ON A FUNCTION MODELING N-STEP SELF AVOIDING WALK

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ABSTRACT. We introduce and study the needle function. We prove that this function is a function modeling n-step self avoiding walk. We show that the total length of the l-step self-avoiding walk modeled by this function is of the order

$$\ll \frac{n^{\frac{3}{2}}}{2}\bigg(\max\{\sup(x_j)\}_{1\leq j\leq \frac{l}{2}}+\max\{\sup(a_j)\}_{1\leq j\leq \frac{l}{2}}\bigg).$$

1. Introduction

Self avoiding walk, roughly speaking, is a sequence of moves on the lattice that does not visit the same point more than once. It is somewhat akin to the graph theoretic notion of a path. It is a mathematical problem to determine a function that models self avoiding walks of any given number of steps. More formally, the problem states

Conjecture 1.1. Does there exist a function that models n-steps self-avoiding walks?

The problem had long been studied from mathematical perspective but unfortunately our understanding was not good enough. For instance the problem has recently been studied from the standpoint of network theory [2]. The problem also has great significance that extends beyond the shores of mathematics and its allied area. For instance studies shows that a good understanding of the underlying problem will certainly have its place in physics and chemistry about the long-term structural movement of substances such as polymers and certain proteins [1],[3]. In this paper we find a function that models an n-step self avoiding walk. We leverage the method of compression and its accompanied estimates to study these things in much more detail. In particular we obtain the following result

Theorem 1.1. *The map* $(\Gamma_{\vec{a_1}}\circ \mathbb{V}_m)\circ(\Gamma_{\vec{a_2}}\circ \mathbb{V}_m)\ldots\circ(\Gamma_{\vec{a_{\frac{l}{2}}}}\circ \mathbb{V}_m):\mathbb{R}^n\longrightarrow \mathbb{R}^n$, *where*

$$(\Gamma_{\vec{a_1}}\circ \mathbb{V}_m)\circ\cdots\circ(\Gamma_{\vec{a_k}}\circ \mathbb{V}_m)$$

is the k-fold needle function with some mixed translation factors $\vec{a_1},\vec{a_2},\ldots,\vec{a_k}\in\mathbb{R}^n$, is a function modeling l-step self avoiding walk.

We also comment very roughly about the total length of the l-step self avoiding walk modeled by the needle function in the following result

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Theorem 1.2. *The total length of the l-step self-avoiding walk modeled by the needle function* $(\Gamma_{\vec{a_1}} \circ \mathbb{V}_m) \circ (\Gamma_{\vec{a_2}} \circ \mathbb{V}_m) \ldots \circ (\Gamma_{\vec{a_{\frac{l}{2}}}} \circ \mathbb{V}_m) : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ *is of order*

$$\ll \frac{n^{\frac{3}{2}}}{2}\left(\max\{\sup(x_j)\}_{1\leq j\leq \frac{l}{2}} + \max\{\sup(a_j)\}_{1\leq j\leq \frac{l}{2}}\right).$$

2. **Preliminary results**

Definition 2.1. By the compression of scale $m \geq 1$ on $\mathbb{R}^n$ we mean the map $\mathbb{V} : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ such that

$$\mathbb{V}_m[(x_1, x_2, \ldots, x_n)] = \left(\frac{m}{x_1}, \frac{m}{x_2}, \ldots, \frac{m}{x_n}\right)$$

for $n \geq 2$ and with $x_i \neq 0$ for all $i = 1, \ldots, n$.

Proposition 2.1. *A compression of scale $m \geq 1$ with $\mathbb{V}_m : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a bijective map. In particular the compression $\mathbb{V}_m : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a bijective map of order 2.*

Proof. Suppose $\mathbb{V}_m[(x_1, x_2, \ldots, x_n)] = \mathbb{V}_m[(y_1, y_2, \ldots, y_n)]$, then it follows that

$$\left(\frac{m}{x_1}, \frac{m}{x_2}, \ldots, \frac{m}{x_n}\right) = \left(\frac{m}{y_1}, \frac{m}{y_2}, \ldots, \frac{m}{y_n}\right).$$

It follows that $x_i = y_i$ for each $i = 1, 2, \ldots, n$. Surjectivity follows by definition of the map. Thus the map is bijective. The latter claim follows by noting that $\mathbb{V}_m^2[\vec{x}] = \vec{x}$. ☐

Remark 2.2. The notion of compression is in some way the process of re scaling points in $\mathbb{R}^n$ for $n \geq 2$. Thus it is important to notice that a compression pushes points very close to the origin away from the origin by certain scale and similarly draws points away from the origin close to the origin.

