# COUNTING SELF AVOIDING WALKS OF LENGTH N

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Abstract. This paper investigates properties of Self Avoiding Walks. We review their asymptotic behavior and state some general conjectures about their exact asymptotic growth. We then explain the Pivot algorithm, a Markov chain which is the primary method for numerical verification of these conjectures, and prove the ergodicity of this Markov chain. We also discuss an alternate method of studying Self Avoiding Walks through the use of Loops (a term defined later in this paper). Finally, we state some questions and conjectures concerning self intersecting walks.

## 1. Introduction

A simple walk in $\mathbb{Z}^2$ proceeds as follows. Starting at $(0, 0)$ take a unit step in any direction, say to $(0, 1)$. Take another unit step from this new point. Repeat this $n$ times, resulting in $n$ total steps. At each step in the walk, there are four possible directions. Therefore, there are $4^n$ $n$-step simple walks.

**Definition 1.1.** We will refer to directions along a simple walk (or along a loop, as will be used in section 3) as **North** (denoted $N$), **South** (denoted $S$), **East** (denoted $E$), and **West** (denoted $W$).

This paper studies these walks with an additional condition: the walk may not revisit a vertex of $\mathbb{Z}^2$ which it had previously visited. These walks are called Self Avoiding Walks.

The most basic unanswered question about Self Avoiding Walks is:

**Open Question 1.2.** *How many Self Avoiding Walks of length $n$ are there in the integer lattice $\mathbb{Z}^2$?*

Of course, one may ask the same question for the integer lattice $\mathbb{Z}^3$, or any dimension. In fact, one could ask this question where the lattice is a hexagonal lattice, or indeed of any graph. This paper will focus on the two dimensional integer lattice. Note that for the lattice $\mathbb{Z}$, the answer to Question 1.2 is trivially two.

Let $S_n$ be the number of Self Avoiding Walks of length $n$. There are a couple upper and lower bounds we can get on $S_n$ without much work. Firstly, consider the set of Self Avoiding Walks which, for each axis in the $d$-dimensional integer lattice space, only take steps in positive directions. These are all obviously Self Avoiding, and at each point there are $d$ potential choices in direction, so there are $d^n$ such self avoiding walks. Therefore $d^n \leq S_n$.

Now for some quick notation. We denote a walk by $\omega_n$, where the $n$ denotes the length of the walk. We will use the notation $\omega_n = \{w_0, ..., w_n\}$, where $w_i$ is the $i$th vertex of $\omega_n$, with $0 \leq i \leq n$.

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Now consider all walks that never return to the vertex they were at in the previous step, that is, the set of all walks for which $w_{i-1} \neq w_{i+1}$. Then at each vertex after the first there are $2d-1$ possible choices, and therefore there are $2d \cdot (2d-1)^{n-1}$ such walks. All Self Avoiding Walks have this property, so there are at most $2d \cdot (2d-1)^{n-1}$ Self Avoiding Walks. Thus $d^n \leq S_n \leq 2d \cdot (2d-1)^{n-1}$.

From these computations, it is natural to guess that $S_n \sim C^n$, where $\sim$ is defined as follows.

**Definition 1.3.** Let $f(x)$ and $g(x)$ be functions. We say that $f(x)$ is asymptotic to $g(x)$, written $f(x) \sim g(x)$, if $\lim_{x\to\infty} \frac{f(x)}{g(x)} = 1$.

It turns out, however, that $S_n \nsim C^n$. Instead, we use the following weaker notion of asymptotic.

**Definition 1.4.** Let $f(x)$ and $g(x)$ be functions. We say that $f(x)$ is logarithmically asymptotic to $g(x)$, written $f(x) \approx g(x)$, if $\lim_{x\to\infty} \frac{\log f(x)}{\log g(x)} = 1$.

The following theorem is well-known. The proof we present can be found in [2].

**Theorem 1.5.** *The limit* $\lim_{n\to\infty} S_n^{1/n}$ *exists, which implies that* $S_n \approx C^n$ *for some* $C$.

Before proving this theorem, we prove the following lemma:

**Lemma 1.6.** *Let* $(a_n)_{n=1}^{\infty}$ *be a sequence of real numbers such that* $a_{n+m} \leq a_n + a_m$*, a property we will refer to as subadditive. Then*

$$\lim_{n\to\infty} \frac{a_n}{n} = \inf_{n\geq 1} \frac{a_n}{n}.$$

*Proof.* We first show that

$$\limsup_{n\to\infty} \frac{a_n}{n} \leq \frac{a_k}{k} \tag{1.7}$$

for all $k$.

Fix $k$. Then for a given $n \in \mathbb{N}$, let $m$ be the largest integer less than $\frac{n}{k}$. Then $n = km + r$ for some $r$ with $1 \leq r \leq k$. Therefore we have

$$a_n \leq a_{km} + a_r \tag{1.8}$$

by subadditivity. Let $b_k = \max_{1\leq r\leq k} a_r$. By induction one can show that $a_{km} \leq m \cdot a_k$. Thus 1.8 becomes

$$a_n \leq m \cdot a_k + a_r < \frac{n}{k} \cdot a_k + b_k,$$

Dividing both sides by $n$ and taking the limit superior gives

$$\limsup_{n\to\infty} \frac{a_n}{n} \leq \limsup_{n\to\infty} \left(\frac{a_k}{k} + \frac{b_k}{n}\right) = \frac{a_k}{k}$$

which is 1.7.

