Self-avoiding walks and tilted-line hits

Matthew Green
Supervised by Professor Tom Kennedy

May 30, 2005

Introduction.
The first objective of this project was to develop an understanding of the pivot algorithm to simulate self avoiding walks (SAW) on a rectangular lattice. A second objective was to calculate the cumulative distribution functions for some random variables associated with properties of the SAW. The second objective can be pursued in two ways: (1) Using computer simulations, (2) Using a result from Schramm-Lowner Evolution (SLE) theory. Both methods were used to obtain the cumulative distribution function for the random variable that takes on the value of the lowest point at which a SAW, starting at the origin, intersects a tilted line in the complex, upper-half plane.

The first part of this paper will be concerned with describing the pivot algorithm and Monte Carlo method used to determine the cumulative distribution function for the tilted-line random variable. The second part will give a primitive interpretation of SLE theory and will state the results used to obtain a cumulative distribution function for the tilted-line random variable.

Pivot Algorithm and Monte Carlo method.
All SAWs we will be concerned with take place on a two-dimensional, rectangular lattice. Furthermore, all SAWs begin at the origin and are finite-length. Let the symbol $\mathbf{W}$ stand for the set of SAWs of finite length N. Clearly, $\mathbf{W}$ is a finite set. The pivot algorithm takes as input a SAW $\omega_n \in \mathbf{W}$ and randomly produces another SAW $\omega_{n+1} \in \mathbf{W}$. The actual implementation of the pivot algorithm developed by Professor Tom Kennedy that we used in this project is very complicated, and we give only a basic, conceptual description of the algorithm here (which has been taken directly from Madras and Slade):

Let G be the group of two-dimensional lattice symmetries. G has 8 elements: 4 rotations, two axis reflections, and two diagonal reflections.
Step 1. Select any $\omega_0 \in \mathbf{W}$ (the easiest way to do this is to take ω_0 to be a straight line walk, which is obviously self-avoiding).
Step 2. Choose an integer i uniformly from the set $\{0, 1, 2, \ldots, N-1\}$. Call $x = \omega_t(i)$ the pivot site. Select a lattice symmetry g uniformly from the symmetry group G. Set $\bar{\omega}(k) = \omega_t(k)$ for $k \leq i$, and $\bar{\omega}(k) = g(\omega_t(k))$ for $k > i$.
Step 3. If $\bar{\omega}$ is self-avoiding, set $\omega_{t+1} = \bar{\omega}$. Otherwise let $\omega_{t+1} = \omega_t$.

Step 4. Increase t by 1 and go to step 2.

The pivot algorithm, when repeatedly applied, produces a sequence $\{\omega_t : t = 0, 1, 2, \ldots\}$, which is a Markov chain with state space $\mathbf{W}$. This Markov chain is aperiodic and irreducible with uniform stationary distribution π, and is reversible, that is, $\pi(\omega_i) \cdot P(\omega_i, \omega_j) = \pi(\omega_j) \cdot P(\omega_j, \omega_i)$. Since π is uniform, the reversibility condition reduces to $P(\omega_i, \omega_j) = P(\omega_j, \omega_i)$, i.e. the transition probability matrix P is symmetric. It is easy to show that P is symmetric for the pivot algorithm: Suppose there are m ways to move, with one pivot, from a SAW ω to another SAW $\bar{\omega}$. For $i = 1, 2, \ldots, m$, consider the pairs (x_i, g_i), where the first component is a pivot point on the SAW and the second component is a symmetry operation. Each pair gives a transition, using the pivot algorithm, from ω to $\bar{\omega}$. Thus the probability of making a transition from ω to $\bar{\omega}$ is

$$P(\omega, \bar{\omega}) = \sum_{i=1}^{m} P(g = g_i) \cdot P(x = x_i). \tag{1}$$

Notice that the pairs (x_i, g_i^{-1}), for $i = 1, 2, \ldots, m$ give one step transitions from $\bar{\omega}$, and that $P(g = g_i) = P(g = g_i^{-1})$ because g is chosen uniformly. Therefore

$$P(\omega, \bar{\omega}) = \sum_{i=1}^{m} P(g = g_i) \cdot P(x = x_i) = \sum_{i=1}^{m} P(g = g_i^{-1}) \cdot P(x = x_i) = P(\bar{\omega}, \omega). \tag{2}$$

This shows the symmetry of P. It is harder to show that the pivot algorithm is irreducible (see Madras and Slade for a proof).

