Exponential growth rates of directed combs

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Introduction

The enumeration of self-avoiding walks of various sorts is an important topic in combinatorics and statistical mechanics. A recent paper investigated a lattice model of comb polymers and their growth rates. [1]

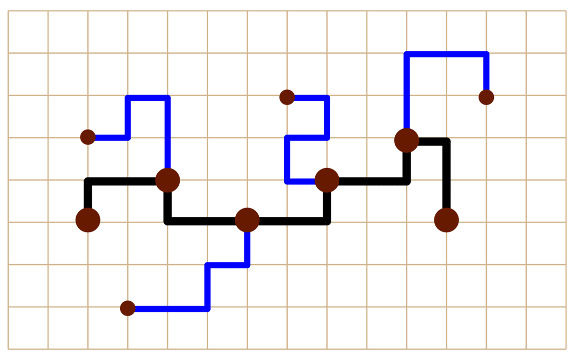

Figure 1. Comb polymer in square lattice[1]

In this poster, we aim to investigate a directed lattice model of comb polymers and try to derive the growth constant for the number of self-avoiding combs.

Preliminaries

Comb polymers are a type of branched polymer that features a long backbone with side chains called teeth attached to nodes on the backbone. The nodes are evenly spaced on the backbone. The parameters for a comb are the length of the teeth (m_a), the spacing between each node (m_b) and the amount of teeth (t).

These comb polymers will be in the $\mathbb{Z}^2$ lattice. The step set $\mathcal{S}$ for a class of walks in a lattice is a collection of vectors that represent the possible directions that a walk can take. For this model, we will use the step set $\mathcal{S} = \{(1,1),(1,-1)\}$.

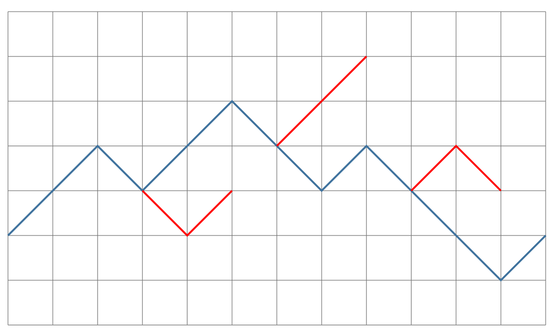

Figure 2. A comb with $m_a = 2, m_b = 3, t = 3$

We denote the number of combs with parameters m_a, m_b, t as $g(m_a, m_b, t)$. To obtain the exponential growth constant of the number of combs, we can compute the limit

$$\zeta(m_a, m_b) = \lim_{t\to\infty} \frac{1}{(m_a+m_b)t} \log g(m_a, m_b, t)$$

The growth constant μ of combs is defined by $e^{\zeta(m_a,m_b)}$

We define the n-th segment of a comb as the section of the comb starting from the n-th node to the next node. We can use segments to establish recurrence relations between $g(m_a, m_b, t+1)$ and $g(m_a, m_b, t)$

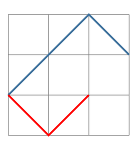

Figure 3. 1st segment of Fig 1

Case 1: $m_a \leq m_b$

In this case, we note that each segment is independent from the other, as the teeth are not long enough to go into the next segment. So, all that is left to do is to count the number of possible segments.

Each segment will consist of 2 non-intersecting walks with lengths m_a and m_b starting from the initial node. Since the walks only go to the right, we can consider it as 2 non-intersecting walks with both lengths m_a and a single walk of length $m_b - m_a$.

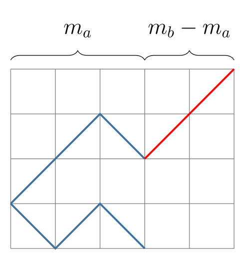

Figure 4. A segment of a comb with $m_a = 3$ and $m_b = 5$

Trivially, there are $2^{m_b - m_a}$ single walks of length $m_b - m_a$. However, the number of paired non-intersecting walks of length m_a is non-trivial. To find this, we will introduce generating function methods.

Let W be the set of paired non-intersecting walks. For $\varphi \in W$, let $|\varphi|$ denote the length of the walk and let $d(\varphi)$ denote half the distance between the walks. This gives us the generating function

$$P(x,s) = \sum_{\varphi\in W} x^{|\varphi|} s^{d(\varphi)}$$

For every walk that ends with distance d, we can create 1 more walk with distance $d+2$, 2 walks with distance d, and 1 walk with distance $d-2$.

