Existence and bounds of growth constants for restricted walks, surfaces, and generalisations

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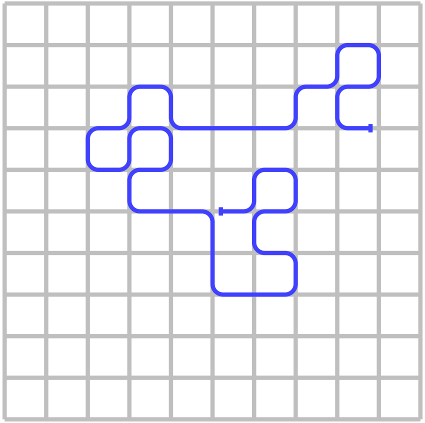
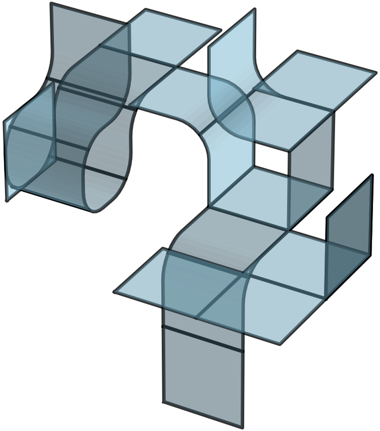


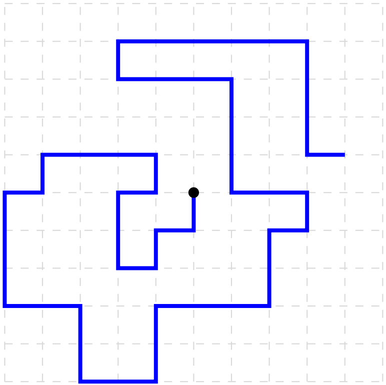


Outline

1. Self-osculating walks and other restricted walks
   - Connective constant μ
   - Some physical motivation
   - Automata method for upper bounding connective constants
2. Self-avoiding surfaces, self-osculating surfaces and generalisations
   - Upper bounds and existence of growth constants μ
   - Twig method for improved upper bounds on μ

Self-avoiding walks

- A self-avoiding walk (SAW) on a graph is a sequence of neighbouring vertices starting from v_0 such that no vertex is visited twice
- Its length n is the number of vertices in the sequence, not counting v_0
- In this talk: triangular ($\triangle$), hexagonal (honeycomb, ⬡), and hypercubic lattices $\mathbb{Z}^{d\geq 2}$ ($\square$, ⧉, ⧉, $\ldots$)



Connective constant

- How does the number of SAWs grows with n?
- Must be exponentially bounded, since for random walks, $c_n = \kappa^n$ (κ is coordination number) and SAWs are a subset
- Connective constant $\mu := \lim_{n\to\infty} \mu_n$, where $\mu_n := c_n^{1/n}$
- Only known exactly on the hexagonal (honeycomb) lattice:

Theorem (Duminil-Copin and Smirnov, 2012)

$$\mu_{\hexagon}^{\mathrm{SAW}} = \sqrt{2+\sqrt{2}}$$

Upper bounding μ

- Any SAW of length $(n+m)$ can be split into a SAW of length n and m, but not all SAWs of length n and m can be joined to become a valid SAW. Therefore

$$c_{n+m} \leq c_n c_m. \tag{1}$$

- Therefore sequence $(\ln c_n)_n$ is subadditive by definition.
- Fekete's lemma $\implies$ μ exists
- In fact $\mu_{2n} \leq \mu_n$, so any μ_n gives an upper bound of μ (but inefficient)
- Current state of the art bounds for $\mu_{\square}^{\mathrm{SAW}}$:

Theorem (Beyer and Wells, 1972, Couronné, 2022)

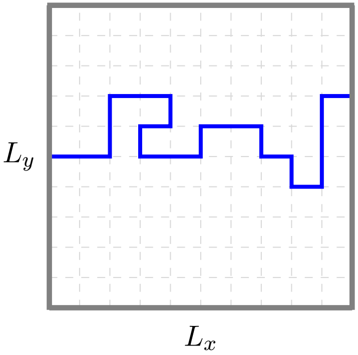
$$2.62002 \leq \mu_{\square}^{\mathrm{SAW}} \leq 2.66235$$

