.T. Chayes, 'Ornstein-Zernike behavior for self-avoiding walks at all noncritical temperatures', *Comm. Math. Phys.*, 105, pp. 221-238, 1986.

[4] J.M. Hammersley, 'The number of polygons on a lattice', *Proc. Camb. Phil. Soc.* 57, pp. 516-523, 1961.

[5] H. Kesten, ‘On the number of self-avoiding walks’, *J. Math. Phys.* 4, pp. 960-969, 1963.

[6] A.J. Guttmann, ‘On two-dimensional self-avoiding random walks’, *J. Phys. A*, 17, pp. 455-468, 1984.

[7] J.F. Le Gall, ‘Propriétés D’intersection des Marches Aléatoires’, *Comm. Math. Phys.* 104, pp. 509-528, 1986.

[8] N. Pippenger, ‘Knots in random walks’, unpublished manuscript, 1987.

[9] S. Hemmer and P.C. Hemmer, ‘An average self-avoiding random walk on the square lattice lasts 71 steps’, *J. Chem. Phys.* 81, pp. 584-585, 1984.

[10] P.C. Hemmer, ‘Trapping of genuine self-avoiding walks’, *Phys. Rev. A* 34, pp. 3304-3308, 1986.

[11] C. Aragao de Carvalho and S. Caracciolo, ‘A new Monte Carlo approach to the critical properties of self-avoiding random walks’, *J. Physique*, 44, pp. 323-331, 1983.

[12] C. Brender, D. Ben-Avraham, and S. Havlin, ‘Study of Monte-Carlo methods for generating self-avoiding walks’, *J. Stat. Phys.*, 31, pp. 661-670, 1983.

[13] B.L. Myers, N.L. Enrick, R. R. Edmond, and J.H. Lindgren, ‘A Monte Carlo approach for the solution of the simple quadratic and cubic self-avoiding random walk’, *Simuletter, Special interest group on simulation, ACM*, 14, pp. 44-63, 1983.

[14] A. Berretti and A.D. Sokal, ‘New Monte Carlo method for the self-avoiding walk’, *J. Stat. Phys.* 40, pp. 483-531, 1985.

[15] A. Sariban, K. Binder, and D.W. Heermann, ‘Monte Carlo test of the Flory-Huggins theory for polymer mixtures’, *Phys. Rev.* B, 35, pp. 6873-6876, 1987.

[16] M. Lal, 'Monte Carlo computer simulation of chain molecules I', *Molec. Phys.* 17, pp. 57-65, 1969.

[17] O.F. Olaj and K.H. Pelinka, 'Pair distribution function and pair potential of lattice model of chains under theta conditions - 1', *Makromol. Chem.* 177, pp. 3413-3425, 1976.

[18] B. MacDonald, N. Jan, D.L. Hunter, and M.O. Steinitz, 'Polymer conformations through wiggling', *J. Phys. A*, 18, pp. 2627-2631, 1985.

[19] D.L. Hunter, N. Jan, and B. Macdonald, 'On the correction-to-scaling exponent of linear polymers in two dimensions', *J. Phys. A*, 19, pp. L543-L545, 1986.

[20] S.D. Stellman and P.J. Gans, 'Efficient computer simulation of polymer conformation - I. Geometric properties of the hard-sphere model', *Macromolecules*, 5, pp. 516-525, 1972.

[21] S.D. Stellman and P.J. Gans, 'Efficient computer simulation of polymer conformation - II. Distribution function for polymers with excluded volume', *Macromolecules*, 5, pp. 720-729, 1972.

[22] J.J. Freire and A. Horta, 'Mean reciprocal distances of short polymethylene chains. calculations of the translational diffusion coefficient of n-alkanes', *J. Chem. Phys.*, 65, pp. 4049-4053, 1976.

[23] N. Madras and A.D. Sokal, 'The pivot algorithm: a highly efficient monte carlo method for the self-avoiding walk', preprint, 1987.

[24] H.S.M. Coxeter, *Introduction to Geometry*, John Wiley & Sons, New York, p. 209, 1969.

[25] G.F. Lawler and A.D. Sokal, 'Bounds on the L^2 spectrum for Markov chains and Markov Processes: a generalization of Cheeger's inequality', preprint, 1987.