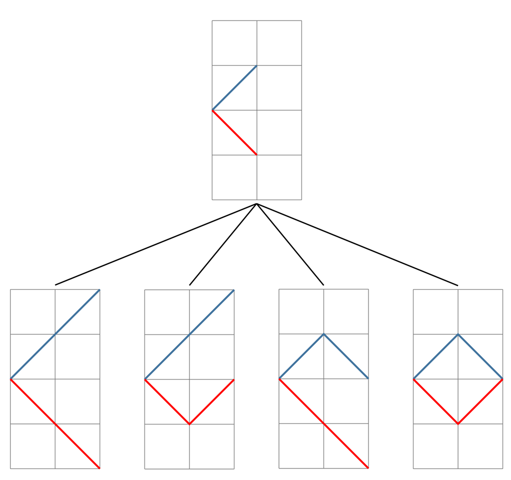

Figure 5. The 4 options for extending a walk

Case 1: $m_a \leq m_b$

This relationship can be represented with a functional equation

$$P(x,s) = xs + x\left(s + 2 + \frac{1}{s}\right)P(x,s) - x[s^1]P(x,s)$$

We will use the kernel method [4] to solve this equation. Rearranging, we get

$$K(x,s)P(x,s) = xs - x[s^1]P(x,s), \quad K(x,s) = \left[1 - x\left(s + 2 + \frac{1}{s}\right)\right]$$

$K(x,s)$ is called the kernel. We find solutions to $K(x,s) = 0$ to remove the left hand side of the equation. The solutions are

$$\hat{s}_{+,-} = \frac{-2x + 1 \pm \sqrt{1-4x}}{2x}$$

We use these solutions to find the $x[s^1]P(x,s)$ term and substitute back to find the main generating function. If we try $\hat{s}_+$, we get

$$P_+(x,s) = -1 - \frac{1}{s}x + O(x^2)$$

So, we reject $\hat{s}_+$, as we require positive integer coefficients for our power series. Substituting $\hat{s}_-$ and $s = 1$, we get

$$P(x,1) = \sum_{\varphi\in W} x^{|\varphi|} = \frac{1}{2}((1-4x)^{-\frac{1}{2}} - 1) = \sum_{n=1}^{\infty} \binom{2n-1}{n} x^n$$

This tells us that there are $\binom{2n-1}{n}$ non-intersecting pairs of walks of length n. We multiply this result by 2 to get $\binom{2n}{n}$, as the top walk can be either backbone or tooth.

Combining this with the previous result, we have $\binom{2m_a}{m_a}2^{m_b - m_a}$ unique segments. Since each comb consists of an initial walk of length m_b followed by t segments, we have

$$g(m_a, m_b, t) = 2^{m_b}\left(\binom{2m_a}{m_a}2^{m_b-m_a}\right)^t$$

Evaluating the growth constant,

$$\mu = e^{\zeta(m_a,m_b)} = \binom{2m_a}{m_a}^{\frac{1}{m_a+m_b}} 2^{\frac{m_b-m_a}{m_b+m_a}}$$

Now, we can look at some asymptotics of the growth rate. If we hold m_a constant and let m_b go to infinity,

$$\lim_{m_b\to\infty} \binom{2m_a}{m_a}^{\frac{1}{m_a+m_b}} 2^{\frac{m_b-m_a}{m_b+m_a}} = \binom{2m_a}{m_a}^0 2^1 = 2$$

This is the expected result, as the resulting comb approaches a similar structure of a self-avoiding walk, which has growth constant 2. If we also take m_a to infinity, we can use Stirling's approximation to evaluate the limit.

$$\lim_{\substack{m_a,m_b\to\infty \\ m_a = o(m_b)}} \mu = \lim_{\substack{m_a,m_b\to\infty \\ m_a = o(m_b)}} \left(\frac{2^{2m_a}}{\sqrt{m_a\pi}}\right)^{\frac{1}{m_b+m_a}} 2^{\frac{m_b-m_a}{m_b+m_a}} = 1 \cdot 2^1 = 2$$

This is a surprising result, as it tells us that the amount of disallowed combs (intersecting combs) does not affect the exponential growth in the long run.

