Efficient experimental mathematics for combinatorics and number theory

Alin Bostan

Inria

Vienna Summer School of Mathematics

Weissensee, Austria

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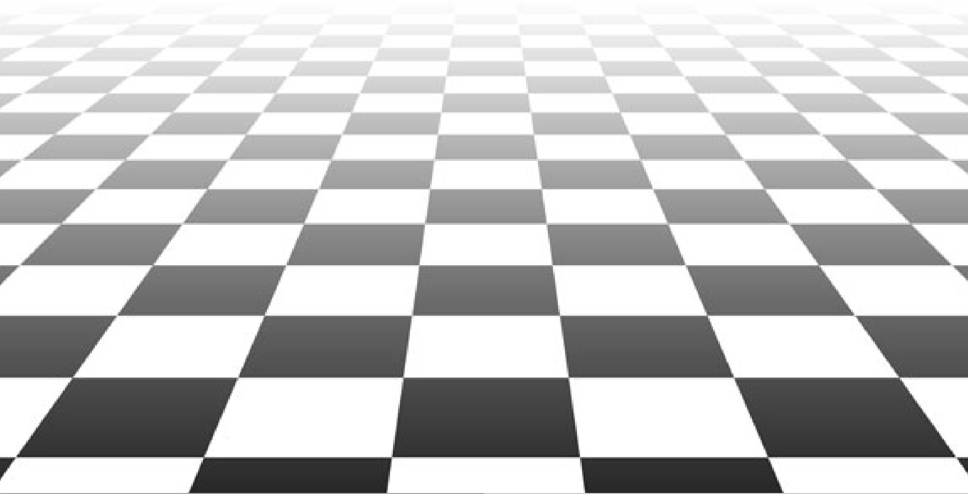
Overview

Lecture 1: Context, Motivation, Examples

Lecture 2: Exp. Math. for Combinatorics

Lecture 3: Inside the Exp. Math. Toolbox

Lecture 2: Exp. Math. for Combinatorics



Computer Algebra for Enumerative Combinatorics: a showcase of Experimental Mathematics

Enumerative Combinatorics: science of counting

Area of mathematics primarily concerned with counting discrete objects.

▷ Main outcome: theorems

Computer Algebra: effective mathematics

Area of computer science primarily concerned with the algorithmic manipulation of algebraic objects.

▷ Main outcome: algorithms

Computer Algebra for Enumerative Combinatorics $\subset$ Experimental Math.

Today: Algorithms for proving Theorems on Lattice Paths Combinatorics.

An (innocent looking) combinatorial question

Let $\mathscr{S} = \{\uparrow, \leftarrow, \searrow\}$. An $\mathscr{S}$-walk is a path in $\mathbb{Z}^2$ using only steps from $\mathscr{S}$. Show that, for any integer n, the following quantities are equal:

(i) number a_n of n-steps $\mathscr{S}$-walks confined to the upper half plane $\mathbb{Z} \times \mathbb{N}$ that start and finish at the origin $(0,0)$ (*excursions*);

(ii) number b_n of n-steps $\mathscr{S}$-walks confined to the quarter plane $\mathbb{N}^2$ that start at the origin $(0,0)$ and finish on the diagonal of $\mathbb{N}^2$ (*diagonal walks*).

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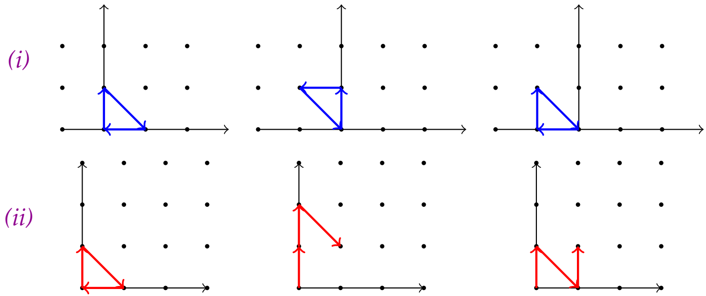
For instance, for $n = 3$, this common value is $a_3 = b_3 = 3$:



Teasers

Teaser 1: This "exercise" is non-trivial

Teaser 2: It can be solved using Experimental Math and Computer Algebra

Teaser 3: ...by two robust and efficient algorithmic techniques,
Guess-and-Prove and Creative Telescoping

Why care about counting walks?

Many objects can be encoded by walks:

- probability theory (voting, games of chance, branching processes, . . .)
- discrete mathematics (permutations, trees, words, urns, . . .)
- statistical physics (Ising model, . . .)
- operations research (queueing theory, . . .)

Counting walks is an old topic: the ballot problem [Bertrand, 1887]

Suppose that candidates A and B are running in an election. If a votes are cast for A and b votes are cast for B, where $a > b$, then the probability that A stays ahead of B throughout the counting of the ballots is $(a - b)/(a + b)$.

Lattice path reformulation: find the number of paths in $\mathbb{Z}^2$ with a upsteps $\nearrow$ and b downsteps $\searrow$ that start at the origin and never touch the x-axis

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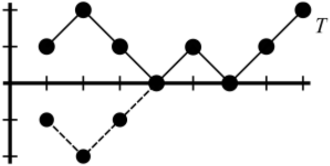
Lattice path reformulation: find the number of paths in $\mathbb{Z}^2$ with $a-1$ upsteps $\nearrow$ and b downsteps $\searrow$ that start at $(1,1)$ and never touch the x-axis

Reflection principle [Aebly, 1923]: *paths in* $\mathbb{Z}^2$ *from* $(1,1)$ *to* $T(a+b, a-b)$ *that do touch the x-axis* are in bijection with *paths in* $\mathbb{Z}^2$ *from* $(1,-1)$ *to* T



Answer: $$\underbrace{(\textit{paths in } \mathbb{Z}^2 \textit{ from } (1,1) \textit{ to } T)}_{\binom{a+b-1}{a-1}} - \underbrace{(\textit{paths in } \mathbb{Z}^2 \textit{ from } (1,-1) \textit{ to } T)}_{\binom{a+b-1}{b-1}}$$

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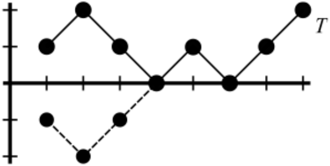

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$$\binom{a+b-1}{a-1} - \binom{a+b-1}{b-1} = \frac{a-b}{a+b}\binom{a+b}{a}$$

…but it is still a very hot topic

Lot of recent activity; many recent contributors:

Arquès, Bacher, Banderier, Beaton, Bernardi, Bostan, Bousquet-Mélou, Buchacher, Budd, Chyzak, Cori, Courtiel, Denisov, Dreyfus, Du, Duchon, Dulucq, Duraj, Fayolle, Fisher, Flajolet, Fusy, Garbit, Gessel, Gouyou-Beauchamps, Guttmann, Guy, Hardouin, van Hoeij, Hou, Iasnogorodski, Johnson, Kauers, Kenyon, Koutschan, Krattenthaler, Kreweras, Kurkova, Lecouvey, Malyshev, Melczer, Miller, Mishna, Niederhausen, Owczarek, Pech, Petkovšek, Prellberg, Raschel, Rechnitzer, Roques, Sagan, Salvy, Sheffield, Singer, Tarrago, Viennot, Wachtel, Wallner, Wang, Wilf, D. Wilson, M. Wilson, Yatchak, Xu, Yeats, Zeilberger, …

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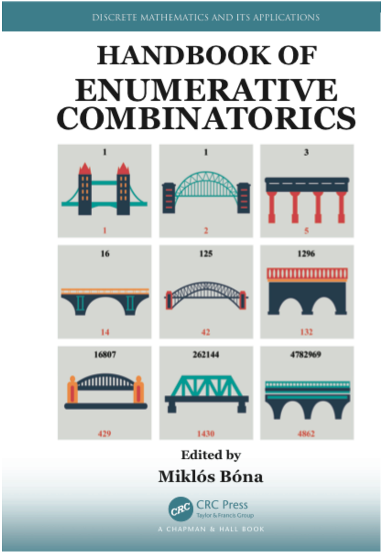
Specific question
Ad hoc solution → **Systematic approach**