2.1. **The mass and the gap of compression.**

Definition 2.3. By the mass of a compression of scale $m \geq 1$ we mean the map $\mathcal{M} : \mathbb{R}^n \longrightarrow \mathbb{R}$ such that

$$\mathcal{M}(\mathbb{V}_m[(x_1, x_2, \ldots, x_n)]) = \sum_{i=1}^{n} \frac{m}{x_i}.$$

Proposition 2.2. *Let $(x_1, x_2, \ldots, x_n) \in \mathbb{N}^n$, then the estimates holds*

$$m\log\left(1 - \frac{n-1}{\sup(x_j)}\right)^{-1} \ll \mathcal{M}(\mathbb{V}_m[(x_1, x_2, \ldots, x_n)]) \ll m\log\left(1 + \frac{n-1}{\operatorname{Inf}(x_j)}\right)$$

for $n \geq 2$.

Proof. Let $(x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$ for $n \geq 2$ with $x_j \geq 1$. Then it follows that

$$\begin{aligned}\mathcal{M}(\mathbb{V}_m[(x_1, x_2, \ldots, x_n)]) &= m\sum_{j=1}^{n} \frac{1}{x_j} \\ &\leq m\sum_{k=0}^{n-1} \frac{1}{\operatorname{Inf}(x_j) + k}\end{aligned}$$

and the upper estimate follows by the estimate for this sum. The lower estimate also follows by noting the lower bound

$$\mathcal{M}(\mathbb{V}_m[(x_1,x_2,\ldots,x_n)]) = m\sum_{j=1}^{n}\frac{1}{x_j} \geq m\sum_{k=0}^{n-1}\frac{1}{\sup(x_j)-k}.$$

□

Definition 2.4. Let $(x_1,x_2,\ldots,x_n)\in\mathbb{R}^n$ with $x_i\neq 0$ for all $i=1,2\ldots,n$. Then by the gap of compression of scale m $\mathbb{V}_m$, denoted $\mathcal{G}\circ\mathbb{V}_m[(x_1,x_2,\ldots,x_n)]$, we mean the expression

$$\mathcal{G}\circ\mathbb{V}_m[(x_1,x_2,\ldots,x_n)] = \left|\left|\left(x_1-\frac{m}{x_1},x_2-\frac{m}{x_2},\ldots,x_n-\frac{m}{x_n}\right)\right|\right|$$

Proposition 2.3. *Let $(x_1,x_2,\ldots,x_n)\in\mathbb{R}^n$ for $n\geq 2$ with $x_j\neq 0$ for $j=1,\ldots,n$, then we have*

$$\mathcal{G}\circ\mathbb{V}_m[(x_1,x_2,\ldots,x_n)]^2 = \mathcal{M}\circ\mathbb{V}_1\left[\left(\frac{1}{x_1^2},\ldots,\frac{1}{x_n^2}\right)\right] + m^2\mathcal{M}\circ\mathbb{V}_1[(x_1^2,\ldots,x_n^2)] - 2mn.$$

In particular, we have the estimate

$$\mathcal{G}\circ\mathbb{V}_m[(x_1,x_2,\ldots,x_n)]^2 = \mathcal{M}\circ\mathbb{V}_1\left[\left(\frac{1}{x_1^2},\ldots,\frac{1}{x_n^2}\right)\right] - 2mn + O\bigg(m^2\mathcal{M}\circ\mathbb{V}_1[(x_1^2,\ldots,x_n^2)]\bigg).$$

Proposition 2.3 offers us an extremely useful identity. It allows us to pass from the gap of compression on points to the relative distance to the origin. It tells us that points under compression with a large gap must be far away from the origin than points with a relatively smaller gap under compression. That is to say, the inequality

$$\mathcal{G}\circ\mathbb{V}_m[\vec{x}] \leq \mathcal{G}\circ\mathbb{V}_m[\vec{y}]$$

if and only if $||\vec{x}||\leq||\vec{y}||$ for $\vec{x},\vec{y}\in\mathbb{N}^n$. This important transference principle will be mostly put to use in obtaining our results.

