

SOME OBSERVATIONS ON SELF-AVOIDING WALKS

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1 Introduction

Self-avoiding walks have been extensively studied and analyzed in the scientific community due to their significant applications in the fields of physics, chemistry, and biology. They are an important model for describing the behavior of polymer chains, and protein folding, and are used in DNA conformational analysis [6] all of which have a similar characteristic of not allowing self-intersections. Further details about self-avoiding walks can be found in [4] [8], [2], [9], and [5].

Initially, a random walk was used to model linear polymers. However, the presence of a monomer at position x prohibits any other part of the polymer from getting too close to x , meaning that other monomers are excluded from a certain volume of space. This is the excluded volume effect. Taking this effect into account reveals that a self-avoiding walk is a more suitable model for a linear polymer than a random walk.

In this article, we address three things. First, we show the number of self-avoiding walks of length n grows exponentially with n . Secondly, we describe an algorithm called the pivot algorithm through which one can generate a self-avoiding walk from another self-avoiding walk. We then consider the growing self-avoiding walk (GSAW) model and find out the mean trapping length of a walk.

Layout: The rest of the article is organized as follows. We shall begin in the next section (2) by defining the model precisely and stating the main result (Theorem 2.3) that specifies the growth rate of the self-avoiding walk. We then proceed to bound the number of the self-avoiding walk for a given n . In the next section (3) we describe the pivot algorithm and discuss Theorem 3.1 stating that the algorithm is ergodic. In the next section (4), we discuss the model of the growing self-avoiding walk and we find the mean trapping length by running simulations. We then describe the collapse transition. In the last section (5), we provide a proof of Theorem (2.3) and discuss the symmetry operations involved in the pivot algorithm.

2 Counting Self-Avoiding Walks

Let \mathbb{Z}^d be the integer lattice. We begin by defining the self-avoiding walk:

Definition 2.1. *An N -step self-avoiding walk can be defined as a function $\omega : \{0, 1, \dots, N\} \rightarrow \mathbb{Z}^d$, beginning at the site x , i.e. $\omega(0) = x$, satisfying*

$$|\omega(j+1) - \omega(j)| = 1, \text{ and } \omega(i) \neq \omega(j) \forall i \neq j$$

We write $|\omega| = N$ to denote the length of ω , and we denote the components of $\omega(j)$ by $\omega_i(j)$ where $i = 1, \dots, d$. Let C_N denote the number of N -step self-avoiding walks beginning at the origin. By convention, $C_0 = 1$.

Let $\log C_n = a_n$.

Proposition 2.2. *The self-avoiding walk is subadditive, i.e., $a_{n+m} \leq a_m + a_n$.*

Now we prove Proposition 2.2 using the following intuitive idea: 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 but the concatenations of every n and m length walk is not self-avoiding.

Proof of Proposition 2.2. : Let S_{n+m} , S_n , and S_m be the set of self-avoiding walks of length $n + m$, n , and m respectively. Consider the function $f : S_{n+m} \rightarrow (S_n \times S_m)$ defined by $f(\omega) = (\omega^{(1)}, \omega^{(2)})$ where $\omega \in S_{n+m}$, $\omega^{(1)} \in S_n$, $\omega^{(2)} \in S_m$

$$\text{and } \omega^{(1)} : \{0, 1, \dots, n\} \rightarrow \mathbb{Z}^d, \omega^{(1)}(k) = \omega(k), k = 0, 1, \dots, n$$

,

$$\omega^{(2)} : \{0, 1, \dots, m\} \rightarrow \mathbb{Z}^d, \omega^{(2)}(0) = \omega^{(1)}(n)$$

.

$$\omega^{(2)}(k) = \omega(k + n) - \omega(n), k = 0, 1, \dots, m$$

. It is clear that f is injective. Therefore $C_{n+m} = |S_{n+m}| \leq |S_n||S_m| = C_n C_m$. \square

We now state a theorem based on the definition above, in order to understand how self-avoiding walks of a specified length n grow with increasing n .

Theorem 2.3. : As $n \rightarrow \infty$, $\frac{a_n}{n} \rightarrow c$ i.e.

$$\lim_{n \rightarrow \infty} \frac{a_n}{n} = c$$

. This shows that as n increases the total number of self-avoiding walks of length n grows exponentially.

The limit μ was first shown to exist by Hammersly and Morton [1]. Roughly, C_n is of order μ^n for large n , so μ is the average number of possible next steps for a long self-avoiding walk. The key idea used to prove this is the subadditivity of the self-avoiding walks.