Self-avoiding walks as a statistical physics model

- Partition function $Z^{\mathrm{SAW}}(\beta) := \sum_w e^{-\beta|w|}$
- Finite for $\beta > \beta_c = \ln \mu$
- More physical situation: modelling an interface: $w_1 = (1, y_1)$, $w_n = (L_x, y_n)$, $x_i \in [1, L_x]$, $y_i \in [1, L_y]$ $\forall i \in [1, n]$. Then:

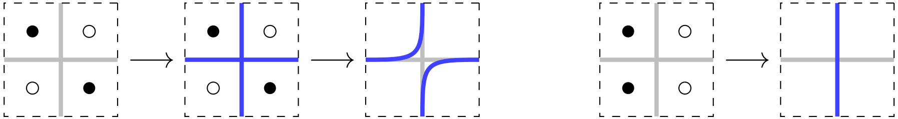
$$Z^{\mathrm{SAW}}_{\mathrm{interface}}(\beta) \leq L_y \sum_{w:|w| \geq L_x}^{L_x L_y} e^{-\beta|w|} \leq \frac{L_y e^{-(\beta-\beta_c)(L_x + o(L_x))}}{1 - \mu e^{-\beta}},$$

If $\beta > \beta_c = \ln \mu$. 'Bulk' information useful for systems with boundaries!



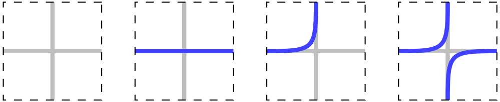
Domain walls

- Interfaces naturally arise as domain walls between regions of different configurations (ex. $\{\circ, \bullet\}$ with boundary conditions)
- For $\kappa \geq 4$, Crossings can occur
- Idea: modify crossings such that they 'osculate'

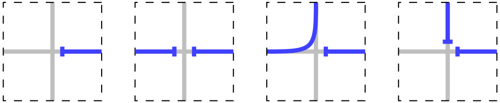


Self-osculating walks (SOWs)

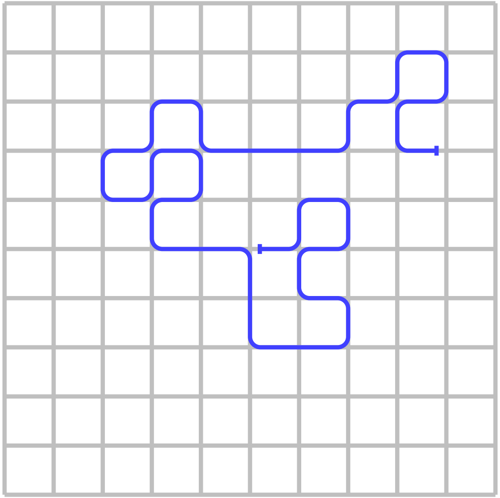
- Superset of self-avoiding walks (SAWs) where walks are allowed to ‘osculate’
- Defined in terms of vertex configurations



- ‘Boundary’ vertex configurations can be obtained by truncation

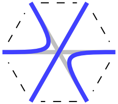
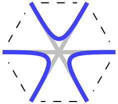


- Like self-osculating polygons but not closed (Jensen and Guttmann, 1998)



Caveat

- Changing crossings to osculating configurations not always the same as those arising from previous procedure (domain walls): ex. the triangular lattice

 is not allowed by ODW, while  $\longrightarrow$  is.

- It is the same on the square lattice
- Call vertex configurations generated by domain wall procedures as osculating domain wall walks (ODWs)
- ODWs relevant in quantum information (2D quantum error correcting codes; P. Kim and McGinley, 2025)

Upper bound on the connective constant

- Previous arguments also apply to self-osculating walks (SOWs)
- A trivial upper bound is $\mu_{\square}^{\mathrm{SOW}} \leq 3$ (subset of Non-Reversing Walks)
- Improved upper bound by adapting the *automata method* of (Pönitz and Tittmann, 2000)

Theorem (SWPK and GP, 2025)

The connective constant for SOWs on the square lattice satisfies

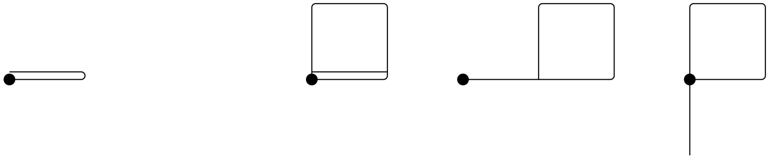
$$\mu_{\square}^{\mathrm{SOW}} \leq 2.73911$$

