

COMPUTABILITY AND COMPLEXITY IN ANALYTIC COMBINATORICS

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University of Waterloo



Moonlight, Waning Winter, Homer Watson (1924)

HOMER WATSON

Introduction

Enumerative Combinatorics

We study **discrete objects** using **sequences** which could

- **count** objects in a combinatorial class

Example: c_n is the number of ways to make change for n dollars using pennies, nickels, dimes, and quarters

- capture the **probability** that an event occurs

Example: p_n is the probability that two numbers in $\{1, \dots, n\}$ are coprime

- track the **runtime** of an algorithm

Example: q_n is the average number of comparisons performed by quicksort on all permutations of $1, \dots, n$

- encode a class with **parameters**

Example: $b_{k,n}$ is the number of binary trees on n nodes with k leaves

Goal:

Say something
interesting about
the sequence

Exact Formulas

A THEOREM ON TREES.

By Prof. CAYLEY.

THE number of trees which can be formed with $n + 1$ given knots $\alpha, \beta, \gamma, \dots$ is $= (n + 1)^{n-1}$; for instance $n = 3$, the number of trees with the 4 given knots $\alpha, \beta, \gamma, \delta$ is $4^2 = 16$

A. Cayley. A Theorem on Trees. Quart. J. Pure Appl. Math. Vol 23, 376–378, 1889.

It's **unreasonable** to expect this to always occur — not all combinatorial sequences have *simple* formulas, and even if they do they can be hard to prove!

Efficient Algorithms

```
1 M = Matrix(ZZ, 2, 2, [1, 1, 1, 0])
2
3 def bin_pow(n):
4     if n == 1: return M
5     elif n%2 == 0: return bin_pow(n/2)^2
6     else: return bin_pow((n-1)/2)^2*M
7
8 def fib(n): return add(bin_pow(n)[1])
9
10 timeit('fib(10^6)') # 208,987 digits long!
```

25 loops, best of 3: 10.1 ms per loop

Gathering data can be useful for studying sequences, and conjecturing formulas, but doesn't fully *capture behaviour*.

Asymptotics

Instead of exact enumeration, focus on **large-scale behaviour** by **approximating** f_n for large n .

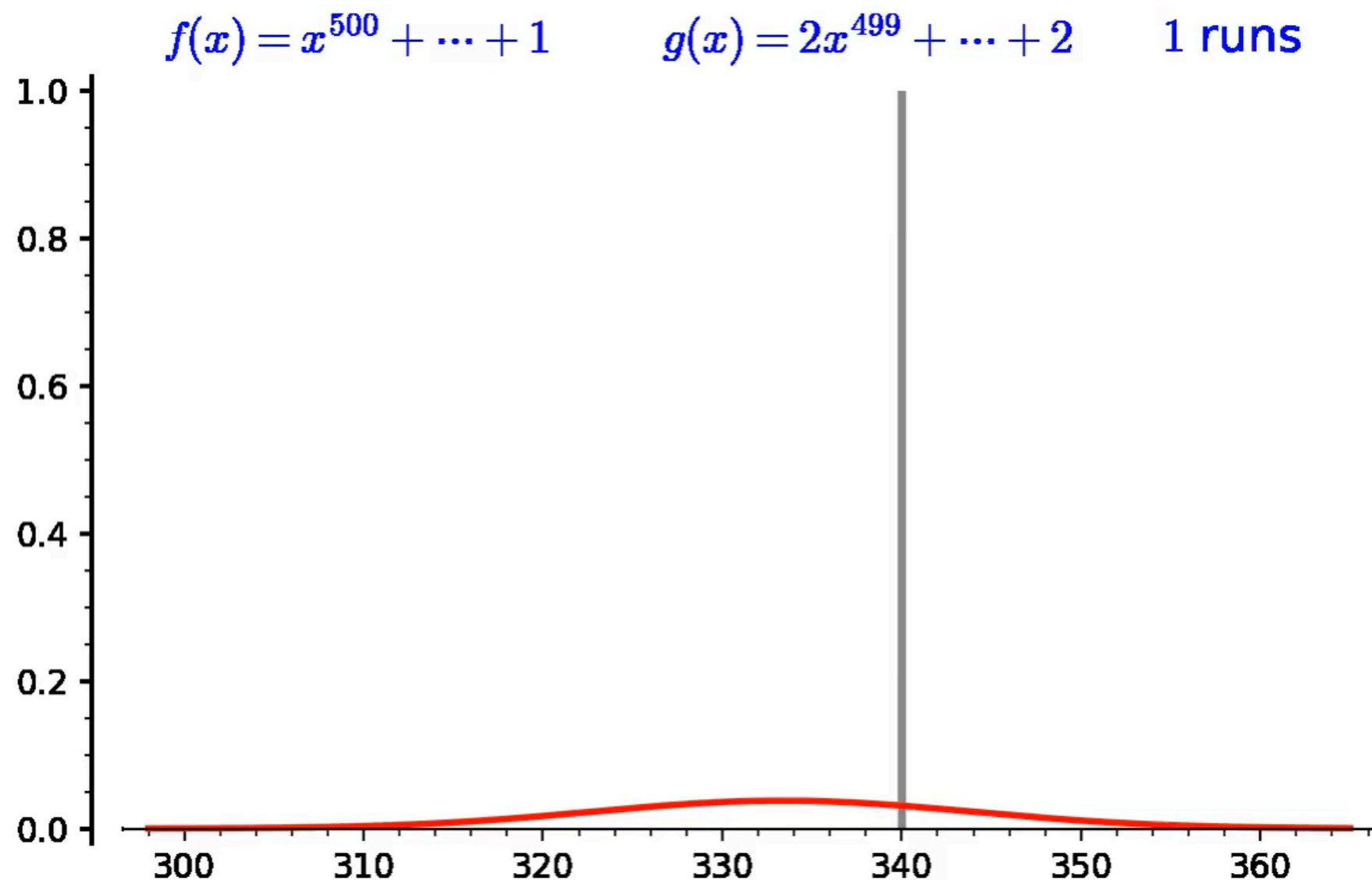
$$\# \text{ partitions of } n \sim \frac{1}{4n\sqrt{3}} \exp\left(\pi\sqrt{\frac{2n}{3}}\right)$$

$$\begin{array}{l} \text{average quicksort cost} \\ \text{on permutation of size } n \end{array} \sim 2n \log n$$

$$\# \text{ unlabelled graphs on } n \text{ nodes} \sim \frac{2^{\binom{2n}{n}}}{n!}$$

Limit Theorems

We can capture the large-scale behaviour of parameters through *limit theorems*



Number of divisions when running Euclidean algorithm on pairs of polynomials in $\mathbb{Z}_3[x]$ with larger polynomial monic of degree 500

Generating Functions

The **generating function (GF)** of f_n is

$$F(z) = \sum_{n \geq 0} f_n z^n$$

Example

The GF for binary strings counted by length is

$$F(z) = 1 + 2z + 4z^2 + \dots = \frac{1}{1 - 2z}$$

Example

The GF for integer partitions is

$$F(z) = \prod_{k \geq 1} \frac{1}{1 - z^k}$$

Generating Functions

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$$F(z) = \sum_{n \geq 0} f_n z^n$$

Algebraic / differential / functional equations for F form a data structure for f_n

First, Let the Relation of each Term to the two preceding ones be expressed in this manner, viz. Let C be $= m B r - n A r r$; and let D likewise be $= m C r - n B r r$, and so on: Then will the sum of that Infinite Series be equal to $\frac{A + B - m r A}{1 - m r + n r r}$.

Generating Function Classes

D-ALGEBRAIC

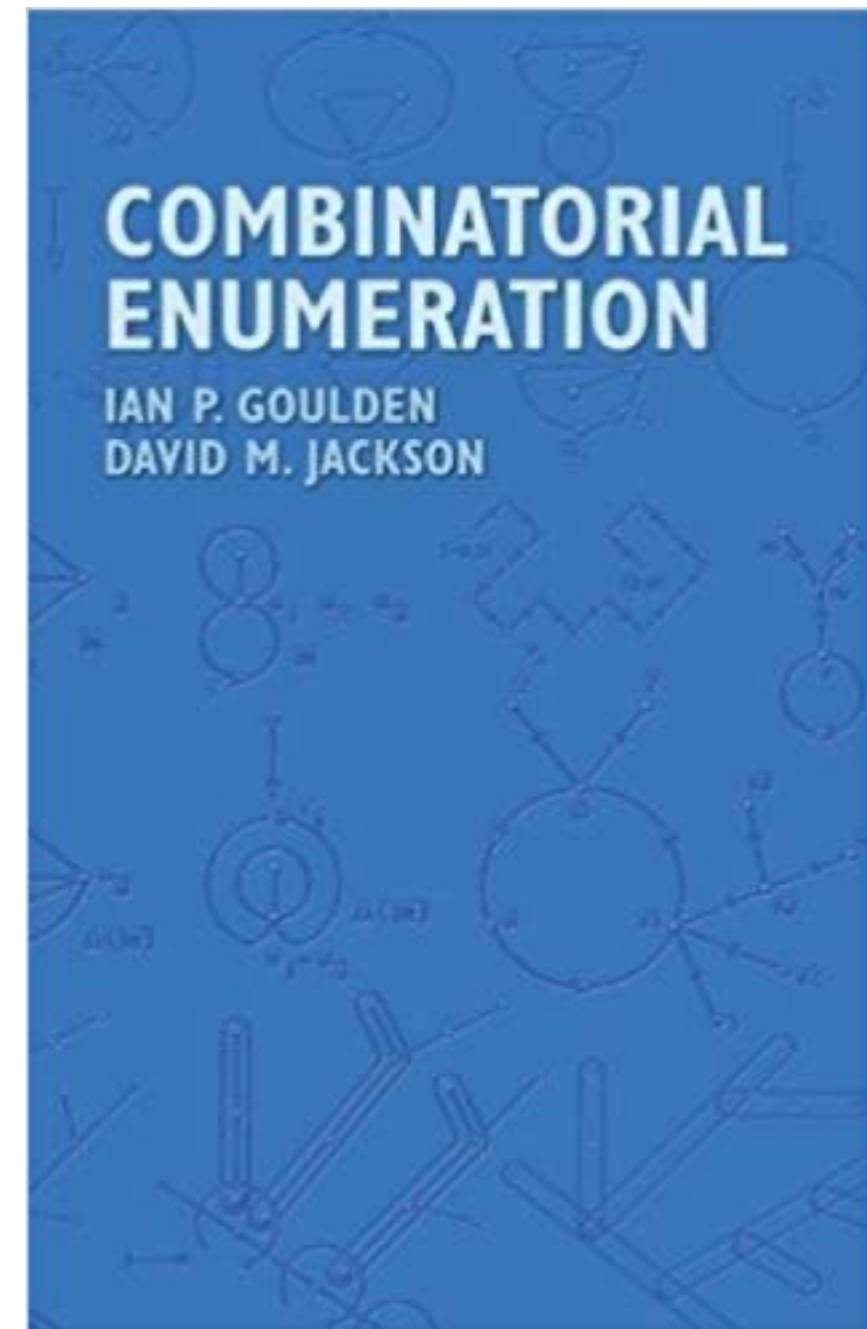
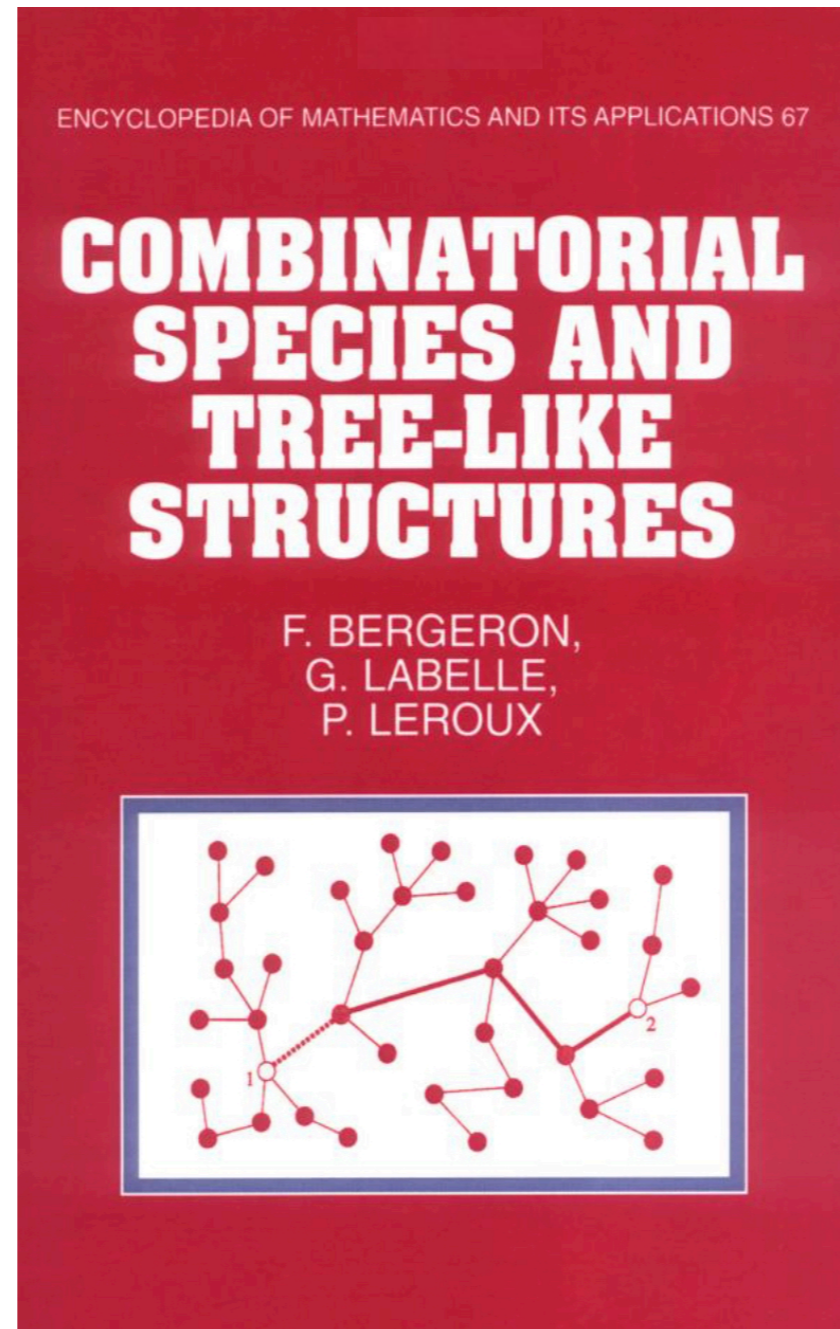
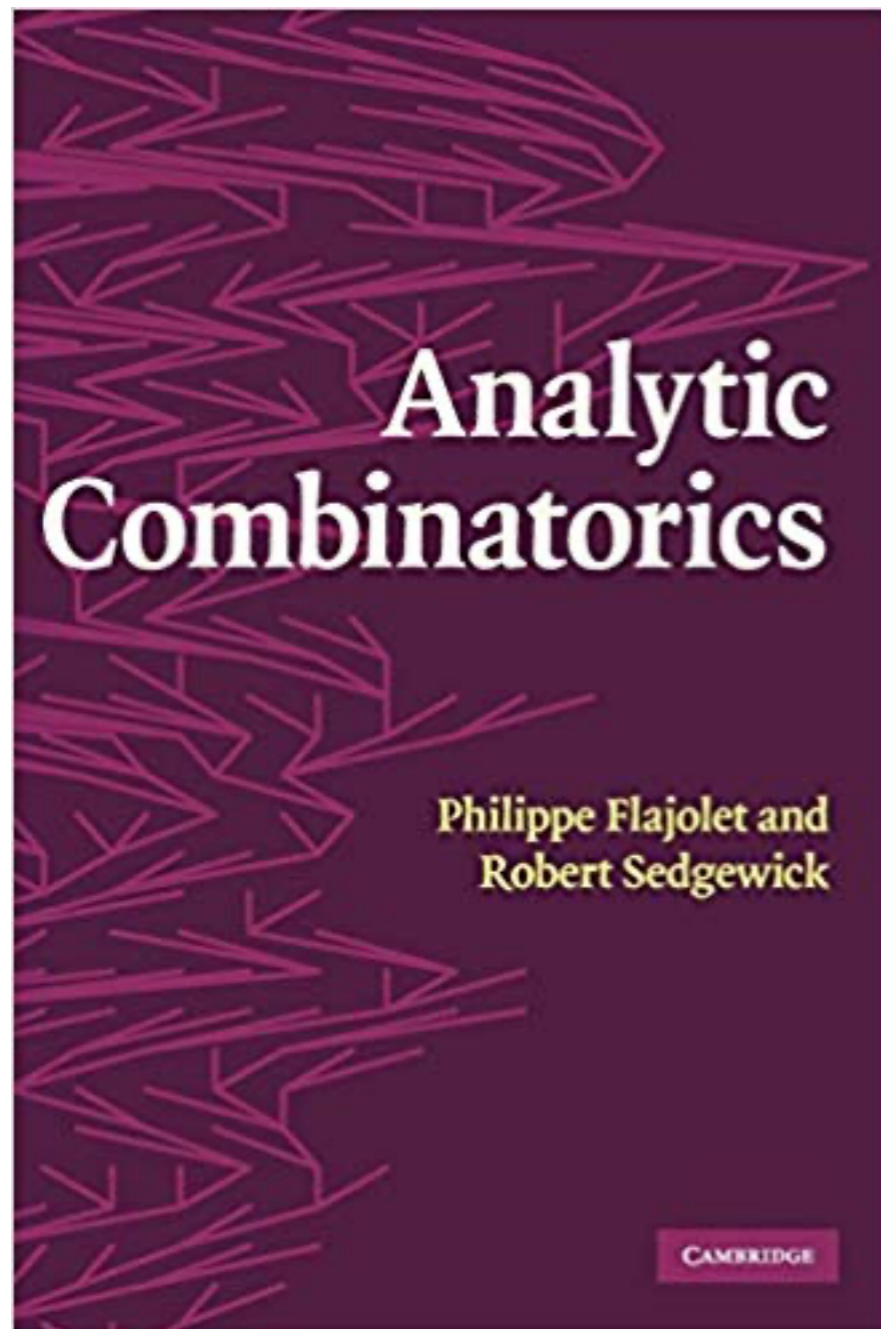


D-FINITE

ALGEBRAIC

RATIONAL

Combinatorial definitions often automatically translate to GF equations



Alternating Permutations

An **alternating permutation** is a permutation π of *odd length* such that $\pi_1 > \pi_2 < \pi_3 > \dots$

The alternating permutations of length three: 213 and 312

$$A(z) = \sum_{k \geq 0} \frac{a_{2k+1}}{(2k+1)!} z^{2k+1}$$

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$$A(z) = \sum_{k \geq 0} \frac{a_{2k+1}}{(2k+1)!} z^{2k+1} = \tan z$$

ANALYSE MATHÉMATIQUE. — Développements de $\sec x$ et de $\tan x$. Note de M. D. ANDRÉ, présentée par M. Hermite.

« On n'a point donné jusqu'à présent, du moins à ma connaissance, de développement, suivant les puissances de x , soit de $\tan x$, soit de $\sec x$, où les coefficients aient une définition simple, nette, indépendante de tout autre développement. L'objet de la présente Note est de combler cette lacune.