We now discuss some bounds of C_n , i.e., the total number of self-avoiding walks of length n .

Lower Bound: Consider the set of self-avoiding walks in the d -dimensional integer lattice space which, for each axis, only take steps in positive directions. These are all obviously self-avoiding, and at each point, there are d possible choices of directions, so there are d^n such self-avoiding walks. Thus, $C_n \geq d^n$.

Upper Bound: Now consider all walks of length n that never return to the site they were at in the previous step, that is, the set of all walks for which $\omega(j-1) \neq \omega(j+1)$ for $j = 1, \dots, n-1$. Then at each site after the initial one, there are $2d-1$ possible choices, and therefore there are $2d(2d-1)^{n-1}$ such walks. All self-avoiding walks have this property, so there are at most $2d(2d-1)^{n-1}$ self-avoiding walks.

Therefore we have $d^n \leq C_n \leq 2d(2d-1)^{n-1}$.

3 The pivot-algorithm

We shall be using the pivot algorithm [5] to generate self-avoiding walks from a self-avoiding walk. The idea behind the pivot algorithm is to start with a self-avoiding walk and then make small perturbations to its shape by rotating segments and reflecting segments around pivot points while ensuring that the resulting path remains self-avoiding.

3.1 Algorithm

The pivot algorithm is implemented as follows:

1. First a self-avoiding walk is created.
2. A pivot point k along the walk ($0 \leq k \leq N - 1$) is chosen according to any preset strictly positive probabilities p_0, \dots, p_{N-1} .
3. Let G be the group of orthogonal transformations (about the origin) that leave \mathbb{Z}^d invariant. Then the symmetry operation $g \in G$ can be chosen according to any preset probability distribution $\{p_g\}_{g \in G}$ that satisfies $p_g = p_g^{-1}$ for all g , and has enough nonzero entries to ensure ergodicity. Now we apply this operation to the walk from the pivot point k onwards. Elements of G are described in the appendix.
4. Now we check if our generated walk is still valid. If it is, then we find another self-avoiding walk. Otherwise, the initial walk is counted again in the sample.

Theorem 3.1. *The pivot algorithm is ergodic for self-avoiding walks on \mathbb{Z}^d provided that all axis reflections, and either all 90° rotations or all diagonal reflections are given nonzero probability. In fact, any N -step self-avoiding walk can be transformed into a straight rod by some sequence of $2N-1$ or fewer such pivots.*

Notation: Let $\omega = (\omega(0), \omega(1), \dots, \omega(N))$ be a self-avoiding walk of length N with $w(0)$ not necessarily equal to 0. Let $B(w)$ be the smallest rectangular box containing w . So, $B(w) = \{(x_1, \dots, x_d) : m_i < x_i < M_i\}$ where $m_i = \min\{w_i(j), j = 0, 1, \dots, N\}$ and $M_i = \max\{w_i(j), j = 0, 1, \dots, N\}$ are the minimum and the maximum values of the i^{th} co-ordinate.

A face of $B(\omega)$ is any set of the form $\{x \in B(\omega) : x_i = m_i\}$ or $\{x \in B(\omega) : x_i = M_i\}$ for some $i = 1, 2, \dots, d$

Let $D(\omega) = \sum_{i=1}^d M_i - m_i$ and $A(\omega) = |\{i : 0 \leq i \leq N, \omega_i = \frac{1}{2}(\omega_{i-1} + \omega_{i+1})\}|$. So $D(\omega)$ is the l^1 diameter and $A(\omega)$ is the number of straight internal angles of ω .

Here is the plan of the proof: We will partition into two subsets:

$A = \{\omega \text{ such that } \omega(0), \omega(N) \notin \{x \in B(\omega) : x_i = m_i\} \text{ for some } i\}$

$B = \{\omega \text{ for which the endpoints } \omega(0) \text{ and } \omega(N) \text{ are in opposite corners of } B(\omega)\}.$

Note that if ω is not in A then it must be that the endpoints together touch each face of $B(\omega)$ (which is subset B).