. . . but it is still a very hot topic



Chapter 10

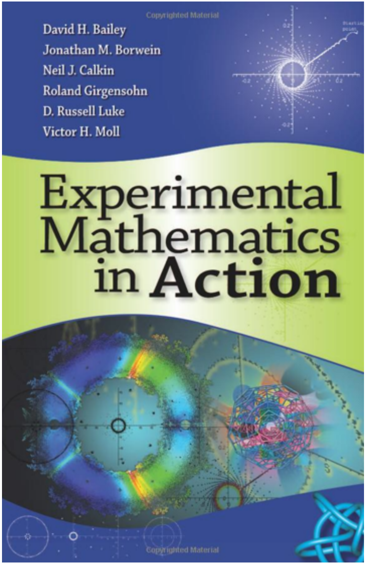
Lattice Path Enumeration

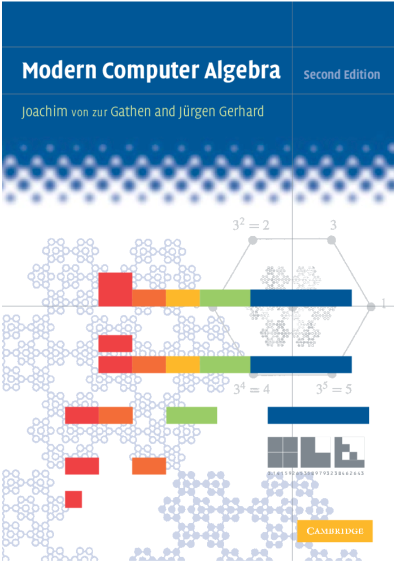
Christian Krattenthaler

Universität Wien

CONTENTS

Our approach: Experimental Mathematics using Computer Algebra





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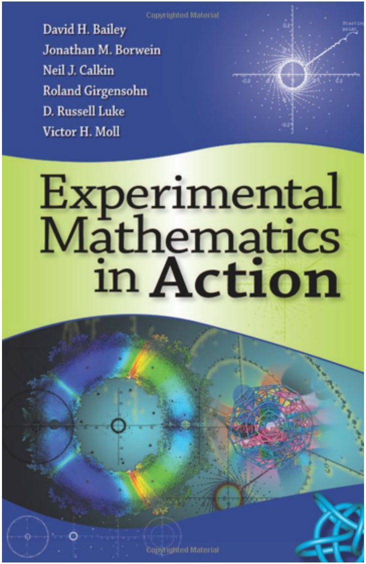

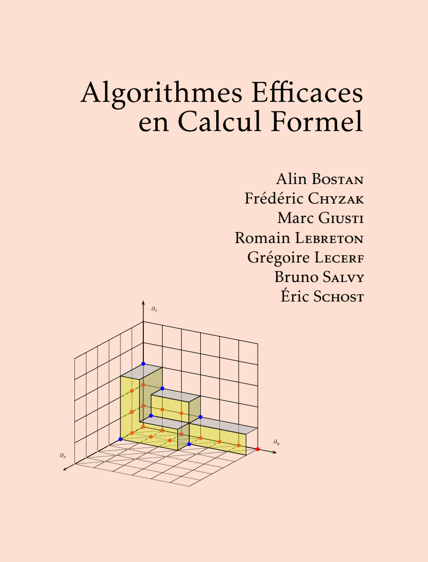

▷ Nearest-neighbor walks in the quarter plane:
$\mathscr{S}$-walks in $\mathbb{N}^2$: starting at $(0,0)$ and using steps in a *fixed* subset $\mathscr{S}$ of

$$\{\swarrow, \leftarrow, \nwarrow, \uparrow, \nearrow, \rightarrow, \searrow, \downarrow\}$$

▷ Counting sequence $q_{\mathscr{S}}(n)$: number of $\mathscr{S}$-walks of length n

▷ Generating function:

$$Q_{\mathscr{S}}(t) = \sum_{n=0}^{\infty} q_{\mathscr{S}}(n) t^n \ \in \mathbb{Z}[[t]]$$

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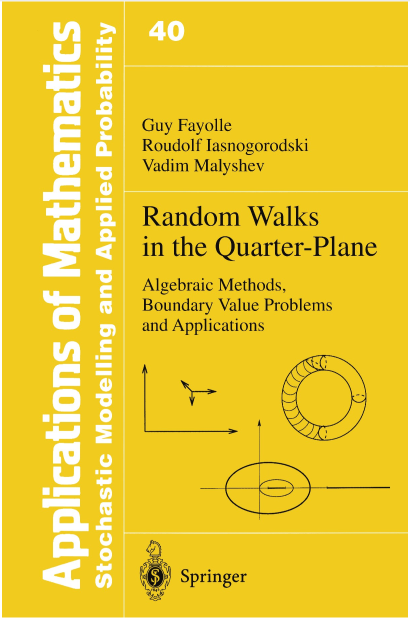
$$\{\swarrow, \leftarrow, \nwarrow, \uparrow, \nearrow, \rightarrow, \searrow, \downarrow\}$$

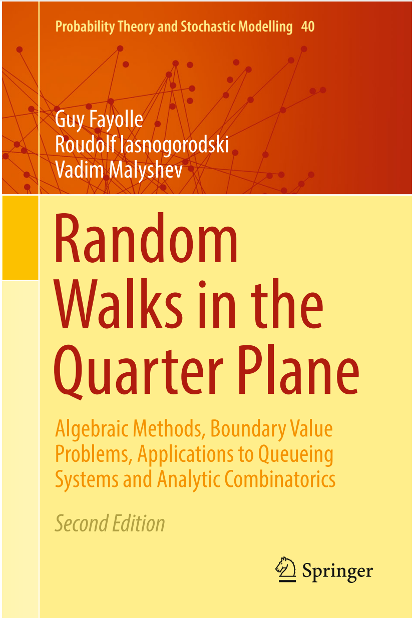
▷ Counting sequence $q_{\mathscr{S}}(i,j;n)$: number of walks of length n ending at (i,j)

▷ Complete generating function (with "catalytic " variables x, y):

$$Q_{\mathscr{S}}(x,y;t) = \sum_{i,j,n=0}^{\infty} q_{\mathscr{S}}(i,j;n) x^i y^j t^n \ \in \mathbb{Z}[[x,y,t]]$$

Entire books dedicated to small step walks in the quarter plane!





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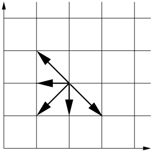

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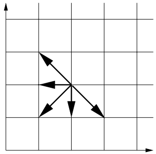

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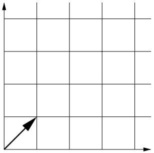

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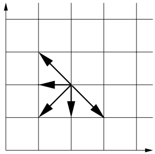

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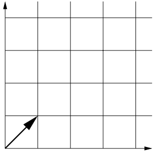

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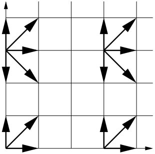

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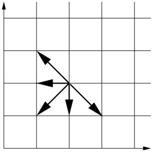

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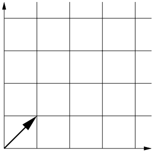

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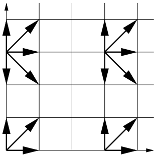

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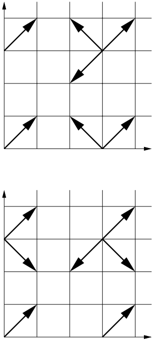

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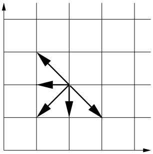

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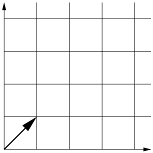

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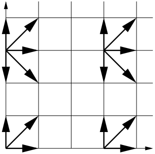

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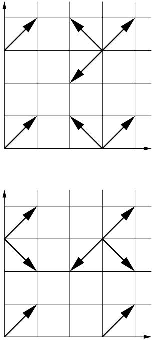

