PIVOT ALGORITHM AND THE SELF AVOIDING WALK

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1. Introduction

1.1. **Self Avoiding Walks.** The majority of this paper deals with self-avoiding walks (SAWs). The N step SAW ω beginning at point x on the lattice $\mathbb{Z}^d$–the d dimensional hypercubic lattice–can be defined as a sequence of sites $(\omega(0), \omega(1), ..., \omega(N))$ with $\omega(0) = x$ satisfying $|\omega(i+1) - \omega(i)| = 1$ and $\omega(i) \neq \omega(j)$ for $i \neq j$[2]. The length of ω is denoted as $|\omega| = N$.

Denote the number of SAWs of length N beginning at the origin by c_N. There is a lot of empirical evidence to suggest that

$$c_N \sim A\mu^N N^{\gamma-1} \tag{1.1}$$

where $\sim$ is defined for $f(N), g(N) : \mathbb{Z}^+ \to \mathbb{Z}^+$ to be

$$f(N) \sim g(N) \iff \lim_{N\to\infty} \frac{f(N)}{g(N)} = 1$$

and A, μ are lattice dependent constants while γ is a dimension dependent constant[2]. The constant μ is known as the growth constant and it can be shown that the limit $\mu = \lim_{N\to\infty} c_N^{1/N}$ exists. The constant γ is referred to as a critical exponent and in addition to characterizing the asymptotic behaviour of c_N it provides a measure of the probability that two N-step SAWs starting at the same point do not intersect[2]. This paper is concerned with providing estimates of both μ and γ. Furthermore there are several statistics that one may gather on all SAWs of a given length N. Indeed, the most important statistic is c_N itself[6]; however, through the clever use of probabilistic arguments–specifically Monte Carlo methods–one may estimate c_N by gaining a measure on a less expensive statistic to compute. In particular, the statistics of interest in this paper are referred to as atmospheres and are discussed in more detail below.

1.2. **Self Avoiding Polygons.** The $2N$ ($N \geq 2$) step SAP centered at the point x on the $\mathbb{Z}^d$ lattice is composed of a SAW ω starting at the point x of length $2N - 1$ satisfying $|\omega(2N-1) - x| = 1$ with the condition $\omega(2N) = x$. It should be noted that the SAW which composes the SAP is not unique; in fact two $2N$-step SAPs are said to be equivalent up to translation if there is a vector $v \in \mathbb{R}^d$ such that translating by v defines a one-to-one correspondence between the bonds in one SAP to the other. It can be shown that the growth constant for SAPs is the same as the growth constant μ for SAWs[3].

2. Atmospheres

For the purposes of this paper the discussion here is limited to SAPs and SAWs in $d \in \{2, 3\}$. In fact, there are more rigorous results known for $d \geq 4$; however, these low dimensions remain to be the most difficult to analyze.

2.1. **Endpoint Atmosphere.** The endpoint atmosphere $a_e(\omega)$ of a SAW $\omega = (\omega(0), \omega(1), ..., \omega(N))$ is defined to be the number of ways an edge may be appended to the end of a SAW to form another SAW ($a_e(\omega) = \left|\left\{x \in \mathbb{Z}^d : (\omega(0), ..., \omega(N), x) \text{ is a SAW}\right\}\right|$.) The endpoint atmosphere has the property that $\sum_{|\omega|=N} a_e(\omega) = c_{N+1}$ and as a direct consequence the average atmosphere of all SAWs of length N is

$$\begin{aligned}\langle a_e \rangle_N &= \sum_{|\omega|=N} \frac{a_e(\omega)}{c_N} \\ &= \frac{c_{N+1}}{c_N}.\end{aligned}$$

Assuming the conjectured asymptotic form 1.1 and its uniform convergence, we have that

$$\begin{aligned}\lim_{N\to\infty} \langle a_e \rangle_N &= \lim_{N\to\infty} \frac{c_{N+1}}{c_N} \\ &= \lim_{N\to\infty} \frac{c_{N+1}}{A\mu^{N+1}(N+1)^{\gamma-1}} \cdot \frac{A\mu^N N^{\gamma-1}}{c_N} \cdot \frac{A\mu^{N+1}(N+1)^{\gamma-1}}{A\mu^N N^{\gamma-1}} \\ &= \mu \lim_{N\to\infty} \left(\frac{N+1}{N}\right)^{\gamma-1} \\ &= \mu\end{aligned}$$

