Monte Carlo Tests of SLE Predictions for the 2D Self-Avoiding Walk

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Abstract

The conjecture that the scaling limit of the two-dimensional self-avoiding walk (SAW) in a half plane is given by the stochastic Loewner evolution (SLE) with \( \kappa = 8/3 \) leads to explicit predictions about the SAW. A remarkable feature of these predictions is that they yield not just critical exponents, but probability distributions for certain random variables associated with the self-avoiding walk. We test two of these predictions with Monte Carlo simulations and find excellent agreement, thus providing numerical support to the conjecture that the scaling limit of the SAW is SLE\( _{8/3} \).

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A variety of two dimensional models in statistical physics are expected to have conformally invariant scaling limits. This conformal invariance has made it possible to determine critical exponents for these two dimensional models. Recently, Schramm introduced a two dimensional conformally invariant random process which he called stochastic Loewner evolution \([1]\). This process depends on a parameter \(\kappa\), and so is denoted SLE\(_{\kappa}\). The qualitative behavior of the process changes with the parameter and it appears that for different values of \(\kappa\), the process is related to the scaling limit of various two dimensional models.

Schramm’s SLE process is defined in a half plane as follows. Let \(B_t\) be a standard one-dimensional Brownian motion. We define a complex-valued function \(g_t(z)\) for \(z\) in the upper half of the complex plane by the following differential equation,

\[
\frac{\partial_t g_t(z) - \sqrt{\kappa}B_t}{g_t(z)} = 2,
\]

along with the initial condition \(g_0(z) = z\). The SLE trace is the curve defined by

\[
\gamma(t) = \lim_{z \to 0} g_t^{-1}(z + \sqrt{\kappa}B_t).
\]

(The limit is only over \(z\) in the upper half plane. \(g_t^{-1}\) can be obtained by solving the differential equation backwards in time.) The limit exists and gives a continuous curve. This has been proved for \(\kappa \neq 8\), and is believed to be true for all \(\kappa\) [1, 2]. For \(\kappa = 8/3\) it is conjectured that this SLE trace gives the scaling limit of the SAW restricted to the half plane [3].

Schramm showed that if the loop-erased random walk has a conformally invariant scaling limit, then that limit must be SLE\(_2\) [1]. He also conjectured that the scaling limit of percolation should be related to SLE\(_6\), and the scaling limit of uniform spanning trees is described by SLE\(_2\) and SLE\(_8\). Smirnov has proved the conformal invariance conjecture for critical percolation on the triangular lattice and that SLE\(_6\) describes the limit [1]. Lawler, Schramm and Werner used SLE\(_6\) to rigorously determine the “intersection exponents” for Brownian motion and proved a conjecture of Mandelbrot that the outer boundary of a Brownian path has Hausdorff dimension \(4/3\) [5, 6, 7, 8]. Rohde and Schramm conjectured that the random cluster representation of the Potts model for \(0 < q < 4\) is related to the SLE process as well [2].

By using stochastic calculus it is possible to compute many quantities related to SLE. A remarkable feature of these calculations is that they can yield not just critical exponents, but
FIG. 1: The random variables $X$ and $Y$ that we study are illustrated for a SAW. (Even though it appears the path intersects itself, when viewed at a smaller resolution one sees that it does not.)

entire probability distributions for certain random variables. In this paper we will consider two examples of such random variables, illustrated in figure 1. For SLE$_{8/3}$ one can explicitly compute the probability distributions of $X$ and $Y$. We will compare these explicit distributions with Monte Carlo simulations of the random variables for the SAW.

To define the first random variable we fix a point $(c, 0)$ on the horizontal axis. Given an SLE trace or a SAW with lattice spacing $\delta$, we consider the distance from the curve to the point $(c, 0)$. We define $X$ to be the ratio of this distance to $c$.

$$X = \frac{1}{c} \min_{t \geq 0} ||\gamma(t) - (c, 0)||$$

(3)

So $X$ takes values in $(0, 1]$. SLE is invariant under dilations, so the distribution of $X$ is independent of $c$. In the scaling limit ($\delta \to 0$) the distribution of $X$ for the SAW should also be independent of $c$.