- Idea: count all walks without 'loops' of size k or less, giving a superset of a desired set of restricted walks

Automata method

Outline

- A *loop* of size k, γ, is a path of length k that is *disallowed*, but such that every proper subpath of γ is allowed.
- ex. Loops of size 2 and 5 for SOWs:



- Find a transfer matrix $M_{\leq k}$ to count all states after n steps without loops of size $\leq k$:

$$c_{n,k} = \kappa \vec{1}^{\intercal} \left(M_{\leq k}\right)^{n-1} v_1$$

- Largest eigenvalue of $M_{\leq k}$ yields an upper bound for $\mu_{\square}^{\mathrm{SOW}}$

Algorithm

Given a restricted walk with a rule R

- Find all loops of size $\leq k$ (up to rotations and reflections):

$$\Gamma_{\leq k} = \{\gamma \mid \gamma \text{ is a loop of size } \leq k\}$$

- Find all subpaths starting from the origin:

$$\mathcal{C}_k = \left\{ \gamma_{[0:l]} \mid \gamma \in \Gamma_{\leq k},\ 1 \leq l \leq \mathrm{len}(\gamma) - 1 \right\}$$

- For each element in $c \in \mathcal{C}_k$, consider all possible evolutions one step further (neglecting loops) and identify it with another element of $\mathcal{C}_k$.
- Each evolution c' is identified with the longest 'suffix' belonging to $\mathcal{C}_k$: that is,

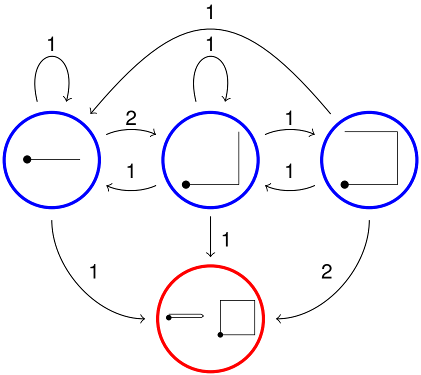
$$c' \sim c'_{\left[\min\{ m : c'_{[m,\mathrm{len}(c')]} \in \mathcal{C}_k \},\mathrm{len}(c')\right]}$$

- $c \to c'$ can be represented by the matrix $M_{\leq k}$.
- Same identification for all elements in $\mathcal{C}_k$

Example: self-avoiding walk

- For loop of size up to 4:

$$M_{\leq 4} = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{2}$$

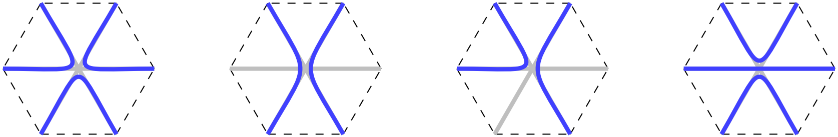


- Largest eigenvalue already gives upper bound

$$\mu_{\square}^{\mathrm{SAW}} \leq 2.83118$$

Generalisations

- Method can be used for restricted walks defined by vertex configurations



- Each subset of these vertex configurations is allowed (up to rotation/reflection).

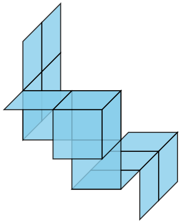
Theorem (SWPK and GP, 2025)

The connective constant for SOWs on the triangular lattice satisfies

$$\mu_{\triangle}^{\mathrm{SOW}} \leq 4.44867 \tag{3}$$

Self-avoiding surfaces (SASs)

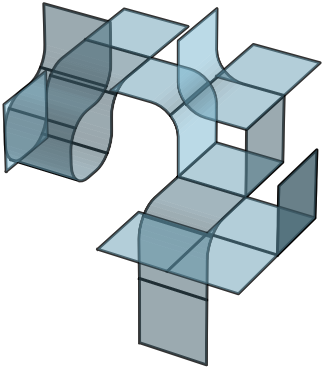
- For general hypercubic lattice $\mathbb{Z}^d$
- $\mathrm{SAS}_{\mathbb{Z}^d} \ni \Sigma$: set of faces such that
  - No two more than two faces neighbour the same edge
  - There is one connected component (two faces are connected if they neighbour the same edge)
  - SASs are identified up to translation
  - Each face has unit area