We can further exploit 1.1 to assert that

$$\langle a_e \rangle \sim \mu \left(1 + \frac{\gamma - 1}{N} + \dots\right)$$

by using the binomial series expansion. Also we may conclude

$$\log \langle a_e \rangle_N \sim \log \mu + (\gamma - 1) \log \left(\frac{N+1}{N}\right). \tag{2.1}$$

By obtaining an estimate on the statistic $\langle a_e \rangle_N$ over a range of increasing values of N it is possible to fit the data to estimate both μ and γ for SAWs. It is, however, unclear how to extend this definition to SAPs. Indeed, this statistic can be improved upon since the standard deviation in the samples to obtain an estimate on $\langle a_e \rangle_N$ is found to be higher than in the statistics used below.

2.2. **Generalized Atmospheres.** In an effort to address the issues with the endpoint atmosphere a_e defined in the previous section–that is to facilitate a definition that holds for SAPs as well as a statistic which has a lower standard deviation in sampling–one can define a positive atmosphere a^+ and a negative atmosphere a^- for either SAWs or SAPs such that $\sum_{|\omega|=N} a^+(\omega) = \sum_{|\omega|=N+1} a^-(\omega)$. The motivation for this is that then

$$\begin{aligned}\frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}} &= \frac{\sum_{|\omega|=N} \frac{a^+(\omega)}{c_N}}{\sum_{|\omega|=N+1} \frac{a^-(\omega)}{c_{N+1}}} \\ &= \frac{c_{N+1}}{c_N}\end{aligned}$$

and we can use the methods of the previous section to obtain estimates for both μ and γ. The difficulty lies in choosing a^+, a^- that are cheap to compute and satisfy the condition. In this paper the choice of a^+, a^- for a SAW $\omega = (\omega(0), \omega(1), ..., \omega(N))$ are the number of ways an edge may be inserted anywhere in the SAW to produce another valid SAW, and the number of ways an edge may be deleted from the SAW to produce another valid SAW respectively, or equivalently (note that in the definitions that follow i is the place of insertion/deletion and x is the unit vector direction of the insertion/deletion):

$$\begin{aligned} a^+(\omega) &= |\{(x,i) \in \mathbb{Z}^d \times \mathbb{Z}^{\geq 0} : |x| = 1, 0 \leq i \leq N, \\ &\quad (\omega(0), \ldots, \omega(i), \omega(i)+x, \omega(i+1)+x, \ldots, \omega(N)+x) \text{ is a SAW}\}| \\ a^-(\omega) &= |\{i : 0 \leq i \leq N-1, x = \omega(i+1) - \omega(i), \\ &\quad (\omega(0), \ldots, \omega(i-1), \omega(i+1)-x, \ldots, \omega(N)-x) \text{ is a SAW }\}|. \end{aligned}$$

For a SAP $\omega = (\omega(0), \omega(1), ..., \omega(2N))$ the value a^+ is the number of ways 2 edges may be inserted into the SAP to produce another valid SAP and a^- is the number of ways 2 edges may be deleted from the SAP to produce another valid SAP, or equivalently:

$$\begin{aligned} a^+(\omega) &= |\{(x,i,j) \in \mathbb{Z}^d \times \mathbb{Z}^{\geq 0} \times \mathbb{Z}^{\geq 0} : |x| = 1, 0 \leq i < j \leq 2N, \\ &\quad (\omega(0), \ldots, \omega(i), \omega(i)+x, \ldots, \omega(j)+x, \omega(j), \ldots, \omega(2N)) \text{ is a SAP}\}| \\ a^-(\omega) &= |\{(i,j) : 0 \leq i < j \leq 2N-1, x = \omega(i+1) - \omega(i), \\ &\quad (\omega(0), \ldots, \omega(i-1), \omega(i+1)-x, \ldots, \omega(j)-x, \omega(j+1), \ldots, \omega(2N)) \text{ is a SAP }\}|. \end{aligned}$$