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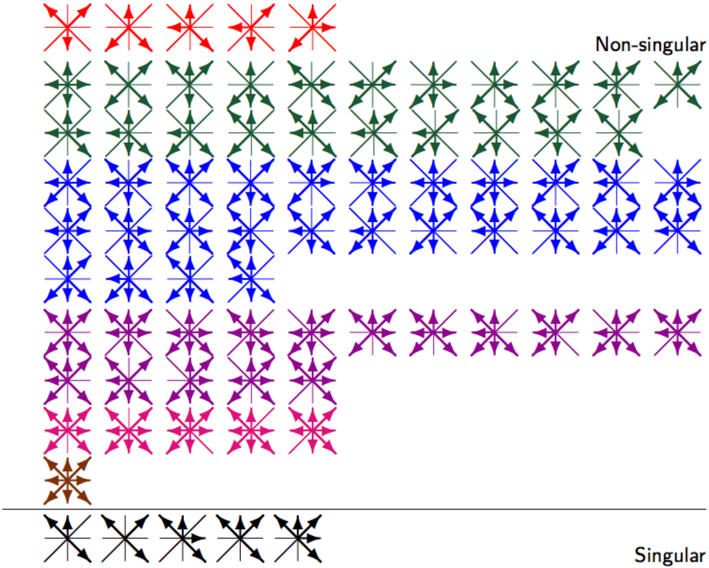
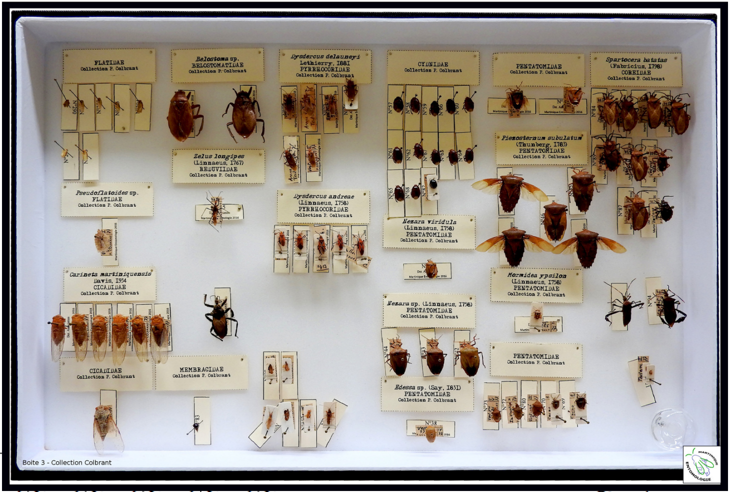
One is left with 79 interesting distinct models.

The 79 small steps models of interest

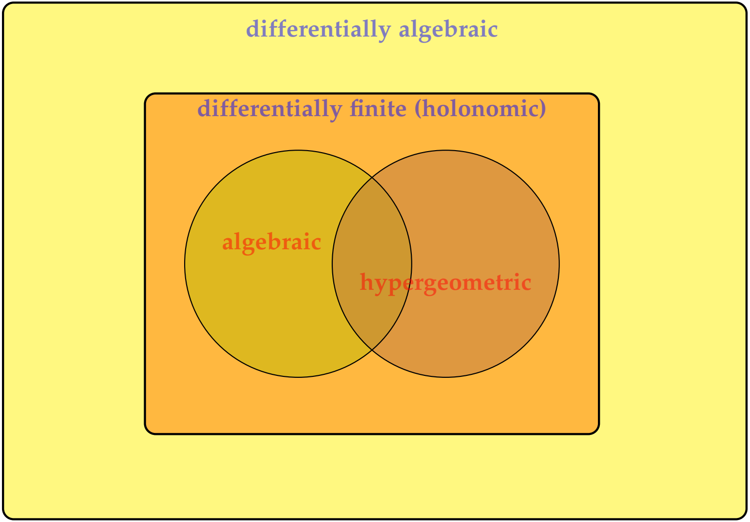


Non-singular



Singular

Classification criterion: properties of generating functions



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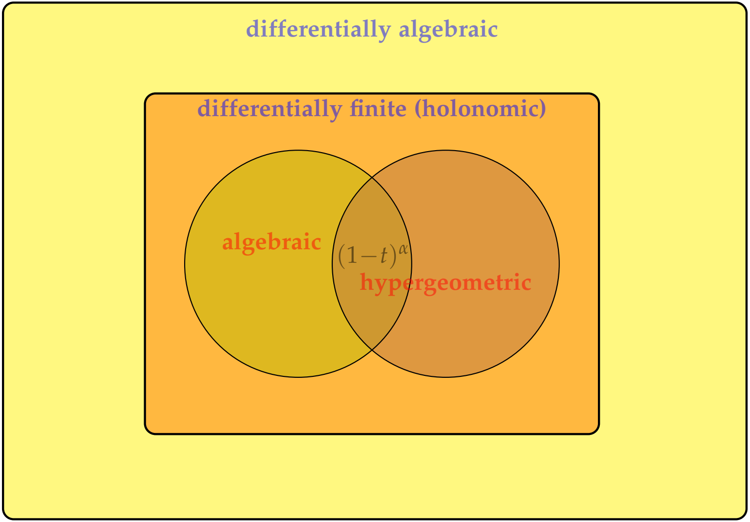

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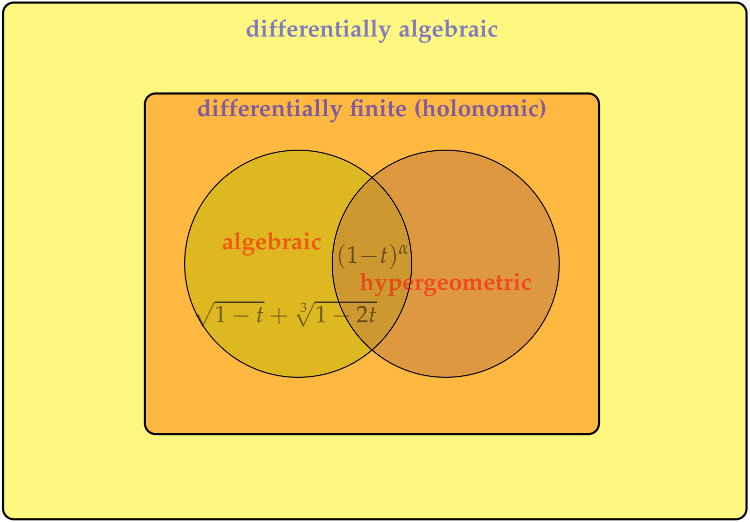

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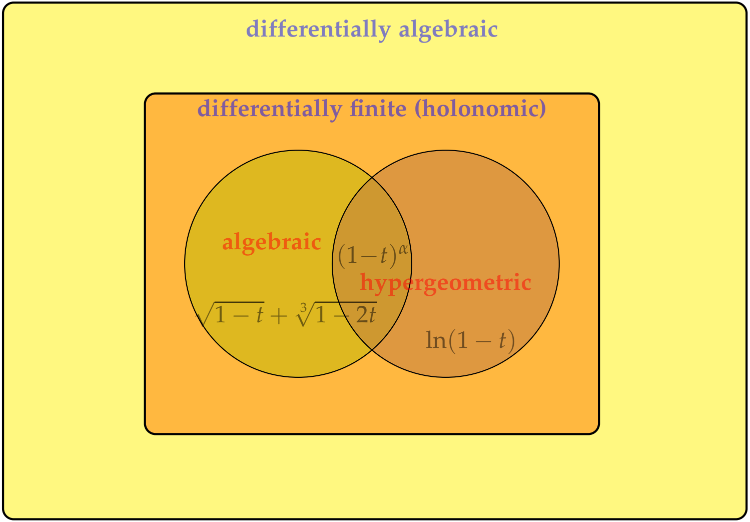