To see that $\lim_{n\to\infty} \frac{a_n}{n}$ exists, simply take the limit inferior of both sides of 1.7 to get that

$$\limsup_{n\to\infty} \frac{a_n}{n} \leq \liminf_{k\to\infty} \frac{a_k}{k}.$$

We may conclude that $\lim_{n\to\infty} \frac{a_n}{n}$ exists. To show that this limit equals $\inf_{n\geq 1} \frac{a_n}{n}$, simply take the infimum of both sides of 1.7. Therefore, the lemma holds.

□

We are now properly equipped to prove the theorem.

*Proof of Theorem 1.5.* Let $(a_n)_{n=1}^{\infty}$ be a sequence, and let $a_n = \log(S_n)$. We first show that

$$S_{n+m} \leq S_n S_m. \tag{1.9}$$

Equation 1.9 holds because every Self Avoiding Walk of length $n+m$ may be split into two smaller Self Avoiding Walks; one of length $n$ and one of length $m$. In more detail, let $A_{n+m}$, $A_n$, and $A_m$ be the set of Self Avoiding Walks of length $n+m$, $n$, and $m$ respectively. Then there exists a function $f : A_{n+m} \to (A_n \times A_m)$ defined by splitting the walk after $n$ steps and sending the $n$ step walk to $A_n$ and the $m$ step walk to $A_m$. This function is injective since concatenation yields a left inverse. Therefore $S_{n+m} = |A_{n+m}| \leq |A_n| \cdot |A_m| = S_n \cdot S_m$.

Taking the logarithm of both sides of 1.9 gives

$$\log(S_{n+m}) \leq \log(S_n S_m) = \log(S_n) + \log(S_m)$$

and therefore the sequence $(a_n)_{n=1}^{\infty}$ is subadditive. We may therefore apply Lemma 1.6 and find that

$$\lim_{n\to\infty} \frac{\log(S_n)}{n} = \inf_{n\geq 1} \frac{\log(S_n)}{n}. \tag{1.10}$$

Therefore the limit $\lim_{n\to\infty} \frac{\log(S_n)}{n}$ exists. Letting $\log(\mu) = \lim_{n\to\infty} \frac{\log(S_n)}{n}$ yields

$$\mu = \lim_{n\to\infty} S_n^{1/n} \tag{1.11}$$

since $\frac{\log(S_n)}{n} = \log(S_n^{1/n})$.

From this one can see that $S_n \approx \mu^n$ by taking the logarithm of both sides of 1.11.

□

Many computer programs have been created to test these results and to help propose generalizations. The following similarity has been hypothesized:

$$S_n \sim A \cdot \mu^n \cdot n^{\gamma},$$

where $A$ and $\gamma$ are constants. Note that since $\log(\mu) = \inf_n \frac{\log(S_n)}{n}$, we may conclude that $\mu^n \leq S_n$ for all $n \geq 1$. This is equivalent to saying that $\gamma \geq 0$.

As for bounds on $\mu$, the current best lower bound is 2.61987, the best upper bound is 2.69576, and the best estimate for $\mu$ in two dimensions is $2.6381585 \pm 0.0000010$. Also, it is conjectured that $\gamma = \frac{43}{32}$.

## 2. The Pivot Algorithm

Another question one may ask about Self Avoiding Walks is: On average, how far away from the origin do they get? Let $E(|\omega(n)|^2)$ be the expected distance (squared) from the origin of a walk $\omega(n)$ of length $n$. Then

$$E(|\omega(n)|^2) = \frac{1}{S_n} \sum_{|\omega|=n} |\omega_n|^2. \tag{2.1}$$

This definition is well know, though here we use the formulation found in [3].

It has been hypothesized that $E(|\omega(n)|^2) \sim B \cdot N^{2\nu}$ where $B$ and $\nu$ are constants. It is conjectured that $\nu = \frac{3}{4}$, but no definitive proof has been found. The Pivot algorithm is one efficient algorithm for estimating the value of $\nu$, and indeed for numerically investigating most any conjecture about Self Avoiding Walks.

The Pivot Algorithm was first invented by Lal in 1969 and later studied by Neal Madras and Alan D. Sokal [3], which takes a Self Avoiding Walk and twists it into another Self Avoiding Walk. The process is as follows. Let $\omega = \{w_0, w_1, ..., w_n\}$ be a Self Avoiding Walk of length $n$. Pick a vertex $w_i$ where $0 < i < n$. This divides our walk of length $n$ into two walks of length $i$ and $n - i$. Then, fixing vertex $w_i$, apply a rotation or reflection (or some combination thereof) to the Self Avoiding Walk $\{w_{i+1}, ..., w_n\}$ to get a new walk $\omega'$. If this walk is self avoiding, we may repeat this process on the new walk. If this walk is not self avoiding, it is ignored and we take the original walk $\omega$ once again.