Lemma 2.5 (Compression estimate)**.** *Let $(x_1,x_2,\ldots,x_n)\in\mathbb{N}^n$ for $n\geq 2$, then we have*

$$\mathcal{G}\circ\mathbb{V}_m[(x_1,x_2,\ldots,x_n)]^2 \ll n\sup(x_j^2) + m^2\log\left(1+\frac{n-1}{\mathrm{Inf}(x_j)^2}\right) - 2mn$$

and

$$\mathcal{G}\circ\mathbb{V}_m[(x_1,x_2,\ldots,x_n)]^2 \gg n\mathrm{Inf}(x_j^2) + m^2\log\left(1-\frac{n-1}{\sup(x_j^2)}\right)^{-1} - 2mn.$$

Proof. The estimates follows by leveraging the estimates in Proposition 2.2 and noting that

$$n\mathrm{Inf}(x_j^2) \ll \mathcal{M}\circ\mathbb{V}_1\left[\left(\frac{1}{x_1^2},\ldots,\frac{1}{x_n^2}\right)\right] \ll n\sup(x_j^2).$$

□

3. Compression lines

In this section we study the notion of lines induced under compression of a given scale. We first launch the following language.

Definition 3.1. Let $\vec{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$ with $x_1 \neq 0$ for $1 \leq i \leq n$. Then by the line $L_{\mathbb{V}_m[\vec{x}]}$ produced under compression $\mathbb{V}_m : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ we mean the line joining the points $\vec{x}$ and $\mathbb{V}_m[\vec{x}]$ given by

$$\vec{r} = \vec{x} + \lambda(\vec{x} - \mathbb{V}_m[\vec{x}])$$

where $\lambda \in \mathbb{R}$.

Remark 3.2. Next we show that the lines produced under compression of two distinct points not on the same line of compression cannot intersect at the corresponding points and their images under compression.

Lemma 3.3. *Let $\vec{a} = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$ with $\vec{a} \neq \vec{x}$ and $a_i, x_j \neq 0$ for $1 \leq i, j \leq n$. If the point $\vec{a}$ lies on the corresponding line $L_{\mathbb{V}_m[\vec{x}]}$, then $\mathbb{V}_m[\vec{a}]$ also lies on the same line.*

Proof. Pick arbitrarily a point $\vec{a}$ on the line $L_{\mathbb{V}_m[\vec{x}]}$ produced under compression for any $\vec{x} \in \mathbb{R}^n$. Suppose on the contrary that $\mathbb{V}_m[\vec{a}]$ cannot live on the same line as $\vec{a}$. Then $\mathbb{V}_m[\vec{a}]$ must be away from the line $L_{\mathbb{V}_m[\vec{x}]}$. Produce the compression line $L_{\mathbb{V}_m[\vec{a}]}$ by join the point $\vec{a}$ to the point $\mathbb{V}_m[\vec{a}]$ by a straight line. Then It follows from Proposition 2.3

$$\mathcal{G} \circ \mathbb{V}_m[\vec{x}] > \mathcal{G} \circ \mathbb{V}_m[\vec{a}].$$

Again pick a point $\vec{c}$ on the line $L_{\mathbb{V}_m[\vec{a}]}$, then under the assumption it follows that the point $\mathbb{V}_m[\vec{c}]$ must be away from the line. Produce the compression line $L_{\mathbb{V}_m[\vec{c}]}$ by joining the points $\vec{c}$ to $\mathbb{V}_m[\vec{c}]$. Then by Proposition 2.3 we obtain the following decreasing sequence of lengths of distinct lines

$$\mathcal{G} \circ \mathbb{V}_m[\vec{x}] > \mathcal{G} \circ \mathbb{V}_m[\vec{a}] > \mathcal{G} \circ \mathbb{V}_m[\vec{c}].$$

By repeating this argument, we obtain an infinite descending sequence of lengths of distinct lines

$$\mathcal{G} \circ \mathbb{V}_m[\vec{x}] > \mathcal{G} \circ \mathbb{V}_m[\vec{a_1}] > \cdots > \mathcal{G} \circ \mathbb{V}_m[\vec{a_n}] > \cdots .$$

This proves the Lemma. □

It is important to point out that Lemma 3.3 is the ultimate tool we need to show that certain function is indeed a function modeling n-step self avoiding walk. We first launch such a function as an outgrowth of the notion of compression. Before that we launch our second Lemma. One could think of this result as an extension of Lemma 3.3.