Proof idea: If $\omega(0)$ is in subset A , we will show that there exists a pivot point ω_t , and an axis reflection whose result is a SAW ω' with $D(\omega') > D(\omega)$ and $A(\omega') = A(\omega)$. If ω is in subset (b) and is not a straight rod, we will show that there exists a pivot point ω_s and a 90° rotation (or a diagonal reflection) whose result is a SAW ω' with $A(\omega') = A(\omega) + 1$ and $D(\omega') \geq D(\omega)$. From this, we conclude that for every N -step

SAW ω that is not a rod, there exists a SAW ω' that may be obtained from ω by a single pivot, and satisfies $A(\omega') + D(\omega') > A(\omega) + D(\omega)$. Since $0 < A < N - 1$ (since there can be at most $N-1$ straight angles in an N -step self avoiding walk) and $0 < D < N$ for every N -step SAW, and $A + D = 2N - 1$ if and only if the walk is a rod, it follows that any N -step SAW can be transformed into a rod by a sequence of at most $2N - 1$ pivots.

Proof. Case 1: ω is in subset A.

Suppose that there exist $i \in \{1, 2\}$ and $j \in \{1, 2, \dots, d\}$ such that neither ω_0 nor ω_N lies in the face $\{x \in B : x_j = m_j^i\}$. Let $t = \min\{k : X_j(\omega_k) = m_j^i\}$. Now reflect $\omega_{t+1}, \dots, \omega_N$ through the hyperplane $x_j = m_j^i$, yielding the walk $\omega' = (\omega'_0, \dots, \omega'_N)$ defined by:

$$\begin{aligned} &\text{for } k \leq t, \omega'_k = \omega_k \\ &\text{for } k > t, X_l(\omega'_k) = X_l(\omega_k) \\ &\text{for } l \neq j \quad X_j(\omega'_k) = 2m_j^i - X_j(\omega_k) \end{aligned}$$

We now show that ω' is a self-avoiding walk. We are required to show that for $k > t$, ω'_k is not in the set $\{\omega_0, \dots, \omega_t\}$. We break it down into two cases: (i) If $X_j(\omega_k) = m_j^i$, then $\omega'_k = \omega_k$. (ii) If $X_j(\omega_k) \neq m_j^i$, then $\omega'_k \notin B(\omega)$ therefore, ω'_k is not in $\{\omega_0, \dots, \omega_t\}$.

Note, that $A(\omega') = A(\omega)$ since right angles are preserved by axis reflections. Now, we show that $D(\omega') > D(\omega)$. Observe that $M_l(\omega') = M_l(\omega)$ for $l \neq j$.

Define $Q_{r,s}(\omega)$ be the extension in the j th coordinate direction of the subwalk $\omega_r, \omega_{r+1}, \dots, \omega_s$, i.e., $Q_{r,s}(\omega) = \max\{X_j(\omega_k) : r \leq k \leq s\} - \min\{X_j(\omega_k) : r \leq k \leq s\}$.

Then, $M_j(\omega) = \max(Q_{0,t}(\omega), Q_{t,N}(\omega))$ while, $M_j(\omega') = Q_{0,t}(\omega) + Q_{t,N}(\omega)$

By definition, $Q_{0,t}(\omega)$ and $Q_{t,N}(\omega)$ are strictly positive so $M_j(\omega') > M_j(\omega)$. Hence, $D(\omega') > D(\omega)$.

Case 2: ω is in subset B and is not a rod. Then $A(\omega) < N - 1$, i.e., ω contains at least one right angle, so we choose our pivot point ω_s to be the last right angle of ω , i.e., $s = \max\{k : 0 < k < N, \omega_k \neq \frac{1}{2}(\omega_{k-1} + \omega_{k+1})\}$. Thus $(\omega_s, \omega_{s+1}, \dots, \omega_N)$ lie on a straight line perpendicular to the line segment joining ω_{s-1} with ω_s . Let j' and j'' be the (unique) coordinates satisfying $X_{j'}(\omega_s) \neq X_{j'}(\omega_N)$ and $X_{j''}(\omega_{s-1}) \neq X_{j''}(\omega_s)$. Now perform a 90° rotation (or diagonal reflection) at j' to get a new SAW ω' with $\omega'_k = \omega_k$ for $k \leq s$, and $(\omega_{s-1}, \omega_s, \dots, \omega_N)$ all on one straight line. Since $\omega'_{s+1}, \dots, \omega'_N \in B(\omega)$, ω' is a SAW.

