Self Avoiding Walks

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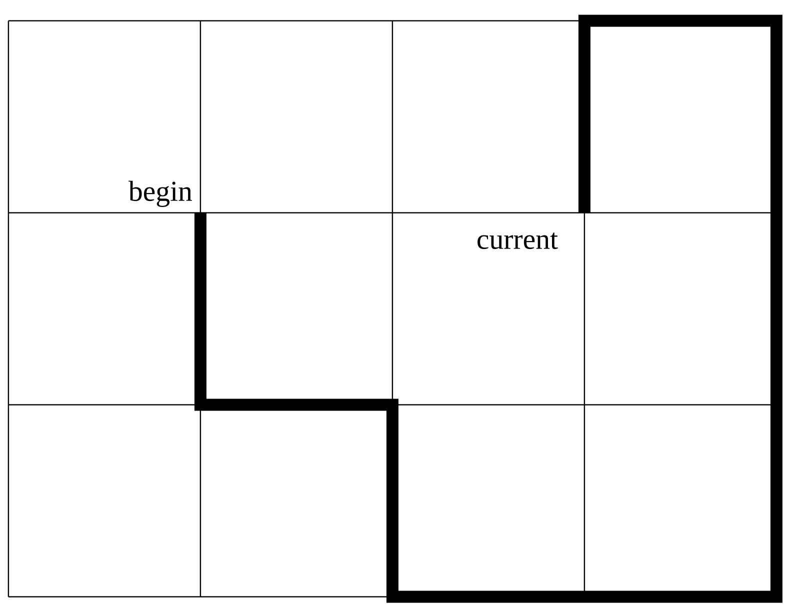
The Scenario:

Suppose you're standing on the plane and you take integer steps in any of the four N,S,E,W directions for a total of n steps with the following restriction: you cannot visit the same grid point more than once. A walk of this form is called a *Self Avoiding Walk (SAW)*. For example, you're walk might look something like this:



The Problem:

Suppose every walk begins at the origin. Let c_n *be the total number of self avoiding walks of size* n *in the space* $\mathbf{Z}^d, d \geq 2$*. What is the numerical value for* c_n*?*

Some Formalism:

Think about the n step SAW as a sequence of points $(w_1, \ldots, w_n)$ where $w_i \in \mathsf{Z}^d, |w_{i+1} - w_i| = 1$, and $w_i \neq w_j$ for all $i \neq j$.

A Quick Bound:

To get an upper bound that will help us later, consider walks that do not go through immediate reversals, $w_{i+2} \neq w_i$. There are $2d$ possible moves for the first step and $(2d - 1)$ choices for the remaining $n - 1$ steps. Note, for large

n, there will be plenty of non-SAWs. TOTAL $= 2d(2d-1)^{n-1}$.

The lower bound will be taken to be the SAWs that take a step in the positive direction each time. There are d positive directions for dimension d, and since we have n total steps, TOTAL $= d^n$.

Thus,

$$d^n \leq c_n \leq 2d(2d-1)^{n-1}$$

Monotonicity of SAWs:

George L. O'Brien (1989) proves that c_n is an increasing function in n.

Random Walks and SAWs:

Let X be a random varialbe which describes the final location of a SAW and give X a uniform distribution; $P(X = \omega_n) = 1/c_n$. Then *mean squared displacement* from the origin is given by,

$$E(X^2) = \frac{1}{c_n}\sum_{\omega_n} |\omega_n|^2$$

Again, calculations become terribly frustrating, however, it is worth while to compare $E(X^2)$ with that of an simple *random* walk. Here we can let X_i go in any of the $1/2d$ directions independently with probability $1/2d$, and let $S_n = X_1 + \cdots + X_n$ denote the final location of the random walk. We then have,

$$E(S_n^2) = \sum_{i,j=1}^{n} E(X_i X_j) = N$$

Since when $i \neq j$ we have $E(X_i X_j) = E(X_i)E(X_j) = 0$ using independence and $E(X_i^2) = 1$ with respect to the Euclidean norm.

Two Conjectures:

It is believed that the number and the mean squared displacement of SAWs behave as,

$$c_n \sim A\mu^n n^{\gamma-1} \quad (1)$$

$$E(X^2) \sim Dn^{2\nu} \quad (2)$$

where A, D, μ, γ, ν are all positive constants which depend upon which dimension we are working in.