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> series(tan(z), z, 20):

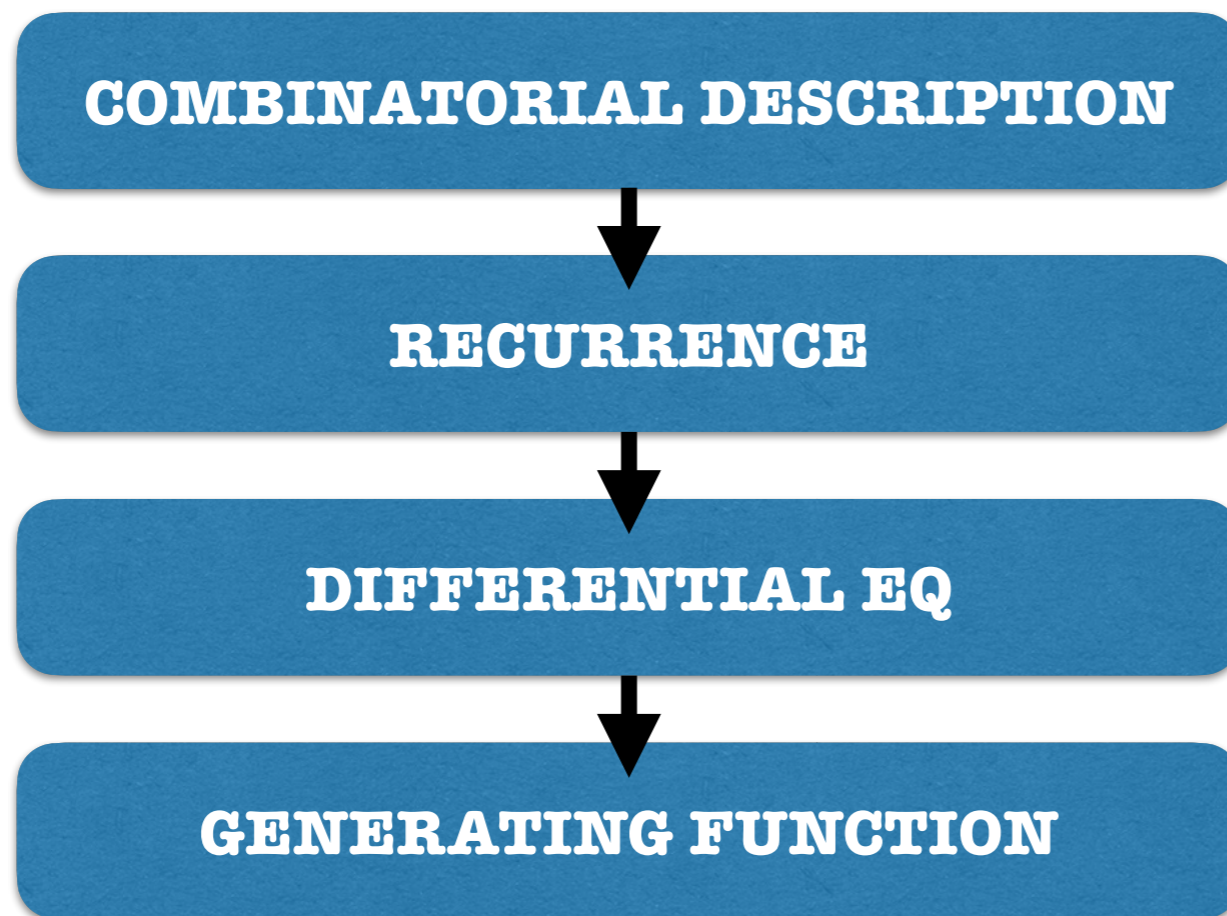
add(coeff(% , z, k) * factorial(k) * z^k / ('factorial'(k)), k=0..15);

$$\frac{z}{1!} + \frac{2z^3}{3!} + \frac{16z^5}{5!} + \frac{272z^7}{7!} + \frac{7936z^9}{9!} + \frac{353792z^{11}}{11!} + \frac{22368256z^{13}}{13!} + \frac{1903757312z^{15}}{15!}$$

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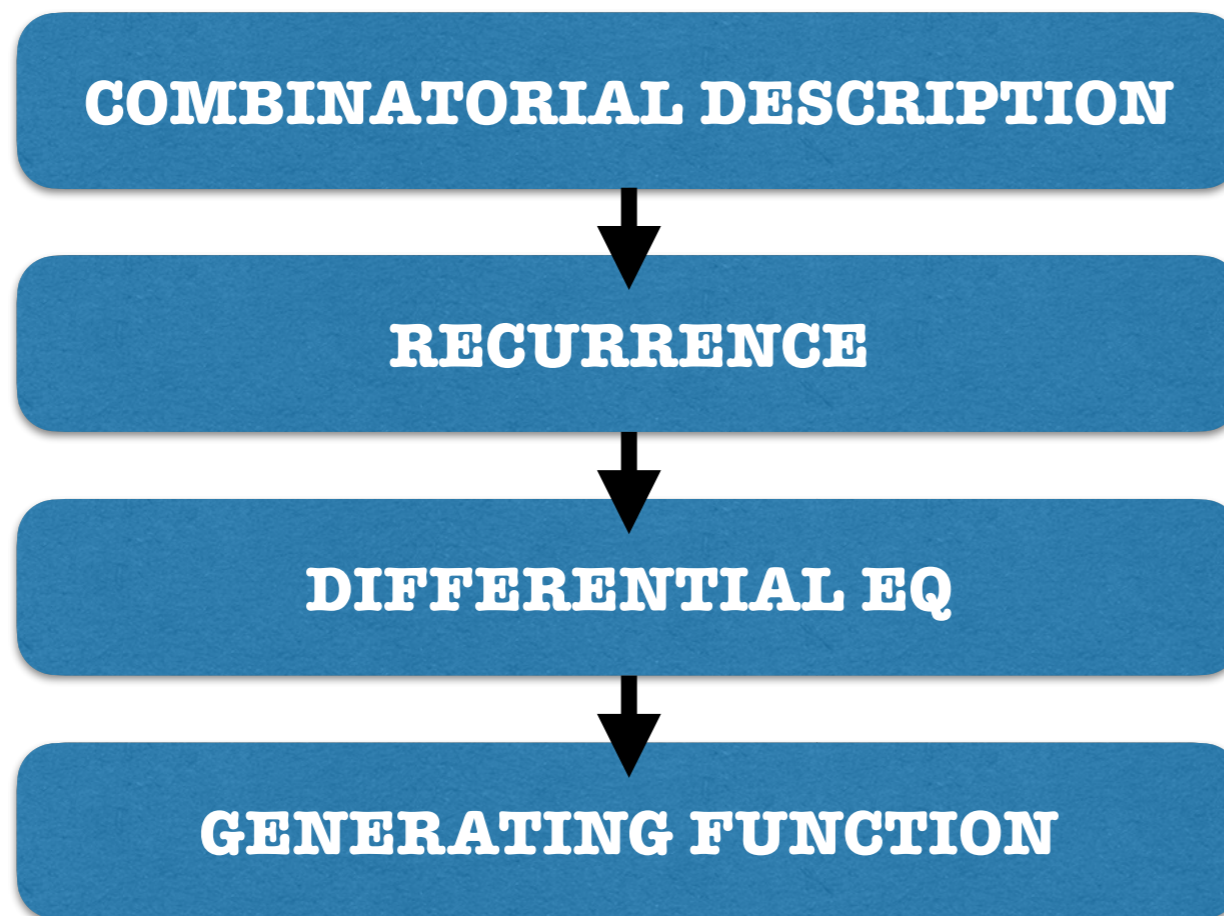
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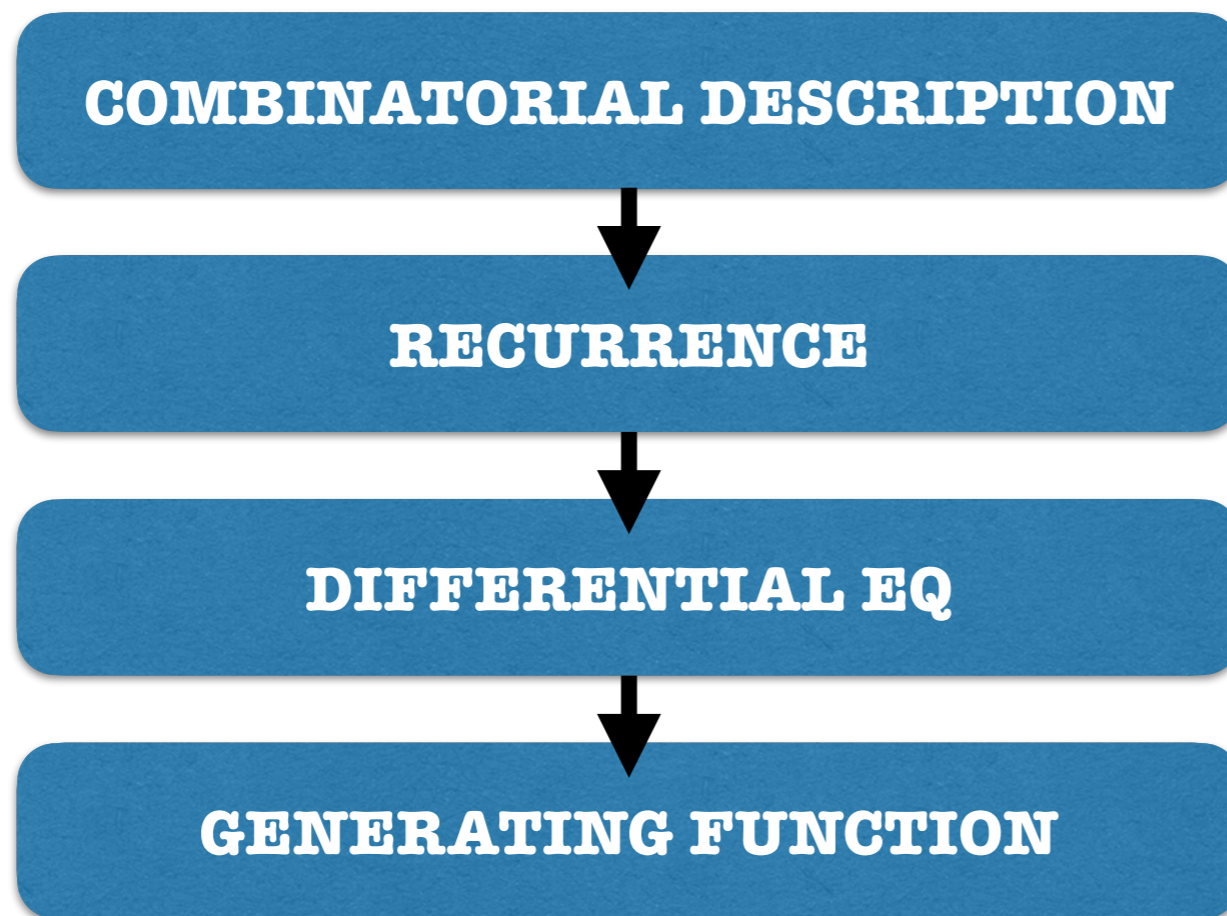


$$a_{2k+1} = \sum_{j \geq 0} \binom{2k}{j} a_j a_{2k-j}$$

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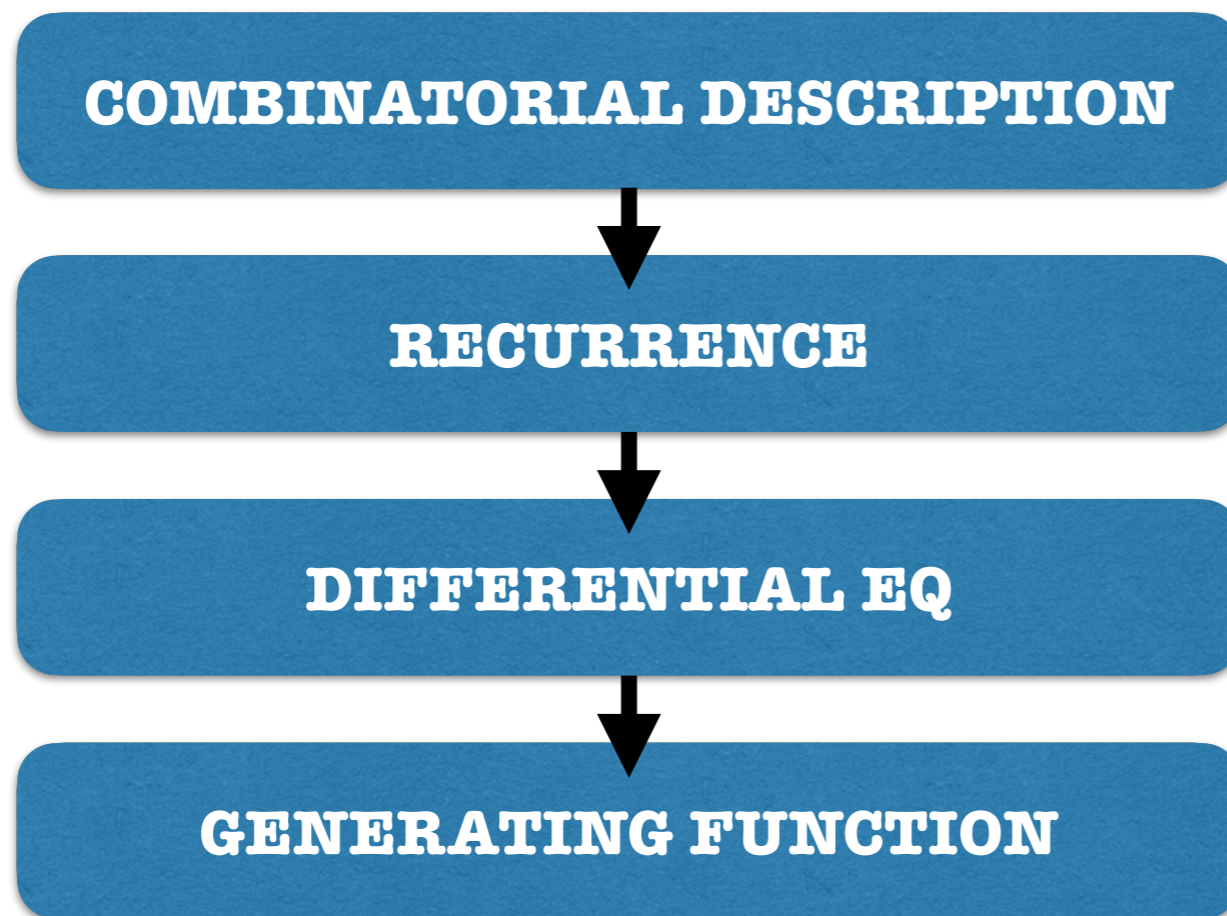
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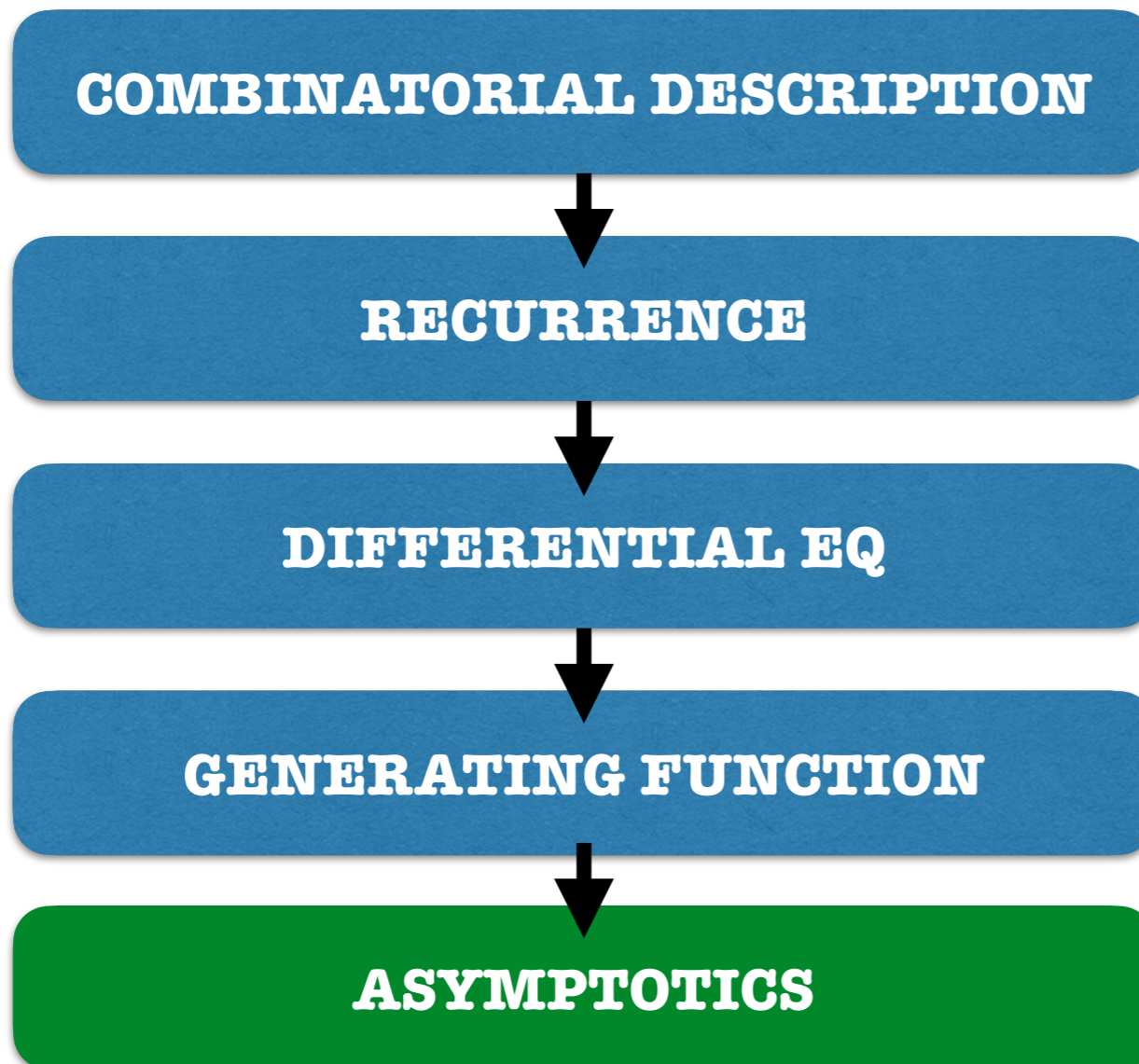
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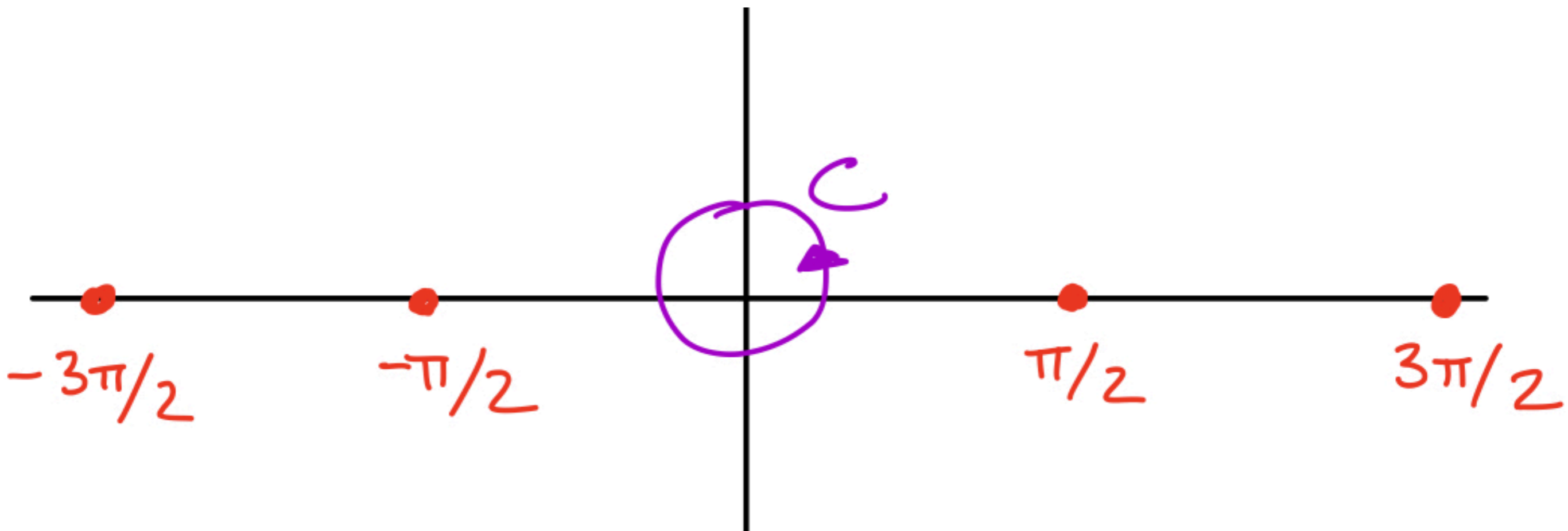
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Asymptotics of Alternating Permutations