- c_n: number of SASs with area n. μ is known as the growth constant
- $\mathrm{SAS}_{\mathbb{Z}^d}(h)$: SASs with h boundary components (ex. $h = 0$ are closed surfaces)
- $d = 2$: also known as polyominoes
- Can be generalised to (d, k)-self-avoiding manifolds (SAMs) of k-area n

Self-osculating surfaces

- More than two faces can neighbour an edge
- If there are two faces neighbouring an edge, they are deemed to be connected
- If there are more than two, then connection between faces must be specified
- Therefore it is a set of faces and (possibly) specified connections
- In the latter case, allow the configurations if they obey the 'osculating condition'



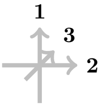
- Can generalise to $(d, k \leq d)$-self-osculating manifolds (SOMs)
- If $(d, k = d)$, only two up to k-faces can neighbour a $(k-1)$-edge
  $\implies \mathrm{SAM}_{(d,d)} = \mathrm{SOM}_{(d,d)}$

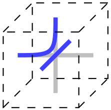
Shopping for orientations

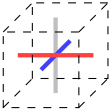
- Consider center coordinates of vertices, edges, faces, cubes, ...
  - Vertices have integer coordinates
  - Edges have one half-integer coordinates
  - faces have two half-integer coordinates (also refer to them as orientations), ...
- In general k-faces have k half-integer dimensions / orientations $|\mathrm{HalfInt}(f)| = k$
- **'trade':** Two k-faces can connect if they share $k-1$ orientations
- **'buy':** A k-face f can neighbour a $(k+1)$-cube b if $\mathrm{HalfInt}(b)$ is one new dimension compared to $\mathrm{HalfInt}(f)$
- **'sell':** A k-face f can neighbour a $(k-1)$-edge l if $\mathrm{HalfInt}(l)$ is $\mathrm{HalfInt}(f)$ with one orientation taken away

Definition (Osculating condition)

- Consider two pairs of hyperfaces, with center coordinates $(\boldsymbol{f}_1, \boldsymbol{f}_2)$, $(\boldsymbol{f}_3, \boldsymbol{f}_4)$, neighbouring the same $(k-1)$-edge at $\boldsymbol{g}$
- Let $\boldsymbol{e}_{i_a} = (\boldsymbol{f}_a - \boldsymbol{g})/\|\boldsymbol{f}_a - \boldsymbol{g}\|$: normalised vectors to from hyperedge to hyperface ($\|\cdot\|$: Euclidean norm)
- Require that:
  - All $\{\boldsymbol{e}_a\}_{a=1}^4$ are different
  - If the normalised vectors are parallel, $\boldsymbol{e}_1 = -\boldsymbol{e}_2$ (i.e. $\boldsymbol{f}_1$ and $\boldsymbol{f}_2$ have the same orientation), then only allow the connections if $\boldsymbol{e}_3 \perp \boldsymbol{e}_4$
- If there are odd number of hyperfaces: is osculating if any new hyperface can be paired with the lone hyperface to fulfill above







Existence and bounds for μ in restricted manifolds

- Cannot use Fekete's lemma as we don't have subadditivity
- (Wilker and Whittington, 1979): If c_n is exponentially upper bounded and $c_n c_m \leq c_{n+y(m)}$ (pseudo-subadditive) such that $\lim_{m\to\infty} y(m)/m = 1$, then μ exists
- Strategy
  1. Exponentially upper bound c_n by finding a labelling scheme for a surface Σ (Use for upper bound of μ later)
  2. Find an injection $\Sigma_n \times \Sigma_m \rightarrowtail \Sigma_{n+m+\mathrm{cst.}}$ via the concatenation procedure $\implies c_n c_m \leq c_{n+m+\mathrm{cst.}}$

Theorem (SWPK and GP, 2025)

The growth constant exists for (d,k)-self-avoiding manifolds, (d,k)-self-osculating manifolds, and (d,k)-fixed polyominoids

Theorem (SWPK and GP, 2025)