3. Pivot Algorithm

3.1. **Introduction.** The pivot algorithm falls under the classification of a dynamic Monte Carlo method and provides a means to sample the set of all SAWs or SAPs of a given length N efficiently. One then may assume the Central Limit Theorem to hold and thus produce estimates on averages of any of the atmospheres–or any statistic at that–described above. In fact the pivot algorithm can be shown to produce "effectively independent" SAWs or SAPs in $O(N \log N)$ time[4]. This of course is extremely efficient considering it takes $O(N)$ time just to write down a SAW or SAP.

3.2. **Overview of Implementation.** The algorithm is implemented as follows. First an initial SAW of the input length N is picked for the starting point. In this implementation this is just the straight line walk in any direction. At each step in the algorithm the SAW length is conserved but a new SAW is reached by choosing a "pivot site" uniformly at random along the current walk. At this site the SAW is broken into two pieces, and a randomly chosen symmetry operation of $\mathbb{Z}^d$ is applied to one piece, using the site as the origin. The result is accepted if an only if it is a SAW. Repeating this an appropriate number of times will produce SAWs that are "effectively independent" from each other and atmospheres may be measured to gain an estimate of the true mean atmosphere.

3.3. **Results for SAWs.** Since 2.1 is the asserted form of the quantity we are interested in as $N \to \infty$ we should expect some corrections required to the form in order to get a good fit. In fact, there is strong evidence[6] from series analysis to suggest that 2.1 requires corrections of the form

$$\log \frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}} \approx \log \mu + (\gamma - 1) \log \left(\frac{N+1}{N} \right) + \frac{const}{N^2}. \tag{3.1}$$

The results of the pivot algorithm for SAWs can be seen in figure 3.1 and 3.2 where clearly a horizontal asymptote is visible in the empirical data on the left and

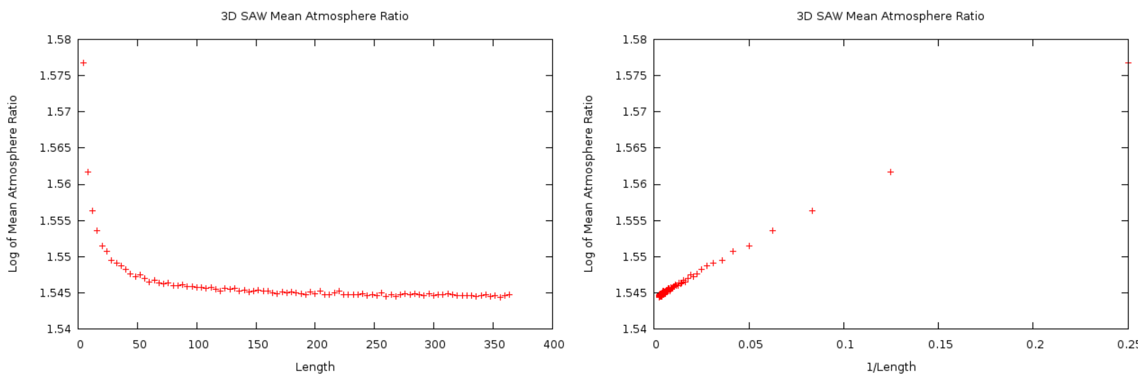

FIGURE 3.1. The pivot algorithm results graphed for the SAW estimates on $\log \frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}}$ with $d = 3$

on the right we see a limit point forming. Using 3.1 to fit the data we obtain the results of table 1.

The estimates of mean atmospheres are produced based on 10^6 samples for values of $N \in \{4, 8, 12, \ldots, 252, 256\}$. The fits themselves discard lower values of N which empirically produces better results. It should be noted that the results were obtained on a regular PC and better results can be expected with more computing power.