The Cauchy integral formula implies

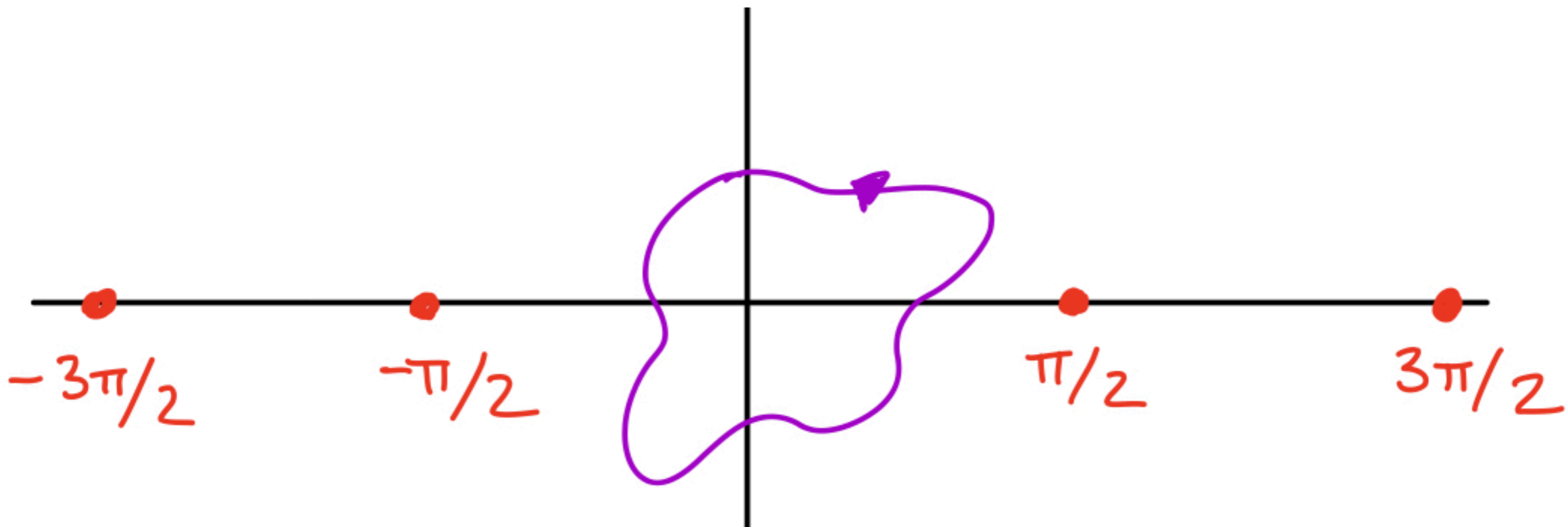
$$\frac{a_n}{n!} = [z^n] \tan z = \frac{1}{2\pi i} \int_C \frac{\tan z}{z^{n+1}}$$



Asymptotics of Alternating Permutations

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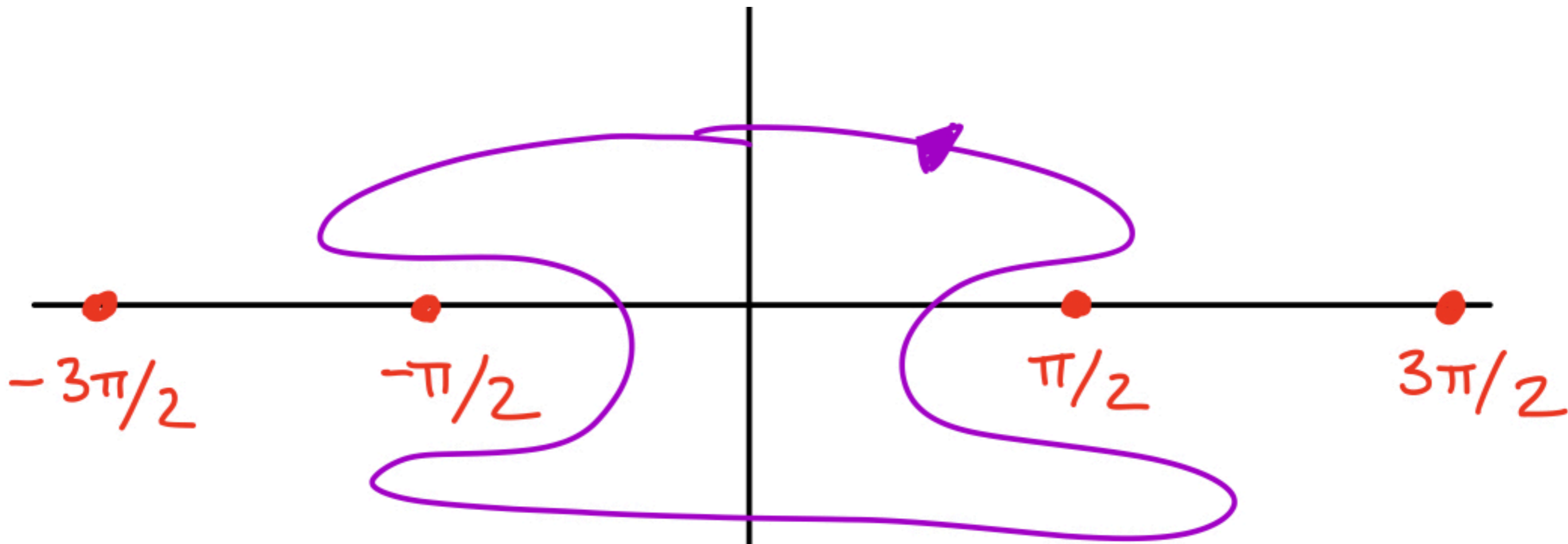
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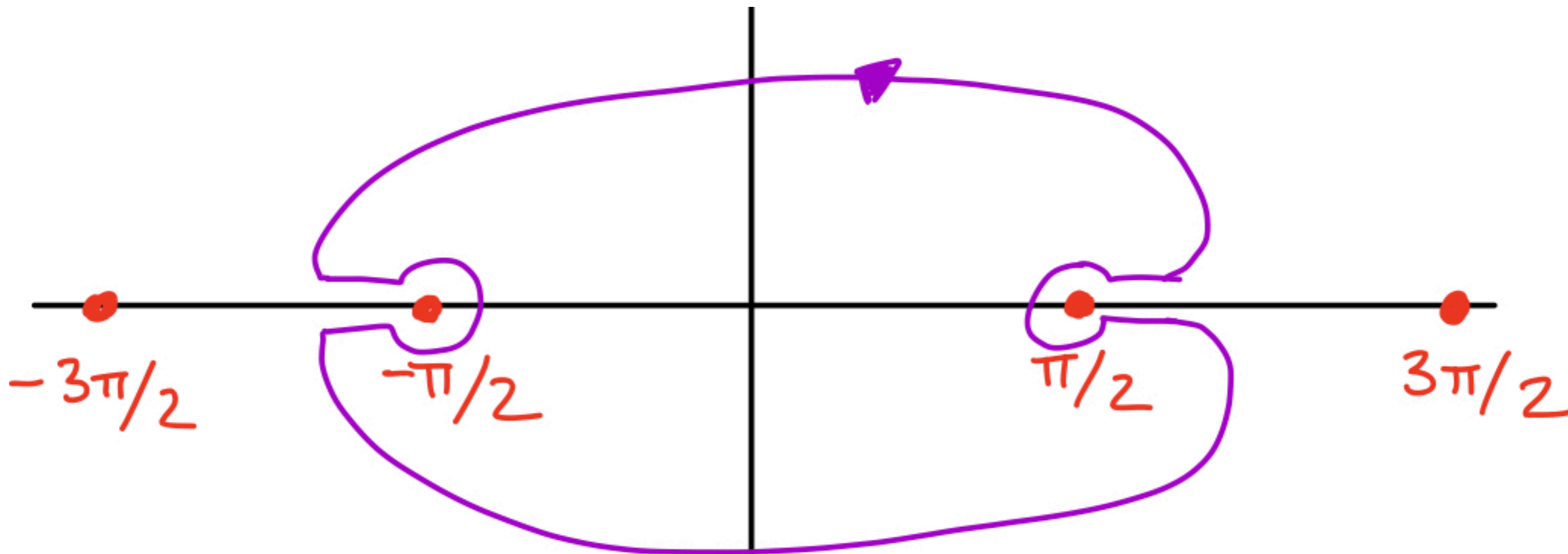
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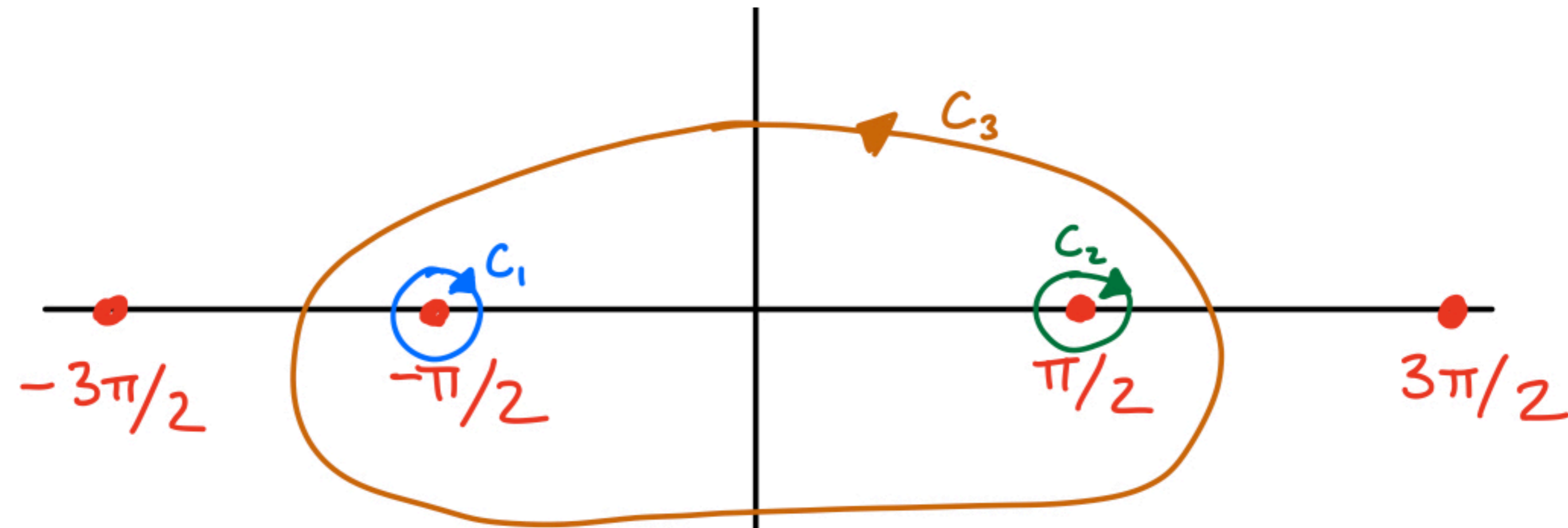
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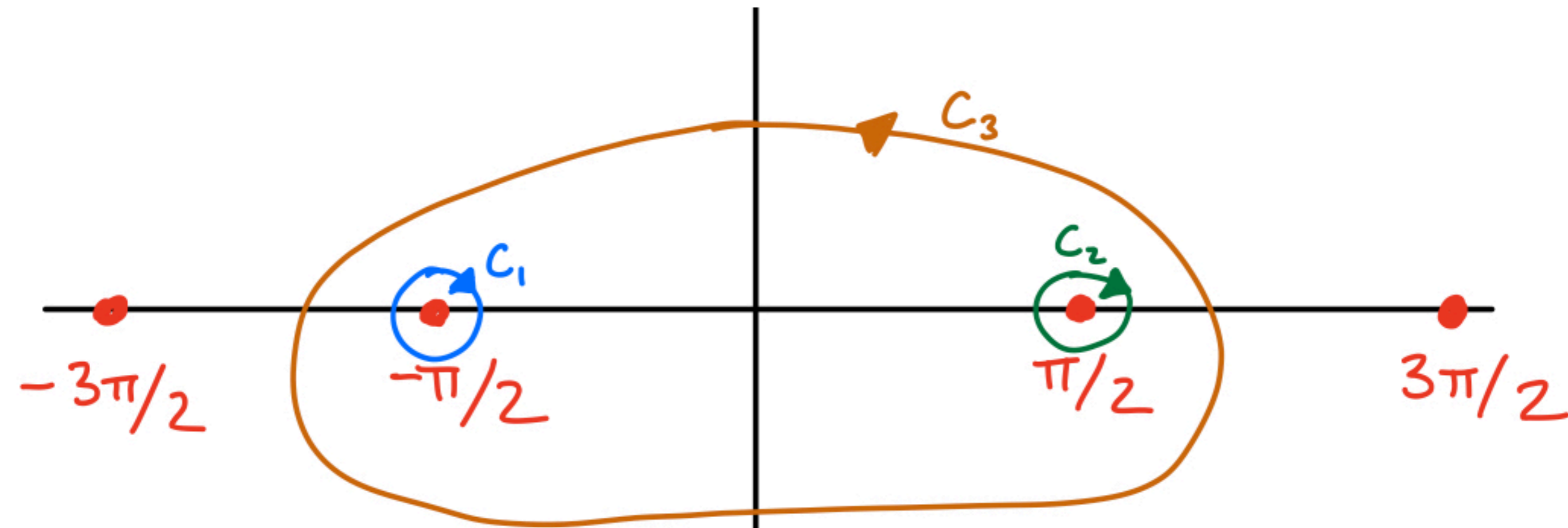
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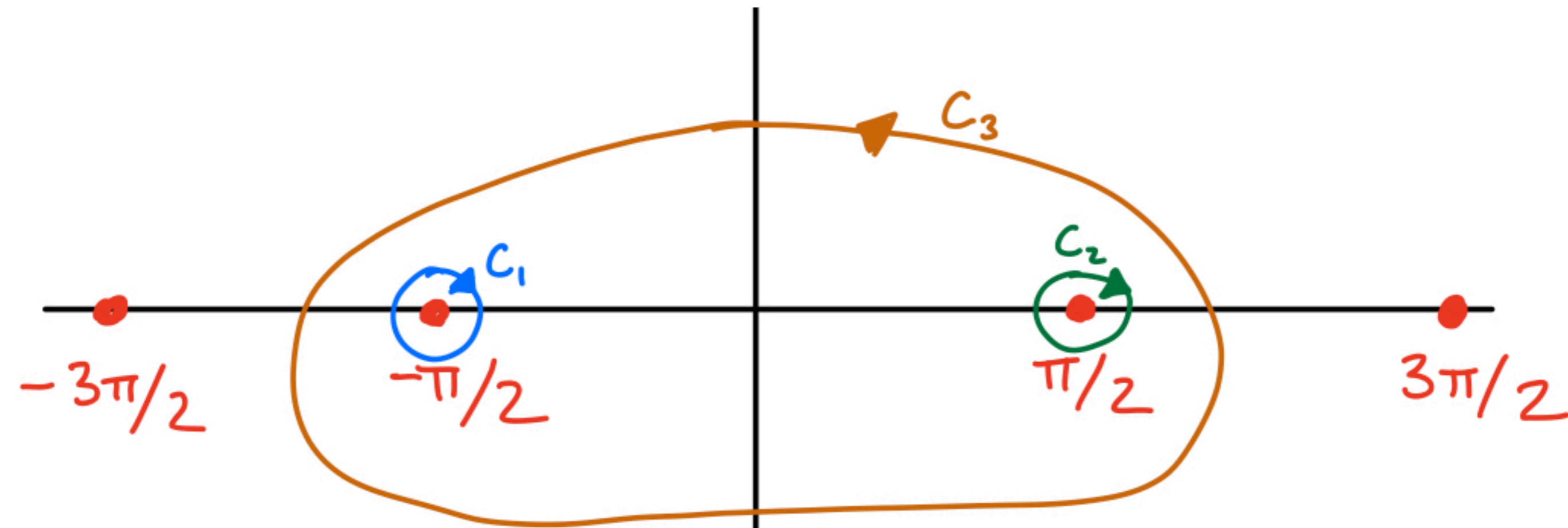
Asymptotics of Alternating Permutations

$$\frac{a_n}{n!} = \frac{1}{2\pi i} \int_{C_1} \frac{\tan z}{z^{n+1}} dz + \frac{1}{2\pi i} \int_{C_2} \frac{\tan z}{z^{n+1}} dz + \frac{1}{2\pi i} \int_{|z|=\pi} \frac{\tan z}{z^{n+1}} dz$$



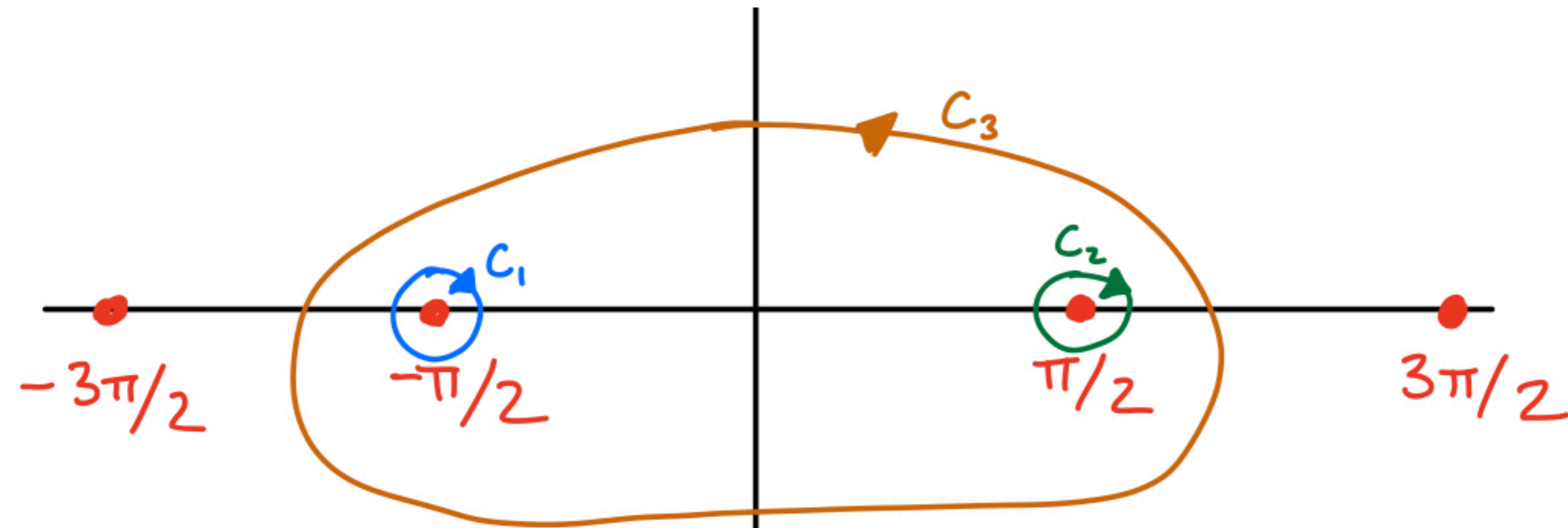
Asymptotics of Alternating Permutations

$$\frac{a_n}{n!} = \left(\frac{-2}{\pi}\right)^{n+1} \operatorname{Res}_{z=-\pi/2}(\tan z) + \left(\frac{2}{\pi}\right)^{n+1} \operatorname{Res}_{z=\pi/2}(\tan z) + O\left(\left(\frac{1}{\pi}\right)^n\right)$$



