Walks crossing a square and the gerrymander sequence

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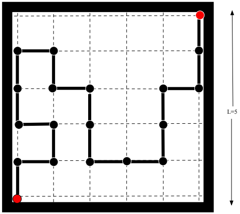
Computer Algebra for Functional Eqns. in Combinatorics and Physics

Collaborators:
Mireille Bousquet-Mélou, Iwan Jensen, Aleks Owczarek, Stu Whittington.

Outline of seminar

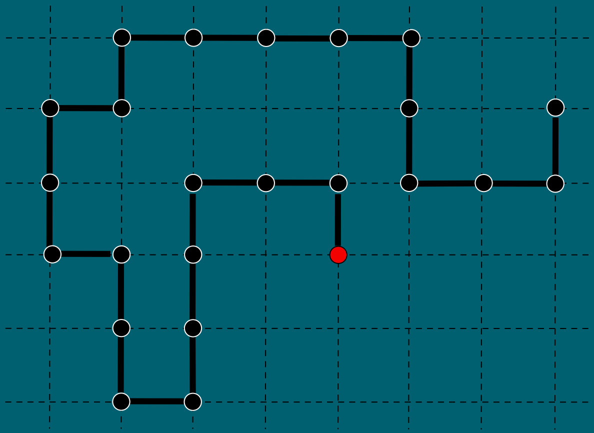
- Self-avoiding walks on an infinite lattice.
- Self-avoiding walks crossing a square (WCAS) and generalisations, including the gerrymander sequence.



- History of WCAS
- Generalisations and proof outlines.
- Enumeration. By hand, by computer (dumb), by computer (smart), then very smart. (Another seminar)
- Analysing numerical data. (Another seminar).
- Related work.
- Hexagonal lattice calculations (G and Jensen).
- Gerrymanders (A348456) and connection to WCAS (and another seminar).

Square lattice Self-avoiding walks (SAW)

A square lattice SAW



SAW without any restriction

- The number of SAWs c_n of length n, grows as

$$c_n \sim const \cdot \mu^n n^{\gamma-1}.$$

- Metric properties, e.g. the mean-square end-to-end distance:

$$\langle R^2 \rangle_n \sim const \cdot n^{2\nu},$$

  where (TBNP) $\gamma = 43/32$ and $\nu = 3/4$.
- Growth constant μ is lattice dependent. Known only for the hexagonal lattice (Neinhuis '82, Duminil-Copin and Smirnov '12). It is $\mu_{hex} = \sqrt{2+\sqrt{2}}$.
- The best estimate for the square lattice is $\mu = 2.63815853032790(3)$ (Jacobsen, Scullard and G, 2016)

A SERIES OF SAW PROBLEMS

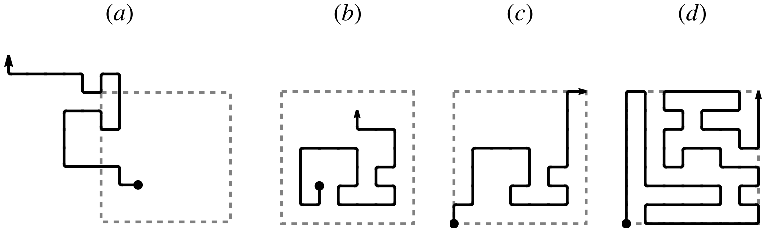
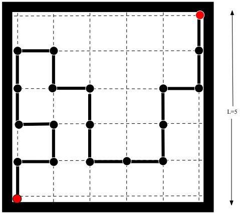


Figure: Example SAWs with increasing degree of confinement to a box of side length $L = 8$. (a) Unconfined, (b) confined to the box, (c) crossing a square (our model) and (d) a Hamiltonian path crossing a square.

SAW crossing a Square I

- Consider SAWs with end points fixed at $(0,0)$ and (L,L) in a square of side L. All sites lie in or on the boundary of the square where

$$2L \le n \le L^2 + 2L.$$



The problem has arisen in (at least) four separate incarnations.

- As a rook's tour problem (see Stephen Finch's book).
- As a telecommunications network problem.
- As a classical problem in combinatorics, initiated in the '70s by Knuth, and studied by Abbott and Hansen (1978).
- As a model of phase transitions in statistical mechanics, introduced as such in the early '90s (G and Whittington).