Suppose that our two-dimensional lattice is embedded in the complex plane, and consider the ray

$$R(s) = c + se^{i\pi\alpha}, s \in [0, \infty), \tag{3}$$

where c is a positive real number and $\alpha \in (0, 1)$. Define a random variable $T(\omega)$, which takes the value of the magnitude of the closest point to zero where the SAW ω intersects the ray $R(s)$. We wish to find the cumulative distribution function $F(l)$ for T. To do this we choose a finite length N and generate, using the pivot algorithm, lots of SAWs of length N. For each SAW we calculate the point where the SAW hits the ray $R(s)$. To calculate the probability that a SAW hits the ray $R(s)$ at a length along the ray less than $l = |R(a)|$ we simply count the number k of SAWs intersecting the set $\{R(s) : 0 \leq s < a\}$, and then, since SAWs were chosen uniformly (in the limit), we have $F(l) = \frac{k}{|W|}$ where $|W|$ is the number of SAWs of length N.

SLE and the exact CDF.
Another way to find the cumulative distribution function (CDF) for the random variable T is to use a powerful result from SLE theory. An SLE is a continuous curve γ in the complex plane, and may be thought of as the continuous limit of a SAW as the lattice spacing approaches zero. So we can think of SAW as a

discrete approximation of SLE, and what is true of SLE is approximately true of SAW. The random variable T in the case of SLE is defined in exactly the same way as it was in the case of SAW. For the case of SLE, we call the CDF of T the exact CDF. As with SAWs, we are concerned only with SLEs starting at the origin and taking place entirely in the upper-half plane H.

Theorem. Let A be a compact subset of $\bar{H}$, which does not contain 0 and such that $H \setminus A$ is simply connected. Let Φ_A be the conformal map from $H \setminus A$ onto H which fixes 0 and ∞ and has $\Phi'_A(\infty) = 1$. For $\kappa = 8/3$, SLE in a half plane satisfies

$$P(\gamma[0,\infty) \cap A = \emptyset) = \Phi'_A(0)^{5/8}. \tag{4}$$

We won't worry about the details of this theorem. The main point here is that this gives us a way to determine the exact CDF for the random variable T.

Let $L_a = \{R(s) : 0 \leq s \leq a\}$ be the line segment along the ray $R(s)$ of length a. An SLE hits the tilted ray $R(s)$ at a point between $R(0)$ and $R(a)$ if and only if it intesects the set L_a. The theorem above tells us that if we can find the appropriate conformal map Φ_a, which maps $H \setminus L_a$ onto H, fixes 0 and ∞, and has $\Phi'_a(\infty) = 1$, for each $a \in [0, \infty)$, then the CDF of T is given by the formula

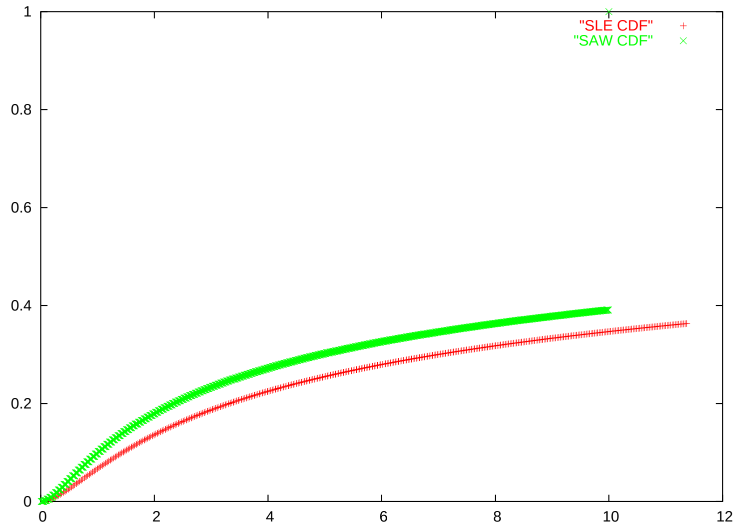
$$F(a) = 1 - \Phi'_a(0)^{5/8}. \tag{5}$$

The inverse map, Φ_a^{-1} taking H to $H \setminus L_a$, can be given explicitly by the formula

$$\Phi_a^{-1}(z) = a \left(\frac{z-c}{a} + 1 - \alpha \right)^{1-\alpha} \left(\frac{z-c}{a} - \alpha \right)^{\alpha} + c. \tag{6}$$

For our purposes we may take $c = 1$, since the results of the theorem above are invariant with respect to scaling. We numerically calculated the values z_0 (which are real) such that $\Phi_a^{-1}(z_0) = 0$, for each a, so that we could then calculate $\Phi'_a(0) = 1 \,/\, \Phi_a^{-1\prime}(z_0)$ (this equality follows from the inverse function theorem).

We plotted both the exact CDF for the random varibale T with $\alpha = 0.25$ and an approximate CDF using Professor Kennedy's implementation of the pivot algorithm to see how closely the two plots match. For the pivot algorithm we used 250,000 step SAWs, and plotted the CDF $F(a)$ for $0 < a \leq 10$. Here are the results:



It is easily seen that the two plots deviate from each other. We have found that the SAW plot differs by a factor of root 2 from the SLE plot. It is very likely that this discrepancy is due to an error in the program that calculates the function $\Phi_a^{-1\prime}(z_0)$. So with a careful debugging the problem could be fixed.