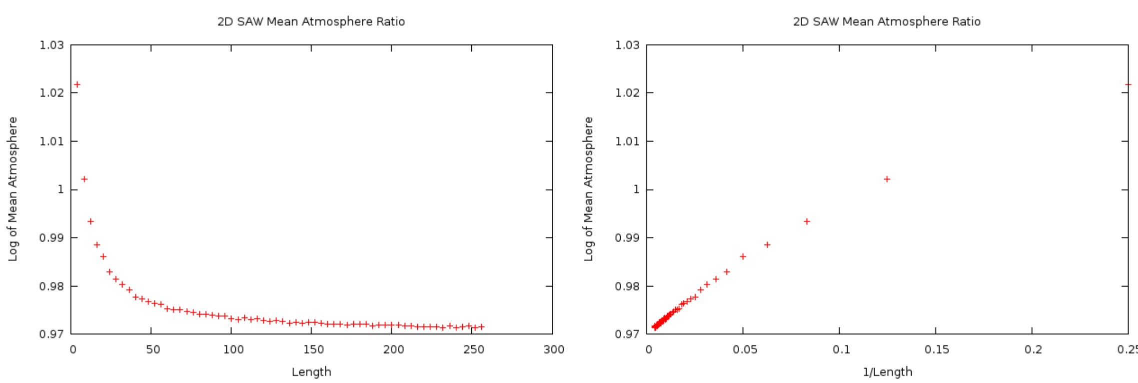

FIGURE 3.2. The pivot algorithm results graphed for the SAW estimates on $\log \frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}}$ with $d = 2$

d	μ fit	γ fit	Best estimate known for μ	Best estimate known for γ
2	2.63833754 ± 0.00018	1.32937 ± 0.012	2.63815853034[1]	43/32
3	4.683988544 ± 0.00023	1.16357 ± 0.012	4.6839066 ± 0.0002	1.162...

TABLE 1. Estimates with SAW data obtained from the Pivot Algorithm

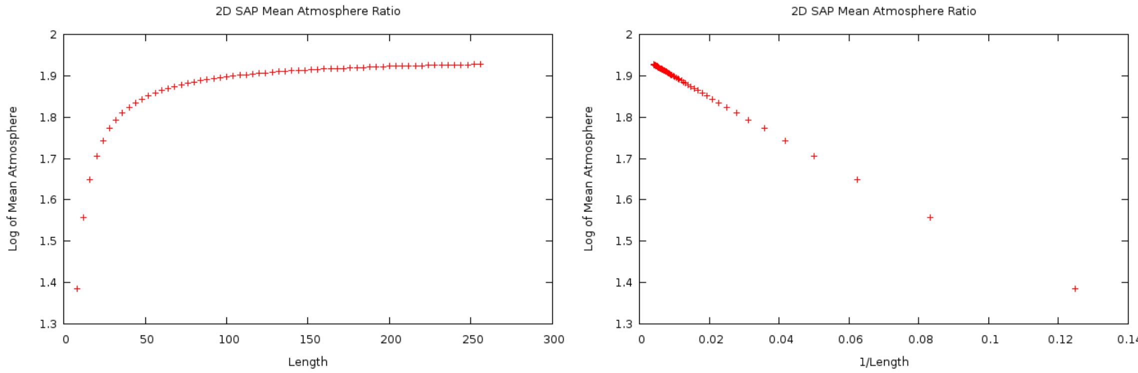

FIGURE 3.3. The pivot algorithm results graphed for the SAP estimates on $\log \frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}}$ with $d = 2$