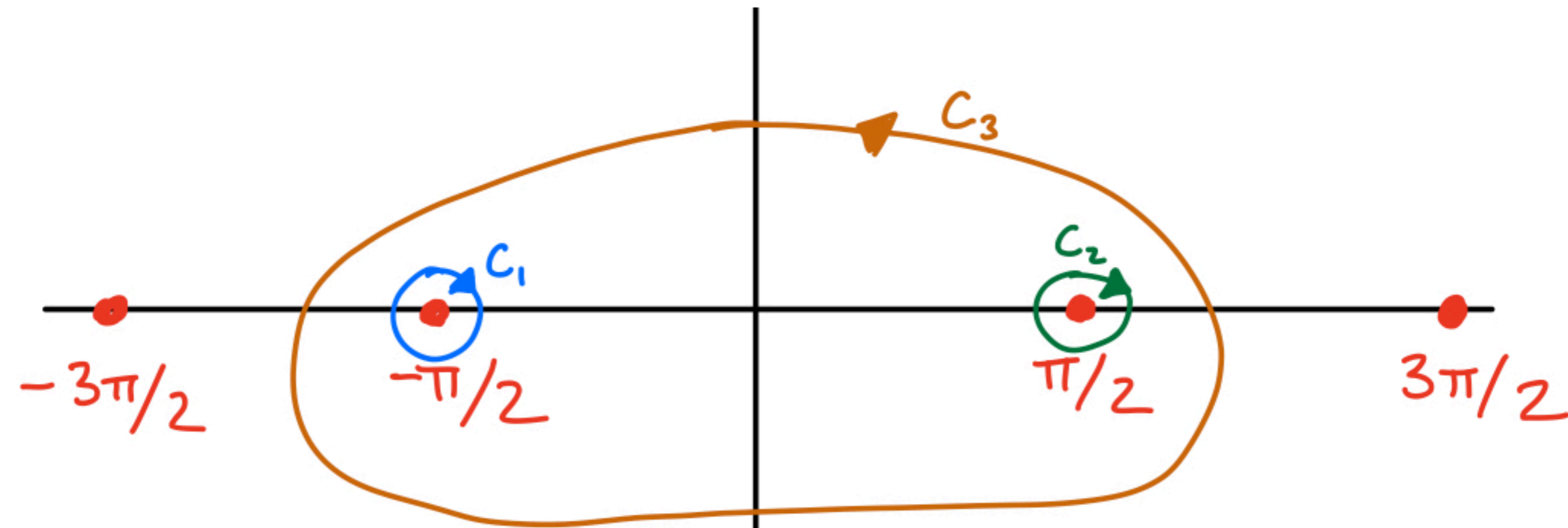
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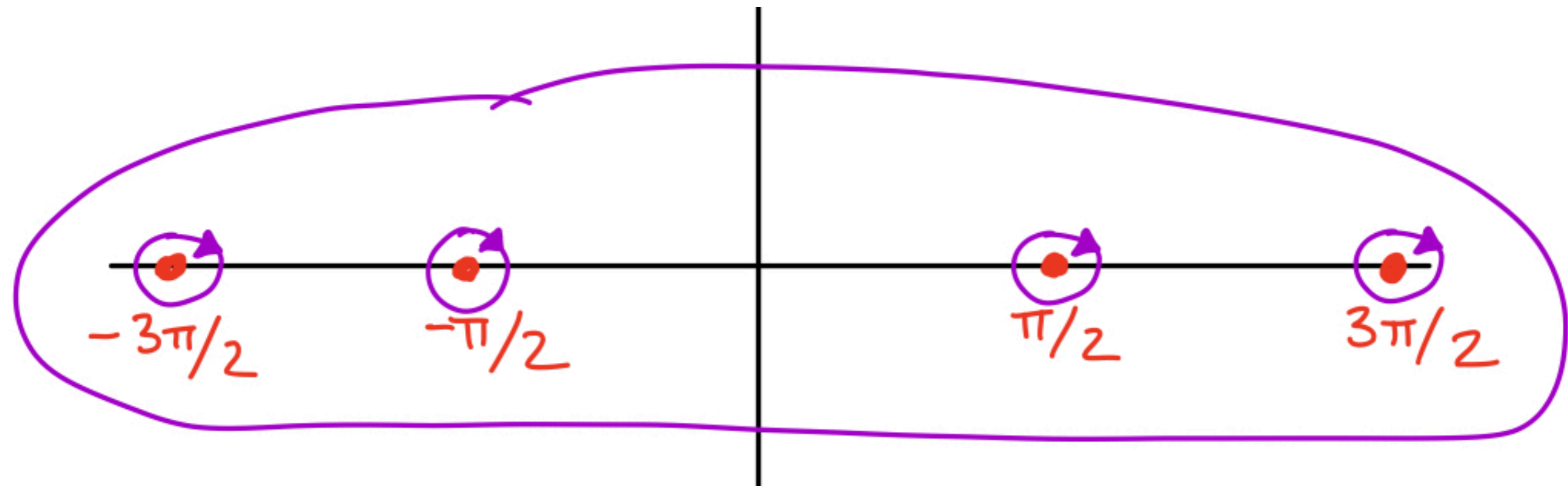
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$$\frac{a_n}{n!} = 2 \left(\frac{2}{\pi} \right)^{n+1} + O \left(\left(\frac{1}{\pi} \right)^n \right) \quad (n \text{ odd})$$



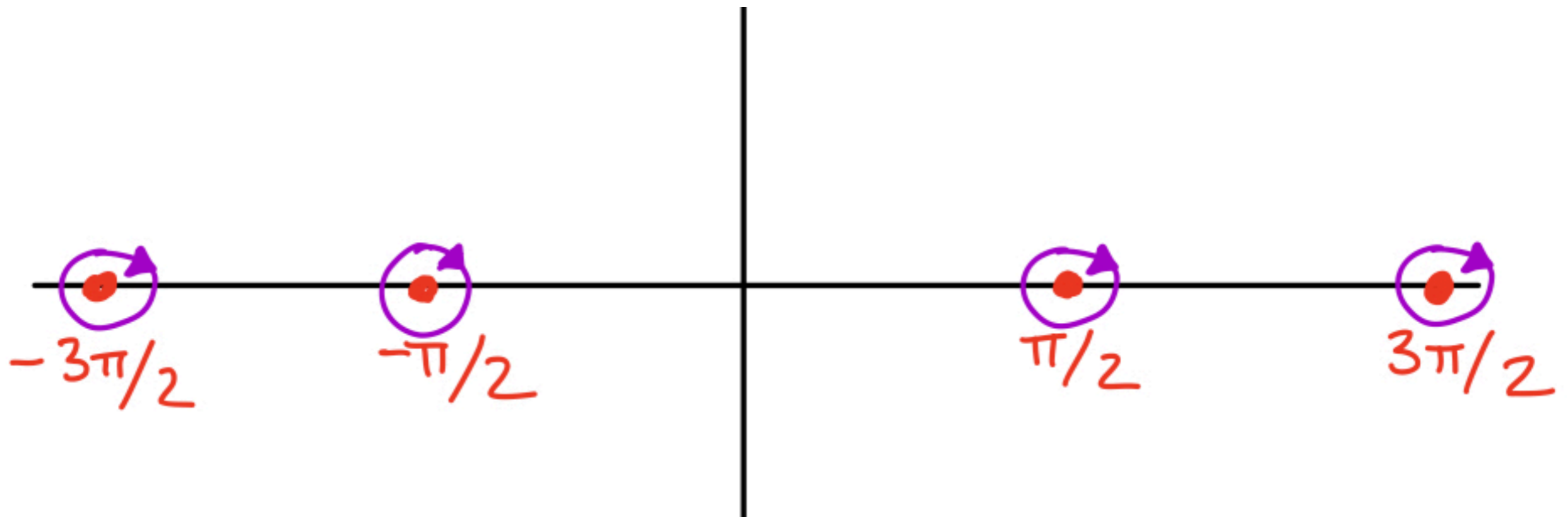
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$$\frac{a_n}{n!} = 2 \left(\frac{2}{\pi} \right)^{n+1} + 2 \left(\frac{2}{3\pi} \right)^{n+1} + O \left(\left(\frac{2}{5\pi} \right)^n \right) \quad (n \text{ odd})$$



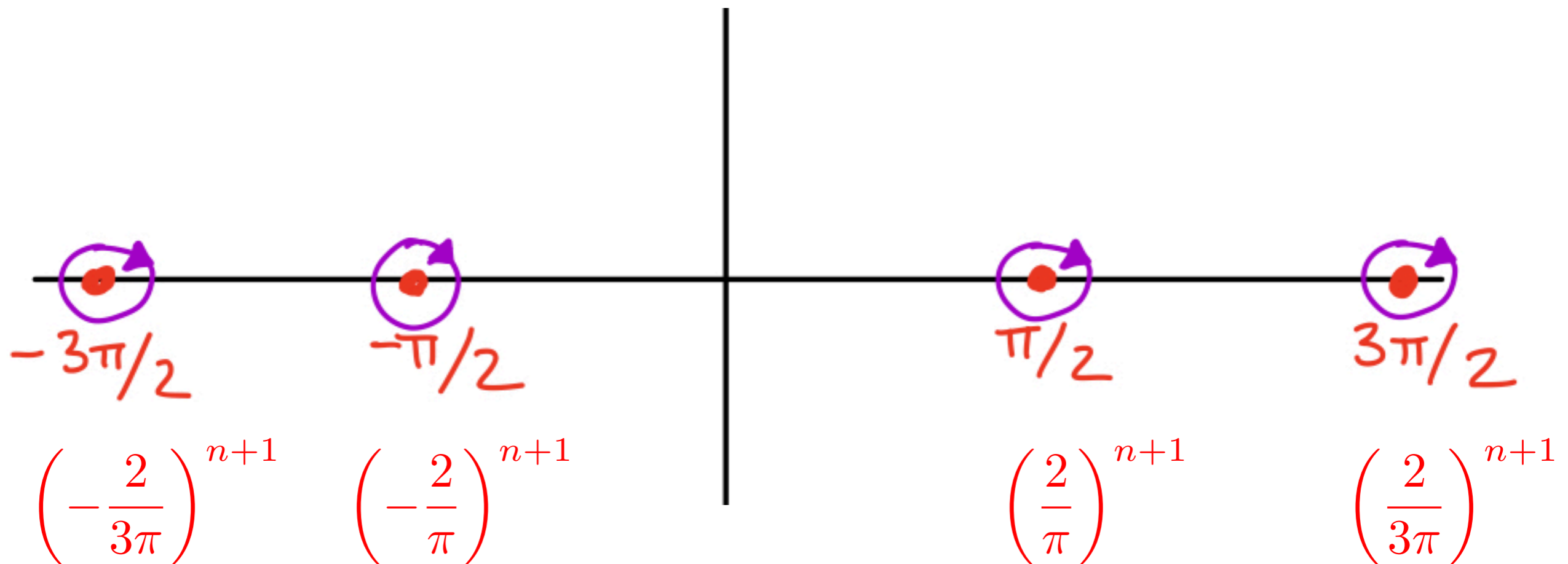
Asymptotics of Alternating Permutations

$$\frac{a_n}{n!} = 2 \left(\frac{2}{\pi} \right)^{n+1} \sum_{k \geq 0} \frac{1}{(2k+1)^{n+1}} \quad (n \text{ odd})$$



Asymptotics of Alternating Permutations

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Analytic Combinatorics

Main Takeaways:

- Each **singularity** gives contribution
- Those singularities **closest to the origin** affect dominant asymptotics
- The contributions of each can be determined by a **local analysis** of the generating function

There are many **known formulas** for different types of singularities

$$F(z) \sim (1 - z)^\alpha \left(\log \frac{1}{1 - z} \right)^\beta \implies f_n \sim \frac{n^{-\alpha-1}}{\Gamma(-\alpha)} (\log n)^\beta$$

*C-Finite Sequences and
Rational Functions*

C-Finite Sequences

A sequence

$$(f_n) = f_0, f_1, \dots$$

is **C-finite** if it satisfies a **linear recurrence relation with constant coefficients**

$$f_{n+r} = c_{r-1}f_{n+r-1} + c_{r-2}f_{n+r-2} + \dots + c_0f_n \quad (n \geq 0)$$

Example: The **Virahanka-Fibonacci** numbers are defined by

$$f_0 = 0, \quad f_1 = 1$$

$$f_{n+2} = f_{n+1} + f_n \quad (n \geq 0)$$

C-Finite Sequences

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$$f_{n+r} = c_{r-1}f_{n+r-1} + c_{r-2}f_{n+r-2} + \dots + c_0f_n \quad (n \geq 0)$$

Theorem: (f_n) is C-finite iff its generating function is rational.

Proof:

$$[z^{n+r}] \left(\sum_{n \geq 0} f_n z^n \right) (1 - c_{r-1}z - \dots - c_0z^r) = f_{n+r} - c_{r-1}f_{n+r-1} - \dots - c_0f_n.$$

A Closed Expression

Back to the **Virahanka-Fibonacci** numbers,

$$F(z) = \frac{z}{1 - z - z^2}$$

A Closed Expression

$$\phi = \frac{-1 + \sqrt{5}}{2}, \quad \tau = \frac{-1 - \sqrt{5}}{2}$$

Back to the **Virahanka-Fibonacci** numbers,

$$F(z) = \frac{z}{1 - z - z^2} = \frac{1}{\sqrt{5}} \left(\frac{1}{1 - z/\phi} - \frac{1}{1 - z/\tau} \right)$$

so

$$f_n = \frac{1}{\sqrt{5}} (\phi^{-n} - \tau^{-n})$$

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Theorem: If $F(z) = G(z)/H(z)$ is rational and H has roots $\sigma_1, \dots, \sigma_m \in \mathbb{C}$ then there exist $P_1(n, x), \dots, P_m(n, x) \in \mathbb{Q}[n, x]$ such that

$$f_n = \sum_{j=1}^m P_j(n, \sigma_j) \sigma_j^{-n}.$$

A Closed Expression

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Corollary: If H has a unique dominant singularity

$$|\sigma_k| < |\sigma_j| \text{ for all } j \neq k$$

then

$$f_n \sim C n^r \sigma_k^{-n}$$

DANIELIS BERNOVLLI, IO. Fil.
 OBSERVATIONES DE SE-
 RIEBVS

QVAE FORMANTVR EX ADDITIONE
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1728

13. Exemplum capiemus ab hac aequatione

$$1 = -2x + 5xx - 4x^3 + x^4.$$

fiat series incipiendo a quatuor numeris arbitrariis
 (quia scilicet aequatio proposita totidem habet dimen-
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$$f_{n+4} = -2f_{n+3} + 5f_{n+2} - 4f_{n+1} + f_n$$

$$f_0 = f_1 = f_2 = f_3 = 1$$

```
> fsolve(1+2*x-5*x^2+4*x^3-x^4);  
      -0.2720196495, 2.272019650  
> evalf(-341/1243);  
      -0.2743362832
```

Look-and-Say Digit Sequence

Consider the sequence

1, 11, 21, 1211, 111221, ...

Look-and-Say Digit Sequence

Consider the sequence

1, 11, 21, 1211, 111221, ...

Conway (1987): GF for # of digits in the n th term is

$$F(z) = \frac{G(z)}{H(z)} = \frac{1 + z + \dots + 18z^{77} - 12z^{78}}{1 - z + \dots - 9z^{71} + 6z^{72}}$$

```
In [4]: # Get a linear recurrence satisfied by the digit counting sequence
digitseq.recurrence_repr()
```

```
Out[4]: 'homogeneous linear recurrence with constant coefficients of degree 72: a(n+72) = a(n+71) + a(n+70) + a(n+69) - a(n+68) - 3*a(n+67) + a(n+65) + 2*a(n+64) - 3*a(n+59) - 3*a(n+58) + 2*a(n+57) + 5*a(n+56) + 8*a(n+55) - 7*a(n+54) - a(n+53) - 8*a(n+52) + 5*a(n+50) - 8*a(n+49) + 12*a(n+48) + 4*a(n+47) + a(n+46) - 18*a(n+44) + 4*a(n+43) - 2*a(n+42) + 13*a(n+41) + 7*a(n+40) - 19*a(n+39) + 14*a(n+38) - 14*a(n+37) + 6*a(n+36) + 4*a(n+35) - 13*a(n+34) + 9*a(n+33) + 7*a(n+32) - 4*a(n+31) + 8*a(n+30) - 7*a(n+29) - 5*a(n+28) - 7*a(n+27) + 12*a(n+26) - 17*a(n+25) + 22*a(n+24) - 8*a(n+23) + 7*a(n+22) - 16*a(n+21) + 6*a(n+20) + 7*a(n+19) + 6*a(n+18) - 3*a(n+17) - 19*a(n+16) + 5*a(n+15) + 5*a(n+14) + 14*a(n+13) - 8*a(n+12) - 2*a(n+11) - 7*a(n+10) + 5*a(n+9) - a(n+8) + 8*a(n+7) - 14*a(n+6) + 11*a(n+5) - 16*a(n+4) + 18*a(n+3) - 9*a(n+2) + 9*a(n+1) - 6*a(n), starting a(0...) = [1, 2, 2, 4, 6, 6, 8, 10, 14, 20, 26, 34, 46, 62, 78, 102, 134, 176, 226, 302, 408, 528, 678, 904, 1182, 1540, 2012, 2606, 3410, 4462, 5808, 7586, 9898, 12884, 16774, 21890, 28528, 37158, 48410, 63138, 82350, 107312, 139984, 182376, 237746, 310036, 403966, 526646, 686646, 894810, 1166642, 1520986, 1982710, 2584304, 3369156, 4391702, 5724486, 7462860, 9727930, 12680852, 16530884, 21549544, 28091184, 36619162, 47736936, 62226614, 81117366, 105745224, 137842560, 179691598, 234241786, 305351794, 398049970, 518891358, 676414798, 881752750, 1149440192, 1498380104, 1953245418]'
```