SAW crossing a Square II

Let the number of such SAW be s_L .
It has been proven (AH 1978 and GW 1990) that the limit

$$\lambda_S = \lim_{L\to\infty} s_L^{1/L^2}$$

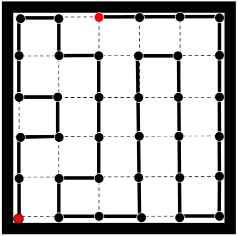
exists so that $s_L = \lambda_S^{L^2+o(L^2)}$.
The best estimate of this growth constant until recently was (Bousquet-Mélou, G. and Jensen 2005) $\lambda_S = 1.744550(5)$

Hamiltonian walks

Hamiltonian walks visit every vertex of a finite lattice.
Let the number of such walks be h_L. The limit

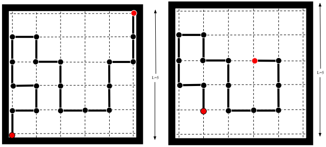
$$\mu_H = \lim_{L \to \infty} h_L^{1/L^2}$$

exists and has been estimated as $\mu_H = 1.472801(1)$ (B-MGJ 2005)



SAW IN A BOX WITH DIFFERENT ENDPOINT CONDITIONS

1. walks whose endpoints lie at opposing corners of the square counted as s_L;
2. walks whose endpoints lie anywhere within the square (Bradly and Owczarek) counted as a_L.



THE LIMIT OF INTEREST

We are interested in the existence of the limit

$$\lambda_A = \lim_{L\to\infty} a_L^{1/L^2} \ .$$

and comparing its value to the previously considered

$$\lambda_S = \lim_{L\to\infty} s_L^{1/L^2} = 1.744550(5) \ .$$

One can in fact prove (G, Jensen, Owczarek 2023) that

$$\lambda_A = \lambda_S.$$

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- Minato developed an improved data structure, extending the series to 26×26 in 2017.
- G and Jensen considered other geometries, and similar problems on the hexagonal lattice in '21-'22.

Growth of WCAS as a function of L

- Knuth (1976) asked how many walks pass through the central vertex of a 10×10 square?
- Let $c_n(L) =$ # of n-step WCAS in an $L \times L$ square, with ogf $C_L(x) := \sum_{n=0}^{L(L+2)} c_n(L) x^n$.
- $C_L(1)$ is just the total number of SAW from $(0,0)$ to (L,L).
- AH and later GW proved that $C_L(1) \sim \kappa^{L^2+o(L^2)}$.
- GW were interested in the phase transition as one varies the weight x associated with the walk length.
- When x is small, the g.f. is dominated by short walks.
- At a critical value, x_c, the average walk length changes from $\Theta(L)$ to $\Theta(L^2)$.
- Whittington has recently proved that $C_L(1) \sim \kappa^{L^2+O(L)}$.
- He proved the same result for polygons crossing a square.

- The value of κ is not known on any lattice, though both bounds and estimates were given by AH and GW.
- GW proved that the critical fugacity $\geq 1/\mu$, and conjectured to be $x_c = 1/\mu$ exactly. Subsequently proved by Madras ('95).
- At x_c we believe (unproved) that the length is $\Theta(L^{1/\nu}) = \Theta(L^{4/3})$.

- AH considered the more general problem of SAWcrossing an $L \times M$ lattice, asking how many paths exist from $(0,0)$ to (L,M)?
- Let the number of such paths be $C_{L,M}$. For M finite, the paths can be generated by a finite dimensional transfer matrix.
- Hence the generating function is rational (Stanley).
- Indeed, AH proved that

$$G_2(x) = \sum_{M \geq 0} C_{2,M} x^M = \frac{1 - x^2}{1 - 4x + 3x^2 - 2x^3 - x^4},$$

- It follows that $C_{2,M} \sim \text{const.}\kappa_2^{2M}$, where $\kappa_2 = \sqrt{\frac{2}{\sqrt{13}-3}} = 1.81735\ldots$.

To get good bounds on κ, we introduced two generalisations of the problem.