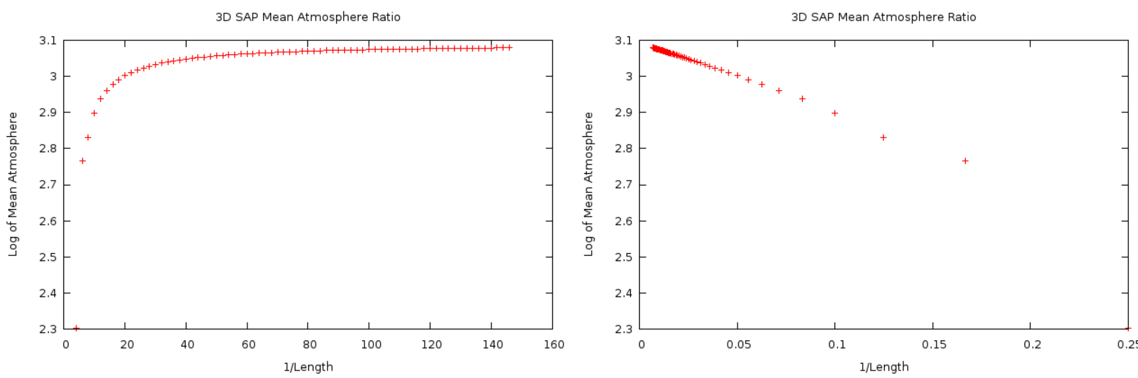

FIGURE 3.4. The pivot algorithm results graphed for the SAP estimates on $\log \frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}}$ with $d = 3$

3.4. **Results for SAPs.** For SAPs we derive a similar fit equation to (3.1) taking care that the values of N for SAPs increment by 2 instead of 1. We arrive at the fit equation

$$\log \frac{\langle a^+ \rangle_N}{\langle a^- \rangle_{N+1}} \approx 2 \log \mu + (\alpha - 3) \log \left(1 + 2\frac{1}{N} \right) + \frac{const}{N^\theta}$$

where α is some constant, and the correction term $\theta \approx .5$ is obtained from the asymptotic form[5]. We obtain the following results for $d = 2, 3$ in table 3.4. The estimates for α are somewhat dissapointing since the value for α in the 2D case should be $\alpha \approx 1/2$.

3.5. **Atmosphere Histograms.** In this section I provide graphs of the histograms of the atmospheres (both positive and negative) for SAWs and SAPs in $d = 2, 3$.