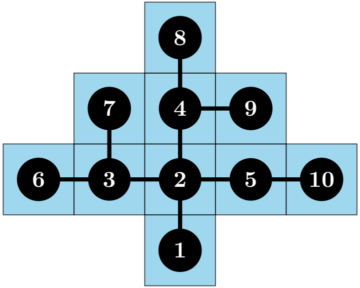
The growth constants are upper bounded by

$$\mu^{\mathrm{SAM}}_{(d,k)} \leq \mu^{\mathrm{SOM}}_{(d,k)} \leq \frac{(2k-1)^{2k-1}}{(2k-2)^{2k-2}}(2(d-k)+1)$$

- ex. self-avoiding surfaces in $\mathbb{Z}^3$: $\mu^{\mathrm{SAS}}_{\square} \leq 20.25$
- Already improved over previous upper bound 31.2504 of (Rensburg and Whittington, 1989); improve further using the twig method

Labelling of self-avoiding manifolds I

- Given Σ, pick lexicographically lowest face as $f^{(1)}$ (the 'bottom' face)
- Take all of its edges in some consistent order (ex. lexicographical, or around clockwise). If there is an unlabeled face attached to it, label it using increasing indices $(f^{(2)}, f^{(3)}, \dots)$
- Surface can be viewed as a tree



- Can generalise to (d, k)-manifolds (face $\leftrightarrow$ k-face, edge $\leftrightarrow$ $(k-1)$-edge)

Labelling of self-avoiding manifolds II

- Can produce any Σ using the following scheme:
  - Choose $f^{(1)}$; it has $\binom{d}{k}$ orientations
  - At each edge (there are $2k-1$ edges except for one it was entered from), if there is a face attached, turn on a boolean variable, then choose from one of $2(d-k)+1$ orientations to attach
  - Final surface has $(n-1)$ boolean variables turned on
  - Caveat: first face has all $2k$ edges that can be turned on

$$
\begin{aligned}
c^{\mathrm{SOM}}_{(d,k),n} &\leq \binom{d}{k}\binom{(2k-1)(n-1)+1}{n-1}(2(d-k)+1)^{n-1} \\
&\leq \binom{d}{k}\left(\frac{(2k-1)^{2k-1}}{(2k-2)^{2k-2}}\right)^{n}(2(d-k)+1)^{n-1}
\end{aligned}
$$

Other restricted manifolds

- Recall that for self-osculating manifolds, neighbouring faces are not necesarily connected
- Above labelling scheme also works for self-osculating manifolds, since we only turn on the boolean at each edge only if the faces are connected, not just neighbouring
- ‘polyominoids’: multiple faces can be connected to an edge; again, label them consistently

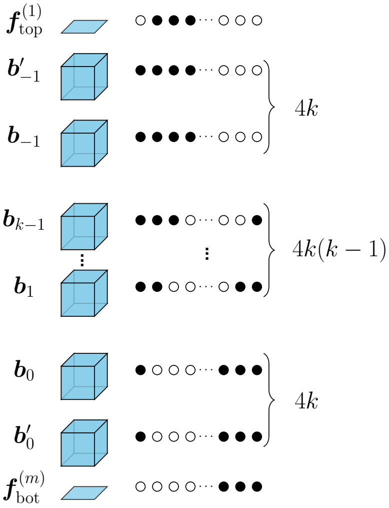
Concatenation procedure

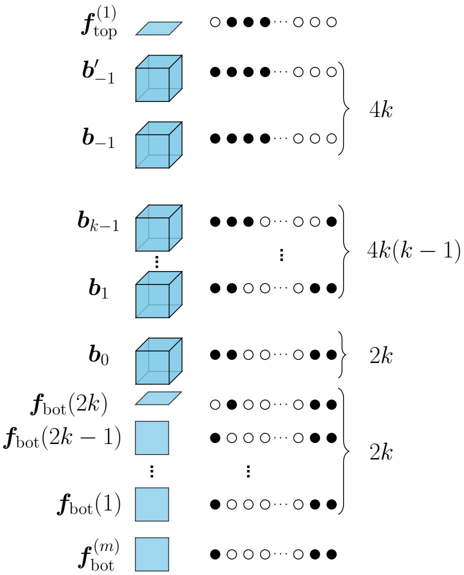
- Idea: concatenate two k-manifolds Σ_{top} Σ_{bot} together via a 'bridge' connecting $f_{\text{top}}^{(1)}$ to $f_{\text{bot}}^{(m)}$ (adapting Rensburg and Whittington, 1989 for general (d, k))
- Two k-faces can be connected via some $(k+1)$-cubes
- Two $(k+1)$-cubes can be connected if they share at least k orientations
  1. Add 'buffer' faces such that future faces don't interact with other existing faces
  2. Add orientation matching faces to make the two surfaces compatible