Note that choosing the above pivot increases the number of straight-line angles by 1, i.e., $A(\omega') = A(\omega) + 1$. From above, we also get that the j'' th coordinate of the new walk increases by $N - s$. Thus, $M_{j''}(\omega') = M_{j''}(\omega) + (N - s)$. Also, $M_{j'}(\omega') \geq M_{j'}(\omega) - (N - s)$ since the j' th coordinate decreases at most by $N - s$ from the old walk. $M_j(\omega') = M_j(\omega)$ for all other $j \in \{1, 2, \dots, d\}$. Thus, $D(\omega') \geq D(\omega)$. \square

Theorem 3.2. *The pivot algorithm is ergodic for self-avoiding walks on \mathbb{Z}^2 provided that the 180° rotation, and either both 90° rotations or both diagonal reflections, are*

given nonzero probability.

Proof. It is enough to show that any ω with $A(\omega) < N - 1$ can be transformed into a self-avoiding walk ω' with $A(\omega') = A(\omega) + 1$ by some finite sequence of allowed pivots. Let ω be an N step SAW. Then WLOG, assume that ω_N and ω_{N-1} differ on the y co-ordinate, i.e. $\omega_N = \omega_{N-1} + -(0, 1)$. If $m_1^1(\omega) = m_1^2(\omega)$, i.e. the maximum of the x coordinate is equal to the minimum of the x co-ordinate, then ω is a straight rod. So, assume that $m_1^1 < m_1^2$. Choose $i \in \{1, 2\}$ so that $X_1(\omega_0) \neq m_1^i$.

Case 1. If $X_1(\omega_N) = m_1^i$, then let ω_s be the last right angle in ω , i.e., $s = \max\{k : 0 < k < N, \omega_k \neq \frac{1}{2}(\omega_{k-1} + \omega_{k+1})\}$. Then a 90° rotation (or a diagonal reflection) at ω_s gives a new walk ω' in which $\omega'_s, \dots, \omega'_N$ lie on a straight line $x_2 = \text{constant}$, and $A(\omega') = A(\omega) + 1$.

Case 2. If $X_1(\omega_N) \neq m_1^i$, let $z = \min\{x_2 : (m_1^i, x_2) \in \{\omega_0, \dots, \omega_N\}\}$ and let t be the unique index such that $\omega_t = (m_1^i, z)$. We can rotate the walk by 180° at ω_t , to get a new SAW ω'' with $X_1(\omega_{N-1}) = X_1(\omega_N)$. Again, $A(\omega'') = A(\omega)$ since rotation by 180° doesn't change the number of straight line angles. \square

4 Collapse transition and theta-point

4.1 Phase Transition

The main references for this section are [3] and [7].

A transition between the swollen and collapsed states is observed on self-avoiding walks on lattices where poor-solvent interactions are incorporated into the model by introducing an associated energy based on the number of nearest-neighbor contact between non-adjacent sites on each walk.

Thus, if there are n available steps, then the probability of the i th step is given by

$$p_i = \frac{e^{-\beta F_i}}{\sum_{j=1}^n e^{-\beta F_j}}, \quad i \in \{1, 2, \dots, d\}$$

where

$$\beta = \frac{1}{T}, \quad F_i = -m_i$$

where m_i is the number of non-adjacent nearest-neighbor occupied sites.

The number of non-adjacent nearest-neighbor occupied sites is explained below with the following example:

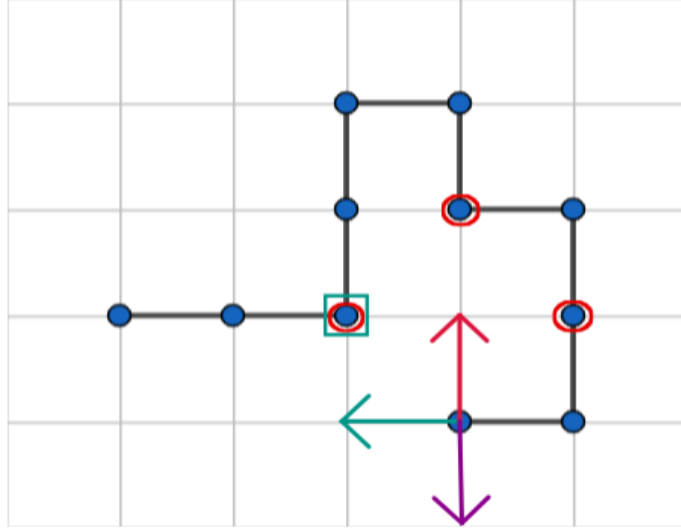


Figure 1:

The number of non-adjacent nearest-neighbor occupied sites (m_i) for the step marked in red is 3 (marked in red circles). Thus the probability of taking the step marked in red is:

$$\frac{e^{\frac{3}{T}}}{\sum_{i=1}^n e^{\frac{m_i}{T}}}$$

The number of non-adjacent nearest-neighbor occupied sites (m_i) for the step marked in green is 1 (marked as a green square). Thus the probability of taking the step marked in green is:

$$\frac{e^{\frac{1}{T}}}{\sum_{i=1}^n e^{\frac{m_i}{T}}}$$

The number of non-adjacent nearest-neighbor occupied sites (m_i) for the step marked in purple is 0. Thus the probability of taking the step marked in purple is:

$$\frac{e^{\frac{0}{T}}}{\sum_{i=1}^n e^{\frac{m_i}{T}}}$$

Note that the sum of these probabilities is 1, i.e.,

$$\frac{e^{\frac{3}{T}}}{1 + e^{\frac{1}{T}} + e^{\frac{3}{T}}} + \frac{e^{\frac{1}{T}}}{1 + e^{\frac{1}{T}} + e^{\frac{3}{T}}} + \frac{e^{\frac{0}{T}}}{1 + e^{\frac{1}{T}} + e^{\frac{3}{T}}} = 1$$

When $\beta = 0$, $p_i = \frac{1}{\text{number of unoccupied sites}}$. Thus, the probability of having an N-step walk is $\prod_{i=1}^N p_i$.

The metric we use to study the transition from an expanded state to a collapsed state in the above described model is the radius of gyration, R_g , which is the standard deviation of the position of every node in the walk, relative to the center-of-mass

position. If (x_i, y_i) is the co-ordinate of the i^{th} step of the walk, then

$$R_g = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + (y_i - \bar{y})^2}{n}}$$

5 Appendix

5.1 Proof of Theorem 2.2

Here is a plan of proof. Using the subadditivity property, in Claim 2.1, we establish that for $n = mq + r$ where n is the length of the walk and m is a fixed integer, $\frac{a_n}{n} \leq \frac{qa_m}{n} + \frac{a_r}{n}$. In Claims 2.2 and 2.3, we show that as $n \rightarrow \infty$, $\frac{qa_m}{n}$ goes to $\frac{a_m}{m}$ and $\frac{a_r}{n}$ goes to 0. Finally in Claim 3.7, we prove that the largest limit point of $\frac{a_n}{n}$ is less than or equal to the largest limit point of $\frac{qa_m}{n} + \frac{a_r}{n}$. Using these claims, we show that as $n \rightarrow \infty$, $\frac{a_n}{n}$ goes to $\inf\{\frac{a_m}{m} | m \geq 1\}$ which we call c .

Proof of Theorem 2.3. : Here we show that as n increases, the number of self-avoiding walks of length n grows exponentially. We prove this using the following four claims.

Claim 5.1. : $a_{kn} \leq ka_n$

Proof. : Fix n . Base case. For $k = 2$, $a_{2n} \leq 2a_n$ from (i)

Let the claim be true for $k = p$, i.e., $a_{pn} \leq pa_n$

Proof for $k = p + 1$: We know $a_{(p+1)n} = a_{pn+n} \leq a_{pn} + a_n$ Again $a_{pn} + a_n \leq pa_n + a_n = (p+1)a_n$ Therefore, $a_{kn} \leq ka_n \forall k \geq 1$

Let $n = mq + r$ where m is a fixed integer and $0 \leq r \leq m - 1$ Now, $a_n = a_{mq+r} \leq a_{mq} + a_r \leq qa_m + a_r$, therefore,

$$\frac{a_n}{n} \leq \frac{qa_m}{n} + \frac{a_r}{n} \quad (1)$$

□

Claim 5.2. : As $n \rightarrow \infty$,

$$\frac{qa_m}{n} \rightarrow \frac{a_m}{m}$$

Proof. : Let $\epsilon > 0$ be given. To show: $|\frac{q}{n} - \frac{1}{m}| < \epsilon$ whenever $n \geq N$.

$$|\frac{q}{n} - \frac{1}{m}| = |\frac{n-r}{mn} - \frac{1}{m}| = |\frac{1}{m} - \frac{r}{mn} - \frac{1}{m}| = |\frac{r}{mn}| \leq \frac{1}{n} \text{ since } \frac{r}{m} \leq 1$$

Now $\frac{1}{n} < \epsilon$ whenever $n \geq [\frac{1}{\epsilon}] + 1$.