One can assign to each vertex between $w_0$ and $w_n$ a probability of being selected. One can also assign to each element of the symmetry group $G$ a probability as well. This defines a Markov chain on the set of Self Avoiding Walks.

**Definition 2.2.** A **Markov chain** is a sequence of random variables with the Markov Property, which is as follows. If $\{X_n\}$ is our sequence of random variables, and $P(A \mid B)$ is the probability of $A$ given $B$, then $\{X_n\}$ has the Markov Property if $\mathbb{P}\{X_{n+1} = x \mid X_k, k \neq n\} = \mathbb{P}\{X_{n+1} = x \mid X_n\}$. Moreover, we will only discuss **time homogeneous** Markov Chains, which is to say that for all $m, n$ we have $\mathbb{P}\{X_{n+1} = x \mid X_n = y\} = \mathbb{P}\{X_{m+1} = x \mid X_m = y\}$.

We first define a few key concepts when discussing Markov chains.

**Definition 2.3.** Let $\{X_n\}$ be a Markov chain. We say that $\{X_n\}$ is **irreducible** if for all states $x$ and $y$ there exists an $n$ such that $\mathbb{P}\{X_n = x \mid X_0 = y\} > 0$.

**Definition 2.4.** Let $\Omega$ be the state space. A Markov Chain is said to be **aperiodic** if there does not exist a partition $\Omega_1, ..., \Omega_n$ where $\Omega_i \cap \Omega_j = \emptyset$ for all $i \neq j$, $\Omega = \bigcup_{i=1}^n \Omega_i$, and $\mathbb{P}\{X_1 \in \Omega_{k'} \mid X_0 \in \Omega_k\} = 1$ where $k' \equiv k + 1 \pmod{n}$.

**Definition 2.5.** A Markov chain is said to be **ergodic** if it is both irreducible and aperiodic.

An important theorem in the study of the Pivot algorithm is that if group operations occur with nonzero probability, then the Pivot algorithm is ergodic. The proof of this can be found in [1, Section 4.7]. This theorem allows for accurate estimations of various desirable constants, such as the ones listed at the top of page 17 in [2].

Here we will reproduce the proof that, if all the probabilities mentioned above are nonzero (i.e., for each vertex $w_i$ with $0 < i < n$ there is positive probability that it is picked for the Pivot algorithm, and likewise for each element of $G$) then the Pivot algorithm is ergodic. We first show that the Pivot algorithm is aperiodic.

We first define diagonal reflections in $\mathbb{Z}^d$ for $d \geq 3$.

**Definition 2.6.** Let $d \geq 3$. Let $a_1, ..., a_d$ be diagonals in $\mathbb{Z}^d$, meaning that $a_1$ is a line through $(0, ..., 0)$ and $(1, ..., 1)$, $a_2$ is a line through $(0, ..., 0)$ and $(-1, 1, ..., 1)$, and so on. A **diagonal reflection** in $\mathbb{Z}^d$ is a reflection over each $(d-1)$-dimensional subspace spanned by $(d-1)$ of the lines $a_1, ..., a_d$.

The following two theorems were first formulated and proved in [3].

**Theorem 2.7.** *Let $G$ be the symmetry group on the integer lattice $\mathbb{Z}^d$. Suppose that all reflections over each $(d-1)$-dimensional subspace spanned by $(d-1)$ coordinate axies have a nonzero probability of being used, and suppose that either all $90°$ rotations around the coordinate axies or all diagonal reflections in $G$ have a nonzero probability of being used. Then the Pivot Algorithm is aperiodic.*

*Proof.* Let $\omega_n$ be a Self Avoiding Walk. Take the vertex $w_i$. Note that there exists either a rotation (or diagonal reflection) or a reflection over an axis that would result in $w_{i-1} = w_{i+1}$. Because this walk is not self avoiding, it would be thrown out, and $\omega_n$ would be taken again. Thus, given any partition of the state space, it is possible that the walk does not change and thus does not advance into a new subset of the state space proving aperiodicity. □

To prove ergodicity we must prove that the Pivot Algorithm is irreducible on walks in $\mathbb{Z}^d$.

**Theorem 2.8.** *Let $G$ be the symmetry group on the integer lattice $\mathbb{Z}^d$. Suppose that all reflections over an axis have a nonzero probability of being used, and suppose that either all $90°$ rotations or all diagonal reflections in $G$ have a nonzero probability of being used. Then the Pivot Algorithm is irreducible. Furthermore, any Self Avoiding Walk of length $n$ may be twisted into a straight line via the Pivot Algorithm in at most $2n-1$ steps.*

*Proof.* Let $\omega_n = \{w_0, w_1, ..., w_n\}$ be a Self Avoiding Walk of length $n$ which is not a straight line. Let $m_j = \min\{e(w_i)_j | 0 \leq i \leq n\}$ where $e(w_i)_j$ is the $j$th coordinate of the vertex $w_i$. Let $M_j = \max\{e(w_i)_j | 0 \leq i \leq n\}$. Let $R(\omega_n) = \{x \in \mathbb{Z}^d \mid m_j \leq e(x)_j \leq M_j\}$. Then $R(\omega_n)$ contains $\omega_n$. Let $B(\omega_n)$ be the set of vertices of $\omega_n$ that are not at right angles, that is, $B(\omega_n) = \{w_i \in \omega_n \mid 0 < i < n$ and $w_i = \frac{1}{2}(w_{i-1} + w_{i+1})\}$. Finally, let $C(\omega_n) = \sum_{j=1}^{d} \left(M_j - m_j\right)$.