Lemma 3.4. *Let $\vec{a} = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$ and $\vec{b} = (b_1, b_2, \ldots, b_n) \in \mathbb{R}^n$ with $\vec{a} \neq \vec{b}$ and $a_i, b_j \neq 0$ for $1 \leq i, j \leq n$. If the corresponding lines $L_{\mathbb{V}_m[\vec{a}]} : r_1 = \vec{a} + \lambda(\vec{a} - \mathbb{V}_m[\vec{a}])$ and $L_{\mathbb{V}_m[\vec{b}]} : r_2 = \vec{b} + \mu(\vec{b} - \mathbb{V}_m[\vec{b}])$ for $\mu, \lambda \in \mathbb{R}$ intersect, then*

$$\vec{a} - \mathbb{V}_m[\vec{a}] \parallel \vec{b} - \mathbb{V}_m[\vec{b}].$$

Proof. First consider the points $\vec{a} = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$ and $\vec{b} = (b_1, b_2, \ldots, b_n) \in \mathbb{R}^n$ with $\vec{a} \neq \vec{b}$ and $a_i, b_j \neq 0$ for $1 \leq i, j \leq n$ with corresponding lines $L_{\mathbb{V}_m[\vec{a}]}$: $r_1 = \vec{a} + \lambda(\vec{a} - \mathbb{V}_m[\vec{a}])$ and $L_{\mathbb{V}_m[\vec{b}]} : r_2 = \vec{b} + \mu(\vec{b} - \mathbb{V}_m[\vec{b}])$ for $\mu, \lambda \in \mathbb{R}$. Suppose they intersect at the point $\vec{s}$, then it follows that the point $\mathbb{V}_m[\vec{s}]$ lies on the lines $L_{\mathbb{V}_m[\vec{a}]} : r_1 = \vec{a} + \lambda(\vec{a} - \mathbb{V}_m[\vec{a}])$ and $L_{\mathbb{V}_m[\vec{b}]} : r_2 = \vec{b} + \mu(\vec{b} - \mathbb{V}_m[\vec{b}])$ and the result follows immediately. □

Lemma 3.3 combined with Lemma 3.4 tells us that the line produced by compression on points away from other lines of compression are not intersecting. We leverage this principle to show that a certain function indeed models a self-avoiding walk.

4. **The needle function**

Definition 4.1. By the needle function of scale m and translation factor $\vec{a}$, we mean the composite map

$$\Gamma_{\vec{a}} \circ \mathbb{V}_m : \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

such that for any $\vec{x} \in \mathbb{R}^n$

$$\Gamma_{\vec{a}} \circ \mathbb{V}_m[\vec{x}] = \vec{y}$$

where $\vec{x} = (x_1, x_2, \ldots, x_n)$ with $x_i \neq 0$ for $1 \leq i \leq n$ and $\Gamma_{\vec{a}}[\vec{x}] = (x_1 + a_1, x_2 + a_2, \ldots, x_n + a_n)$.

Definition 4.2. The needle function $\Gamma_{\vec{a}} \circ \mathbb{V}_m : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a bijective function of order 2.

Proof. We remark that the translation with translation factor $\vec{a}$ for a fixed $\vec{a}$ given by $\Gamma_{\vec{a}} : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a bijective map. The result follows since the composite of bijective maps is still bijective. □

Theorem 4.3. *The map* $(\Gamma_{\vec{a_1}} \circ \mathbb{V}_m) \circ (\Gamma_{\vec{a_2}} \circ \mathbb{V}_m) \ldots \circ (\Gamma_{\vec{a_{\frac{l}{2}}}} \circ \mathbb{V}_m) : \mathbb{R}^n \longrightarrow \mathbb{R}^n$, *where*

$$(\Gamma_{\vec{a_1}} \circ \mathbb{V}_m) \circ \cdots \circ (\Gamma_{\vec{a_k}} \circ \mathbb{V}_m)$$

is the k-fold needle function with mixed translation factors $\vec{a_1}, \vec{a_2}, \ldots, \vec{a_k} \in \mathbb{R}^n$, *is a function modeling l-step self avoiding walk.*