Case 2: $m_a = 2m_b$

$m_a > m_b$ in general is difficult to tackle in one go, so we will focus on this first case of $m_a = 2m_b$. For $m_a > m_b$, teeth from previous segments can interact with the current segment. In this case, each segment past the 2nd will consist of 3 walks, with the third walk coming from the previous segment.

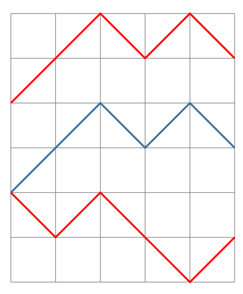

Figure 6. A segment of comb with $m_a = 10$ and $m_b = 5$

We can construct a functional equation for this scenario and solve it with the obstinate kernel method [3]. WLOG, let the top walk be the walk from the previous segment. For $\varphi \in W$, we denote $d_1(\varphi)$ and $d_2(\varphi)$ as the half-distance between the top and middle path and the middle and bottom path subtracted by 1. This gives us the generating function

$$P(x,r,s) = \sum_{\varphi\in W} x^{|\varphi|} r^{d_1(\varphi)} s^{d_2(\varphi)}$$

This time, we can extend each walk in 8 directions instead of 4, and we will eliminate any walks that result in $d_1 < 0$ or $d_2 < 0$, giving us this functional equation

$$P(x,r,s) = xr^k + \frac{x(r+1)(s+1)(r+s)}{rs}P(x,r,s) - \frac{x(s+1)}{r}P(x,0,s) - \frac{x(r+1)}{s}P(x,r,0)$$

Using the kernel method from earlier, we have

$$K(x,r,s)P(x,r,s) = xr^k - \frac{x(s+1)}{r}P(x,0,s) - \frac{x(r+1)}{s}P(x,r,0),$$

$$K(x,r,s) = 1 - \frac{x(r+1)(s+1)(r+s)}{rs}$$

The kernel is symmetric under these transformations

$$\Phi : (r,s) \mapsto (s,r), \Psi : (r,s) \mapsto \left(r, \frac{r}{s}\right)$$

We can use these to create a family of 12 symmetries, but we will focus on 3 relevant ones: $(r,s) \mapsto (r,s), (r,s) \mapsto \left(r, \frac{r}{s}\right), (r,s) \mapsto \left(\frac{1}{s}, \frac{r}{s}\right)$. Substituting the solution of the kernel $\hat{r}$ and applying these 3 transformations, we get a system of equations. Solving these 3 equations and substituting $s = 1$, we get

$$2x(P(x,0,1) + P(x,1,0)) = x\hat{r} + x\hat{r}^{k+1}(1-\hat{r})$$

Case 2: $m_a = 2m_b$

Substituting $r = s = 1$ into our functional equation, we get

$$(1-8x)P(x,1,1) = x - 2x(P(x,0,1) + P(x,1,0))$$

Combining these two and substituting in the value of $\hat{r}$, we get

$$P(x,1,1) = \frac{x}{1-8x}\left(\frac{1-8x-\sqrt{1-8x}}{4x}\right)\left(1 - \left(\frac{1-4x-\sqrt{1-8x}}{4x}\right)^{k+1}\right)$$

There is a clear singularity at $x = \frac{1}{8}$, so $[x^n]P(x,1,1) \bowtie 8^n$. So, $[x^n]P(x,1,1) = \theta(k,n)8^n$, where $\theta(k,n)$ is subexponential w.r.t n. We note that $\theta(k,n) \leq 1$, as 8^n is the maximum amount of triples of walks. Let W_t be the set of combs with t teeth and $m_a = 2m_b$, with the added condition that extra teeth right of the backbone are removed. Then, $|W_t| = \frac{1}{2^{m_b}}g(m_a, m_b, t)$. For $\varphi \in W_t$, let $k(\varphi)$ denote the half-distance between the last tooth and the path nearest to it subtracted by 1. For $\varphi \in W_t$, we can extend φ to $\theta(k(\varphi), m_b)8^{m_b}$ more combs with $t+1$ teeth. So,

$$g(m_a, m_b, t+1) = 2^{m_b} \sum_{\varphi\in W_t} \theta(k(\varphi), m_b)8^{m_b}$$

Let $\sigma(t, m_b)$ be the average of $\theta(k(\varphi), m_b)$ over all $\varphi \in W_t$. We note that $\sigma(t, m_b)$ is also subexponential and less than or equal to 1. From the previous expression, we have

$$g(m_a, m_b, t+1) = 2^{m_b}\sigma(t, m_b)|W_t|8^{m_b} = \sigma(t, m_b)8^{m_b}g(m_a, m_b, t)$$