We split the proof into two cases.

(1) There is a face of $R(\omega_n)$ which contains neither $w_0$ nor $w_n$.
(2) The vertices $w_0$ and $w_n$ are on opposite corners of $R(\omega_n)$.

We will start by examining the first case. Let $A$ be the face of $R(\omega_n)$ such that $w_0, w_n \notin A$. Then $A = \{x \in \mathbb{Z}^d \mid e(w_i)_j = m_j\}$ or $A = \{x \in \mathbb{Z}^d \mid e(w_i)_j = M_j\}$ for all $i$ with $0 \leq i \leq n$ and for some $j$ with $1 \leq j \leq d$. Suppose without loss of generality that the second set equivalence holds.

Then define $p = \min\{k \mid e(w_k)_j = M_j\}$, that is, $p$ is the index number of the first vertex of $\omega_n$ on face $A$. This will be our pivot point. The symmetric group operation $g$ is a flip across the face of $A$, creating the following walk:

If $k \leq p$, then $g(e(w_k)_{j'}) = e(w_k)_{j'}$ for all $j'$.

If $p < k$ and $j' \neq j$ then $g(e(w_k)_{j'}) = e(w_k)_{j'}$.

If $p < k$ and $j' = j$ then $g(e(w_k)_{j'}) = 2M_j - e(w_k)_{j'}$.

Call the new walk $\omega_n'$.

We shall now see if there was any change in $B$ or $C$, and that the resulting walk is self avoiding. First, suppose there exists an $i$ and $k'$ such that $w_i = w_{k'}$ with $i \neq k'$. Then there are three possibilities.

a) $i, k' \leq p$ ($w_i$ and $w_{k'}$ were not changed by the operation $g$. In this case the original walk $\omega_n$ would not have been self avoiding, which is a contradiction.
b) $p \leq i, k'$. This implies that the new walk $\{w_{p'}, ..., w_{n'}\}$ is not self avoiding, which implies that $\{w_{p'}, ..., w_{n'}\}$ is not self avoiding. This implies that $\omega_n$ is not self avoiding, which is a contradiction.
c) $i < p < k'$ (the following proof can be applied to the case $k' < p < i$ too). This case, however, is impossible since after reflection $e(w_i)_j \leq e(w_{k'})_j$. Obviously strict inequality cannot hold, and if they're equal then vertex $w_k$ was not changed by the transformation $g$, which implies that $\omega_n$ is not self avoiding, a contradiction.

Therefore, the resulting walk $\omega_n'$ is self avoiding.

Note that this flip didn't change any right angles between vertices in the part of the walk $\{w_0, ..., w_{p-1}\}$, since the transformation was euclidean. Also note that the flip didn't change any right angles in the part of the walk $\{w_{p+1}, ..., w_n\}$ for similar reasons. Finally, note that because $w_p$ is the first vertex of $\omega_n$ to be in the face $A$, then $w_p$ must be attached to a right angle. One of the two sides forming this right angle would be on face $A$, so it would have been unaffected by the flip. Therefore $B(\omega_n) = B(\omega_n')$.

Finally, we show that $C(\omega_n') > C(\omega_n)$. Note that for all $r \neq j$ we have that $M_r - m_r = M_{r'} - m_{r'}$. So it remains to be shown that $M_j - m_j < M_{j'} - m_{j'}$. This is a consequence of the fact that the face $A$ contains neither $w_0$ nor $w_n$. Therefore since $A$ contains at least two vertices of $\omega_n$, the walk $\omega_n$ must have an edge that leaves $A$, and therefore $M_{j'} > M_j$, and even if $m_{j'} > m_j$ (and since $M_j \neq m_j$) $M_j$ is increased by strictly more than $m_j$ is increased. Therefore, $M_j - m_j < M_{j'} - m_{j'}$, and therefore $C(\omega_n') > C(\omega_n)$.

Now consider the second case. First note that if case 1 does not hold then $w_0$ and $w_n$ must together touch each face of $R(\omega_n)$. The only way this can happen is if they both occupy opposite corners of $R(\omega_n)$.