Proof. Pick arbitrarily a point $\vec{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{N}^n$ for $n \geq 2$ with $x_i \neq 0$ for $1 \leq i \leq n$ and apply the needle function $\Gamma_{\vec{a_1}} \circ \mathbb{V}_m[\vec{x}]$ for a fixed translation factor $\vec{a_1} \neq \vec{O}$ such that the point $\Gamma_{\vec{a_1}} \circ \mathbb{V}_m[\vec{x}]$ with a fixed compression scale m is away from the line $L_{\mathbb{V}_m[\vec{x}]}$. Let us now traverse the line produced under compression to the line produced by translation of the point $\Gamma_{\vec{a_1}}(\mathbb{V}_m[\vec{x}])$ with the starting point $\vec{x}$ to $\mathbb{V}_m[\vec{x}]$ and finally from $\mathbb{V}_m[\vec{x}]$ to $\Gamma_{\vec{a_1}}(\mathbb{V}_m[\vec{x}])$. The upshot is a self avoiding walk of length 2. Since the point $\Gamma_{\vec{a_1}}(\mathbb{V}_m[\vec{x}]) = \vec{z}$ is away from the line $L_{\mathbb{V}_m[\vec{x}]}$ produced under compression on the point $\vec{x}$, the line under compression on the point $\mathbb{V}_m[\vec{x}] = \vec{z}$ given by $L_{\mathbb{V}_m[\vec{z}]}$ cannot intersect the line $L_{\mathbb{V}_m[\vec{x}]}$ produced under compression. For suppose this happens, then by Lemma 3.4 the line $L_{\mathbb{V}_m[\vec{z}]}$ produced under compression on the point $\vec{z}$ must be parallel to the line $L_{\mathbb{V}_m[\vec{x}]}$. This is absurd since the point $\vec{z}$ is away from the line $L_{\mathbb{V}_m[\vec{x}]}$. The upshot is a self avoiding walk of length 3. Again we apply the translation $\Gamma_{\vec{a_2}}$ on the point

$\mathbb{V}_m[\vec{z}]$ with a suitable translation factor $\vec{a_2} \neq \vec{O}$ such that the point $\Gamma_{\vec{a_2}} \circ \mathbb{V}_m[\vec{z}]$ is away from previous lines so constructed and whose corresponding line under compression does not intersect previous lines so constructed under translation, since by Lemma 3.4 and Lemma 3.3 the corresponding line under compression cannot intersect previous lines under compression by the choice of our translation factor. By traversing all these lines starting from the point $\vec{x}$ to $\mathbb{V}_m[\vec{x}]$, $\vec{z} = \mathbb{V}_m[\vec{x}]$ to $\Gamma_{\vec{a_1}}[\vec{z}]$, $\Gamma_{\vec{a_1}}[\vec{z}]$ to $\mathbb{V}_m \circ \Gamma_{\vec{a_1}}[\vec{z}]$ and finally from $\mathbb{V}_m \circ \Gamma_{\vec{a_1}}[\vec{z}]$ to $\Gamma_{\vec{a_2}} \circ \mathbb{V}_m \circ \Gamma_{\vec{a_1}}[\vec{z}]$, we obtain a self avoiding walk of length 4. By continuing this argument $\frac{l}{2}$ number of times and choosing an appropriate translation factor so that the image point under such translation is away from all the previous lines and whose corresponding line under compression does not intersect previous line produced under translation, and noting that this line under compression will certainly not intersect previous lines of compression by appealing to Lemma 3.3 and Lemma 3.4, we produce a self avoiding walk of length l. This completes the proof. □

We remark that we can certainly do more than this by estimating the total length of the self-avoiding walk modeled by this function in the following result.

Theorem 4.4. *The total length of the l-step self-avoiding walk modeled by the needle function $(\Gamma_{\vec{a_1}} \circ \mathbb{V}_m) \circ (\Gamma_{\vec{a_2}} \circ \mathbb{V}_m) \ldots \circ (\Gamma_{\vec{a_{\frac{l}{2}}}} \circ \mathbb{V}_m) : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ for $\vec{a_i} \in \mathbb{R}^n$ is of order*

$$\ll \frac{n^{\frac{3}{2}}}{2}\bigg(\max\{\sup(x_j)\}_{1 \leq j \leq \frac{l}{2}} + \max\{\sup(a_j)\}_{1 \leq j \leq \frac{l}{2}}\bigg).$$

Proof. We note the the total length of the l-step self avoiding walk modeled by the needle function is given by the expression

$$\sum_{i=1}^{\frac{l}{2}} \mathcal{G} \circ \mathbb{V}_m[\vec{x_i}] + \sum_{i=1}^{\frac{l}{2}} ||\vec{a_i}||$$

and the result follows by applying the estimates in Lemma 2.5. □

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