Lemma (SWPK and GP, 2025)

There exists an injection via the concatenation procedure

$$\Sigma_n \times \Sigma_m \rightarrowtail \Sigma_{n+m+2(k^2+3k-1)}$$


$\boldsymbol{f}_{\mathrm{top}}^{(1)}$
$\boldsymbol{b}'_{-1}$
$\boldsymbol{b}_{-1}$
$4k$
$\boldsymbol{b}_{k-1}$
$\boldsymbol{b}_1$
$4k(k-1)$
$\boldsymbol{b}_0$
$\boldsymbol{b}'_0$
$4k$
$\boldsymbol{f}_{\mathrm{bot}}^{(m)}$


$\boldsymbol{f}_{\mathrm{top}}^{(1)}$
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$4k(k-1)$
$\boldsymbol{b}_0$
$2k$
$\boldsymbol{f}_{\mathrm{bot}}(2k)$
$\boldsymbol{f}_{\mathrm{bot}}(2k-1)$
$\boldsymbol{f}_{\mathrm{bot}}(1)$
$2k$
$\boldsymbol{f}_{\mathrm{bot}}^{(m)}$

Twigs

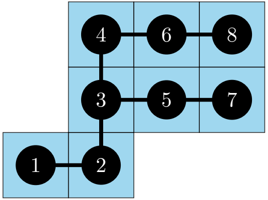
- Adapted the *twigs method* of (Klarner and Rivest, 1973) to $d = 3$

Theorem (SWPK and GP, 2025)

The growth constant for self-avoiding surfaces on the cubic lattice satisfy

$$\mu^{\mathrm{SAS}}_{\square} \leq 17.11728$$

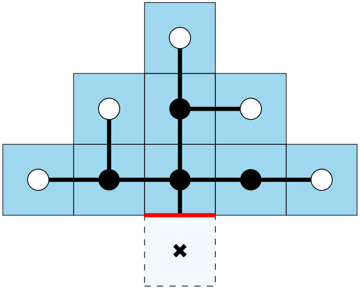
- cf. previous upper bound ≤ 31.2504 (Rensburg and Whittington, 1989)
- Monte Carlo estimates ≈ 12.798 (Glaus, 1986)
- A twig is a subtree of the tree representing the surface



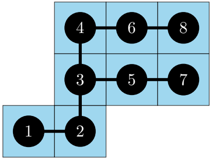
Twigs

Polyominoes ($d = 2$)

- A twig is a collection of connected faces
- Each face is either dead (black circle) or alive (white circle).
- First face is always dead
- First face is possibly connected to living faces at distance ℓ via dead faces
- To connect two twigs, a living face of the first twig overlaps with the first face of the second twig (which is dead)
- Any SAS is a sequence of twigs
- Set of twigs $\mathrm{Twigs}(\ell)$ labelled by level ℓ. It is constructed recursively from level $\ell = 1$

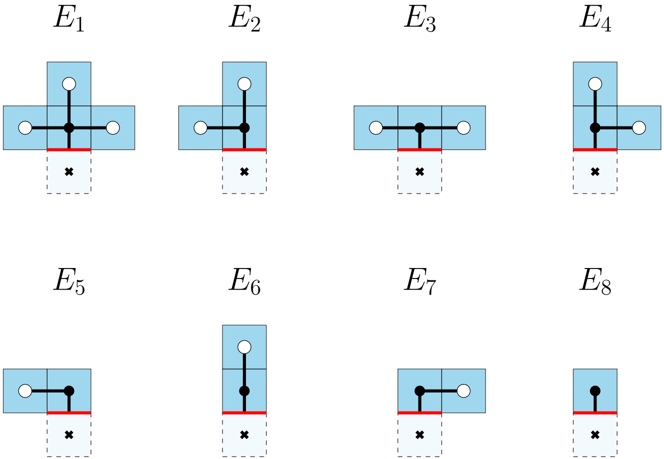


Example: Twig level 1 for $d = 2$



- Sequence of twigs:

$$\begin{array}{ccccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \Sigma = & E_7 & E_5 & E_4 & E_7 & E_6 & E_6 & E_8 & E_8 \end{array}$$