Define $t = \max\{k \mid w_k \text{ is a vertex at a right angle }\}$. Then the walk $\{w_t, ..., w_n\}$ is a straight line, terminating in a corner. Let $E$ be the edge connecting $w_{t-1}$ to $w_t$. There exists a single $\overline{j}$ such that $e(w_{t-1})_{\overline{j}} \neq e(w_t)_{\overline{j}}$ (this $\overline{j}$ corresponds to the dimension along which $E$ lies). Let $q$ be such that $e(w_t)_q \neq e(w_t)_q$ (this $q$ corresponds to the dimension along which the walk $\{w_t, ..., w_n\}$ lies). Rotate $\{w_t, ..., w_n\}$ so that $\{w_{t-1}, w_t, ..., w_n\}$ now all line on a straight line, along the dimension corresponding to $\overline{j}$. Call this new walk $\omega_n'$.

Note that $B(\omega_n') = B(\omega_n) + 1$ since this rotation transforms the last right angle of $\omega_n$ into a straight angle. Also note that $\omega_n'$ is a Self Avoiding Walk for reasons entirely analogous to those given in case 1.

Finally, note that $M_k - m_k = M_{k'} - m_{k'}$ for all $k \neq j'', q'$. Also, the quantity $M_q - m_q$ is increased (or decreased) by at most $n - t - 1$, and the quantity $M_{\overline{j}} - m_{\overline{j}}$ is (depending on what happened to $M_q - m_q$) decreased (or increased) by at most $n - t - 1$, and therefore $(M_q - m_q) + (M_{\overline{j}} - m_{\overline{j}})$ either increases or stays the same after the rotation. Therefore $C(\omega_n) \leq C(\omega_n')$.

From each of these two cases, we may conclude that $B(\omega_n)+C(\omega_n) < B(\omega_n')+C(\omega_n)$ for all Self Avoiding Walks which are not straight lines. Since, in general, $0 \le B(\omega_n) \le n-1$ and $0 \le C(\omega_n) \le n$, we may conclude that it takes at most $2n-1$ steps to take a Self Avoiding Walk of length $n$ and transform it into a Self Avoiding Walk $\overline{\omega_n}$ where $B(\overline{\omega_n}) + C(\overline{\omega_n}) = 2n-1$. But if this last equation holds, then the walk has no right angles and has total diameter $n$, meaning that the walk $\overline{\omega_n}$ must be a straight line. Therefore it takes at most $2n-1$ steps to transform a Self Avoiding Walk of length $n$ into a straight line of length $n$.

Thus, there is a positive probability that any self avoiding walk of length $n$ may be reduced to a straight line via the pivot algorithm. It follows that a straight line of length $n$ may be twisted into any self avoiding walk of length $n$ with positive probability also. Therefore, for each self avoiding walk there is a positive probability that it can be twisted into any other self avoiding walk of length $n$. Thus, the Markov chain $\{\omega_n\}$ is irreducible. □

The following theorem replaces the condition in the above theorem with the 'reflection of axies' condition replaced by $180°$ rotations.

**Theorem 2.9.** *The Pivot Algorithm is irreducible for Self Avoiding Walks in $\mathbb{Z}^2$ if $180°$ rotations, and either $90°$ rotations or diagonal reflections, occur with nonzero probability.*

*Proof.* Let $\omega_n = \{w_0, ..., w_n\}$ be a Self Avoiding Walk of length $n$ in $\mathbb{Z}^2$ that is not a straight line. Let $e(\vec{z})_1$ denote the $x$ component of $\vec{z}$, and let $e(\vec{z})_2$ denote the $y$ component of $\vec{z}$. Much of the notation from the previous theorem is reused here, including the definitions of $R(\omega_n)$, $B(\omega_n)$, $C(\omega_n)$, $M_j$, and $m_j$. We assume that $e(w_0)_1 \ne M_1$. If $e(w_0)_1 = M_1$ then the same proof applies with $M_1$ replaced with $m_1$ ($m_1 < M_1$ since $\omega_n$ is not a straight line).

We also assume, without loss of generality, that $e(w_{n-1})_1 = e(w_n)_1$.

We split this proof into two cases.

(1) $e(w_n)_1 = m_1$.
(2) $e(w_n)_1 \ne M_1$.

Consider the first case. Define $t = \max\{k \mid w_k \text{ is a vertex at a right angle }\}$, just as in the previous theorem. Then the walk $\{w_t, ..., w_n\}$ is a straight line, and in a proof similar to the one given in the above theorem, we may rotate $\{w_t, ..., w_n\}$ by $90°$ to get a new Self Avoiding Walk $\omega_n'$ where $B(\omega_n') = B(\omega_n) + 1$.

It is enough that each walk $\omega_n$ may be turned into a walk $\omega_n'$ where $\omega_n'$ has one right angle less than $\omega_n$, i.e.,

$$B(\omega_n') = B(\omega_n) + 1. \tag{2.10}$$

This is because we can then repeat this process until we get a walk $\overline{\omega_n}$ where $A(\overline{\omega_n}) = n-1$, and therefore, $\overline{\omega_n}$ is a straight line.

Now, consider the second case. We show that one can apply a $180°$ rotation that results in a self avoiding walk. The pivot point is the point $w_i = (x, y)$ where $x = M_1$ and $y = \min\{z \mid (M_1, z) \in \omega_n\}$ (so $w_i$ is the point farthest to the right that is lowest). We rotate the walk $\{w_i, ..., w_n\}$ around this point by $180°$.