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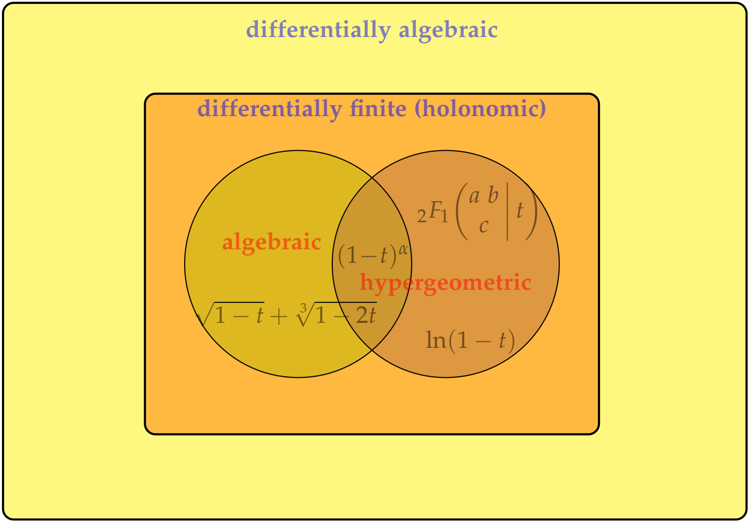
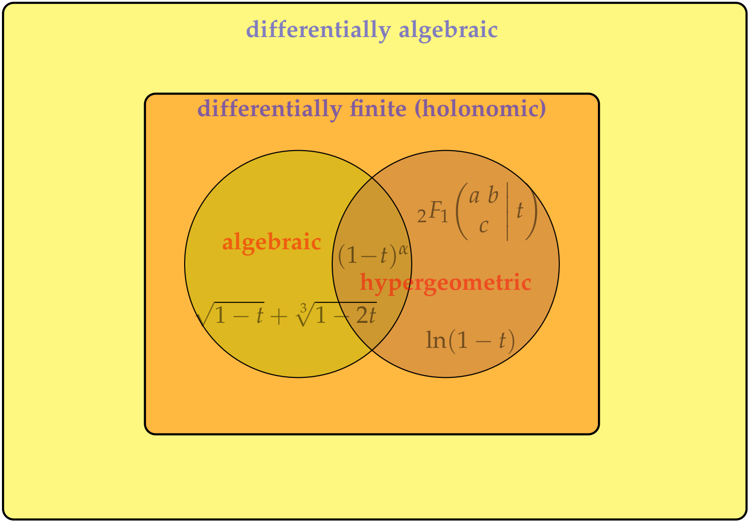


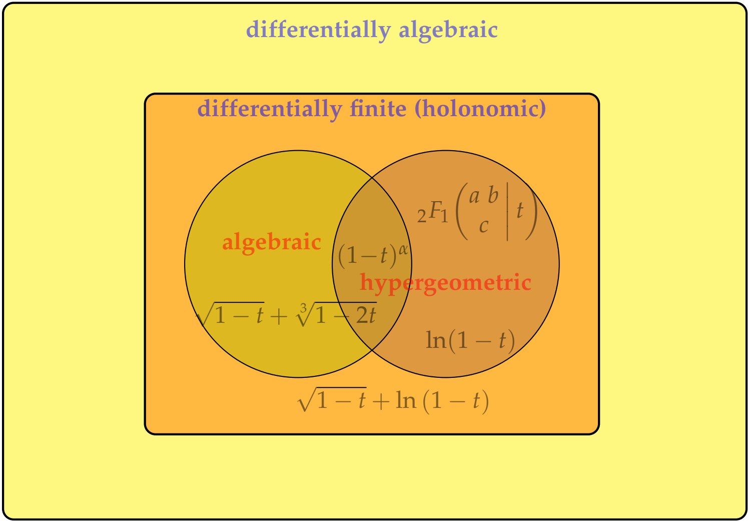
$$ {}_2F_1\left(\begin{matrix} a\ b \\ c \end{matrix}\,\middle|\, t\right) := \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n}\frac{t^n}{n!}, \quad \text{where} \quad (a)_n = a(a+1)\cdots(a+n-1). $$

Classification criterion: properties of generating functions



E.g., $(1-t)^\alpha = {}_2F_1\left(\begin{matrix} -\alpha\ 1 \\ 1 \end{matrix} \middle| t\right), \quad \ln(1-t) = -t \cdot {}_2F_1\left(\begin{matrix} 1\ 1 \\ 2 \end{matrix} \middle| t\right) = -\sum_{n=1}^{\infty} \frac{t^n}{n}$

Classification criterion: properties of generating functions



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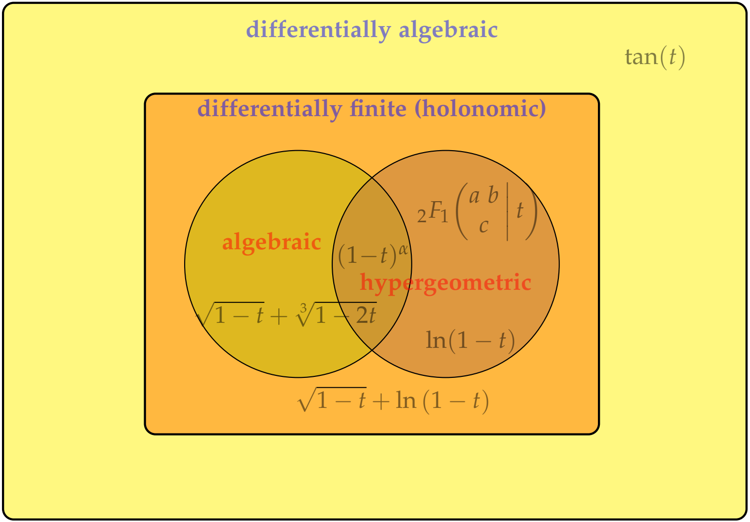

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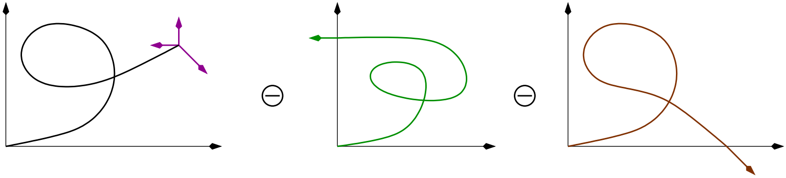
Algebraic reformulation of main task: solving a functional equation

Generating function: $Q(x,y) \equiv Q(x,y;t) = \sum_{i,j,n=0}^{\infty} q(i,j;n)x^i y^j t^n \in \mathbb{Z}[[x,y,t]]$

Recursive construction yields the *kernel equation*

$$Q(x,y) = 1 + t\left(y + \frac{1}{x} + x\frac{1}{y}\right)Q(x,y) - t\frac{1}{x}Q(0,y) - tx\frac{1}{y}Q(x,0)$$



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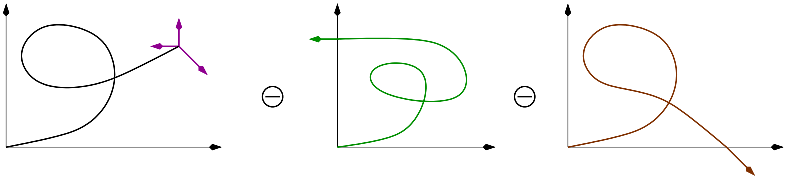
$$\left(1 - t\left(y + \frac{1}{x} + x\frac{1}{y}\right)\right) xyQ(x,y) = xy - tyQ(0,y) - tx^2Q(x,0)$$



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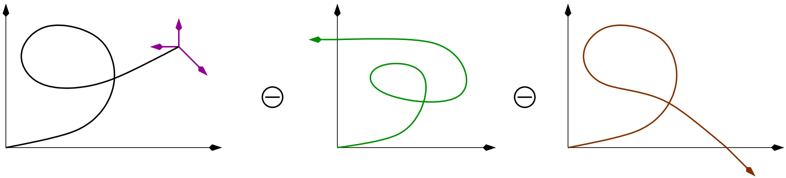

New task: Solve this functional equation!