Look-and-Say Digit Sequence

Consider the sequence

1, 11, 21, 1211, 111221, ...

```
In [6]: # Find the closed form of the sequence
asm = digitseq.closed_form()
asm
```

```
Out[6]: 2.042160076857881? * 1.303577269034297? ^ n - (1.304638747964804? - 0.1269290081499280? * I) * (1.059673936824031? + 0.06193785064242932? * I) ^ n - (1.304638747964804? + 0.1269290081499280? * I) * (1.059673936824031? - 0.06193785064242932? * I) ^ n + (0.02805004006256416? - 0.6707565233085509? * I) * (1.032508921516637? + 0.2788945601052167? * I) ^ n + (0.02805004006256416? + 0.6707565233085509? * I) * (1.032508921516637? - 0.2788945601052167? * I) ^ n - (0.12331055512333749? + 1.201334126923233? * I) * (1.020231387488337? + 0.1732885609934655? * I) ^ n - (0.12331055512333749? - 1.201334126923233? * I) * (1.020231387488337? - 0.1732885609934655? * I) ^ n + (0.0981439660979499? - 0.01577626267857238? * I) * (0.9814594704741177? + 0.3758720971778864? * I) ^ n + (0.0981439660979499? + 0.01577626267857238? * I) * (0.9814594704741177? - 0.3758720971778864? * I) ^ n + (0.03481179854242824? - 0.1121258670026815? * I) * (0.9161602225609649? + 0.6457963110326476? * I) ^ n + (0.03481179854242824? + 0.1121258670026815? * I) * (0.9161602225609649? - 0.6457963110326476? * I) ^ n + (1.628877576705379? + 1.686352734102582? * I) * (0.9104733616787827? + 0.1519984821535185? * I) ^ n + (1.628877576705379? - 1.686352734102582? * I) * (0.9104733616787827? - 0.1519984821535185? * I) ^ n - (0.003919639533825015? + 0.2266456462319149? * I) * (0.8567209043332170? + 0.449031756082565? * I) ^ n - (0.003919639533825015? - 0.2266456462319149? * I) * (0.8567209043332170? - 0.449031756082565? * I) ^ n - (0.0407290929829635? + 0.07087511881818378? * I) * (0.8399666788300980? + 0.6003062158802451? * I) ^ n - (0.0407290929829635? - 0.07087511881818378? * I) * (0.8399666788300980? - 0.6003062158802451? * I) ^ n - (0.2840300502107521? - 0.3004542497948497? * I) * (0.678827751775423? + 0.6478304904047382? * I) ^ n - (0.2840300502107521? + 0.3004542497948497? * I) * (0.678827751775423? - 0.6478304904047382? * I) ^ n - (0.4893153413442025? + 0.5778030774135450? * I) * (0.594227321547377? + 0.7225690549852261? * I) ^ n - (0.4893153413442025? - 0.5778030774135450? * I) * (0.594227321547377? - 0.7225690549852261? * I) ^ n + (0.3874848481654065? + 0.2054814416473357? * I) * (0.5675536121973295? + 0.8341522109021707? * I) ^ n + (0.3874848481654065? - 0.2054814416473357? * I) * (0.5675536121973295? - 0.8341522109021707? * I) ^ n - (0.02549605434774883? - 0.02408173751335947? * I) * (0.542332767099137? + 0.9258485990610539? * I) ^ n - (0.02549605434774883? + 0.02408173751335947? * I) * (0.542332767099137? - 0.9258485990610539? * I) ^ n - (0.1292061890592742? - 0.2764105281976084? * I) * (0.4177076932836939? + 0.9981509518397633? * I) ^ n - (0.1292061890592742? + 0.2764105281976084? * I) * (0.4177076932836939? - 0.9981509518397633? * I) ^ n + (0.044188346162900112? - 0.287266422170110062? * I) * (0.21641502562061022? + 0.059227210600111102? * I) ^ n + (0.044188346162900112? + 0.287266422170110062? * I) * (0.21641502562061022? - 0.059227210600111102? * I) ^ n
```

Look-and-Say Digit Sequence

Consider the sequence

1, 11, 21, 1211, 111221, ...

Conway (1987): GF for # of digits in the n th term is

$$F(z) = \frac{G(z)}{H(z)} = \frac{1 + z + \dots + 18z^{77} - 12z^{78}}{1 - z + \dots - 9z^{71} + 6z^{72}}$$

Knowing H has a single dominant singularity $\lambda = 0.767119\dots$
where $H'(\lambda) \neq 0$ implies

$$f_n \sim \frac{-G(\lambda)}{\lambda H'(\lambda)} \lambda^{-n} \approx (2.042\dots)(1.30357\dots)^n.$$

The Skolem Problem

Theorem (Skolem, 1933)

The indices of zeroes of a C-finite sequence over \mathbb{Q} form a **finite set** together with a **finite set of arithmetic progression**

Open Problem 1

Is there an algorithm that takes any C-finite sequence and determines whether it has a zero term?

Open Problem 2

Is there an algorithm that takes any C-finite sequence and determines whether it is positive?

The Skolem Problem

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Open Problem 1

Is there an algorithm that takes any C-finite sequence and determines whether it has a zero term?

Open Problem 2'

Is there an algorithm that takes any C-finite sequence and determines whether it is **eventually** positive?

N-Rationality

The generating functions of **regular languages** form the **N-rational functions**. This is the class that

- contains 1 and x
- is closed under addition, multiplication, and $f \mapsto 1/(1 - xf)$

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Berstel (1971): If F is \mathbb{N} -rational then its dominant singularities differ by multiples of roots of unity.

Corollary: If F is \mathbb{N} -rational then there is **predictable periodic behaviour**.

N-Rationality

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- contains 1 and x
- is closed under addition, multiplication, and $f \mapsto 1/(1 - xf)$

Berstel (1971): If F is N-rational then its dominant singularities differ by multiples of roots of unity.

I have never met a counting problem that would yield a rational, but not N-rational GF — Mireille Bousquet-Mélou, 2006 ICM

*P-Recursive Sequences and
D-Finite Functions*

Antoni Van Leeuwenhoek

More Microscopical Observations made by the same M. Leeuwenhoek, and promised in Numb. 97. of these Tracts; Com-

I Have divers times endeavoured to see and to know, what parts the *Blood* consists of; and at length I have observ'd, taking some Blood out of my own hand, that it consists of small round globuls driven thorough a Crystalline humidity or water: Yet, whether all Blood be such, I doubt.

Fig: 1.

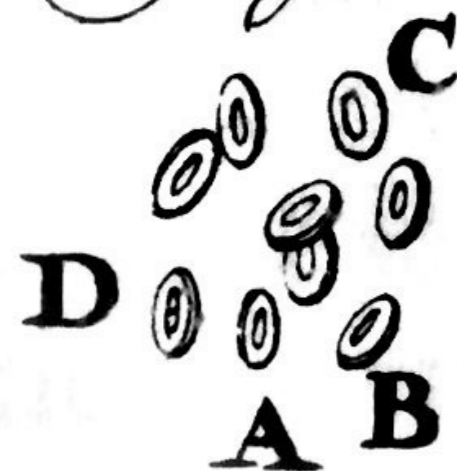
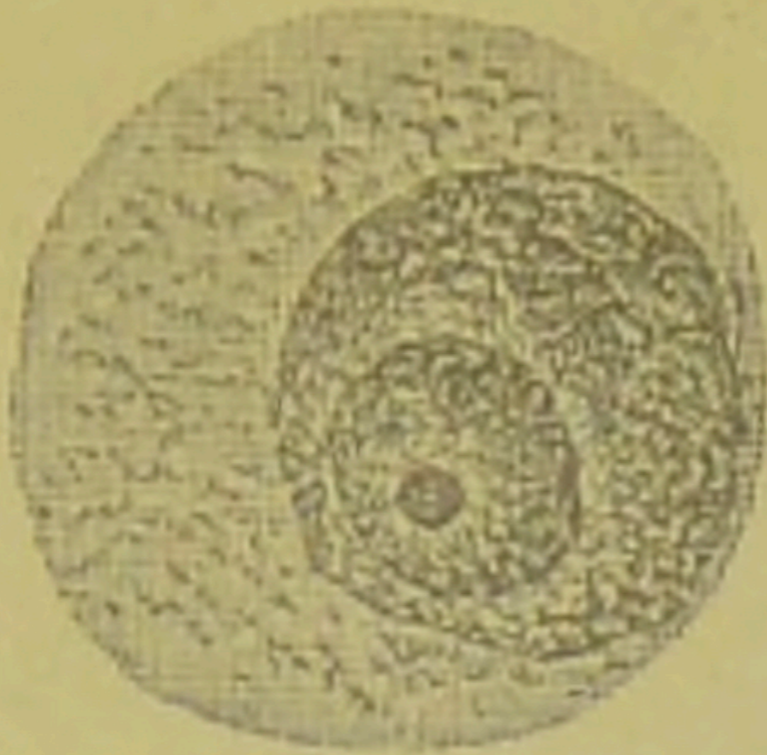


Fig: 2.

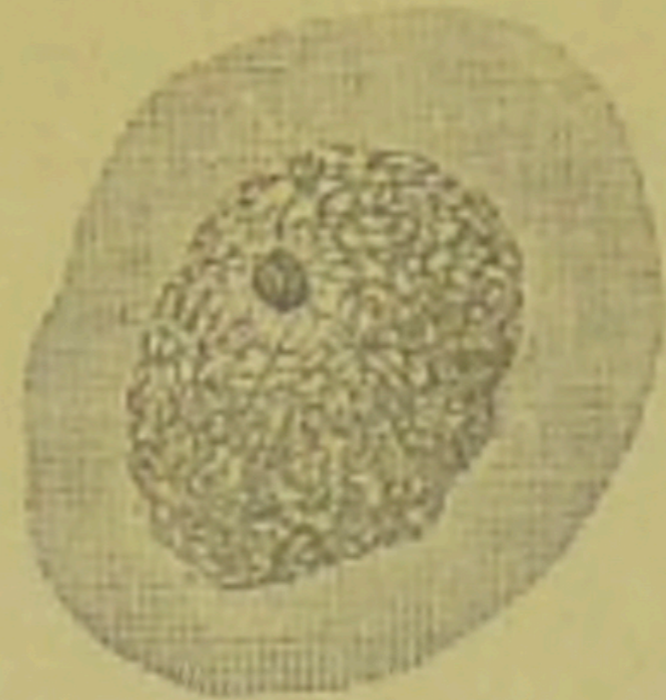


Fig: 3.





Young red corpuscle. Frog. Formation of coloured portion. X 1800



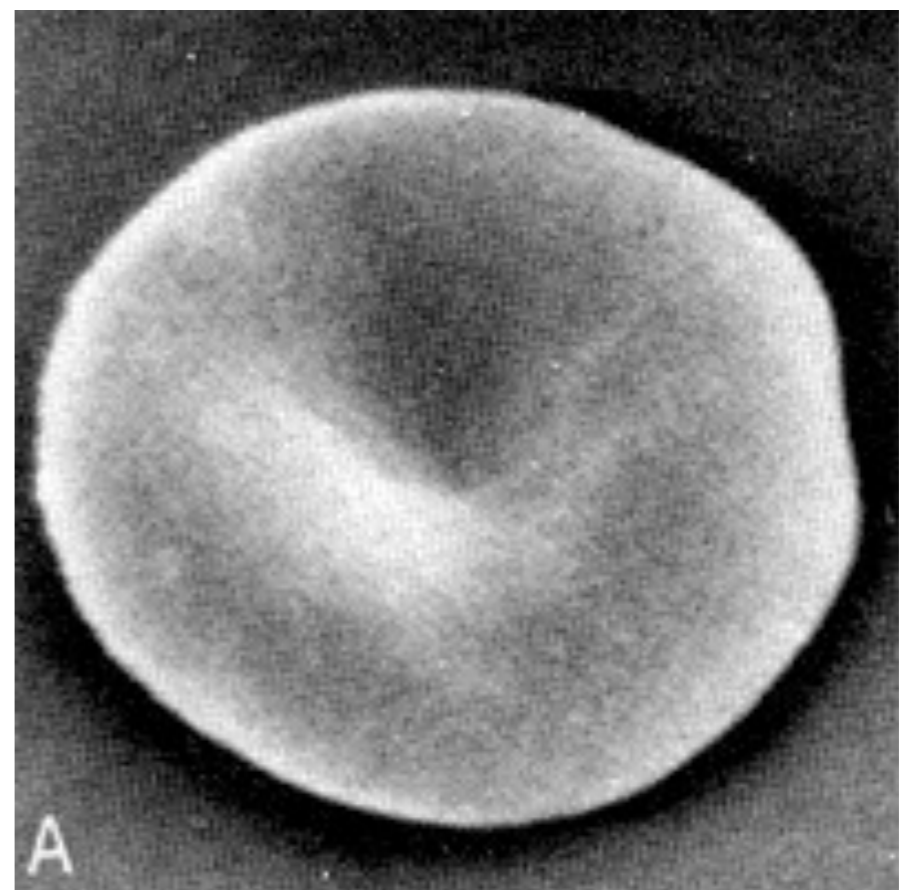
Young red corpuscle. Part of coloured portion fully formed. X 1800.



WHERE DOES THIS SHAPE COME FROM?



Human Cells



Canine Cell

J. Theoret. Biol. (1970) **26**, 61–81

The Minimum Energy of Bending as a Possible Explanation of the Biconcave Shape of the Human Red Blood Cell

P. B. CANHAM

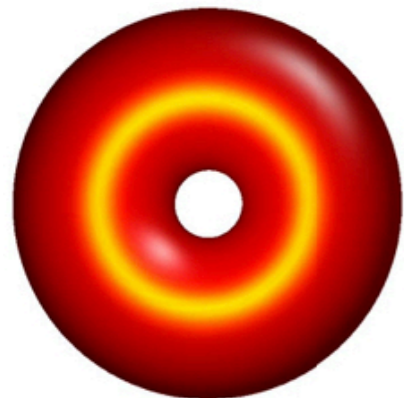
*Department of Biophysics,
University of Western Ontario, London, Ontario, Canada*

Lindström (1963) reported that cells resumed their equilibrium form within a fraction of a second after emerging from very small blood vessels. Rand (1964*b*) showed that a cell released from a micropipette returned to the biconcave shape within a few seconds. **These observations imply that the biconcave form requires the least energy to be maintained. We believe the energy minimized is the bending energy of the membrane, and that the membrane is solely responsible for the cell's shape.**

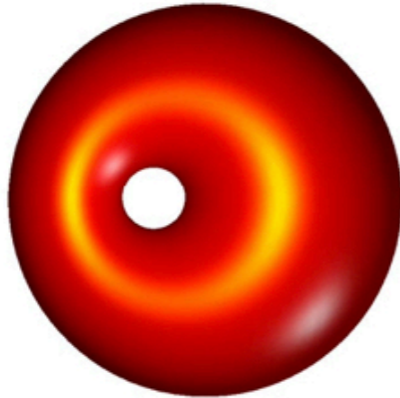
Genus 1 Canham Model

Canham Problem: For fixed genus g and fixed *isoperimetric ratio* ι_0 find the surface S minimizing $\int_S (\kappa_1 + \kappa_2)^2 dA$

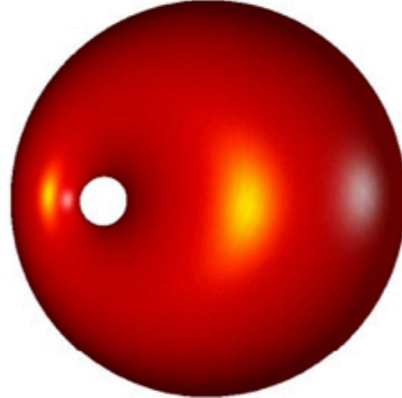
$\iota(S) = 0.71$



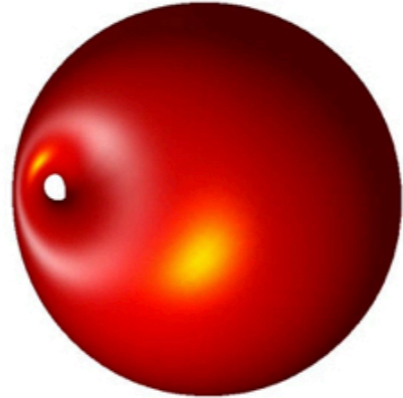
$\iota(S) = 0.75$



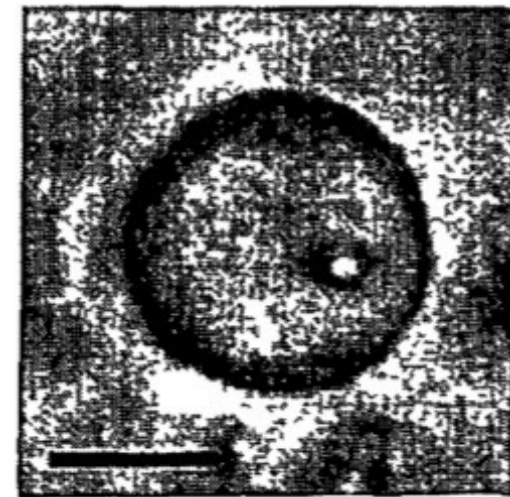
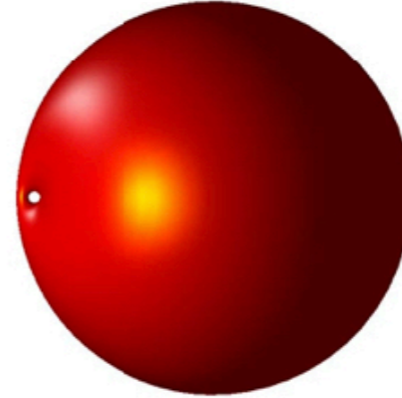
$\iota(S) = 0.85$



$\iota(S) = 0.95$



$\iota(S) = 0.99$



Yu and Chen (2020): Let (d_n) be the following sequence. There is a **unique** solution in genus one if all terms of (d_n) are positive, where

d_n is defined by the recurrence

$$0 = r_7(n)d_{n+7} + r_6(n)d_{n+6} + \cdots + r_0(n)d_n$$

with

$$(d_0, \dots, d_6) = \left(72, 1932, 31248, \frac{790101}{2}, \frac{17208645}{4}, \frac{338898609}{8}, \frac{1551478257}{4} \right)$$

and

$$\begin{aligned} r_0(n) &= -(n+8)(n+7)(12232n^3 + 298144n^2 + 2412586n + 6469077)(n+6)^2 \\ r_1(n) &= (n+8)(183480n^6 + 7655560n^5 + 131977142n^4 + 1202876299n^3 + 6112196895n^2 + 16418149668n + 18219511026) \\ r_2(n) &= -(n+8)(941864n^6 + 38326904n^5 + 644300514n^4 + 5727711699n^3 + 28407144241n^2 + 74557779538n + 80949464718) \\ r_3(n) &= (1993816n^7 + 97303624n^6 + 2021855198n^5 + 23184921987n^4 \\ &\quad + 158457515673n^3 + 645518710454n^2 + 1451619424860n + 1390493835900) \\ r_4(n) &= (-1993816n^7 - 98090344n^6 - 2054897438n^5 - 23758375953n^4 \\ &\quad - 163720428321n^3 - 672459054524n^2 - 1524577250976n - 1472211879228) \\ r_5(n) &= (n+6)(941864n^6 + 40789672n^5 + 730497394n^4 + 6921881565n^3 + 36590122947n^2 + 102300885158n + 118218544398) \\ r_6(n) &= (n+6)(183480n^6 + 7756760n^5 + 135519142n^4 + 1252328453n^3 + 6456460129n^2 + 17612930492n + 19872693550) \\ r_7(n) &= (n+7)(n+6)(12232n^3 + 215600n^2 + 1256970n + 2435511)(n+8)^2 \end{aligned}$$

P-Recursive Sequences

A sequence

$$(f_n) = f_0, f_1, \dots$$

is **P-recursive** if it satisfies a **linear recurrence relation with polynomial coefficients**

$$0 = c_r(n)f_{n+r} + c_{r-1}(n)f_{n+r-1} + \dots + c_0(n)f_n$$

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Example: If $f_n = n!$ then

$$f_0 = 1, \quad f_{n+1} = (n+1)f_n$$

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Example: If $f_n = n!$ then

$$f_0 = 1, \quad f_{n+1} = (n+1)f_n$$

Theorem: f_n is P-recursive iff $F(z)$ is **D-finite**

$$0 = p_s(z)F^{(s)}(z) + p_{s-1}(z)F^{(s-1)}(z) + \dots + p_0(z)F(z)$$

M. and Mezzarobba (2021)

Theorem 1: The dominant asymptotic term of d_n is positive

Theorem 2: If $n > 1000$ then the dominant asymptotic term is larger than all subdominant terms

Theorem 3: The terms d_0, \dots, d_{1000} are positive

Corollary: The genus one Canham problem has a **unique** solution when $\tau \leq \iota_0 < 1$.