The resulting walk (call it $\omega_n'$) is self avoiding. If not, let $w_{u'} = w_{v'}$ be two vertices which intersect after the $180°$ rotation. There are three cases, just as in the proof of Case 1 in the theorem above, and the arguments are entirely similar.

Note that $B(\omega_n) = B(\omega'_n)$. But this rotation did help us, because now note that $M_{1'} > M_1$ (the walk has been extended in the positive $x$ direction). This should make sense because all vertices of $\omega_n$ have $x$ coordinate less than or equal to $M_1$, so after rotating them $180°$ they are all on the other side of $M_1$, and therefore have $x$ coordinate greater than or equal to $M_1$.

We may now check to see whether $e(w_{n'})_1$ equals $M_{1'}$ or not. If $e(w_{n'})_1 = M_{1'}$, then we can apply the rotation in Case 1 to get a new Self Avoiding Walk in which some form of Equation 2.10 holds. If $e(w_{n'})_1 \neq M_{1'}$ then we repeat Case 2. After at most $n$ steps in Case 2 we will be able to use Case 1, so this process eventually terminates.

By repeating, where appropriate, Case 1 and Case 2, we see that the Pivot Algorithm is ergodic on Self Avoiding Walks in $\mathbb{Z}^2$.

$\square$

Since after each use of Case 1 (there may be at most $n$ such uses) we may need to use Case 2 at most $n$ times, the required number of pivots to turn a Self Avoiding Walk in $\mathbb{Z}^2$ into a straight line is at most $n^2$.

Thus, the Pivot Algorithm is ergodic in either of these cases.

## 3. Loops

We define a loop (in $\mathbb{Z}^2$ on the integer lattice) as follows.

**Definition 3.1.** A **loop** of length $2k$ is a walk that intersects itself exactly once, that point of intersection being the first vertex and the last vertex. If the set of vertices of the loop were to be written $\{w_0, w_1, ..., w_{2k}\}$, then $w_0 = w_n$.

It is worth studying these loops because walks which are not self avoiding have loops imbedded in them. If we count the number of loops we may deduce the number of self avoiding walks. Let $C_{2k}$ be the number of loops of length $2k$.

We introduce the notation $\ell_{2n}$ for a loop of length $2n$. We do this because there is no such thing of a loop that has an odd number of edges, since to return to the point one starts at, every step in the $N$ direction must eventually be undone by an $N^{-1}$ step. The same holds for the $E/E^{-1}$ direction. To write the actual steps of the loop, we write the edges rather than the vertices. For example, one way to denote the square loop would be $ENE^{-1}N^{-1}$. Starting at $(0, 0)$, one takes a single step East. Then one takes a step North, then West (denoted by $E^{-1}$), then South (denoted by $N^{-1}$). For a rectangle with six sides on the perimeter, one could denote it $E^2NE^{-2}N^{-1}$. The $E^2$ term means take two steps in the east direction, while the $E^{-2}$ means take two steps in the west direction.

We write $\nu^{p(1)}\mu^{q(1)} \cdots \nu^{p(n)}\mu^{q(n)}$ as the most general way to write a loop of length $2n$. Note that for any such loop, the following equation holds.

$$\sum_{i=1}^{n} p(i) = \sum_{i}^{n} q(i) = 0.$$

Note that $\nu^{p(1)}\mu^{q(1)} \cdots \nu^{p(n)}\mu^{q(n)}$ is a word in the free group on two generators, those two generators being $N$ and $E$. In fact, a loop is a walk written in word form that, when commutativity is allowed, reduces to the empty word, though no strict cyclic sub-string of the loop may have this property. If one wanted to check that a given random walk was indeed a Self Avoiding Walk, one would write down the non-reduced word form of the walk, and then search for an embedded word which, with commutativity, could be reduced to the empty word.

When describing a loop in the notation of a word, we always go counterclockwise around it for consistency of notation. However, if one wanted to describe a loop $\nu^{p(1)}\mu^{q(1)}\dots\nu^{p(n)}\mu^{q(n)}$ by going clockwise, the resulting loop would just be

$$\mu^{-q(n)}\nu^{-p(n)}\cdots\mu^{-q(1)}\nu^{-p(1)}.$$

**Theorem 3.2.** *Any loop of length $2n$ may be created from a loop of length $2(n-1)$ by adding two edges.*

*Proof.* Let $\ell_{2n} = \nu^{p(1)}\mu^{q(1)},...,\nu^{p(n)}\mu^{q(n)}$ be a loop of length $2n$. Then it is enough to show that there exists two edges in $\ell_{2n}$ that may be deleted, and the resulting loop is still a loop (only intersects itself on the first and last vertex).

Deleting a pair of edges from $\ell_{2n}$ involves removing them from the word that represents $\ell_{2n}$. Note that either an $N, N^{-1}$ pair or an $E, E^{-1}$ pair must be chosen. By choosing two such edges, one essentially splits the loop $\ell_{2n}$ into two pieces.