- Firstly, let SAWs start anywhere on the left edge and end anywhere on the right edge; these are walks *traversing* the square.
- Secondly, allow several independent SAW, each starting and ending on the perimeter of the square, but not allowed to take steps along the perimeter. Such walks partition the square into distinct regions and by colouring the regions alternately black and white we get a *cow-patch* pattern.
- Recall $C(L) = C_L(1)$ is the number of WCAS. Similarly define $P(L)$ for cow-patch walks, and $T(L)$ for *transverse* walks.
  We can prove

$$\lim C(L)^{1/L^2} = \lim T(L)^{1/L^2} = \lim P(L)^{1/L^2} = \kappa.$$

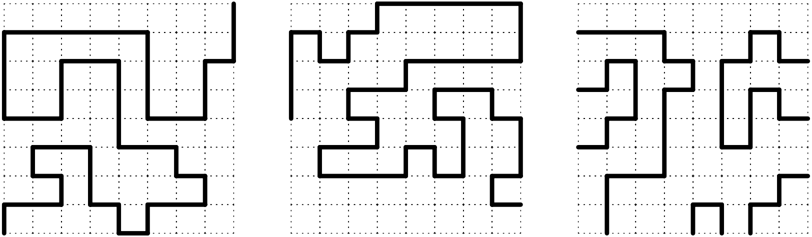

Figure: An example of a SAW configuration crossing a square (left panel), traversing a square from left to right (middle panel) and a cow-patch (right panel).

We can break the lattice up into a grid of smaller squares, and combine smaller WCAS or transverse walks into a WCAS.

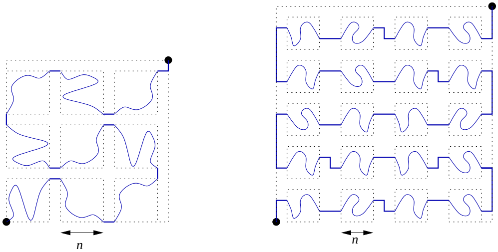

Figure: Dense packings of walks crossing or traversing a square ($k = 3$).

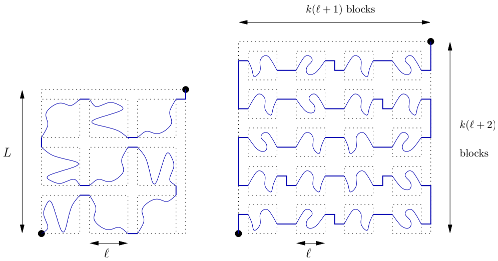

Figure: Dense packings of walks crossing or traversing a square ($k = 3$).

In this way we can obtain the bound

$$C(l)^{1/(l+1)^2} \leq \kappa.$$

A stronger lower bound comes from transverse walks.

$$\kappa \geq T(l)^{1/((l+1)(l+2))}.$$

Upper bounds

AH obtained an upper bound on κ by recasting the problem in a matrix setting. We'll give an alternative method based on cowpatch configurations.

- Following AH, label each unit square in the WCAS by 1 if it lies to the right of the path, and by 0 if it lies to the left.
- This provides a $1:1$ correspondence between paths and a subset of $L \times L$ matrices with elements 0 or 1.
- Matrices corresponding to allowed paths are *admissible*, otherwise *inadmissible*.
- There are 2^{L^2} such matrices on an $L \times L$ lattice, so $C_{L,L} \leq 2^{L^2}$.
- Of the 16 possible 2×2 matrices, only 14 correspond to portions of non-intersecting lattice paths.
- Thus $C_{L,L} \leq 14^{(1/L)^2}$, so $\kappa \leq 14^{1/4} = 1.9343...$
- Similarly, for 3×3 lattices we find 320 admissible matrices (out of a possible 512), so $\kappa \leq 320^{1/9} = 1.8982..$

An alternative interpretation follows from the cowpatch walks defined earlier. For cowpatches, colour alternate regions black or white, so that adjacent regions have different colours.
This gives a bijection between cow-patches and *admissible* matrices, previously defined. Thus by arguments similar to the above, we find

$$(2P(L))^{1/L^2} \geq \kappa.$$

This is the same bound found by Abbott and Hanson, but easier to calculate. Our cowpatch counts gave the number of admissible matrices up to 19×19. There are 3.5465202×10^{90} such matrices, hence $\kappa \leq 1.781684$. From transverse walks we get the lower bound $\kappa \geq 1.65657$. So

$$1.65657 \leq \kappa \leq 1.781684.$$

Following GW, Madras in '95 proved a number of results for the hypercubic lattice. Restricting to 2d we have:

- Let

$$\lambda_1(x) := \lim_{L\to\infty} C_L(x)^{1/L} \tag{1}$$

$$\lambda_2(x) := \lim_{L\to\infty} C_L(x)^{1/L^2} \tag{2}$$

Theorem

(i) Both limits exist. (1) is finite for $0 \le x \le 1/\mu$, and is infinite for $x > 1/\mu$. For $0 < x < 1/\mu$, $0 < \lambda_1(x) < 1$ and $\lambda_1(1/\mu) = 1$. (ii) (2) is finite for all $x > 0$. $\lambda_2(x) = 1$ for $0 < x < 1/\mu$ and $\lambda_2(x) > 1$ for $x > 1/\mu$.

The average length of a walk is

$$\langle n(x) \rangle_L := \sum_n n c_n(L) x^n \Big/ \sum_n c_n(L) x^n. \tag{3}$$

Theorem

As $L \to \infty$, we have $\langle n(x) \rangle_L = \Theta(L)$ for $0 < x < 1/\mu$ and $\langle n(x) \rangle_L = \Theta(L^2)$ for $x > 1/\mu$.

- Unknown at $x = 1/\mu$. Compelling numerical evidence that $\langle n(1/\mu) \rangle_L = \Theta(L^{1/\nu})$, as suggested by Madras.

Enumeration

- The basic algorithm used to enumerate WCAS is based on the method of Conway, Enting and G for enumerating SAW.
- SAWs crossing an $L \times L$ square are counted using a TM algorithm. This involves drawing a boundary line through the square, intersecting up to $L+2$ edges.
- For each edge configuration we maintain a count of partially completed walks intersecting the boundary in that pattern.
- WCAS are counted by moving the boundary, adding one vertex at a time (figure coming.)

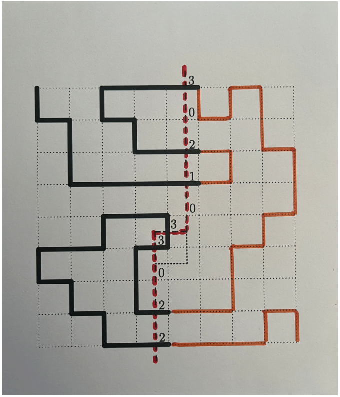

Figure: A WCAS, showing the intersection during TM counting. Walks are enumerated by successive moves of the kink in the boundary, as shown by the dotted line. One vertex at a time is added to the square.

- Squares are built up column by column, sequentially adding one vertex at a time. Configurations are represented by sets of states $\{\sigma_i\}$.
- An empty edge is indicated by $\sigma_i = 0$. An occupied edge is either free (not connected to other edges) or connected to exactly one other edge via a path to the left of the boundary. We indicate this by $\sigma_i = 1$ for a free end, $\sigma_i = 2$ for the lower end of a loop and $\sigma_i = 3$ for the upper end of loop.
- Since we are studying 2d SAWs, this encoding uniquely specifies which ends are paired. Read from the bottom the intersection configuration is $\{2203301203\}$ (prior to move) and $\{2300001203\}$ (after move).

- Time and memory requirements are proportional to the maximal number of distinct configurations along the boundary line.
- When there is no kink in the intersection (a column has just been completed) we can calculate this number, $N_{\text{conf}}(L)$, exactly. Obviously the free end cuts the boundary line into two pieces.
- Each piece consists of '0's and an equal number of '2's and '3's, with the latter forming a perfectly balanced parenthesis.
- Each piece thus correspond to a Motzkin path (map 0 to a horizontal step, 2 to a NE step, and 3 to a SE step).

$$\mathcal{M}(x) = \sum_n M_n x^x = [1 - x - (1 - 2x - 3x^2)^{1/2}]/2x^2. \qquad (4)$$

The number of configurations $N_{\mathrm{conf}}(M)$ is simply obtained by inserting a free end between two Motzkin paths,

$$N_{\mathrm{conf}}(L) = \sum_{k=0}^{L} M_k M_{M-k}. \qquad (5)$$

- When the boundary line has a kink the number of configurations exceeds $N_{\mathrm{conf}}(L)$ but clearly is less than $N_{\mathrm{conf}}(L+1)$.
- From (4) we can show that $N_{\mathrm{conf}}(L)$ grows like 3^L.
- The same is true for the maximal number of boundary configs. and so for the computational complexity of the algorithm.