DMM (2022): Software to do general analysis (with some assumptions)

Singularities of D-finite Functions

The generating function of this sequence satisfies a D-finite equation whose solutions form a **finite-dimensional vector space**.

$$p_3(z)D^{(3)}(z) + p_2(z)D''(z) + p_1(z)D'(z) + p_0(z)D(z) = 0$$

$$\begin{aligned} & (25165779z^{15} - 1702884379z^{14} + 22196217078z^{13} - 108363844374z^{12} + 197744302789z^{11} - 20375892397z^{10} - 35 \\ & 0408306796z^9 + 350408306796z^8 + 20375892397z^7 - 197744302789z^6 + 108363844374z^5 - 22196217078z^4 + 17028 \\ & 84379z^3 - 25165779z^2)Dz^3 + (553647138z^{14} - 36951752165z^{13} + 394079321954z^{12} - 1450287066584z^{11} + 1482 \\ & 230828728z^{10} + 2523313940179z^9 - 6434889690300z^8 + 3026134593192z^7 + 3073463034898z^6 - 3856865346575z^5 \\ & + 1475536731514z^4 - 205218539152z^3 + 9026126068z^2 - 125828895z)Dz^2 + (3523209060z^{13} - 234394065606z^{12} \\ & + 1926843034914z^{11} - 4689642916650z^{10} - 1172674969842z^9 + 19779027227864z^8 - 23096380215644z^7 - 417366056 \\ & 1220z^6 + 24995188572752z^5 - 17824401172934z^4 + 4891640236090z^3 - 415956772498z^2 + 10989056830z - 1006631 \\ & 16)Dz + 6341776308z^{12} - 427012938072z^{11} + 2435594423178z^{10} - 2400915979716z^9 - 10724094731502z^8 + 262725 \\ & 36406048z^7 - 8496738740956z^6 - 30570113263064z^5 + 39394376229112z^4 - 19173572139496z^3 + 3825886272626z^2 \\ & - 170758199108z + 2701126946 \end{aligned}$$

Singularities of D-finite Functions

The generating function of this sequence satisfies a D-finite equation whose solutions form a **finite-dimensional vector space**.

We can compute a **basis** of series solutions centred any point in.

In our example, the series centred at $z = \zeta$ have the form

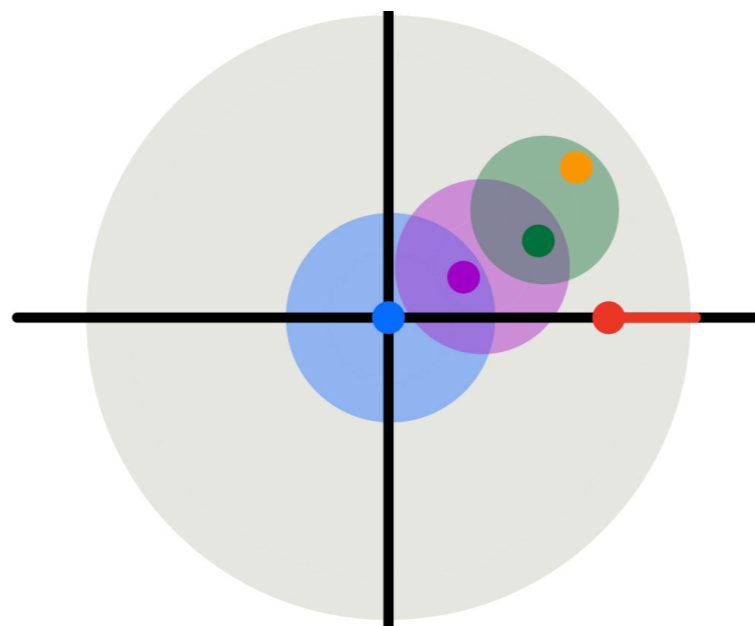
$$(z - \zeta)^\nu \sum_{k=0}^{\kappa} \left(\phi_k(z) \log^k(1 - z/\zeta) \right)$$

These series will **converge** in open disks (potentially with a ray from the centre removed because of log / algebraic powers).

Biomembrane Asymptotics

Techniques from **numeric analysis**, **differential equations**, and **computer algebra** are used to create **practical** algorithms for *numeric analytic continuation*.

We determine the behaviour of the generating function near its singularities in terms of constants that can be **rigorously approximated**. This translates to asymptotic expansions with **explicit error bounds**.



Biomembrane Asymptotics

Ultimately, we obtain

$$D(z) = C_1(z - \rho)^{-4} + C_2(z - \rho)^{-4} \log \frac{1}{1 - z/\rho} + \text{explicit error}$$

for constants

$$C_1 = [0.0598 \pm 4.79 \cdot 10^{-5}] \quad \text{and} \quad C_2 = [0.0420 \pm 3.14 \cdot 10^{-5}]$$

(Note: with efficient algorithms we can determine **1000 decimal places** in Sage in **1 min**)

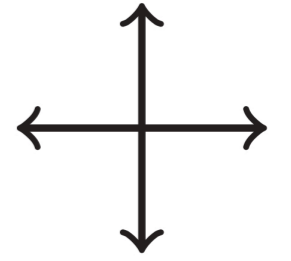
Corollary

For all integers $n \geq 1000$,

$$d_n \geq \rho^{-n} n^2 \log^2 n \left(8.07 \frac{n}{\log n} + 1.37 \frac{n}{\log^2 n} - 1196 \right) > 0.$$

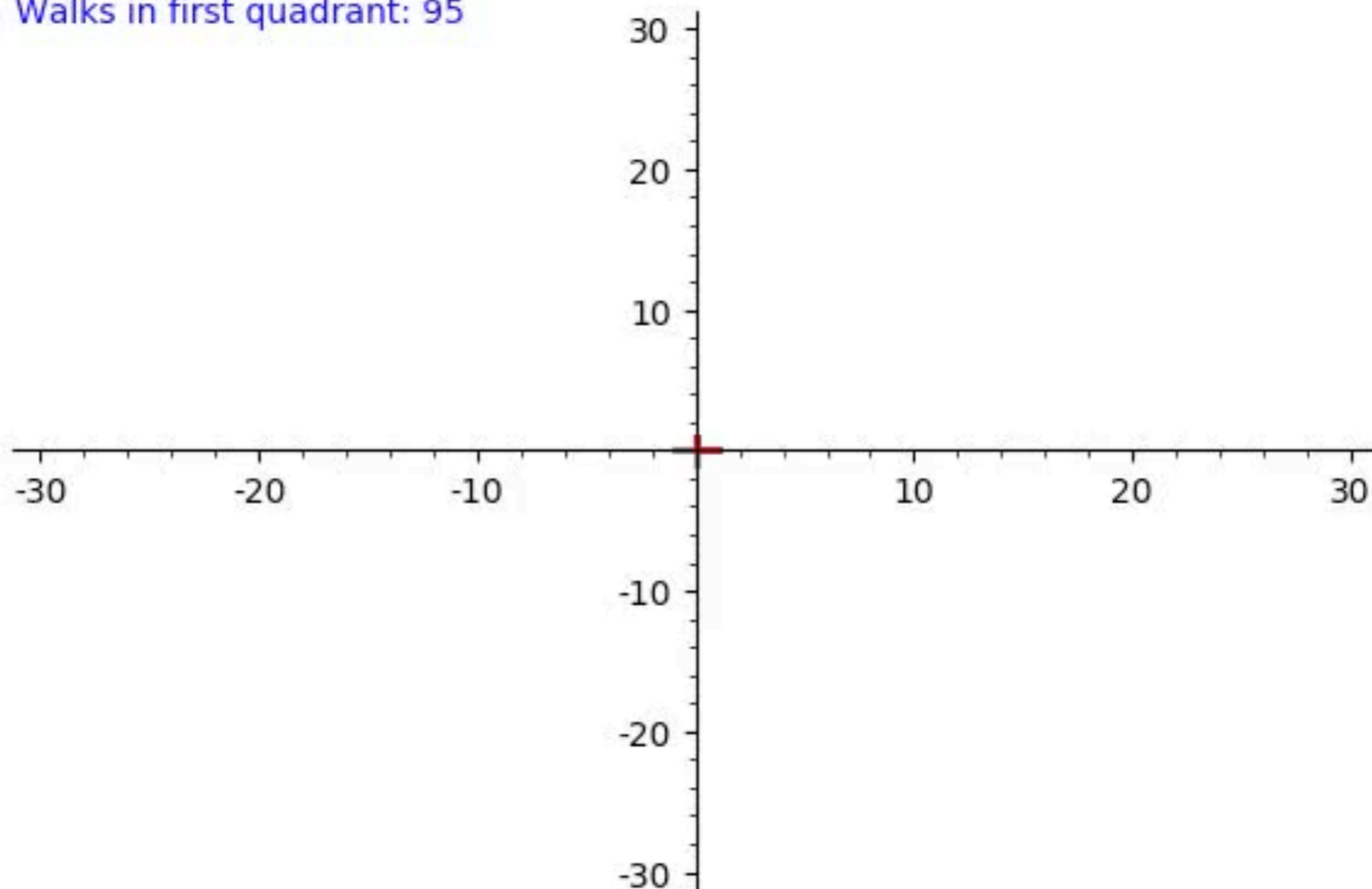
What Can Go Wrong?

Lattice Path Example

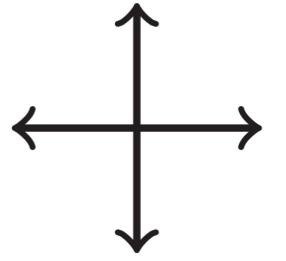


How many lattice paths taking n steps $\{N,S,E,W\}$ start at the origin and stay in the first quadrant?

Number of steps: 1
Walks in first quadrant: 95



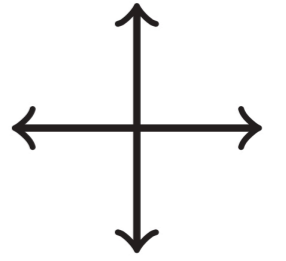
Lattice Path Example



The *kernel method* proves that the generating function for the number of such walks satisfies

$$\begin{aligned} z^2(4z - 1)(4z + 1)Q'''(z) + 2z(4z + 1)(16z - 3)Q''(z) \\ + 2(112z^2 + 14z - 3)Q'(z) + 4(16z + 3)Q(z) = 0 \end{aligned}$$

Lattice Path Example



The *kernel method* proves that the generating function for the number of such walks satisfies

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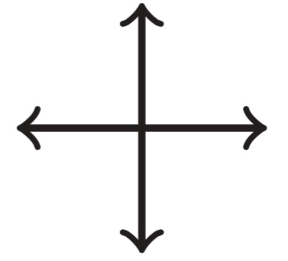
This proves that the number of walks satisfies the recurrence

$$(n + 4)(n + 3)q_{n+2} - 4(2n + 5)q_{n+1} - 16(n + 1)(n + 2)q_n = 0$$

which has a basis of solutions

$$\Phi_1(n) = 4^n n^{-1} \left(1 - \frac{3}{2n} + \dots \right) \quad \Phi_2(n) = (-4)^n n^{-3} \left(1 - \frac{9}{2n} + \dots \right)$$

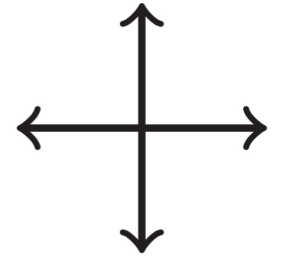
Lattice Path Example



There exist $c_1, c_2 \in \mathbb{C}$ such that $q_n = c_1 \Phi_1(n) + c_2 \Phi_2(n)$, so

$$q_n = c_1 4^n n^{-1} \left(1 - \frac{3}{2n} + \dots \right) + c_2 (-4)^n n^{-3} \left(1 - \frac{9}{2n} + \dots \right)$$

Lattice Path Example



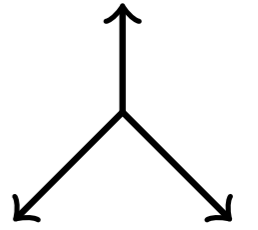
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$$q_n = c_1 4^n n^{-1} \left(1 - \frac{3}{2n} + \dots \right) + c_2 (-4)^n n^{-3} \left(1 - \frac{9}{2n} + \dots \right)$$

We can use **rigorous numeric analytic continuation** to show

$$q_n = (1.273\dots) 4^n n^{-1} \left(1 - \frac{3}{2n} + \dots \right) + (5.092\dots) (-4)^n n^{-3} \left(1 - \frac{9}{2n} + \dots \right)$$

Lattice Path Example 2



Consider walks on the steps $\{N, SE, SW\}$ in \mathbb{N}^2

The number of walks satisfies an **order 6 P-recurrence**.

There is an basis consisting of solutions with expansions

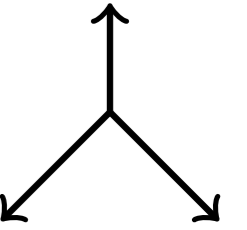
$$3^n n^{-1/2} \left(1 - \frac{33}{16} n^{-1} + \dots \right)$$

$$\left(2\sqrt{2} \right)^n n^{-2} \left(1 - \frac{32\sqrt{2} + 57}{4} n^{-1} + \dots \right)$$

$$\left(-2\sqrt{2} \right)^n n^{-2} \left(1 + \frac{32\sqrt{2} - 57}{4} n^{-1} + \dots \right)$$

with other elements $o\left(\frac{(2\sqrt{2})^n}{n^3}\right)$

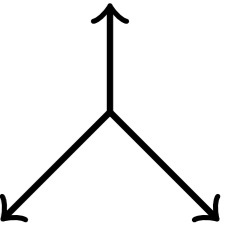
Lattice Path Example 2



One can write

$$q_n = C_1 \frac{3^n}{\sqrt{n}} \left(1 - \frac{33}{16n} + \dots \right) + C_2 \frac{(2\sqrt{2})^n}{n^2} \left(1 - \frac{32\sqrt{2} + 57}{4n} + \dots \right) \\ + C_3 \frac{(-2\sqrt{2})^n}{n^2} \left(1 - \frac{32\sqrt{2} - 57}{4n} + \dots \right) + O\left(\frac{(2\sqrt{2})^n}{n^3}\right)$$

Lattice Path Example 2



One can write

$$q_n = C_1 \frac{3^n}{\sqrt{n}} \left(1 - \frac{33}{16n} + \dots \right) + C_2 \frac{(2\sqrt{2})^n}{n^2} \left(1 - \frac{32\sqrt{2} + 57}{4n} + \dots \right) \\ + C_3 \frac{(-2\sqrt{2})^n}{n^2} \left(1 - \frac{32\sqrt{2} - 57}{4n} + \dots \right) + O\left(\frac{(2\sqrt{2})^n}{n^3}\right)$$

Here we calculate

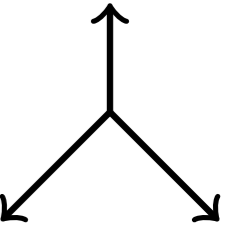
$$C_1 = 0.000\dots \quad C_2 = 10.49\dots \quad C_3 = 0.308\dots$$

We can't **prove** $C_1 = 0$ without bounds on these constants...

Open Problem 3

Can we decide when such *connection coefficients* are exactly zero?

Lattice Path Example 2



One can write

$$q_n = C_1 \frac{3^n}{\sqrt{n}} \left(1 - \frac{33}{16n} + \dots \right) + C_2 \frac{(2\sqrt{2})^n}{n^2} \left(1 - \frac{32\sqrt{2} + 57}{4n} + \dots \right) \\ + C_3 \frac{(-2\sqrt{2})^n}{n^2} \left(1 - \frac{32\sqrt{2} - 57}{4n} + \dots \right) + O\left(\frac{(2\sqrt{2})^n}{n^3}\right)$$

Here we calculate

$$C_1 = 0.000\dots \quad C_2 = 10.49\dots \quad C_3 = 0.308\dots$$

We can't **prove** $C_1 = 0$ without bounds on these constants...

We need **another representation...**

Rational Diagonals

Multivariate Diagonals

Now we start with a multivariate series

$$F(\mathbf{z}) = \sum_{(i_1, \dots, i_d) \in \mathbb{N}^d} f_{i_1, \dots, i_d} z_1^{i_1} \cdots z_d^{i_d} = \sum_{\mathbf{i} \in \mathbb{N}^d} f_{\mathbf{i}} \mathbf{z}^{\mathbf{i}}$$

The **r-diagonal** consists of the coefficients $(f_{n\mathbf{r}}) = f_{\mathbf{0}}, f_{\mathbf{r}}, f_{2\mathbf{r}}, \dots$
Note the coefficient $f_{n\mathbf{r}}$ is defined only if $n\mathbf{r} \in \mathbb{N}^d$

(1, 1) – Diagonal (Main Diagonal)

$$F(x, y) = \frac{1}{1 - x - y} \\ = 1 + x + y + 2xy + x^2 + y^2 + 3x^2y + 3xy^2 + y^3 + 6x^2y^2 + \dots$$

Multivariate Diagonals

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(2, 1) – Diagonal

$$F(x, y) = \frac{1}{1 - x - y} \\ = 1 + x + y + 2xy + x^2 + y^2 + 3x^2y + \cdots + 15x^4y^2 + \cdots$$

Why Diagonals?