So, we choose $N = [\frac{1}{\epsilon}] + 1$

□

Claim 5.3. : As $n \rightarrow \infty$, $\frac{a_r}{n} \rightarrow 0$

Proof. : We know $a_r \leq \max\{a_1, a_2, \dots, a_{m-1}\} = k \quad \forall \quad n \geq 1$

To show: Let $\epsilon > 0$ be given. $|\frac{k}{n} - 0| < \epsilon$ whenever $n > N$. Choose $N = \lceil \frac{k}{\epsilon} \rceil + 1$.

Now, let

$$\alpha_n = \frac{a_n}{n}, \beta_{n,m} = \frac{qa_m}{n} + \frac{a_r}{n}$$

From (1), $\alpha_n \leq \beta_{n,m}$ We know from the previous 2 claims that

$$\lim_{n \rightarrow \infty} \beta_{n,m} = \frac{a_m}{m}$$

where $m \in \mathbb{N}$ is fixed.

Thus α_n and $\beta_{n,m}$ are bounded. □

Limit point of a sequence: A real number p is said to be the limit point of a sequence $\{S_n\}_{n \geq 1}$ if for a given $\epsilon > 0$, $S_n \in (p - \epsilon, p + \epsilon)$ for infinitely many values of n .

We now prove 4 lemmas for the next part of the proof:

Lemma 5.4. Fix m and let $n > m$. Let L be the largest limit point of $\beta_{n,m}$. Then for $\epsilon > 0$, there exists N such that $\beta_{n,m} \leq L + \epsilon \forall n \geq N$

Proof. Let there be infinitely many $\beta_{n,m}$ s above $L + \epsilon$. Then for every $m \in \mathbb{N}$ the sequence $\{\beta_{n,m}\}_{n > m}$ will have a $\beta_{n,m}$ such that $\beta_{n,m} \geq L + \epsilon$. Let x_i be the supremum of the $\{\beta_k\}_{k \geq i}$. Then $x_i \geq L + \epsilon \forall i$. But $L = \lim_{n \rightarrow \infty} \alpha_n = \lim_{n \rightarrow \infty} \beta_{n,m} \geq L + \epsilon$. We get a contradiction, so our assumption must be false. □

Lemma 5.5. If $\alpha_n \leq M \forall n > N, N \in \mathbb{N}$, then the largest limit point of $\alpha_n \leq M$.

Proof. Let M_1 be a limit point of $\alpha_n, M_1 \geq M$. Let $\epsilon = \frac{M_1 - M}{2}$. Since M_1 is a limit point of $\alpha_n, \exists N_1$ such that $M_1 - \epsilon \leq \alpha_n \leq M_1 + \epsilon \forall n \geq N_1$ i.e.

$$M_1 - \frac{(M_1 - M)}{2} \leq \alpha_n \leq M_1 + \frac{(M_1 - M)}{2} \forall n \geq N_1$$

$$\frac{M_1 + M}{2} \leq \alpha_n \leq \frac{3M_1 - M}{2} \forall n \geq N_1$$

Let $N_2 = \max(N_1, N)$. Then $\alpha_n \geq M \forall n > N_2$ and $\alpha_n \leq M \forall n > N_2$ is a contradiction. Therefore, the largest limit point of $\alpha_n \leq M$. □

Lemma 5.6. Largest limit point of $\alpha_n \leq$ largest limit point of $\beta_{n,m}$ ($m \in \mathbb{N}$ is fixed)

Proof. Let the largest limit point of $\beta_{n,m}$ be L . By Lemma 1, there exists N such that $\beta_{n,m} \leq L + \epsilon \forall n \geq N$. Since $\alpha_n \leq \beta_{n,m}$ where m is fixed and $n \geq m$, so there exists N such that

$$\alpha_n \leq L + \epsilon \forall n \geq N$$

. Therefore only finitely many α_n s are above $L + \epsilon$. Using Lemma 2, this implies that the largest limit point of $\alpha_n \leq L + \epsilon$. Since $\epsilon \geq 0$ is arbitrary, the largest limit point of $\alpha_n \leq$ largest limit point of $\beta_{n,m}$ where m is fixed. \square

Lemma 5.7. *If $\{x_n\}$ is a bounded and increasing sequence then $\lim_{n \rightarrow \infty} x_n = \sup\{x_n : n \in \mathbb{N}\}$*