- Since the number a walks grows like κ^{L^2}, our algorithm gives a better than exponential improvement over direct enumeration.
- The integers occurring in the calculation become very large so calculations are performed using modular arithmetic. We repeat the calculation modulo various primes p_i and then reconstruct the full coefficients.
- We used primes of the form $p_i = 2^{30} - r_i$, ($r_i < 1000$). The CRT ensures that any integer has a unique representation in terms of residues.
- The algorithm is easily generalised to include a step fugacity x. The count associated with the boundary line configuration is replaced by a generating function for partial walks. This generating function is just a polynomial of degree L^2 in x.

- The generalisation to traversing walks is also quite simple.
- The generalisation to cow-patch patterns is more complicated but can be overcome with minimal increase in computational complexity.
  Enumeration results
- Proceeding as above, we calculated $c_n(L)$ for all n for $L \leq 17$.
- In addition, we computed $C_{18}(1)$ and $C_{19}(1)$.
- We also computed $P_L(1)$ and $T_L(1)$, the g.f's. for cowpatch and traversing walks respectively, for $L \leq 19$.

BDDs and ZDDs

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- See also the Wikipedia entry on ZDDs, which is very accessible, and gives applications to this problem.

ZDD APPLICATIONS

- For example, the set of five-letter English words, of which there are 5757, can be encoded in a ZDD of size 5020 nodes, which can be used to immediately answer questions such as all words of the form *b*a*t*. It will immediately give you *beast*, *blast boast* etc.

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- In that technical report they went to size 25×25, subsequently improved to 27×27.

Numerical analysis

It has been proved AH,GW that $\lim_{L\to\infty} C_{L,L}^{\frac{1}{L^2}} = \kappa$ exists.

- We expect that the ratios $R_L = C_{L+1,L+1}/C_{L,L}$ are dominated by a term that behaves as κ^{2L}. (Not rigorous). The generating function $\mathcal{R}(x) = \sum_L R_L x^L$ therefore has r.c. $x_c = 1/\kappa^2$, which we can estimate accurately using differential approximants.

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- With the extra data we can refine this to $x_c = 0.3285744(2)$, or that $\kappa = 1.7445498(5)$.
- More precisely, we find

$$C_L(1) \sim \kappa^{L^2+dL+e} \cdot L^g$$

where $\kappa \approx 1.7445498$, $d = -0.04354 \pm 0.0001$, $e \approx 0.5624 \pm 0.0005$ and $g = 0$.

- We have mentioned earlier that the mean number of steps undergoes a transition from $\langle n(x,L)\rangle = \Theta(L)$ to $\langle n(x,L)\rangle = \Theta(L^2)$ at $x = x_c = 1/\mu$.
- Fluctuations in this quantity, $V(x,L) = \langle n^2(x,L)\rangle - \langle n(x,L)\rangle^2$ have also been investigated.
- For fixed L, we find $V(x,L)$ has a single maximum located at $x_c(L)$, which approaches x_c as L approaches infinity.
- More precisely, we find

$$V(x,L) \sim const.L^{2/\nu}U((x-x_c)L^{1/\nu}),$$

  where $U(y)$ is a scaling function, and $\nu = 3/4$.
- It follows that the position and height of the peak scale as $x_c(L) - x_c \sim const.L^{-1/\nu}$ and $V_{max}(L) \sim const.L^{2/\nu}$. Both these results are borne out by our numerical work.

- We can also calculates the number of SAW crossing an $L \times L$ square of length $2L + 2K$ for small values of K.
- For $K = 0$ the answer is $\binom{2L}{L}$.
- For $K = 1$ the answer is $2L\binom{2L}{L+2}$, and we found the result for $K \leq 4$.
- Asymptotically, we can prove that, for $K = \mathrm{o}(L^{1/3})$ the number is

$$\frac{4^L}{\sqrt{L\pi}} \frac{(2L)^K}{K!}.$$

Here the first term is given by the number of ways of choosing the backbone, $\binom{2L}{L} \sim \frac{4^L}{\sqrt{L\pi}}$ and the second is given by the number of ways of placing K defects on a path of length $2L$, which is just $(2L)^K$. The defects are indistinguishable, introducing the factor K!