Algebraic reformulation of main task: solving a functional equation

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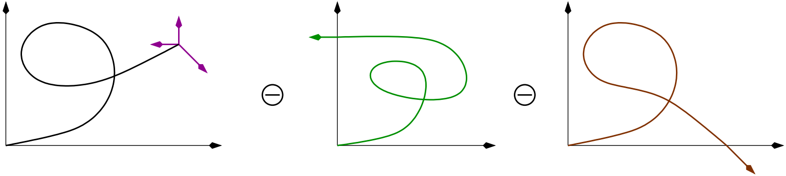
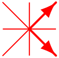
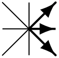


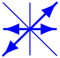
New task: For the other models – solve 78 similar equations!

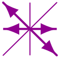
Dyck: 

Motzkin: 

Pólya: 

Kreweras: 

Gessel: 

Gouyou-Beauchamps: 

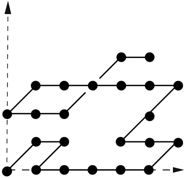
King walks: 

Tandem walks: 

- $g(n)$ = number of n-steps $\{\nearrow, \swarrow, \leftarrow, \rightarrow\}$-walks in $\mathbb{N}^2$
  1, 2, 7, 21, 78, 260, 988, 3458, 13300, 47880, ...

Question: What is the nature of the generating function

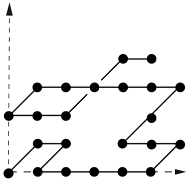
$$G(t) = \sum_{n=0}^{\infty} g(n)\, t^n \text{ ?}$$



- $g(i,j;n)$ = number of n-steps $\{\nearrow, \swarrow, \leftarrow, \rightarrow\}$-walks in $\mathbb{N}^2$ from $(0,0)$ to (i,j)

Question: What is the nature of the generating function

$$G(x,y;t) = \sum_{i,j,n=0}^{\infty} g(i,j;n)\, x^i y^j t^n \ ?$$



Gessel walks (2000)

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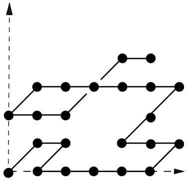

Theorem [B., Kauers, 2010]

$G(x,y;t)$ is an algebraic function†.

▷ computer-driven discovery/proof via *algorithmic Guess-and-Prove*

† Minimal polynomial $P(G(x,y;t); x,y,t) = 0$ has $> 10^{11}$ terms; ≈ 30 Gb (6 DVDs!)

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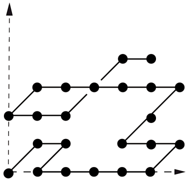
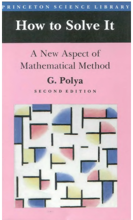


Corollary [B., Kauers, 2010] (former conjecture of Gessel's)

$$(3n+1)\, g(2n) = (12n+2)\, g(2n-1) \quad \text{and} \quad (n+1)\, g(2n+1) = (4n+2)\, g(2n)$$

▷ computer-driven discovery/proof via *algorithmic Guess-and-Prove*

Guess-and-Prove



Guessing and Proving

George Pólya

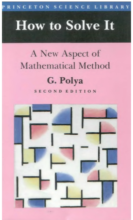
What is “scientific method”? Philosophers and non-philosophers have discussed this question and have not yet finished discussing it. Yet as a first introduction it can be described in three syllables:

Guess and test.

Mathematicians too follow this advice in their research although they sometimes refuse to confess it. They have, however, something which the other scientists cannot really have. For mathematicians the advice is

First guess, then prove.

Guess-and-Prove



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First guess, then prove.

generate data → make conjectures → prove them

Guess-and-Prove: a toy example

Question: Find $B_{i,j}$:= the number of $\{\rightarrow, \uparrow\}$-walks in $\mathbb{N}^2$ from $(0,0)$ to (i,j)

Guess-and-Prove: a toy example

Question: Find $B_{i,j}$:= the number of $\{\rightarrow, \uparrow\}$-walks in $\mathbb{N}^2$ from $(0,0)$ to (i,j)

1. There are 2 ways to get to (i,j), either from $(i-1,j)$, or from $(i,j-1)$:

$$B_{i,j} = B_{i-1,j} + B_{i,j-1}$$

2. There is only one way to get to a point on an axis: $B_{i,0} = B_{0,j} = 1$

▷ These two rules completely determine all the numbers $B_{i,j}$

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(I) Generate data:

⋮							
1	7	28	84	210	462	924	
1	6	21	56	126	252	462	
1	5	15	35	70	126	210	
1	4	10	20	35	56	84	
1	3	6	10	15	21	28	
1	2	3	4	5	6	7	
1	1	1	1	1	1	1	…

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(I) Generate data:

(II) Guess:

⋮								
1	7	28	84	210	462	924		
1	6	21	56	126	252	462		
1	5	15	35	70	126	210		
1	4	10	20	35	56	84	$\longrightarrow$	$\cdots$
1	3	6	10	15	21	28	$\longrightarrow$	$\frac{(i+1)(i+2)}{2}$
1	2	3	4	5	6	7	$\longrightarrow$	$i+1$
1	1	1	1	1	1	1	$\longrightarrow$	1

Guess-and-Prove: a toy example

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1	1	1	1	1	1	1	…

(II) Guess:

$$B_{i,j} \stackrel{?}{=} \frac{(i+j)!}{i!j!}$$

Guess-and-Prove: a toy example

Question: Find $B_{i,j}$:= the number of $\{\to,\uparrow\}$-walks in $\mathbb{N}^2$ from $(0,0)$ to (i,j)

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1	2	3	4	5	6	7	
1	1	1	1	1	1	1	…

(III) Prove: If $C_{i,j} \stackrel{\text{def}}{=} \frac{(i+j)!}{i!j!}$, then

$$\frac{C_{i-1,j}}{C_{i,j}} + \frac{C_{i,j-1}}{C_{i,j}} = \frac{i}{i+j} + \frac{j}{i+j} = 1$$

and $C_{i,0} = C_{0,j} = 1$.

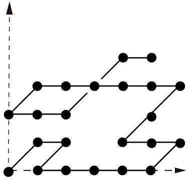
Thus $B_{i,j} = C_{i,j}$

Guess-and-Prove for Gessel walks

- $g(i,j;n)$ = number of n-steps $\{\nearrow, \swarrow, \leftarrow, \rightarrow\}$-walks in $\mathbb{N}^2$ from $(0,0)$ to (i,j)

Question: What is the nature of the generating function

$$G(x,y;t) = \sum_{i,j,n=0}^{\infty} g(i,j;n)\, x^i y^j t^n \ ?$$



Answer: [B., Kauers, 2010] $G(x,y;t)$ is an algebraic function†.

Approach:

1. Generate data: compute G to precision t^{1200} ($\approx$ 1.5 billion coeffs!)
2. Guess: conjecture polynomial equations for $G(x,0;t)$ and $G(0,y;t)$ (degree 24 each, coeffs. of degree $(46,56)$, with 80-bits digits coeffs.)
3. Prove: multivariate resultants of (very big) polynomials (30 pages each)

† Minimal polynomial $P(G(x,y;t);x,y,t) = 0$ has $> 10^{11}$ terms; $\approx 30\,\text{Gb}$ (6 DVDs!)

A typical Guess-and-Prove algorithmic proof

Theorem ["Gessel excursions are algebraic"]

$$g(t) := G(0,0;\sqrt{t}) = \sum_{n=0}^{\infty} \frac{(5/6)_n (1/2)_n}{(5/3)_n (2)_n} (16t)^n \quad \text{is algebraic.}$$

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Proof: First guess a polynomial $P(t,T)$ in $\mathbb{Q}[t,T]$, then prove that P admits the power series $g(t) = \sum_{n=0}^{\infty} g_n t^n$ as a root.

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2. Implicit function theorem: $\exists!$ root $r(t) \in \mathbb{Q}[[t]]$ of P.

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3. $r(t) = \sum_{n=0}^{\infty} r_n t^n$ being algebraic, it is D-finite, and so (r_n) is P-recursive:

$$(n+2)(3n+5)r_{n+1} - 4(6n+5)(2n+1)r_n = 0, \qquad r_0 = 1$$

$\Rightarrow$ solution $r_n = \frac{(5/6)_n(1/2)_n}{(5/3)_n(2)_n}16^n = g_n$, thus $g(t) = r(t)$ is algebraic.