Upper bound on the growth constant

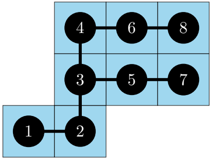
- Recursively generate larger set $\mathrm{Twigs}(\ell)$ from trees of base twig $\in \mathrm{Twigs}(\ell-1)$ and twigs $\in \mathrm{Twigs}(1)$
- Each twig is mapped to $x^{N_c-1}y^{N_\mathrm{b}}$: N_c is the number of faces and N_b is the number of dead faces
- The set of twigs defines a polynomial: $\mathrm{Twigs}(\ell) \mapsto p_\ell(x,y)$
- Generating function at level ℓ:

$$f(x,y;\ell) = \frac{x}{1-p_\ell(x,y)} = \sum_{n,m\geq 0} c_{nm}(\ell)x^n y^m$$

- Polyominoes with n faces $\mapsto x^{n-1}y^n$
- Inverse of the radius of convergence of the diagonal part yields an upper bound

$$f_\ell(z) = \sum_{n\geq 0} c_{nn}(\ell) z^n$$

Back to twig level 1

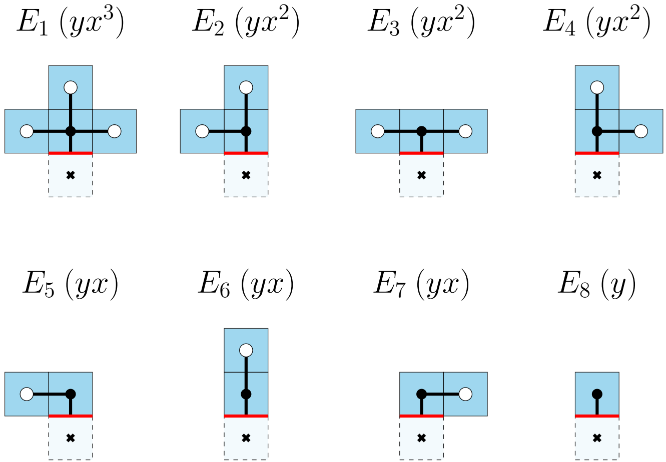


- Sequence of twigs:

$$
\begin{array}{ccccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\Sigma = & E_7 & E_5 & E_4 & E_7 & E_6 & E_6 & E_8 & E_8 \\
 & xy & xy & x^2y & xy & xy & xy & y & y
\end{array}
$$

$$\downarrow$$

$$x^7y^8$$



- Twigs at level 1 correspond to

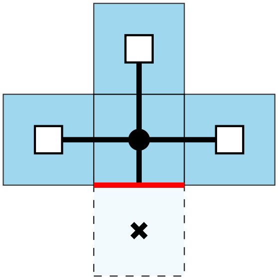
$$p_1(x,y) = y(1+x)^3$$

- The generating function is

$$f(x,y;1) = \frac{x}{1-y(1+x)^3} = \sum_{n,m\geq 0} \binom{3n}{m} x^{m+1} y^n$$

- Diagonal part is

$$f_1(z) = \sum_{n>0} \binom{3n}{n-1} z^n \implies \mu_{\square}^{\mathrm{SAS}} \leq \lim_{n\to\infty} \binom{3n}{n-1}^{1/n} = \frac{27}{4}$$



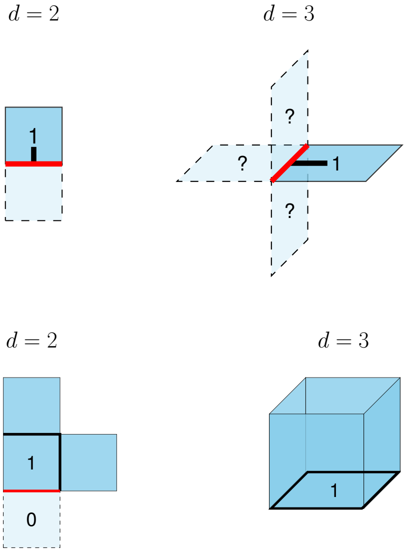
Twigs in $d = 3$

- In $d = 3$, we cannot assign a unique “entering face”
- Need to modify the generating function