Hamiltonian walks

Hamiltonian walks can only exist on $2L \times 2L$ lattices. For lattices with an odd number of edges, one site must be missed.

- A Hamiltonian walk is of length $4L(L+1)$ on a $2L \times 2L$ lattice.
- The number of such walks grows as τ^{4L^2}, where we find $\tau \approx 1.472$ based on exact enumeration up to 17×17 lattices.
- τ is thus about 20% less than κ, the growth constant for all paths.
- In AH it is proved that $2^{1/3} \leq \tau \leq 12^{1/4}$. Numerically, $1.260 \leq \tau \leq 1.861$.
- We can improve on these bounds.

- We define Hamiltonian versions of transverse and cow-patch walks.
- Then the proofs of bounds for Hamiltonian walks follow similarly *mutatis mutandis* from the bounds we established for WCAS.
- In this way, and enumerating the Hamiltonian paths, and their transverse and cow-patch counterparts, we find

$$1.429 < \tau < 1.530.$$

- Having previously proved that $1.6284 < \kappa$, it follows that $\tau < \kappa$.

Other work

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- We find this ratio for all lattices up to size 18×18, and note that it is approaching a constant, remarkably close to $\sqrt{\pi/5}$. How to prove or disprove such a possibility?

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We can proved that $C_L(1) \sim A \cdot \lambda^{L^2}$, where L is the linear dimension of the hexagon. We estimate $\lambda \approx 1.38724951$. But we can't guess its exact value!

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- We first proved that it should grow like $\lambda^{L^2+o(L^2)}$, where L is the linear dimension.
- We estimated that $\lambda \approx 1.7445$ – the same as the growth constant for WCAS!
- We then proved that the growth constants are the same, and also related the sub-dominant asymptotics to those of WCAS.

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- For L even $\mathcal{C}_L$ is twice the gerrymander sequence coefficient.
- In any GGC one (or both) regions has to be a self-avoiding polygon (SAP). This is the key to our efficient enumeration.

- Here are the four distinct cases one has to consider, noting that the grey region is a SAP.

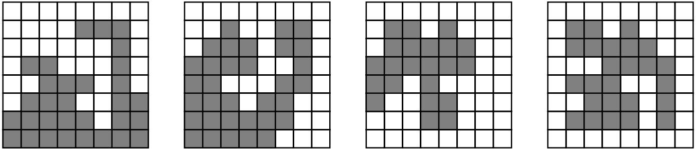

Figure: The four cases of self-avoiding polygons (grey regions) resulting in gerrymander configurations.

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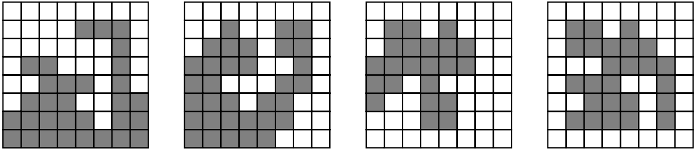

Figure: The four cases of self-avoiding polygons (grey regions) resulting in gerrymander configurations.

- Given the constraint of only two connected regions, it follows that the grey region can be chosen so that it contains either zero, one, or two corners of the square.

Theorem

PCAS have the same growth constant as WCAS.

Theorem

SAPS within a square grow as WCAS.

Theorem

The generalised gerrymander sequence has the same growth constant as WCAS.

We find that the coefficients of A348456 grow as

$$\lambda^{4L^2+dL+e} \cdot L^g$$

where $\lambda = \lambda(WCAS) \approx 1.7445498$, $d = -8.0708 \pm 0.0002$, $e \approx 7.69$, and $g = 3/4$.

CONCLUSION

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Conclusion

- We have unified and extended a number of results in this problem, which provides a nice example of both enumeration techniques and a simply understood mechanism of a phase transition.
- It also offers scope for developing a variety of mathematical techniques, including enumeration algorithms, establishing rigorous bounds, and proving existence theorems.
- It also shows that the statistical mechanics, algebraic combinatorics and computer science communities should talk to one another!