The only vertices we must be concerned with are those pairs of vertices which are within 1 unit of each other (either in the $N/N^{-1}$ or $E/E^{-1}$ direction) but which are not connected by an edge. When we pick our $N, N^{-1}$ pair to delete, it is possible that one piece of the old loop $\ell_{2n}$ will contain a vertex that is within $N/N^{-1}$ of a vertex in the other piece of the old loop $\ell_{2n}$. If this is the case, when these two pieces are combined, the result will not be a loop as it would have a self-intersection. We must show that one can always get around this problem.

To simplify notation, we will say that $(x, y) \leftrightarrow (x', y')$ if they are adjacent to one another in the loop. Additionally, we will say $(x, y) \in \ell_{2n}$ if the point $(x, y)$ occurs in the loop $\ell_{2n}$. Define

$$A = \{(x, y) \in \ell_{2n} \mid \exists_{(x',y')\in\ell_{2n}} \text{ where } |(y - y')| = 1, (x, y) \not\leftrightarrow (x', y')$$

Let $C \subseteq A$ be defined as

$$C = \{(x, y) \in A \mid \forall (x', y') \in A, x \leq x'\}.$$

Now look at the set of vertices and edges of the loop $\ell_{2n}$ which involves $x$ coordinates strictly less than the $x$ coordinates of points in $C$, call this set $B$. There are three cases, involving three separate conditions on $B$. It is worth noting that if $B \neq \emptyset$ (the case $B = \emptyset$ is one of the three cases) then $B$ contains at least three edges, so there must be at least one $N, N^{-1}$ or $E.E^{-1}$ pair of edges in $B$.

Case 1) There are two points in $B$ which are connected via an $N$ edge, and there are two points in $B$ which are connected via an $N^{-1}$ edge. In this case, we can remove these two edges and the result will still be a loop. This is because one piece of loop $\ell_{2n}$ will contain every pair of vertices which are within one unit of each other. Thus, the problem outlined in the previous paragraph is avoided, and the result is a loop of length$\ell_{2(n-1)}$, since two edges were removed.

Case 2) Vertices in $B$ are only connected to edges of the form $E, E^{-1}$, and $N^{-1}$ (instead of $N^{-1}$ we could have $N$ without loss of generality).

In this case we find an $E, E^{-1}$ pair that can be removed. Define

$$B'(u) = \{(x, y) \in B \mid x = u\}.$$

Note that this defines $B'(u)$ as a set of vertices with the same $x$ coordinate (namely, $u$), but with different $y$ coordinates. We let $u'$ be the smallest $x$ value for which $B'(u') \neq \emptyset$. This means that we let $B'(u)$ be the set of vertices and edges which lie in the intersection of the line $x = u$ with the loop $\ell_{2n}$. Then $B'(u')$ is the set of points and edges in $\ell_{2n}$ furthest to the left. We then partition $B'(u')$ into disjoint subsets $\beta_1, ..., \beta_s$ where

$$\bigcup_{i=1}^{s} \beta_i = B'(u'),$$

and if $(x, y), (a, b) \in \beta_i$ then $(x, y)$ is connected to $(a, b)$ by a string of $N^{-1}$ edges.

Then there exists $\beta_{i'}$ which has the vertices with the smallest $y$ coordinates. Let $(x_t, y_t)$ be the vertex with the largest $y$ coordinate of all vertices in $\beta_{i'}$, and let $(x_b, y_b)$ be the vertex with the smallest $y$ coordinate of all vertices in $\beta_{i'}$. Then $(x_t, y_t)$ must be connected to an $E^{-1}$, and $(x_t, y_t)$ must be connected to an $E$.

Delete this $E, E^{-1}$ pair. If this causes $\beta_{i'}$ to intersect $\ell_{2n}$ only at vertices $(x_b, y_b)$ and $(x_t, y_t)$, then we are done. However, this deletion cannot be done if there are vertices one unit to the right of each vertex in $\beta_{i'}$ besides vertices $(x_t, y_t)$ and $(x_b, y_b)$ (imagine a loop shaped like a capitalized $E$).

We may then look at the set of all vertices (and edges) each of which are within one unit of at least one vertex in $\beta_{i'}$. In a similar fashion to how we picked $\beta_{i'}$, take the bottom most string of $N$'s, call it $s(1)$. Look at the endpoints of $s(1)$ and see if one can delete the $E, E^{-1}$ pair without disrupting anything. If not, repeat the process again. Because each of these strings must have length strictly less than the previous one, this process will eventually terminate, if only because the last string will have length 1, being two vertices attached to one $N$ or $N^{-1}$ edge.

Case 3) $B = \emptyset$. This means that each vertex furthest to the right in loop $\ell_{2n}$ is within one $N/N^{-1}$ step of another vertex, though they are not connected via an edge. The method of proof for this case is entirely similar to the method in the previous paragraph. We can partition $C$ into disjoint subsets which are strings of $N^{-1}$'s. Then we can look at the top and bottom vertices of one of these strings and delete the $E^{-1}$ associated with the top vertex, and the $E$ associated with the bottom vertex. If this would cause the string of $N^{-1}$'s to illegally intersect a vertex (and, consequently, a string of $N$'s), then repeat the process with this new string of $N$'s.