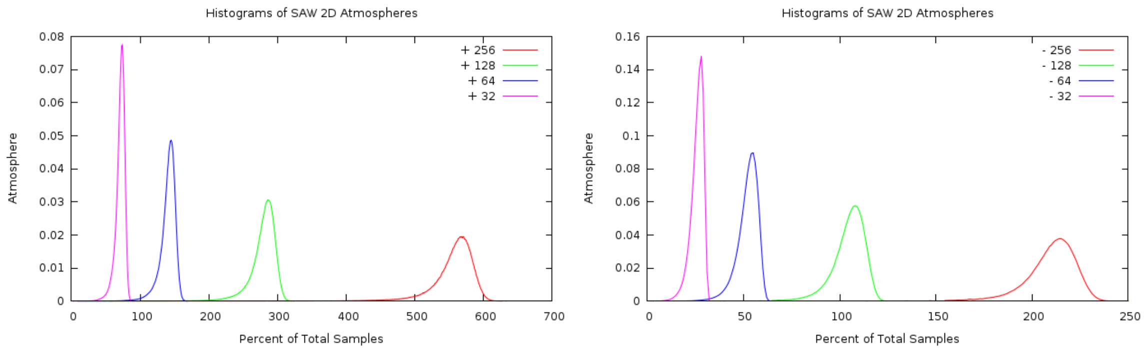

Figure 3.5. Histograms of 2D SAWs

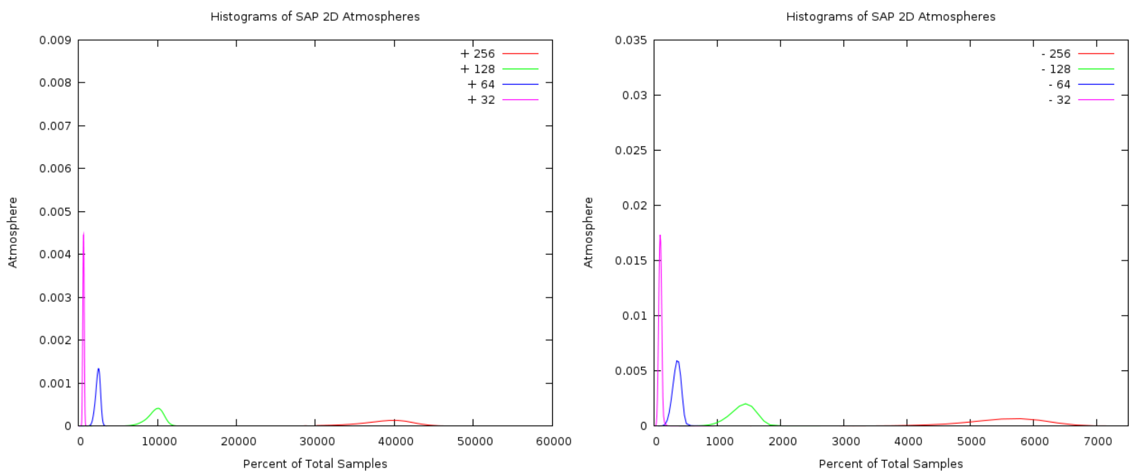

Figure 3.6. Histograms of 2D SAPs

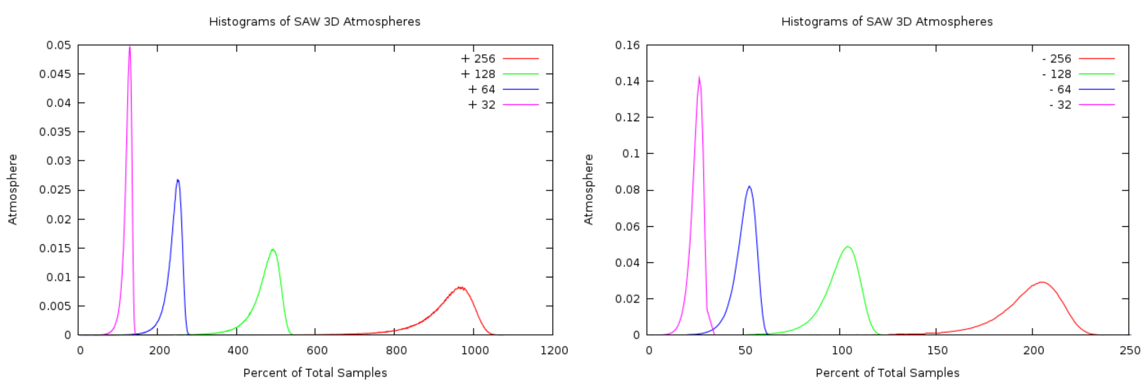

Figure 3.7. Histograms of 3D SAWs

d	μ fit	α fit
2	2.638118569 ± 0.00044	0.443839 ± 0.00347
3	4.461700628 ± 0.031	2.4695 ± 0.04066

TABLE 2. Estimates with SAP data obtained from the Pivot Algorithm

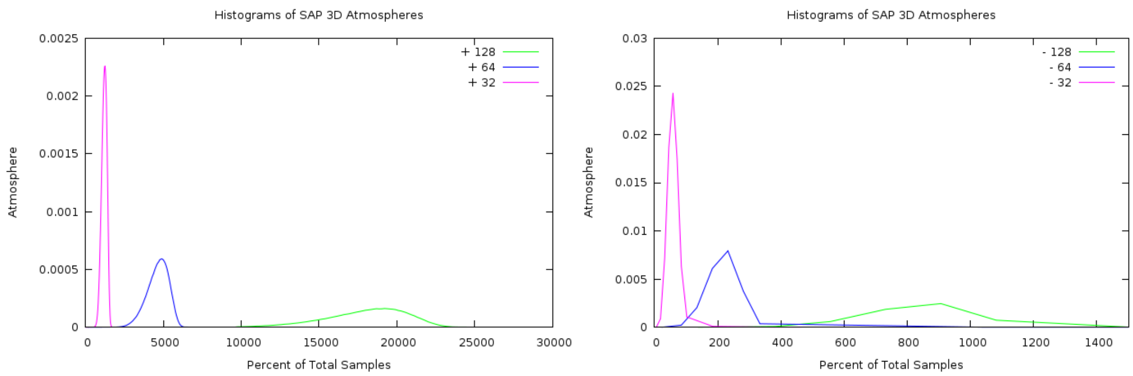

FIGURE 3.8. Histograms of 3D SAPs

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