- **Data structures** for interesting univariate sequences
- **Uniform asymptotics** over *most* directions
- Yield **combinatorial limit theorems** (ask me)

We focus on **rational** (or **meromorphic**) diagonals

- Diagonal of an algebraic function in d variables is the diagonal of a rational function in $2d$ variables

Generating Function Classes

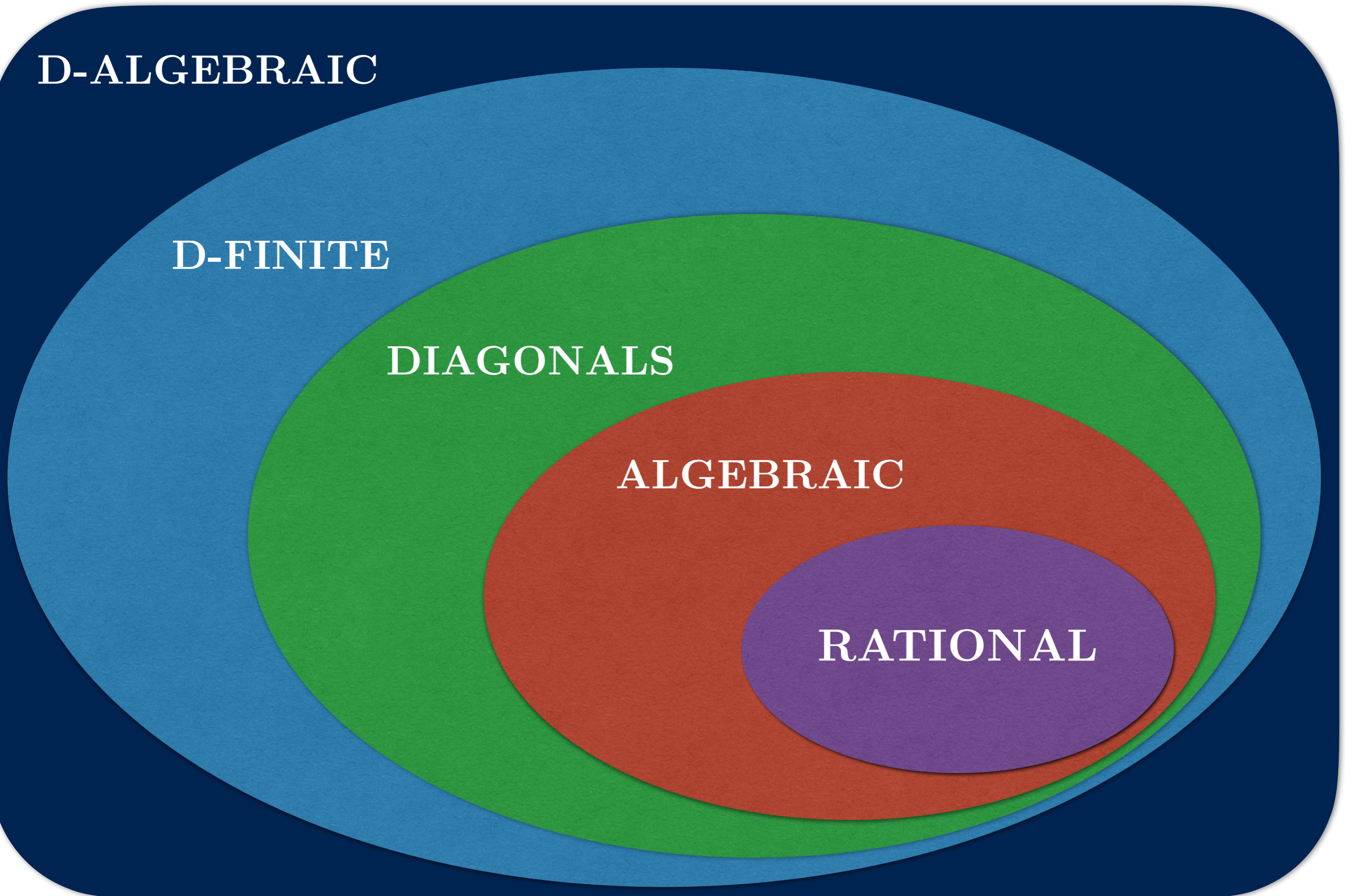
D-ALGEBRAIC

D-FINITE

DIAGONALS

ALGEBRAIC

RATIONAL



Analytic Combinatorics in Several Variables

Assume

$$F(\mathbf{z}) = \frac{G(\mathbf{z})}{H(\mathbf{z})} = \sum_{\mathbf{i} \in \mathbb{N}^d} f_{\mathbf{i}} \mathbf{z}^{\mathbf{i}}$$

converges in a neighbourhood of the origin.

The singularities of $F(\mathbf{z})$ are given by $\mathcal{V} := \{\mathbf{z} : H(\mathbf{z}) = 0\}$.

Singularities **closest** to the origin are called **minimal points**.

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Multivariate Cauchy Integral Formula

$$f_{n\mathbf{r}} = \frac{1}{(2\pi i)^d} \int_{\mathcal{C}} F(\mathbf{z}) \frac{d\mathbf{z}}{\mathbf{z}^{n\mathbf{r}+1}} \quad n\mathbf{r} \in \mathbb{N}^d$$

where \mathcal{C} is a product of circles $|z_i| = \varepsilon$

Difficulties of ACSV

One variable rational (or meromorphic) functions

- Find finite set of singularities closest to the origin
- Add their asymptotic contributions

In more than one variable

- Set of minimal points is infinite
- Singular set can have nontrivial geometry (self-intersections)
- Can deform domain of integration *around* singular set!

Smooth ACSV

Simplest case: Denominator H and its partial derivatives don't simultaneously vanish.

Then **critical points** are defined by

$$H = 0, \quad r_j z_1 H_{z_1} = r_1 z_j H_{z_j} \quad (2 \leq j \leq d)$$

 partial derivative

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Critical points: Asymptotic approximations can be made

Minimal points: Cauchy integral can be deformed close to

The asymptotic contribution of a minimal critical point \mathbf{w} depends on an explicit matrix $\mathcal{M} = \mathcal{M}_{\mathbf{w}}$ built from partial derivatives of H

Main Theorem of Smooth ACSV

(Baryshnikov Pemantle 2011 / BMP 2021)

Suppose that

$$H = 0, \quad r_j z_1 H_{z_1} = r_1 z_j H_{z_j} \quad (2 \leq j \leq d)$$

admits a finite number of solutions. If

- there is exactly one minimal solution, $\mathbf{w} \in \mathbb{C}_*^d$
- $H_{z_d}(\mathbf{w})$ and $\det \mathcal{M}$ are non-zero,

then

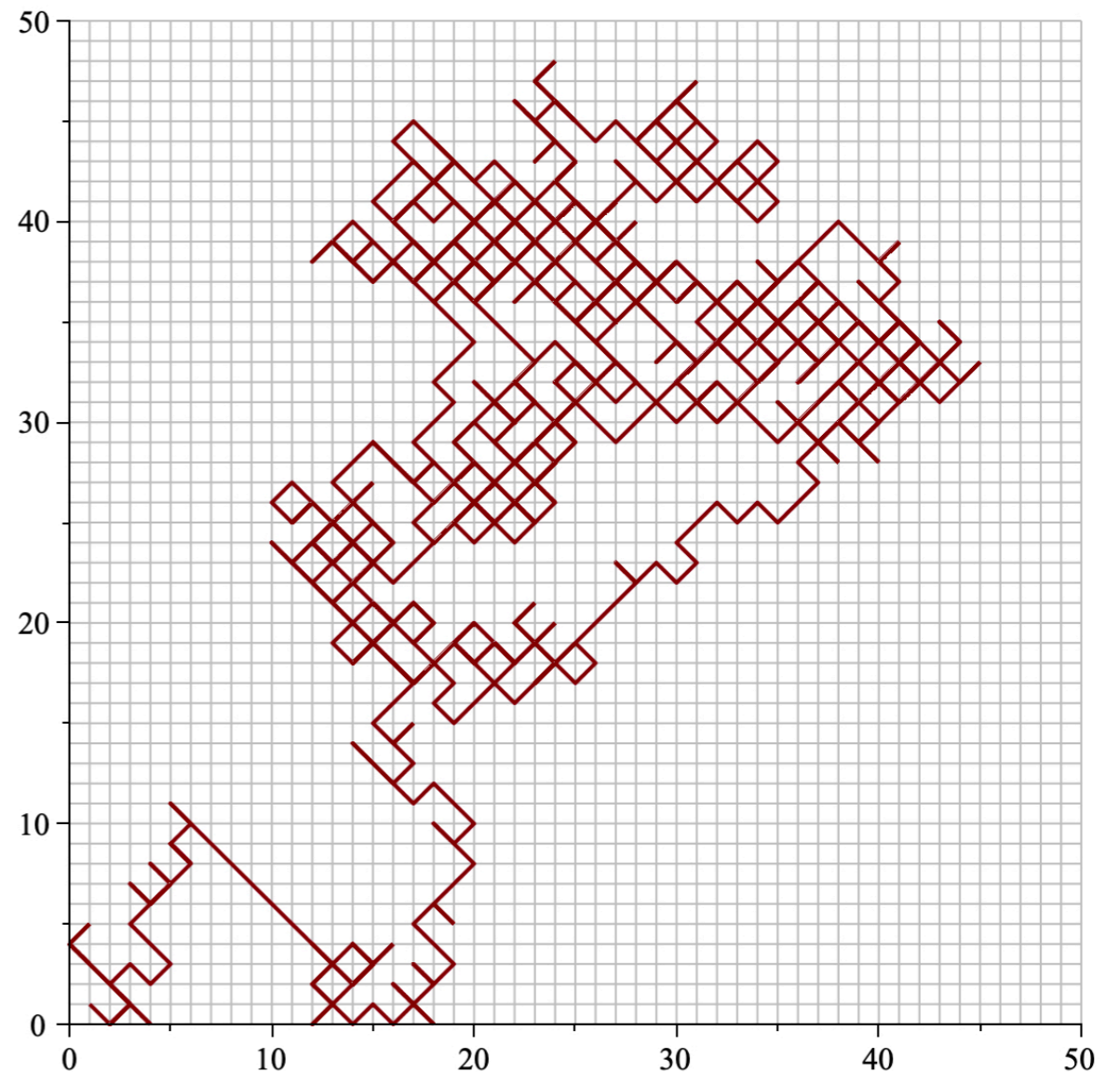
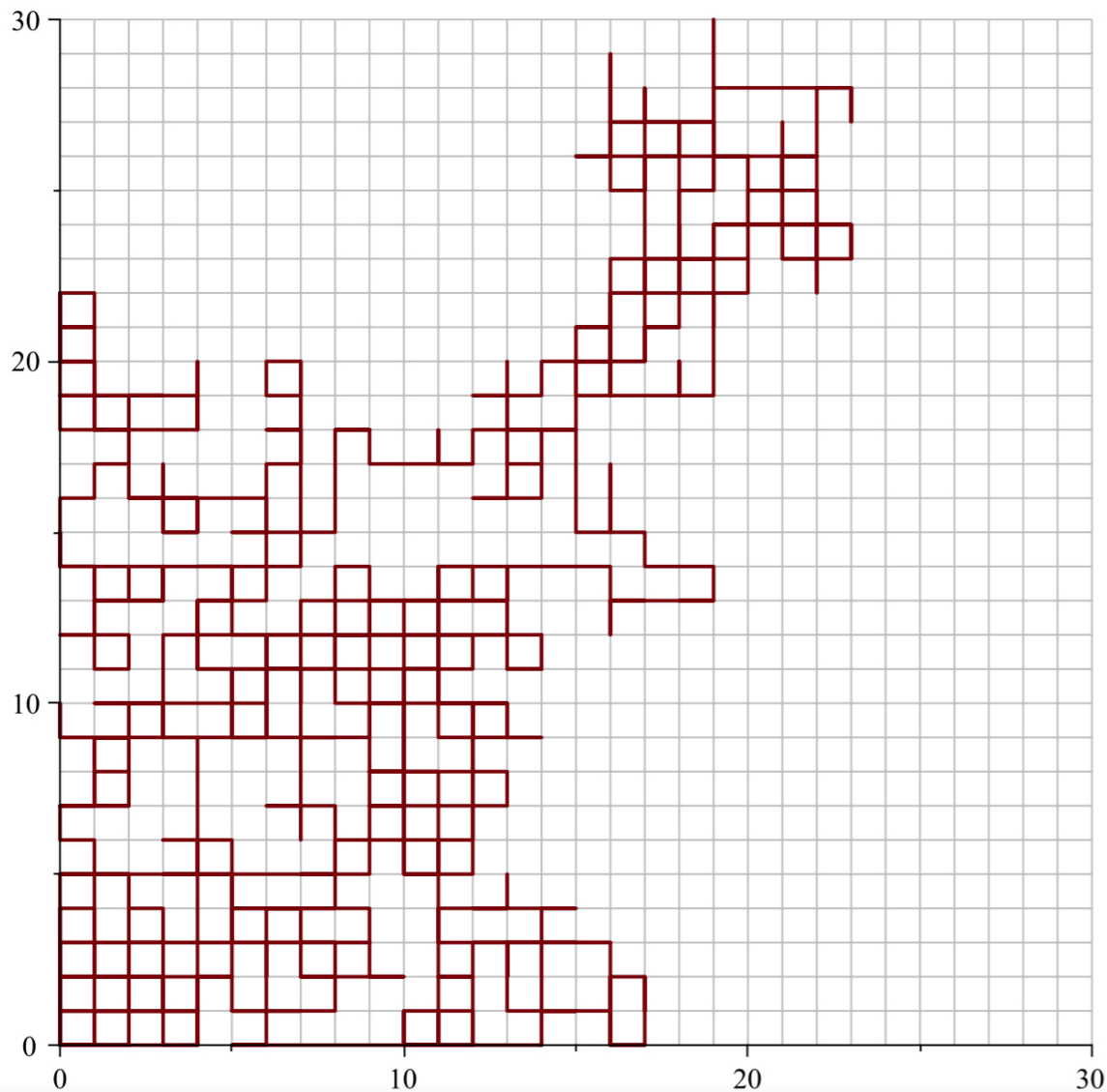
$$[\mathbf{z}^{n\mathbf{r}}] \frac{G(\mathbf{z})}{H(\mathbf{z})} = \mathbf{w}^{-n\mathbf{r}} (nr_d)^{(1-d)/2} (2\pi)^{(1-d)/2} \det(\mathcal{M})^{-1/2} \left(\frac{-G(\mathbf{w})}{w_d H_{z_d}(\mathbf{w})} + O\left(\frac{1}{n}\right) \right)$$

Application: Walks in an Orthant

Uniform diagonal expression for walk models in \mathbb{N}^d whose **step sets** $\mathcal{S} \subset \{\pm 1, 0\}^d$ are **symmetric over every axis**.

$$\frac{(1 + z_1) \cdots (1 + z_d)}{1 - t(z_1 \cdots z_d)S(\mathbf{z})},$$

$$S(\mathbf{z}) = \sum_{\mathbf{i} \in \mathcal{S}} \mathbf{z}^{\mathbf{i}}$$

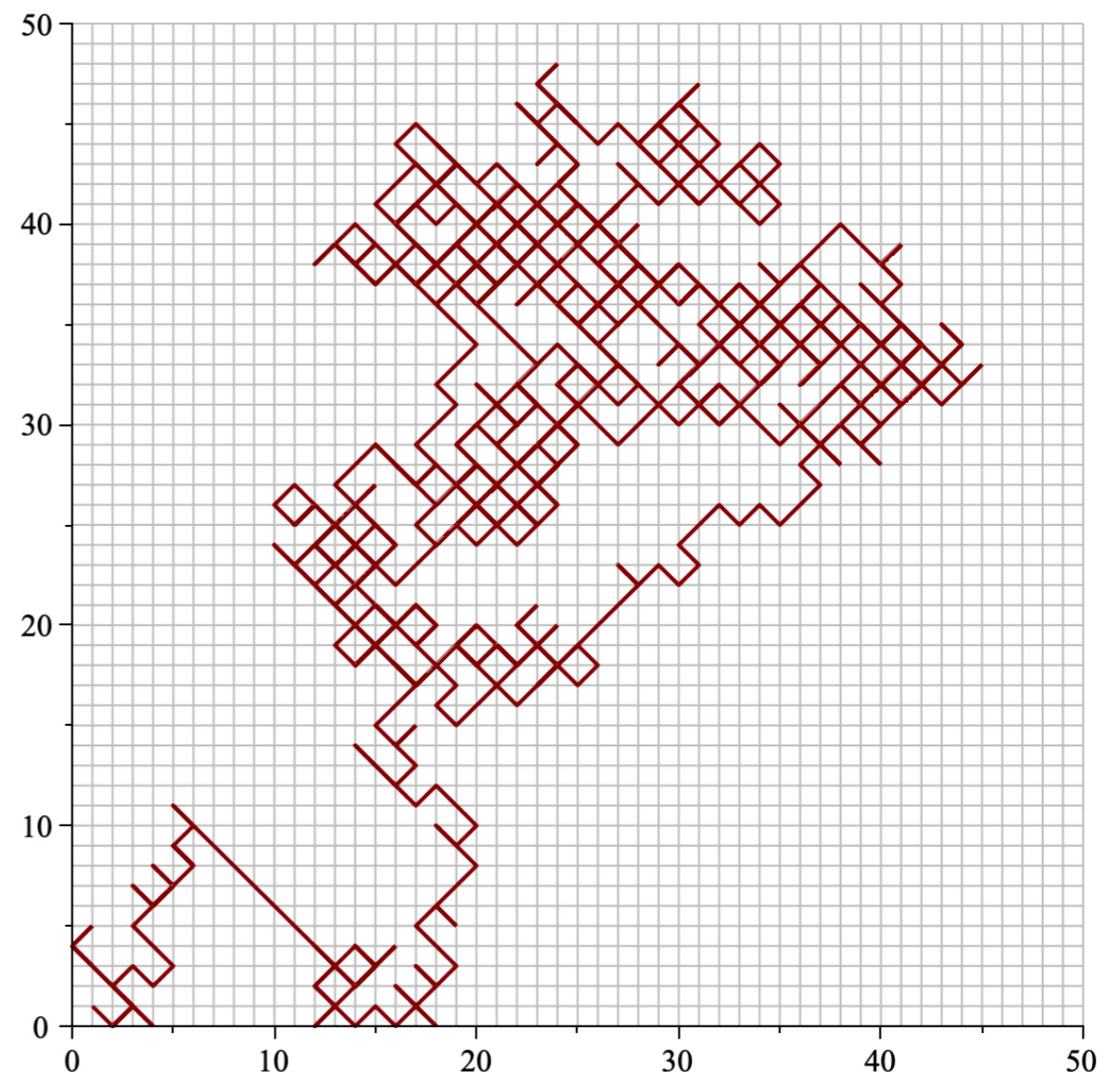
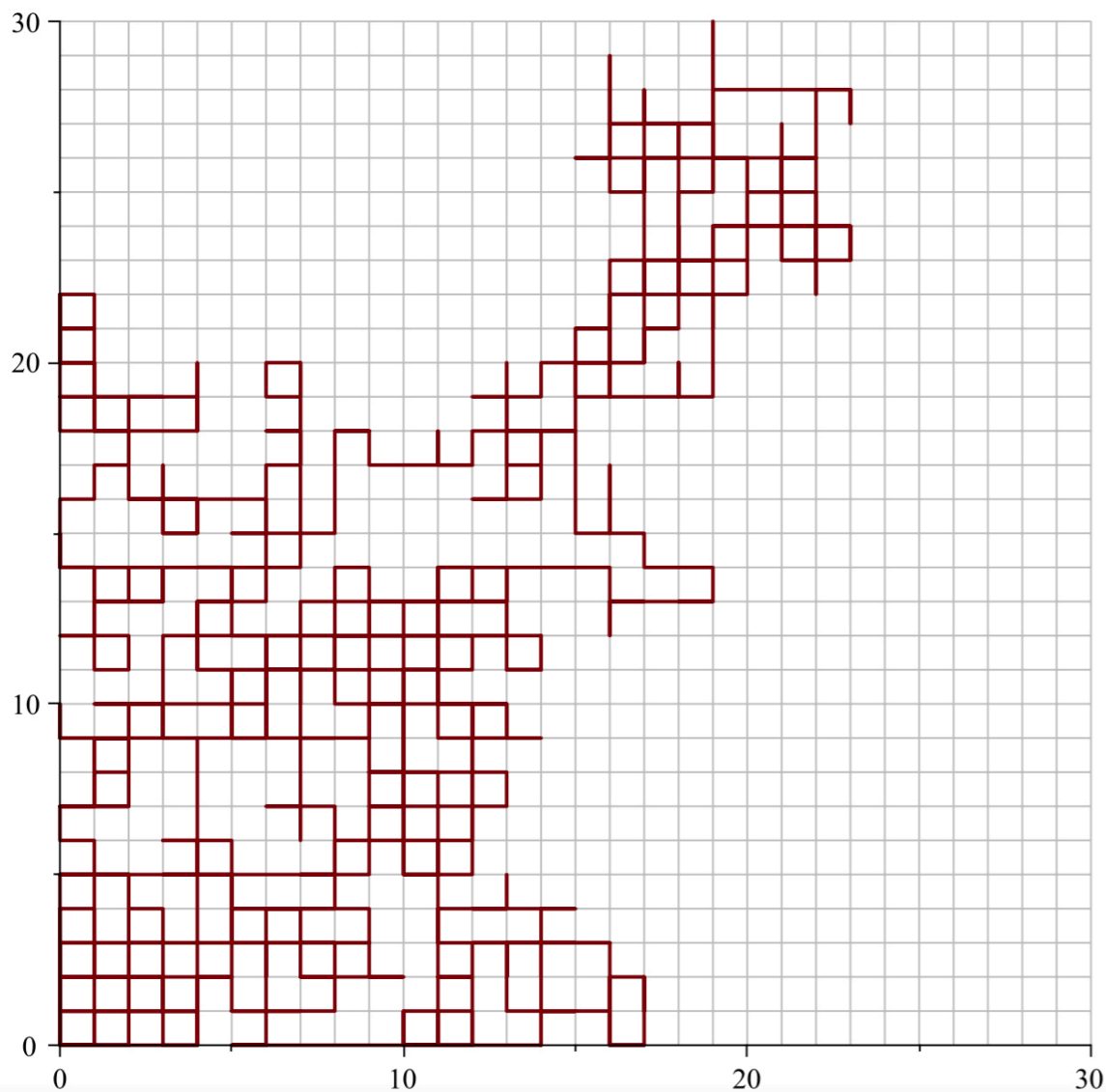


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Uniform diagonal expression for walk models in \mathbb{N}^d whose **step sets** $\mathcal{S} \subset \{\pm 1, 0\}^d$ are **symmetric over every axis**.