Proof. Since $\{x_n\}$ is bounded, there exists a real number M such that $x_n \leq M \forall n \geq N$. Since $\{x_n\}$ is bounded above, $x^* = \sup\{x_n : n \in \mathbb{N}\} \in R$. We will show that $x^* = \lim_{n \rightarrow \infty} x_n$. If $\epsilon \geq 0$ is given then $x^* - \epsilon$ is not an upper bound of the set $\{x_n : n \in \mathbb{N}\}$. Hence $\exists x_k$ such that $x^* - \epsilon < x_k$. $\{x_n\}$ is an increasing sequence implies that $x_k \leq x_n$ whenever $n \geq k$, so

$$x^* - \epsilon < x_k \leq x_n < x^* < x^* + \epsilon \forall n \geq k$$

. Therefore, we have $|x_n - x^*| \leq \epsilon \forall n \geq k$. Since $\epsilon \geq 0$ was arbitrary x_n converges to x^* . \square

Lemma 5.8.

$$\lim_{n \rightarrow \infty} \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\} = \sup_n \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\}$$

Proof. Define $M_n = \inf_{k \geq n} \left\{ \frac{a_k}{k} : k \geq 1 \right\}$. Now $M_n \leq M_{n+1}$, i.e., M_n is an increasing sequence. Since $\lim_{n \rightarrow \infty} M_n = \lim_{n \rightarrow \infty} \inf_{k \geq n} \left\{ \frac{a_k}{k} : k \geq 1 \right\}$. We also know that an increasing sequence which is bounded goes to $\sup_n \inf_{k \geq n} \left\{ \frac{a_k}{k} : k \geq 1 \right\}$ as n goes to ∞ . (By Lemma 4). Therefore,

$$\lim_{n \rightarrow \infty} \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\} = \sup_n \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\}$$

.

\square

Claim 5.9. : *Largest limit point of $\alpha_n \leq \frac{a_m}{m}$ for every m .*

Proof. We know that $\alpha_n \leq \beta_{n,m}$ for every $n \geq m$, where $m \in \mathbb{N}$ is fixed. By Lemma 3, the largest limit point of $\alpha_n \leq$ largest limit point of $\beta_{n,m}$. Since for $n \geq m$, where $m \in \mathbb{N}$ is fixed, we have $\alpha_n \leq \beta_{n,m}$ and $\lim_{n \rightarrow \infty} \beta_{n,m} = \frac{a_m}{m}$, so the largest limit point of $\alpha_n \leq \frac{a_m}{m}$. \square

This implies that the largest limit point of $\alpha_n \leq \inf\left\{ \frac{a_k}{k}, k \geq 1 \right\}$

Claim 5.10. *Smallest limit point of $\alpha_n \geq \inf\left\{ \frac{a_k}{k}, k \geq 1 \right\}$*

Proof. We know, the smallest limit point of $\alpha_n = \lim_{n \rightarrow \infty} \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\}$. From the last lemma, we have $\lim_{n \rightarrow \infty} \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\} = \sup_n \inf_{k \geq n} \left\{ \frac{a_k}{k} \right\}$. Therefore,

$$\sup_n \inf_{k \geq n} \left\{ \frac{a_k}{k} : k \geq 1 \right\} \geq \inf \left\{ \frac{a_k}{k} : k \geq 1 \right\}$$

. Therefore, the smallest limit point of $\alpha_n = \lim_{n \rightarrow \infty} \inf_{k \geq n} \{\frac{a_k}{k}\} = \sup_n \inf_{k \geq n} \{\frac{a_k}{k} : k \geq 1\} \geq \inf\{\frac{a_k}{k} : k \geq 1\}$ \square

The largest limit point of $\alpha_n \leq \inf\{\frac{a_m}{m} | m \geq 1\}$

The smallest limit point of $\alpha_n \geq \inf\{\frac{a_m}{m} | m \geq 1\}$

From the above, the smallest limit point of $\alpha_n \geq$ largest limit point of α_n .

Therefore, smallest limit point = largest limit point of $\alpha_n = \inf\{\frac{a_m}{m} | m \geq 1\} = c$ (say)

Hence,

$$\lim_{n \rightarrow \infty} \frac{\log C_n}{n} = c$$

Thus, $\forall \epsilon > 0 \exists N \in \mathbb{N}$ such that whenever $n \geq N$, $|\frac{\log C_n}{n} - c| < \epsilon$. Take $\epsilon = \frac{c}{2}$, then $\frac{c}{2} \leq \frac{\log C_n}{n} \leq \frac{3c}{2} \implies e^{\frac{nc}{2}} \leq C_n \leq e^{\frac{3nc}{2}}$. Therefore, $C_n \sim e^{nc}$ \square

Thus we can say that C_n increases exponentially with increasing n .