From this recurrence relation, we have

$$g(m_a, m_b, t) = \left(\prod_{i=1}^{t-1} \sigma(i, m_b)8^{m_b}\right) g(m_a, m_b, 1)$$

Calculating $g(m_a, m_b, 1)$ is relatively simple, a comb with one tooth consists of 3 sections, 2 walks with length m_b and a non-intersecting pair of walks of length m_b, giving us

$$g(m_a, m_b, 1) = 2^{m_b}\binom{2m_b}{m_b}2^{m_b} \approx \frac{16^{m_b}}{\sqrt{m_b\pi}}$$

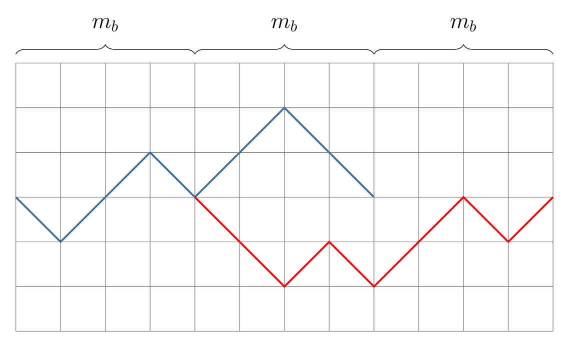

Figure 7. A comb with one tooth for $m_a = 8$ and $m_b = 4$

The growth rate doesn't have a nice closed form expression, so we will investigate its asymptotic behaviour.

$$g(m_a, m_b, t) = \frac{2^{m_b}8^{m_b t}}{\sqrt{m_b\pi}} \prod_{i=1}^{t-1}(\sigma(i, m_b))$$

Computing the limit $\zeta(m_a, m_b)$, we have

$$\zeta(m_a, m_b) = \lim_{t\to\infty} \frac{1}{3m_b t} g(m_a, m_b, t) = \log 2 + \lim_{t\to\infty} \frac{1}{3m_b t} \sum_{i=1}^{t-1} \log(\sigma(i, m_b))$$

We observe that $\log(\sigma(i, m_b)) \leq 0$, so

$$\log 2 + \lim_{t\to\infty} \frac{t-1}{3m_b t} \log(\sigma(j, m_b)) \leq \zeta(m_a, m_b) \leq \log 2,$$

where $\sigma(j, m_b) = \min_{l\in\{1,\dots,t-1\}} \sigma(l, m_b)$ Using the property that $\log(\sigma(j, m_b))$ is subexponential with respect to m_b,

$$\lim_{m_b\to\infty} (\log 2 + \lim_{t\to\infty} \frac{t-1}{3m_b t} \log(\sigma(j, m_b)) = \log 2 + \lim_{m_b\to\infty} \frac{\log(\sigma(j, m_b))}{3m_b} = \log 2$$

By squeeze theorem,

$$\lim_{m_b\to\infty} \zeta(2m_b, m_b) = \log 2$$

So, the growth rate for combs with $m_a = 2m_b$ also approaches 2 as $m_b \to \infty$

Further opportunities

We can use the result for triples of non-intersecting walks to the case where $m_b < m_a < 2m_b$. This case uses largely the same approach as before, but each segment now has a section with only 2 walks. We end up with the same growth rate of 2 as $m_b \to \infty$.

Further cases of $m_a > 2m_b$ requires analysis of 4 or more non-intersecting walks in the lattice, which there are no current methods of solving. However, simulations reveal that the growth rate of n non-intersecting walks approaches 2^n for $n = 4, 5, 6$. Proving this result for general n would imply that growth rate for combs always approaches 2 for all $m_a > m_b$

References

[1] S G Whittington E J Janse van Rensburg. Exponential growth rate of lattice comb polymers. *Journal of Physics A: Mathematical and Theoretical*, 57(48), 2024.

[2] P. Flajolet and R. Sedgewick. *Analytical combinatorics*. Cambridge University Press, 2009.

[3] Rami Tabbara. *Generalised directed walker models of adsorption and gelation*. PhD thesis, The University of Melbourne, 2015.

[4] Thomas Wong. *Enumeration problems in directed walk models*. PhD thesis, The University Of British Columbia (Vancouver), 2015.

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