For the second random variable we consider the intersections of the curve with the vertical line $x = c$. We define $Y$ to be the ratio of the $y$-coordinate of the lowest intersection to $c$.

$$Y = \frac{1}{c} \min \{y : (y, c) = \gamma(t) \text{ for some } t \geq 0\}$$

(4)

So $Y$ takes values in $(0, \infty)$. The distribution of $Y$ should also be independent of $c$.
The distributions of $X$ and $Y$ will follow from a remarkable theorem of Lawler, Schramm and Werner [3], which appears in a survey article by Lawler [9] about their joint results. Let $H$ be the upper half plane, and $\bar{H}$ its closure. Let $A$ be a compact subset of $\bar{H}$ which does not contain 0 and such that $H \setminus A$ is simply connected. Let $\Phi_A$ be the conformal map from $H \setminus A$ onto $H$ which fixes 0 and $\infty$ and has $\Phi'_A(\infty) = 1$.

Theorem (Lawler, Schramm, Werner) For $\kappa = 8/3$, SLE in a half plane satisfies

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

The Riemann mapping theorem says that the conformal map $\Phi_A$ exists, but an explicit formula for it is available in only a few special cases. For the two random variables defined above, the computation of their distributions is just an application of the above theorem for two $A$’s for which there is an explicit conformal map.

We start with the random variable $X$, and take $c = 1$. For $a < 1$, let $A_a$ be the half of the disc centered at $(1,0)$ with radius $a$ that is in the upper half plane. The distance $X$ from $\gamma[0, \infty)$ to $(1,0)$ is less than or equal to $a$ if and only if $\gamma[0, \infty)$ hits $A_a$. So

$$P(X \leq a) = P(\gamma[0, \infty) \cap A_a \neq \emptyset)$$

The conformal map that sends $H \setminus A_a$ onto $H$ is

$$\Phi_{A_a}(z) = z - 1 + \frac{a^2}{z - 1} + 1 + a^2,$$

It is normalized so that it fixes 0 and $\infty$ and has $\Phi'_{A_a}(\infty) = 1$. Since $\Phi'_{A_a}(0) = 1 - a^2$, the theorem says

$$P(X \leq t) = 1 - (1 - t^2)^{5/8}.$$

In figure 2 the solid curve is the above function. The results of our Monte Carlo simulation for the SAW on the square lattice are shown with circles. One cannot see any difference at the scale of this plot.
FIG. 2: The curve is the exact distribution of $X$ for SLE$_{8/3}$. The points are the results of a Monte Carlo simulation for the SAW on the square lattice.

Now we find the distribution of $Y$. Again, we take $c = 1$. Let $L_a$ to be the vertical line segment from $(1, 0)$ to $(1, a)$. The random variable $Y$ is less than or equal to $a$ if and only if the curve hits $L_a$. So

$$P(Y \leq a) = P(\gamma[0, \infty) \cap L_a \neq \emptyset)$$

(9)

The conformal map that takes $H \setminus L_a$ onto the upper half plane is

$$\Phi_{L_a}(z) = i\sqrt{-(z-1)^2-a^2 + \sqrt{1+a^2}}$$

(10)

(The square root is defined with the usual branch cut along the negative $x$-axis.) The map fixes 0 and $\infty$ and has $\Phi'_{L_a}(\infty) = 1$. We have $\Phi'_{L_a}(0) = 1/\sqrt{1+a^2}$, so the theorem says

$$P(Y \leq t) = 1 - (1 + t^2)^{-5/16}$$

(11)

In figure 3 the solid curve is the above function and the results of our Monte Carlo simulation for the SAW on the square lattice are again shown with circles.
FIG. 3: The curve is the exact distribution of $Y$ for SLE$_{8/3}$. The points are the results of a Monte Carlo simulation for the SAW on the square lattice.

We simulate the self-avoiding walk using the pivot algorithm (Expository accounts of this algorithm may be found in \cite{10, 11}. An iteration of this Markov chain algorithm starts by picking a random site on the walk. Then one picks a random lattice symmetry $g$. The section of the walk from the starting point to the randomly chosen site is not changed. The rest of the walk is “pivoted” by applying $g$ to it with respect to the randomly chosen site. If the resulting walk is self-avoiding, it is accepted; otherwise it is rejected. The pivot algorithm can also be used to simulate the SAW restricted to the half plane. When a pivot is proposed, in addition to checking if the pivoted walk is self-avoiding, one must also check if it stays in the half-plane. If both of these conditions are satisfied, then the pivot is accepted.