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```
> P:=gfun:-listtoalgeq([seq(pochhammer(5/6,n)*pochhammer(1/2,n)/
      pochhammer(5/3,n)/pochhammer(2,n)*16^n, n=0..100)], g(t)):
> gfun:-diffeqtorec(gfun:-algeqtodiffeq(P[1], g(t)), g(t), r(n));
```

Algorithmic classification of models with D-Finite $Q_{\mathscr{S}}(t) := Q_{\mathscr{S}}(1,1;t)$

	OEIS	$\mathscr{S}$	Pol size	LDE size	Rec size		OEIS	$\mathscr{S}$	Pol size	LDE size	Rec size
1	A005566		—	(3, 4)	(2, 2)	13	A151275		—	(5, 24)	(9, 18)
2	A018224		—	(3, 5)	(2, 3)	14	A151314		—	(5, 24)	(9, 18)
3	A151312		—	(3, 8)	(4, 5)	15	A151255		—	(4, 16)	(6, 8)
4	A151331		—	(3, 6)	(3, 4)	16	A151287		—	(5, 19)	(7, 11)
5	A151266		—	(5, 16)	(7, 10)	17	A001006		(2, 2)	(2, 3)	(2, 1)
6	A151307		—	(5, 20)	(8, 15)	18	A129400		(2, 2)	(2, 3)	(2, 1)
7	A151291		—	(5, 15)	(6, 10)	19	A005558		—	(3, 5)	(2, 3)
8	A151326		—	(5, 18)	(7, 14)						
9	A151302		—	(5, 24)	(9, 18)	20	A151265		(6, 8)	(4, 9)	(6, 4)
10	A151329		—	(5, 24)	(9, 18)	21	A151278		(6, 8)	(4, 12)	(7, 4)
11	A151261		—	(4, 15)	(5, 8)	22	A151323		(4, 4)	(2, 3)	(2, 1)
12	A151297		—	(5, 18)	(7, 11)	23	A060900		(8, 9)	(3, 5)	(2, 3)

Equation sizes = (order, degree)

▷ Computerized discovery: enumeration + guessing [B., Kauers, 2009]

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Equation sizes = (order, degree)

- ▷ Computerized discovery: enumeration + guessing [B., Kauers, 2009]
- ▷ 1–22: DF confirmed by human proofs in [Bousquet-Mélou, Mishna, 2010]
- ▷ 23: DF confirmed by a human proof in [B., Kurkova, Raschel, 2017]
- ▷ All: explicit eqs. proved via CA [B., Chyzak, van Hoeij, Kauers, Pech, 2017]

Algorithmic classification of models with D-Finite $Q_{\mathscr{S}}(t) := Q_{\mathscr{S}}(1,1;t)$

	OEIS	$\mathscr{S}$	algebraic?	asymptotics		OEIS	$\mathscr{S}$	algebraic?	asymptotics
1	A005566		N	$\frac{4}{\pi}\frac{4^n}{n}$	13	A151275		N	$\frac{12\sqrt{30}}{\pi}\frac{(2\sqrt{6})^n}{n^2}$
2	A018224		N	$\frac{2}{\pi}\frac{4^n}{n}$	14	A151314		N	$\frac{\sqrt{6}\lambda\mu C^{5/2}}{5\pi}\frac{(2C)^n}{n^2}$
3	A151312		N	$\frac{\sqrt{6}}{\pi}\frac{6^n}{n}$	15	A151255		N	$\frac{24\sqrt{2}}{\pi}\frac{(2\sqrt{2})^n}{n^2}$
4	A151331		N	$\frac{8}{3\pi}\frac{8^n}{n}$	16	A151287		N	$\frac{2\sqrt{2}A^{7/2}}{\pi}\frac{(2A)^n}{n^2}$
5	A151266		N	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{3^n}{n^{1/2}}$	17	A001006		Y	$\frac{3}{2}\sqrt{\frac{3}{\pi}}\frac{3^n}{n^{3/2}}$
6	A151307		N	$\frac{1}{2}\sqrt{\frac{5}{2\pi}}\frac{5^n}{n^{1/2}}$	18	A129400		Y	$\frac{3}{2}\sqrt{\frac{3}{\pi}}\frac{6^n}{n^{3/2}}$
7	A151291		N	$\frac{4}{3\sqrt{\pi}}\frac{4^n}{n^{1/2}}$	19	A005558		N	$\frac{8}{\pi}\frac{4^n}{n^2}$
8	A151326		N	$\frac{2}{\sqrt{3\pi}}\frac{6^n}{n^{1/2}}$		$A = 1+\sqrt{2},\ B = 1+\sqrt{3},\ C = 1+\sqrt{6},\ \lambda = 7+3\sqrt{6},$			$\mu = \sqrt{\frac{4\sqrt{6}-1}{19}}$
9	A151302		N	$\frac{1}{3}\sqrt{\frac{5}{2\pi}}\frac{5^n}{n^{1/2}}$	20	A151265		Y	$\frac{2\sqrt{2}}{\Gamma(1/4)}\frac{3^n}{n^{3/4}}$
10	A151329		N	$\frac{1}{3}\sqrt{\frac{7}{3\pi}}\frac{7^n}{n^{1/2}}$	21	A151278		Y	$\frac{3\sqrt{3}}{\sqrt{2}\Gamma(1/4)}\frac{3^n}{n^{3/4}}$
11	A151261		N	$\frac{12\sqrt{3}}{\pi}\frac{(2\sqrt{3})^n}{n^2}$	22	A151323		Y	$\frac{\sqrt{2}3^{3/4}}{\Gamma(1/4)}\frac{6^n}{n^{3/4}}$
12	A151297		N	$\frac{\sqrt{3}B^{7/2}}{2\pi}\frac{(2B)^n}{n^2}$	23	A060900		Y	$\frac{4\sqrt{3}}{3\Gamma(1/3)}\frac{4^n}{n^{2/3}}$

▷ Computerized discovery: convergence acceleration + LLL [B., Kauers, '09]

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2	A018224		N	$\frac{2}{\pi}\frac{4^n}{n}$	14	A151314		N	$\frac{\sqrt{6}\lambda\mu C^{5/2}}{5\pi}\frac{(2C)^n}{n^2}$
3	A151312		N	$\frac{\sqrt{6}}{\pi}\frac{6^n}{n}$	15	A151255		N	$\frac{24\sqrt{2}}{\pi}\frac{(2\sqrt{2})^n}{n^2}$
4	A151331		N	$\frac{8}{3\pi}\frac{8^n}{n}$	16	A151287		N	$\frac{2\sqrt{2}A^{7/2}}{\pi}\frac{(2A)^n}{n^2}$
5	A151266		N	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{3^n}{n^{1/2}}$	17	A001006		Y	$\frac{3}{2}\sqrt{\frac{3}{\pi}}\frac{3^n}{n^{3/2}}$
6	A151307		N	$\frac{1}{2}\sqrt{\frac{5}{2\pi}}\frac{5^n}{n^{1/2}}$	18	A129400		Y	$\frac{3}{2}\sqrt{\frac{3}{\pi}}\frac{6^n}{n^{3/2}}$
7	A151291		N	$\frac{4}{3\sqrt{\pi}}\frac{4^n}{n^{1/2}}$	19	A005558		N	$\frac{8}{\pi}\frac{4^n}{n^2}$
8	A151326		N	$\frac{2}{\sqrt{3\pi}}\frac{6^n}{n^{1/2}}$		$A=1+\sqrt{2}$, $B=1+\sqrt{3}$,	$C=1+\sqrt{6}$,	$\lambda=7+3\sqrt{6}$,	$\mu=\sqrt{\frac{4\sqrt{6}-1}{19}}$
9	A151302		N	$\frac{1}{3}\sqrt{\frac{5}{2\pi}}\frac{5^n}{n^{1/2}}$	20	A151265		Y	$\frac{2\sqrt{2}}{\Gamma(1/4)}\frac{3^n}{n^{3/4}}$
10	A151329		N	$\frac{1}{3}\sqrt{\frac{7}{3\pi}}\frac{7^n}{n^{1/2}}$	21	A151278		Y	$\frac{3\sqrt{3}}{\sqrt{2}\Gamma(1/4)}\frac{3^n}{n^{3/4}}$
11	A151261		N	$\frac{12\sqrt{3}}{\pi}\frac{(2\sqrt{3})^n}{n^2}$	22	A151323		Y	$\frac{\sqrt{2}3^{3/4}}{\Gamma(1/4)}\frac{6^n}{n^{3/4}}$
12	A151297		N	$\frac{\sqrt{3}B^{7/2}}{2\pi}\frac{(2B)^n}{n^2}$	23	A060900		Y	$\frac{4\sqrt{3}}{3\Gamma(1/3)}\frac{4^n}{n^{2/3}}$

- ▷ Computerized discovery: convergence acceleration + LLL [B., Kauers, '09]
- ▷ Asympt. confirmed by human proofs via ACSV in [Melczer, Wilson, 2016]
- ▷ Transcendence proofs via CA [B., Chyzak, van Hoeij, Kauers, Pech, 2017]

Models 1–19: proofs, explicit expressions and transcendence

Theorem [B., Chyzak, van Hoeij, Kauers, Pech, 2017]