Both equations (1) and (2) have been proven to hold only when $d \geq 5$.

Connective Constant, μ:

If we let,

$$\mu = \lim_{n\to\infty} \sqrt[n]{c_n}$$

this limit exists and is called the *connectivity constant*. This provides some justification for equation (1) above.

From this we have a nice bound on the connectivity constant in terms of the dimension of our space,

$$d \leq \mu \leq 2d - 1$$

To see this, note for $a > 0$, $\sqrt[n]{a} \to 1$ as $n \to \infty$, and let $a = 2d/(2d-1)$.

A proof is based on the following observation,

$$c_{n+m} \leq c_n c_m$$

$$\log(c_{n+m}) \leq \log(c_n) + \log(c_m)$$

The sequence $\{\log(c_n)\}$ is called *subadditive* due to the last relation and using the following lemma, we have,

Lemma. *Let* $\{a_n\}$ *be a subadditive sequence of real numbers. Then,*

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

Critical Exponent γ:

Since $\mu^n \leq c_n$ we have $\gamma \geq 1$. It has been proven that for equation (1), $\gamma = 1$ when the dimension $d \geq 5$.

Note, an **open problem** is to prove that γ is finite or find its numerical value when $d = 2, 3, 4$ provided equation (1) holds.

The probability (uniform measure) that two SAWs of length n beginning at the same point **do not** intersect is given by,

$$p = \frac{c_{2n}}{c_n c_n} \sim \frac{2^{\gamma-1}}{A} n^{1-\gamma}$$

To see this, note that if two SAWs do not intersect and begin from the same point, we must choose from the total number of SAWs of length $2n$; also use equation (1) above.

Concerning the cases when $d = 2, 3, 4$ we have,

1. if $\gamma > 1, p \to 0$; their paths cross at infinity. Otherwise, $\gamma = 1, p \sim 1/A > 0$, and there is positive probability that their paths do not cross.

2. for two simple random walks in an analogous situation, it has been proven that $p > 0$ when $d \geq 5$ and $p \to 0$ otherwise.

Critical Exponent, ν:

If we assume the equation (2), mean squared displacement, we have

$$|w_n|^2 \leq n^2 \Rightarrow E(X^2) \leq n^2 \Rightarrow \nu \leq 1$$

Note, an **open problem** is to prove that

$$E(X^2) \;\geq\; Kn \tag{3}$$

for some constant K. This states that the mean squared distance grows as fast as or faster than *diffusion* which is associated to the simple random walk.

This also implies that $\nu \geq 1/2$. It has been proven that $\nu = 1/2$ when $d \geq 5$.

Some Considerations:

1. If W denotes the collection of *all* walks of size n and W_i denotes the subset of walks that intersect themselves exactly i times, then we can partition W as

$$W = W_0 \bigcup W_1 \bigcup \cdots \bigcup W_{n-1}$$

with W_0 being the collection of SAWs. From this we can conclude

(a) If we let $c(n)_i = c_i$ be the cardinality of W_i (c_i is a function of the length of the walks under consideration), we have

$$c_0 = (2d)^n - \sum_{k=1}^{n-1} c_k$$

Also note, $c_{n-1} = 2d$ since if the walk of size n must intersect itself $n-1$ times, it must be of length one and there are only $2d$ of these. Thus we have,

$$c_0 = (2d)^n - \sum_{k=1}^{n-2} c_k - 2d$$

And I believe that the inner sum terms can be calculated in terms of $c(j)_0$ for $j = 1, \ldots, n-2$; that is, we can compute $c(n)_0$ recursively. However, the combinatorics seem to become difficult to calculate even for $n \geq 4$. So this leads me to believe that no only is it difficult to find c_0, but also c_1, c_2, and so on.

2. Recall that O'Brien proved that $c(n)_0$ is monotone in n. Can we prove that $c(n)_i$ is monotone in n for each i? And if so, what will that tell us?

References:

1. Neal Madras and Gordon Slade (1993). The Self Avoiding Walk. Birkhauser.

2. George L. O'Brien (1990). Monotonicity of the Number of Self-Avoiding Walks. *J. Stat. Phys.*, **11**:969-979.