□

To find $C_{2k}$ we need to define what it means for two loops to be equivalent. For example, is the loop $ENE^{-1}N^{-1}$ equivalent to the loop $NEN^{-1}E^{-1}$? In fact, when we say that there are 256 walks of length 4, we count these loops as separate walks.

However, consider loops

$$\ell_{8,1} = E^2NE^{-1}NE^{-1}N^{-2}$$

and

$$\ell_{8,2} = N^{-1}E^{-1}N^2E^2N^{-1}E^{-1}.$$

Geometrically, these two loops are very similar. In fact, if one were to flip $\ell_{8,1}$ across the $x$ axis, apply the appropriate shift to the vertex it starts at, and go around the loop clockwise, one would get $\ell_{8,2}$. This forces us to ask how many different ways a loop of length $2n$ may be written. One may define an equivalence relation on loops where $\ell_{2n} \sim \ell_{2m}$ if one can be rotated, flipped and shifted to get the other.

One can get an upper bound linear on the number of ways to write a loop by the following argument. Let $W(\ell_{2n})$ be the number of ways to write $\ell_{2n}$ as a word. First, associate each vertex to one of the edges touching it so that no two vertices are matched with the same edge. There are exactly two ways to do this. Any loop $\ell_{2n}$ may be written starting from any one of its $2n$ vertices. For an arbitrarily chosen vertex $(u, v)$ one can direct it's associated edge along any of the four possible directions.

Thus, $W(\ell_{2n}) \leq 2 \cdot 4 \cdot (2n) = 16n$. A lower bound is easily obtained by observing that $2n \leq W(\ell_{2n})$ since the word $\ell_{2n}$ could start at any one of it's $2n$ vertices.

One final observation about loops. Recall that when we use the $\nu, \mu$ notation we assume that the walk never revisits a vertex it was just at.

**Theorem 3.3.** *Let $\omega_{2m} = \nu^{p(1)}\mu^{q(1)}, ..., \nu^{p(n)}\mu^{q(n)}$ be a walk (it may or may not be self avoiding). Then one must check up to $(m-1)^2$ sub-words to see if $\omega_{2m}$ has a loop in it.*

*Proof.* Consider the walk $\nu^{p(1)}\mu^{q(1)}\nu^{p(2)}\mu^{q(2)}, ..., \nu^{p(n)}\mu^{q(n)}$.

We would first check the sub-word made up of the first four elements in the word. For example, if $p(1) \geq 4$ (suppose $p(1)$ is positive without loss of generality), the first four elements would be $\nu\nu\nu\nu$. If $p(1) = 2$ and $q(1) = 1$ and $p(2) = -2$ t hen the first four elements would be $\nu\nu\mu\nu^{-1}$. We would then check the sub-word with six elements, starting with the first $\nu$ in walk $\omega_{2m}$. Continuing by adding two elements each time, and checking sub-words that start with the first $\nu$ in $\omega_{2m}$, we would check a total of

$$\frac{2m-2}{2} = m - 1$$

sub-words. We would then repeat the process, but starting with the second element. If $p(1) = 1$ that second element would be $\mu^{\pm 1}$ depending on the sign of $q(1)$. If $p(1) > 1$ then the second element would still be $\nu$. Because the walk is of even length, we would have to check $m - 2$ sub-words (the last checked word being of length $2m - 2$). Starting with the third element, we would have to check $m - 2$ sub-words. The fourth and fifth element would require checking $n - 3$ sub-words each. The $k$th and $k+1$th element would require checking $m - \left(\lfloor \frac{k}{2} \rfloor + 1\right)$ sub-words.

Therefore, for a walk of length $2m$, one would have to check a total of

$$(m-1) + 2\sum_{i=1}^{m-2} i = (m+1) + 2\frac{(m-2)(m-1)}{2} = (m-1)\big(1 + m - 2\big) = (m-1)^2$$

sub-words to see if that walk contained a loop.

□

One way to check whether a given sub-word is indeed a loop is to see if the sum of the powers of $\nu$ equal zero, and if the sum of the powers of $\mu$ equal zero. If both these conditions hold then the walk is not self avoiding (there's some sort of loop in it).

## 4. Further Questions

Some further questions include

(1) Let $\ell_{2n}$ be a loop of length $2n$. What is $W(\ell_{2n})$? At the end of the previous section, we found an upper bound and a lower bound on $W(\ell_{2n})$. Would it be possible to improve either of these bounds? We conjecture that the lower bound may be improved to $2 \cdot (2n) = 4n$, because one would never get a previously found word by going clockwise and counterclockwise at each point.

(2) Is it possible to write down explicitly the number of loops of length $2n$? If not, recall that $S_{2n} \approx \mu^n$ as proved in Theorem 1.5. Can $C_{2n}$ be similarly approximated?

(3) How walks are there of length $k$ which have exactly one loop of length $2n$ embedded in them? How many walks are there which have multiple loops embedded in them?

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