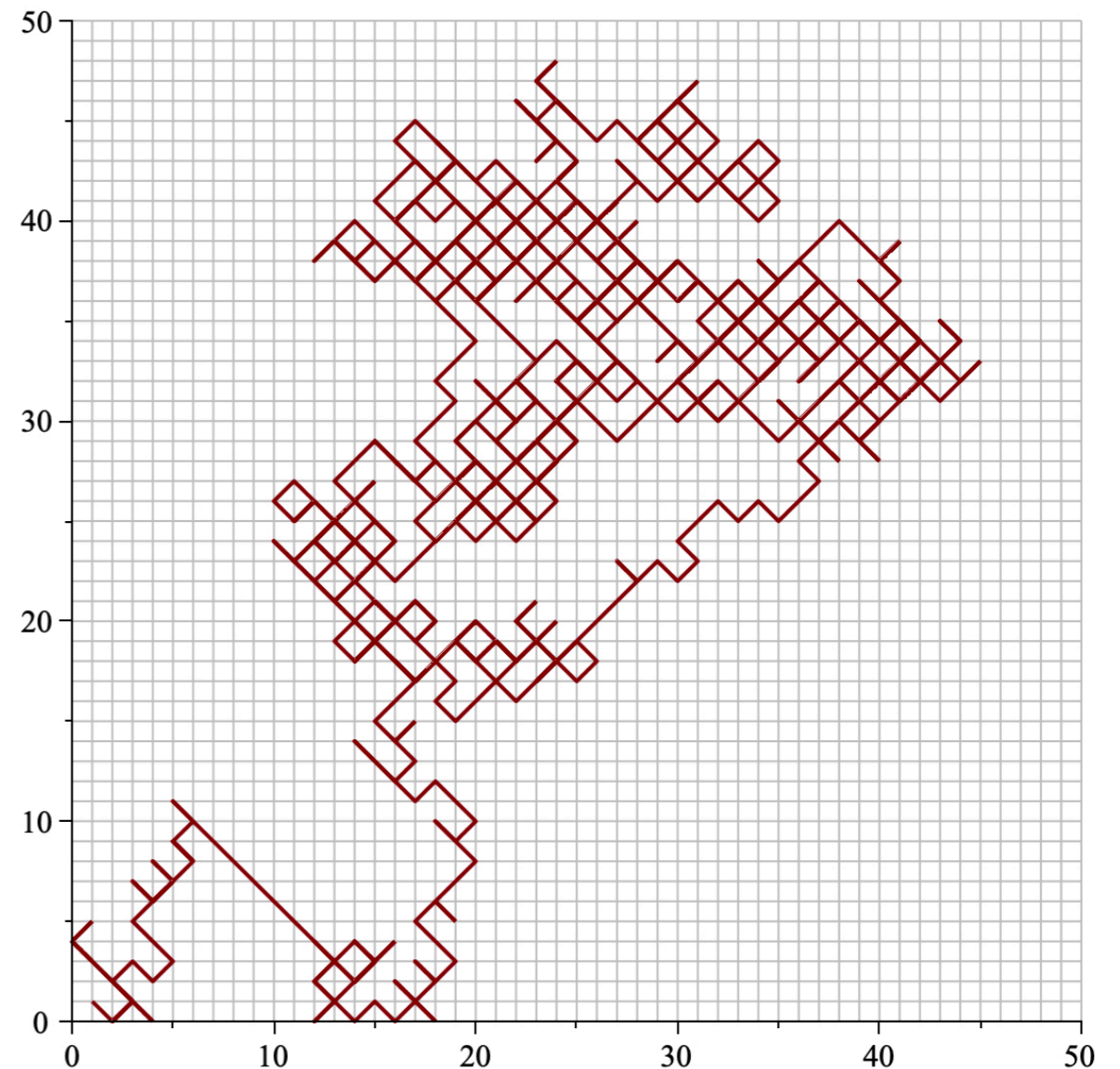
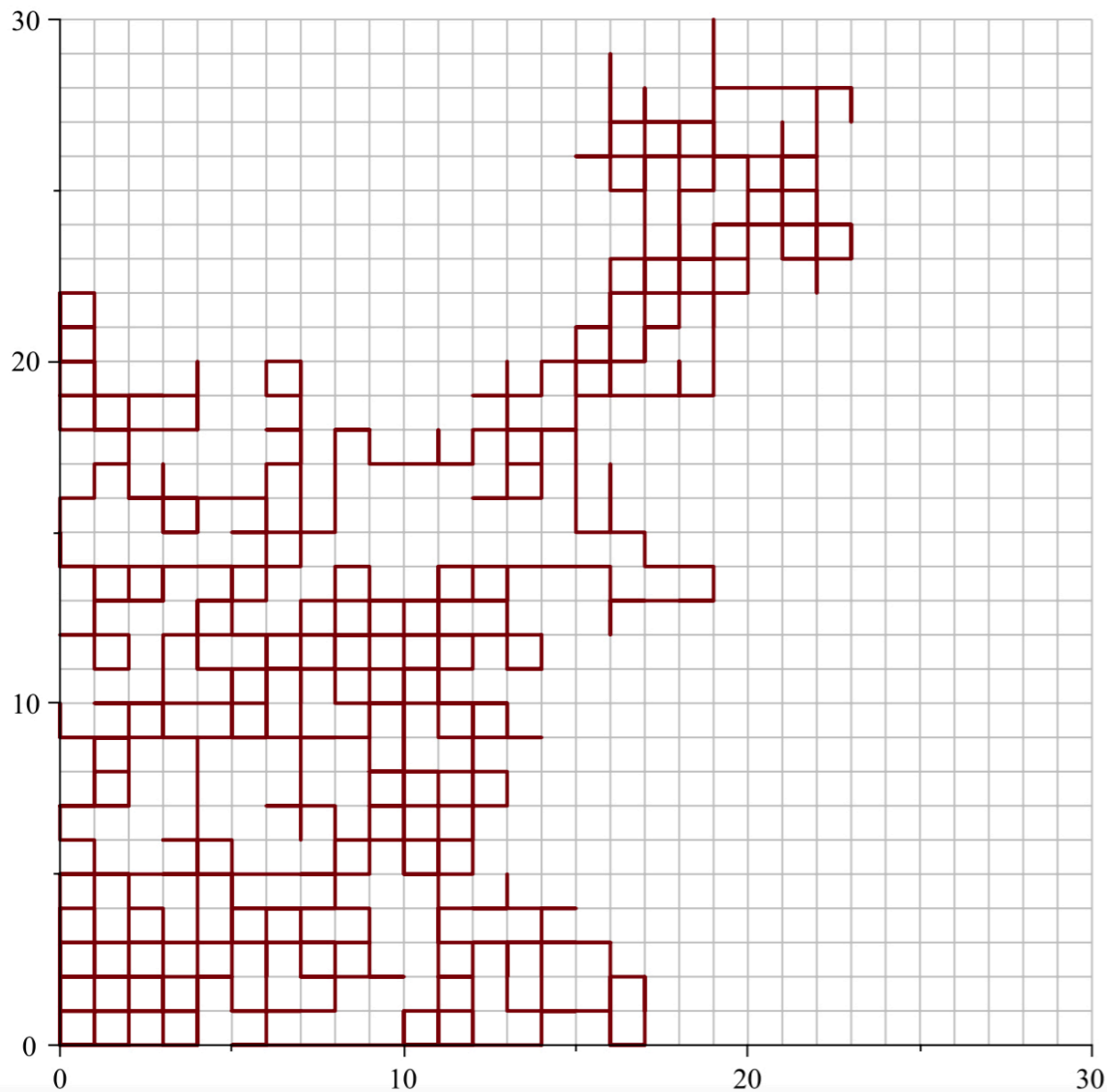
$$\# \text{ walks} \sim |\mathcal{S}|^n \cdot n^{-d/2} \cdot \left(\left(s^{(1)} \dots s^{(d)} \right)^{-1/2} \pi^{-d/2} |\mathcal{S}|^{d/2} + O\left(\frac{1}{n}\right) \right)$$

M. and Mishna, 2016



Application: Walks in an Orthant

M. and Wilson (2019) generalize this to find asymptotics for models with step sets **symmetric over all but one axis** (including the previous example).



Application: Lonesum Matrices

A **lonesum matrix** is a 0 – 1 matrix that is uniquely determined by its row and column sums.

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

NO

$$\begin{array}{ccccc} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \\ & \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{array}$$

YES

Application: Lonesum Matrices

A **lonesum matrix** is a 0 – 1 matrix that is uniquely determined by its row and column sums.

$$F(x, y) = \sum_{n, k \geq 0} \frac{B_{n, k}}{n!k!} x^n y^k = \frac{1}{1 + e^{-x} + e^{-y}}$$

Noncommutative Biology: Sequential Regulation of Complex Networks
Letsou and Cai. PLOS Computational Biology, 2016.

Together with the fact that the reachable configurations are a subset of the staircase matrices, this implies that the **reachable configurations and the lonesum matrices are in fact the same set**, and we have

Theorem 3 *The number of reachable configurations in the (n, m) ratchet network with $l_n = l_m = 1$ and threshold 1 scales as the poly-Bernoulli numbers $B_m^{-n} = B_n^{-m}$.*

Application: Lonesum Matrices

A **lonesum matrix** is a 0 – 1 matrix that is uniquely determined by its row and column sums.

$$F(x, y) = \sum_{n, k \geq 0} \frac{B_{n, k}}{n!k!} x^n y^k = \frac{1}{1 + e^{-x} + e^{-y}}$$

Let $f(t) = t/(1 - e^t) \log(1 - e^{-t})$.

Theorem. If $n, k \rightarrow \infty$ such that $n/k \rightarrow \lambda > 0$ then

$$B_{n, k} = \frac{a^{-n} b^{-n}}{\sqrt{k}} \frac{n!k!}{\sqrt{2\pi a e^{-a} [b e^{-b} + a e^{-a} - ab]}} (1 + O(k^{-1})),$$

where $a = f^{-1}(\lambda)$ and $b = f^{-1}(1/\lambda)$

ACSV Complexity Results

Suppose that $G(\mathbf{z})$ and $H(\mathbf{z})$ have coefficients $\leq 2^h$ and degree q
Suppose also that the power series of $F(\mathbf{z})$ has non-negative coefficients

Theorem (M. and Salvy, 2016)

Under generic and verifiable assumptions one can **find all minimal critical points**, and compute asymptotics in $\tilde{O}(hq^{4d+5})$ bit operations.

Can remove non-negativity assumption, with increased complexity.

Theorem (M. and Salvy, 2021)

Under verifiable assumptions, one can find minimal critical points in $\tilde{O}(hq^{9d+4}2^{3d})$ bit operations.

ACSV Complexity Results

Theorem (M. and Salvy, 2021)

Under verifiable assumptions, one can find minimal critical points in $\tilde{O}(hq^{9d+4}2^{3d})$ bit operations.

General Idea:

- Assumptions imply finite number of critical points
- Use a *univariate (Kronecker) representation* to encode them
- Reduce everything to **polynomial equalities and inequalities with bounded degrees and coefficient sizes**
- Use numerical methods with sufficient precision to test minimality

Irrationality of Zeta(3)

Exercise

Be the first in your block to prove by a 2-line argument that $\zeta(3)$ is irrational.⁷

⑥ Given the definitions of ⑤ show that $a_n b_{n-1} - a_{n-1} b_n = b_n^{-3}$ and $b_n = O(\alpha^n)$ with $\alpha = (1 + \sqrt{2})^4$. Conclude that $\zeta(3)$ is irrational because $\log \alpha > 3$.

A Proof that Euler Missed, Alfred van der Poorten

$$b_n = \sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{k}^2 = [(xyz t)^n] \frac{1}{1 - t(1+x)(1+y)(1+z)(1+y+z+yz+xyz)}$$

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```
> A, U, PRINT := DiagonalAsymptotics(numer(F), denom(F), [a, b, c, z], u, k, useFGb):  
A, U;
```

$$\frac{1}{4} \frac{\left(\frac{2u - 366}{34u + 1458} \right)^k \sqrt{2} \sqrt{\frac{2u - 366}{-96u - 4192}}}{k^{3/2} \pi^{3/2}}, [RootOf(_Z^2 - 366_Z - 17711, -43.27416997969...)]$$

Restricted Factors in Words

The number of *balanced* binary strings with no substring equal to 10101101 and 1110101 is the main diagonal of

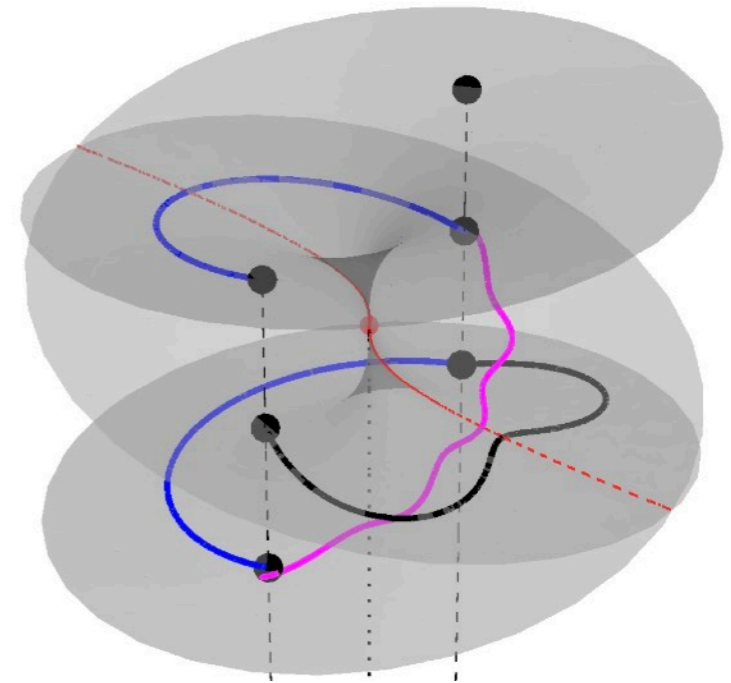
$$\frac{1 - x^3y^6 + x^3y^4 + x^2y^4 + x^2y^3}{1 - x - y + x^2y^3 - x^3y^3 - x^4y^4 - x^3y^6 + x^4y^6}$$

```
> ASM, U := DiagonalAsymptotics( numer(F), denom(F), indets(F), u, k, true, u-T, T) :
ASM;
1/2 ( ( ( 84 u^20 + 240 u^19 - 285 u^18 - 1548 u^17 - 2125 u^16 - 1408 u^15 + 255 u^14 + 756 u^13 + 2509 u^12 + 2856 u^11 + 605 u^10 + 2020 u^9 + 1233 u^8 - 1760 u^7 +
-12 u^20 + 30 u^19 + 258 u^18 + 500 u^17 + 440 u^16 - 102 u^15 - 378 u^14 - 1544 u^13 - 2142 u^12 - 550 u^11 - 2222 u^10 - 1644 u^9 + 2860 u^8 - 1848 u^7 + 123
sqrt( 84 u^20 + 240 u^19 - 285 u^18 - 1548 u^17 - 2125 u^16 - 1408 u^15 + 255 u^14 + 756 u^13 + 2509 u^12 + 2856 u^11 + 605 u^10 + 2020 u^9 + 1233 u^8 - 1760 u^7 + 9
-162 u^18 - 612 u^17 - 902 u^16 - 616 u^15 + 254 u^14 + 548 u^13 + 2054 u^12 + 2156 u^11 + 898 u^10 + 2268 u^9 + 2462 u^8 - 2088 u^7 + 1312 u^6 -
-255 u^16 - 190 u^15 - 19 u^14 + 46 u^13 + 461 u^12 + 628 u^11 + 133 u^10 + 374 u^9 + 161 u^8 - 384 u^7 + 146 u^6 - 138 u^5 - 285 u^4 - 40 u^3 + 91 u^2 - 30 u + 32
+ 756 u^13 + 2509 u^12 + 2856 u^11 + 605 u^10 + 2020 u^9 + 1233 u^8 - 1760 u^7 + 924 u^6 - 492 u^5 - 675 u^4 + 632 u^3 - 249 u^2 + 24 u + 16) )
```

Complexity and Algorithms for ACSV

Lee, M., Smolčić (2022): Algorithms using *polynomial homotopy methods*

```
sys1 = System([u; v; circeqs; J2eqs[2:n]], variables=[x; y; t], parameters=[a; b; v])
init = get_start_solution(sys1, [abvals; 0])
if !isnothing(init)
  res = monodromy_solve(sys1, init, [abvals; 0], show_progress=show_progress)
  if length(real_solutions(results(res))) != 0
    # if any sol has t ∈ (0, 1) the point is not minimal (certify requires square system)
    certs = distinct_certificates(certify(System([u; v; circeqs; J2eqs[2:n]], variables=[x; y; t]
    minimal[idx] &= !check_solutions(certs, 2*n+1, tol)
  end
end
```



Andrew Luo URA (2022): First rigorous implementation with interval arithmetic, and generalization of polynomial methods to *Laurent* expansions

```
# Compute the Kronecker representation of our system
P, Qs = Kronecker(system, u_, λ, vsT, linf_constant)
U, N, kappa = NumericalKronecker(P, Qs)

Qt = Qs[-2] # Qs ordering is H.variables() + [t, λ]
Pd = P.derivative()
```

Conclusion

- For **rational/algebraic** GFs determining asymptotics is (for practical applications) **automatic**
- For **D-algebraic** GFs determining asymptotics is undecidable
- Computability of **D-finite** asymptotics is open due to the **connection problem**
- **Rational diagonals** lie between algebraic and D-finite, and allow new techniques to be applied. Also allow for multivariate analysis (ask me)
- Effective methods for analytic combinatorics answer are **interesting** and find **application** to real problems

The End