If one uses a hash table and checks for self-intersections in the pivoted walk starting from the pivot point and working outwards, then the time required for the pivot algorithm to produce an accepted pivot is believed to be $O(N)$ on average \cite{12}. It has been shown recently that by taking advantage of the nearest neighbor nature of the walk when checking for self-intersections
and using a data structure to store the walk that postpones carrying out the pivots, the pivot algorithm in two dimensions can be implemented so that the time required to produce an accepted pivot is $O(N^q)$ with $q$ less than one [13]. The exact value of $q$ is not known, but it appears to be less than 0.57 for two-dimensional walks.

To study the scaling limit of the SAW walk there are two limits that must be taken. We must let the number of steps, $N$, go to infinity and we must take the lattice spacing to zero. A walk with $N$ steps lives on scale $N^{3/4}$, so to study the random variables $X$ and $Y$ we take $c = sN^{3/4}$. We must take $s$ small to make the effect of the finite length of our walks negligible, and we must take $N$ large to make the lattice spacing small compared to the scale of the random variables. Our simulations are done on the square lattice with $N = 1,000,000$. We study the distribution of $X$ for $s = 0.05$ and $s = 0.1$. For $Y$ we use $s = 0.005$ and $s = 0.01$. We compute $P(X \leq t)$ and $P(Y \leq t)$ for 1,000 values of $t$. For $X$, the values of $t$ range from 0 to 1. For $Y$

FIG. 4: Each curve is the difference between the Monte Carlo computation of the cumulative distribution of $X$ for the SAW and the exact cumulative distribution of $X$ for SLE$_{8/3}$. Error bars of two standard deviations are shown for selected values of $t$. 

\[ P(X < t) \]
FIG. 5: Each curve is the difference between the Monte Carlo computation of the cumulative distribution of $Y$ for the SAW and the exact cumulative distribution of $Y$ for SLE$_{8/3}$. Error bars of two standard deviations are shown for selected values of $t$.

The values range from 0 to 20.

There are 20 billion iterations of the Markov chain in the simulation. Approximately 5% of these proposed pivots are accepted. For some random variables, e.g., the end to end distance of the walk, an accepted pivot produces a radical change in the value of the random variable, and it is expected that each accepted pivot produces an essentially independent sample of the random variable. For our random variables a pivot can change their values only if it occurs in a relatively short segment of the walk near the origin. So the autocorrelation time will be significantly longer than for random variables like the end to end distance.

Since it is impossible to see the difference between the SAW simulations and the SLE curves in figures 2 and 3, we plot the distributions from the SAW simulations minus the SLE$_{8/3}$ distributions in figures 4 and 5. The most important feature of these figures is the scale on the vertical axis. It is $1/100$ of the scale of figures 2 and 3. So the agreement between the SLE
distributions and the simulated SAW distributions is excellent. Since the simulation uses finite length walks with a nonzero lattice spacing, if the simulation was run long enough we would see that the quantity being plotted is not exactly zero. Error bars, based on two standard deviations, are shown in the figures for selected values of $t$. (Different values of $t$ are used for the two curves so the error bars do not overlap.) The error bars are the same order of magnitude as the quantity being plotted, so our simulation is not quite accurate enough to see the finite length and lattice effects for the values of $N$ and $s$ that we use. (In the $s = 0.1$ curve for $X$, the effects might be just beginning to emerge.)

Our simulations of the SAW walk in a half plane have shown that the distributions of two particular random variables related to the walk agree extremely well with the exact distributions of SLE$_{8/3}$ for these random variables. This supports the conjecture that the scaling limit of the SAW is SLE$_{8/3}$. Schramm has recently given a formula for the probability that the SLE curve passes to the right of a fixed point in the half plane for all values of $\kappa$ [1]. We expect that the distributions of many more random variables associated with SLE$_{8/3}$ will be found in the near future.

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