Let $\mathscr{S}$ be one of the models 1–19. Then

- $Q_{\mathscr{S}}(x, y; t)$ is expressible using iterated integrals of ${}_2F_1$ expressions.
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Example (King walks in the quarter plane, A151331)

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$$Q(t) = \frac{1}{t}\int_0^t \frac{1}{(1+4x)^3} \cdot {}_2F_1\left(\begin{matrix}\frac{3}{2} & \frac{3}{2} \\ & 2\end{matrix} \,\middle|\, \frac{16x(1+x)}{(1+4x)^2}\right) dx$$

$$= 1 + 3t + 18t^2 + 105t^3 + 684t^4 + 4550t^5 + 31340t^6 + 219555t^7 + \cdots$$

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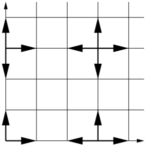
▷ Computer-driven discovery and proof; no human proof yet.
▷ Proof uses: (1) kernel method + (2) creative telescoping.

(1) Kernel method [Bousquet-Mélou, Mishna, 2010]



The kernel $K(x,y;t) := 1 - t \cdot \sum_{(i,j)\in\mathscr{S}} x^i y^j = 1 - t\left(x + \frac{1}{x} + y + \frac{1}{y}\right)$ is left invariant under the change of (x,y) into the elements of

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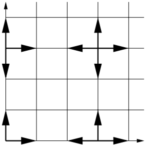

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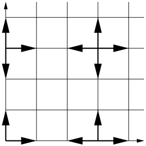

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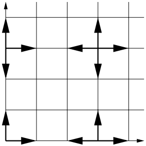

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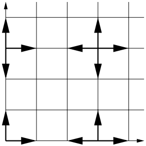

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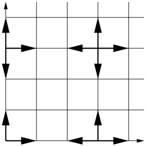

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Summing up yields the orbit equation:

$$\sum_{\theta\in\mathcal{G}} (-1)^{\theta}\theta\big(xy\,Q(x,y;t)\big) = \frac{xy - \frac{1}{x}y + \frac{1}{x}\frac{1}{y} - x\frac{1}{y}}{K(x,y;t)}$$

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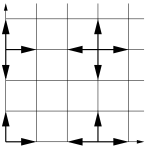

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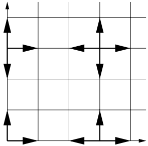

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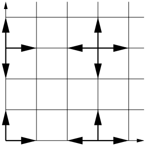

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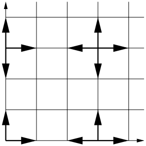

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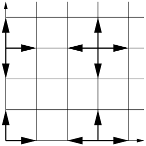

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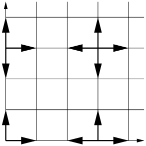
▷ Argument works if $\mathsf{OS} \neq 0$: algebraic version of the reflection principle



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▷ Creative Telescoping finds a differential equation for GF = $\oiint$ RatFrac

(2) Creative Telescoping

"An algorithmic toolbox for multiple sums and integrals with parameters"

Example [Apéry 1978]: $A_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2$ satisfies the recurrence

$$(n+1)^3 A_{n+1} + n^3 A_{n-1} = (2n+1)(17n^2+17n+5) A_n.$$

▷ Key fact used to prove that $\zeta(3) := \sum_{n \geq 1} \frac{1}{n^3} \approx 1.202056903\ldots$ is irrational.

1. Journées Arithmétiques de Marseille-Luminy, June 1978

The board of programme changes informed us that R. Apéry (Caen) would speak Thursday, 14.00 "Sur l'irrationalité de $\zeta(3)$." Though there had been earlier rumours of his claiming a proof, scepticism was general. The lecture tended to strengthen this view to rank disbelief. Those who listened casually, or who were afflicted with being non-Francophone, appeared to hear only a sequence of unlikely assertions.

7. ICM '78, Helsinki, August 1978

Neither Cohen nor I had been able to prove (5) or (5') in the intervening 2 months. After a few days of fruitless effort the specific problem was mentioned to Don Zagier (Bonn), and with irritating speed he showed that indeed the sequence $\{b'_n\}$ satisfies the recurrence (4). This more or less broke the dam and (5') and (5) were quickly conquered. Henri Cohen addressed a very well-attended meeting at 17.00 on Friday, August 18 in the language of the majority, proving (5) and explaining how this implied the

[Van der Poorten, 1979: "A proof that Euler missed"]

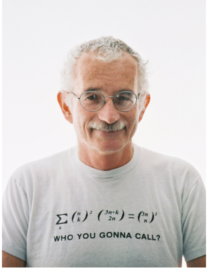
(2) Creative Telescoping

"An algorithmic toolbox for multiple sums and integrals with parameters"

Example [Apéry 1978]: $A_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2$ satisfies the recurrence

$$(n+1)^3 A_{n+1} + n^3 A_{n-1} = (2n+1)(17n^2+17n+5) A_n.$$

▷ Key fact used to prove that $\zeta(3) := \sum_{n \geq 1} \frac{1}{n^3} \approx 1.202056903\ldots$ is irrational.



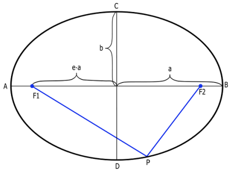
[Zeilberger, 1990: "The method of creative telescoping"]

(2) Creative Telescoping

"An algorithmic toolbox for multiple sums and integrals with parameters"

Example [Euler, 1733]: Perimeter of an ellipse of eccentricity e, semi-major axis 1

$$p(e) = 4\int_0^1 \sqrt{\frac{1-e^2u^2}{1-u^2}}\,\mathrm{d}u = 4 \oint\!\!\oint \frac{\mathrm{d}u\mathrm{d}v}{1-\frac{1-e^2u^2}{(1-u^2)v^2}}$$



Principle: Find algorithmically

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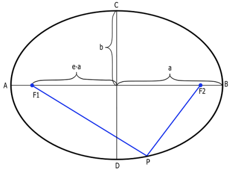

Principle: Find algorithmically

$$\left((e-e^3)\partial_e^2 + (1-e^2)\partial_e + e\right)\cdot\left(\frac{1}{1-\frac{1-e^2u^2}{(1-u^2)v^2}}\right) =$$

$$\partial_u\left(-\frac{e\left(-1-u+u^2+u^3\right)v^2\left(-3+2u+v^2+u^2\left(-2+3e^2-v^2\right)\right)}{\left(-1+v^2+u^2(e^2-v^2)\right)^2}\right)$$