Here, $\lim_{n \rightarrow \infty} C_n^{1/n}$ is known as the connective constant μ .

5.2 Elements of the group of orthogonal transformations

An element $g \in G$ is a $d \times d$ orthogonal matrix with integer entries; so it suffices to specify the columns of g , which are ge_1, ge_2, \dots, ge_d , where e_1, e_2, \dots, e_d are the unit vectors in \mathbb{Z}^d . Hence, an element $g \in G$ can be specified uniquely by giving a permutation π of $1, \dots, d$ and numbers $\sigma_1, \dots, \sigma_d = \pm 1$, and setting $ge_i = \sigma_i e_{\pi(i)}$. It follows that the cardinality of G is $2^d d!$ (each of $d\sigma_i$'s have 2 choices and d numbers have $d!$ permutations).

1. Let $A_{11} \in$, taking $m = 2$, $n_1 = n_2 = 1$ and $A_{21} = -A_{11}$ we have

$$\bigcup_{i=1}^m \bigcap_{j=1}^{n_i} A_{ij} = (A_{11})(-A_{11}) =$$

Hence \in . Taking $m = 1$, $n_1 = 2$ with A_{11} and $A_{12} = -A_{11}$ yields \in .

2. Let $A \in$ and $B \in$, then

$$A = \bigcup_{i=1}^m \bigcap_{j=1}^{n_i} A_{ij} \text{ and } B = \bigcup_{i=1}^s \bigcap_{j=1}^{t_i} B_{ij}$$

Suppose without loss of generality that $m \geq s$, then let $C_{i,j} = A_{i,j}$ if $1 \leq i \leq m$ and $1 \leq j \leq n_j$, and let $C_{i,j+n_j} = B_{i,j}$ if $1 \leq i \leq s$ and $1 \leq j \leq n_j$, and let $v_i = n_i + t_i$ if $1 \leq i \leq s$ and $v_i = n_i$ otherwise, then

$$C = \bigcup_{i=1}^m \bigcap_{j=1}^{v_i} C_{ij} = AB$$

with the m sets $\bigcap_{j=1}^{v_i} C_{ij}$ obviously disjoint. It follows that $C \in$ and hence $AB \in$ if $A, B \in$.

3. Suppose that $A \in$, then there exist A_{ij} such that

$$A = \bigcup_{i=1}^m \bigcap_{j=1}^{n_i} A_{ij} \longrightarrow A^c = \bigcap_{i=1}^m \bigcup_{j=1}^{n_i} A_{ij}^c$$

Take $B_i = \bigcup_{j=1}^{n_i} A_{ij}^c$, note that either $A_{ij} \in$, in which case $(A_{ij}^c)^c \in$ or $A_{ij}^c \in$, it follows that $B_i \in$ (with $m = 1$) for $1 \leq i \leq m$. Now we invoke part (b) (and induction) to conclude that

$$A^c = (B_1 B_2 \cdots B_m) \in$$

4. Finally, let $A, B \in$, then

$$AB = (A^c B^c)^c \in$$

Hence $AB \in$ if $A, B \in$, and therefore is a field.

It follows that is a field such that A , therefore $f()$. To see that $f()$, let $X \in$, then

$$X = \bigcup_{i=1}^m \bigcap_{j=1}^{n_i} A_{ij}$$

where either $A_{ij} \in$ or $A_{ij}^c \in$, note that each $A_{ij} \in f()$ (since each singleton $A_{ij} \in f()$ or $A_{ij}^c \in$, hence $A_{ij}^c \in f()$ and therefore $A_{ij} \in f()$ since $f()$ is closed under complements). Then X is a finite union over finite intersections of sets in $f()$, and is therefore in $f()$ because $f()$ is a field. It follows that $f()$, as required.

$$G = \left\{ \bigcup_{i=1}^m \bigcap_{j=1}^{n_i} A_{ij} : A_{ij} \in \text{ or } A_{ij}^c \in, m \geq 0, n_i \geq 0, \right. \\ \left. \text{and the } \bigcap_{j=1}^{n_i} A_{ij} \text{ are disjoint} \right\}$$

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