$$f(x, y; \ell) = \frac{xy(1 + 3x)^4}{1 - p_\ell(x, y)}$$

- At level $\ell = 2$ we find

$$\mu^{\mathrm{SAS}}_{\square} \leq 17.11728$$



Summary

- Introduced restricted walks and restricted surfaces
- Applied the automata method to find upper bounds for self-osculating walks:

$$\mu^{\mathrm{SOW}}_{\square} \leq 2.73911 \qquad \mu^{\mathrm{SOW}}_{\triangle} \leq 4.44867$$

- Concatenation method to prove the existence of the growth constant for surfaces
- General upper bound:

$$\mu^{\mathrm{SAM}}_{(d,k)} \leq \mu^{\mathrm{SOM}}_{(d,k)} \leq \frac{(2k-1)^{2k-1}}{(2k-2)^{2k-2}}(2(d-k)+1)$$

- Modified twigs method for self-avoiding surfaces in $\mathbb{Z}^3$:

$$\mu^{\mathrm{SAS}}_{\cube} \leq 17.11728$$

Outlook

- Lower bounds?
- Improved sets of twigs?
- Twigs for self-osculating surfaces and fixed polyominoids
- Systematic methods for closed surfaces, and fixed boundaries?
    - Closed surfaces can also be defined for SOSs
- Critical properties? Which universality class? $c_n \sim n^\theta \mu^n$
- Which journal should we publish this to?

Details on diagonal function

Consider a function

$$g(x,y) = \sum_{nm} g_{nm} x^n y^m \,, \tag{4}$$

and its diagonal part

$$g_d(z) = \sum_{n} g_{nn} z^n \,. \tag{5}$$

$g_d(z)$ has the following contour integral representation

$$g_d(z) = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma ds s^{-1} g(s, zs^{-1}) \,, \tag{6}$$

where Γ is a contour in a region where $g(s, zs^{-1})$ is analytic, $|s| < R_x \cup |zs^{-1}| < R_y$, which implies $|z/R_y| < |s| < R_x$.

In our case the function $g(x, y)$ has the form

$$g(x, y) = \frac{q(x, y)}{p(x, y)}, \tag{7}$$

where q and p are polynomials in x, y. Using the fact that

$$p(s, zs^{-1}) = s^{-N_{\mathrm{y}}} \sum_{j=0}^{N_{\mathrm{x}}+N_{\mathrm{y}}} s^j P_j(z) = s^{-N_{\mathrm{y}}} P_{N_{\mathrm{x}}+N_{\mathrm{y}}}(z) \prod_{j=1}^{N_{\mathrm{x}}+N_{\mathrm{y}}} (s - r_j(z)), \tag{8}$$

where P_j is a polynomial of degree j. Singularities of $g_d(z)$ are among the roots of

$$P_{N_{\mathrm{x}}+N_{\mathrm{y}}}(z) \prod_{k=1, k\neq j}^{N_{\mathrm{x}}+N_{\mathrm{y}}} (r_k(z) - r_j(z)) \tag{9}$$

The radius of convergence R_d satisfies:

$$R_d^{-1} \leq 1/r_{\mathrm{min}} \tag{10}$$

from which we can extract the upper bound for the growth constant.

Details on twigs construction

1. Start with the set of twigs from the previous level, $\mathrm{Twigs}(\ell - 1)$.
2. Identify all faces marked with a white circle (alive).
3. Convert each of these alive faces into new dead faces by replacing the white circle with either a black dot or a cross. Store this set of "partial" new twigs.
4. For each new dead face (white circles turned into black dots in Step 3) of the "partial" twig, find all nearest-neighbor faces, excluding:
    - Any faces that have already been marked as dead or with a cross.
    - Neighbors of faces previously marked as dead or with a cross.
5. For each set of valid neighboring faces, consider all possible combinations in which each neighboring face is:
    - Alive (represented by a white circle), or
    - Not part of the polyomino (represented by a cross).

   Each new configuration of faces defines a new twig.
6. Collect all such twigs from Step 5, along with the twigs from all previous levels that contain no white circles (and hence only black dots), to form the full set of twigs at the next level, $\mathrm{Twigs}(\ell)$.