$$+\,\partial_v\left(\frac{2e\left(-1+e^2\right)u\left(1+u^3\right)v^3}{\left(-1+v^2+u^2(e^2-v^2)\right)^2}\right)$$

▷ Conclusion: $(e-e^3)\cdot p''(e) + (1-e^2)\cdot p'(e) + e\cdot p(e) = 0.$

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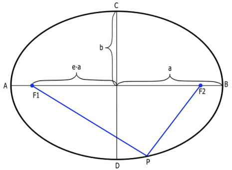

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$$+\,\partial_v\left(\frac{2e(-1+e^2)u(1+u^3)v^3}{(-1+v^2+u^2(e^2-v^2))^2}\right)$$

▷ Conclusion: $p(e) = \frac{\pi}{2}\cdot {}_2F_1\left(\left.\begin{matrix}-\frac{1}{2} & \frac{1}{2}\\ & 1\end{matrix}\right|\, e^2\right) = 2\pi - \frac{\pi}{2}e^2 - \frac{3\pi}{32}e^4 - \cdots.$

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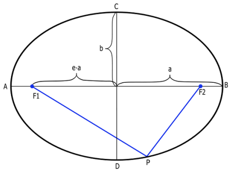

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▷ Drawback: Size(certificate) $\gg$ Size(telescoper).

Algorithm for the integration of rational functions [B., Lairez, Salvy, 2013]

- **Input:** $R(e, \mathbf{x})$ a rational function in e and $\mathbf{x} = x_1, \ldots, x_n$.
- **Output:** A linear ODE $T(e, \partial_e) y = 0$ satisfied by $y(e) = \oint\!\!\oint R(e, \mathbf{x}) d\mathbf{x}$.
- **Complexity:** $\mathcal{O}(D^{8n+2})$, where $D = \deg R$.
- **Output size:** T has order $\leq D^n$ in ∂_e and degree $\leq D^{3n+2}$ in e.

▷ Avoids the (costly) computation of certificates, of size $\Omega(D^{n^2/2})$.

▷ Previous algorithms: complexity (at least) doubly exponential in n.

▷ Very efficient in practice.

A toy *transcendence proof*: blending Guess-and-Prove and CT

Theorem (Apéry's power series is transcendental)

$$f(t) = \sum_n A_n t^n, \quad \text{where } A_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2, \quad \text{is transcendental.}$$

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Proof:

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   $$\left\{ 1 + 5t + O(t^2),\ \ln(t) + (5\ln(t) + 12)t + O(t^2),\ \ln(t)^2 + (5\ln(t)^2 + 24\ln(t))t + O(t^2) \right\}$$

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5. Conclusion: f is transcendental†

---

† f algebraic would imply a full basis of algebraic solutions for $L_f^{\min}$ [Tannery, 1875].

Summary: classification of walks with small steps in $\mathbb{N}^2$

$Q_{\mathscr{S}}$ is D-finite $\iff$ a certain group $\mathcal{G}_{\mathscr{S}}$ is finite (!)

quadrant models $\mathscr{S}$: 79

- $|\mathcal{G}_{\mathscr{S}}| < \infty$: 23
  - orbit sum $= 0$: 4
    - Guess-and-Prove
      - **algebraic**
  - orbit sum $\neq 0$: 19
    - Creative Telescoping
      - **D-finite**
- $|\mathcal{G}_{\mathscr{S}}| = \infty$: 56
  - asymptotics + GB
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    - $\nexists$ decoupling: 47 — diff. Galois — **D-transcendental**

* $\exists U \in \mathbb{Q}(x,t), V \in \mathbb{Q}(y,t)$ s.t. $U(x) + V(y) = xy$ on the kernel $K(x,y;t) = 0$.

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▷ Proofs use various tools: algebra, complex analysis, probability theory, differential Galois theory, computer algebra, etc.

Conclusion

- Enumerative Combinatorics and Computer Algebra enrich one another
- Classification of $Q(x,y;t)$ fully completed for 2D small step walks
- Robust algorithmic methods, based on efficient algorithms:
  - Guess-and-Prove
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- Lack of "purely human" proofs for some results.

- Many beautiful open questions for 2D models with repeated or large steps, and in dimension > 2.

Exercises

1. Explain why $\sum_n F_n t^n$ is rational, where $F_{n+2} = F_{n+1} + F_n, F_0 = 0, F_1 = 1$. Find a general statement.
2. Show that the series $\sum_n \binom{2n}{n} t^n$ and $\sum_n \binom{5n}{n} t^n$ are both algebraic.
3. Prove that the series
   - $\sqrt{1-4t} = 1 - 2\,t - 2\,t^2 - 4\,t^3 - 10\,t^4 - 28\,t^5 - \cdots$
   - $\sqrt[3]{1-9t} = 1 - 3\,t - 9\,t^2 - 45\,t^3 - 270\,t^4 - 1782\,t^5 - \cdots$

   have only integer coefficients. Try to generalize.
4. Prove that $\tan(t) = t + \frac{1}{3}t^3 + \frac{2}{15}t^5 + \frac{17}{315}t^7 + \frac{62}{2835}t^9 + \cdots$ is not D-finite.
5. Let $M_{n,k}$ be the number of $\{(1,1),(1,-1)\}$-walks in $\mathbb{N}^2$ of length n that start at $(0,0)$ and end at vertical altitude k. Let $M(x,y) = \sum_{n,k} M_{n,k} x^n y^k$.
   (a) Show that $(y - x(1+y^2)) \cdot M(x,y) = y - x \cdot M(x,0)$
   (b) Deduce that $M(x,y) = \dfrac{\sqrt{1-4x^2}+2xy-1}{2x(y-x(1+y^2))}$

Bonus

Beyond dimension 2: walks with small steps in $\mathbb{N}^3$

▷ $2^{3^3-1} \approx 67$ million models, of which ≈ 11 million inherently 3D

3D octant models $\mathscr{S}$ with ≤ 6 steps: 20804

- $|\mathcal{G}_{\mathscr{S}}| < \infty$: 170
  - orbit sum $\neq 0$: 108
    - Creative Telescoping
      - **D-finite**
  - orbit sum $= 0$: 62
    - 2D-reducible: 43
      - **D-finite**
    - not 2D-reducible: 19
      - **non-D-finite?**
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[B., Bousquet-Mélou, Kauers, Melczer, 2016] + [Du, Hou, Wang, 2017];
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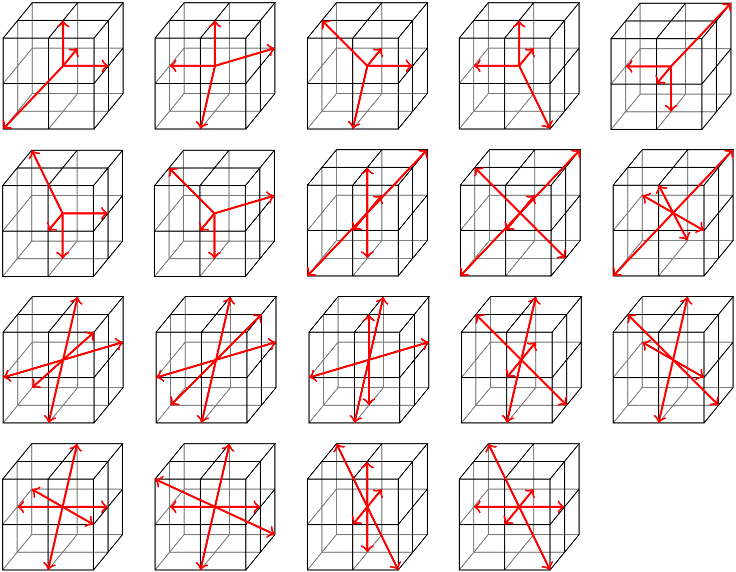
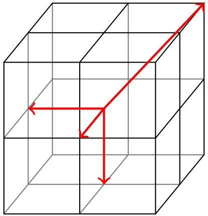
Question: differential finiteness $\Longleftrightarrow$ finiteness of the group?

Answer: probably no

19 mysterious 3D-models: finite $\mathcal{G}_{\mathscr{S}}$ and possibly non-D-finite $Q_{\mathscr{S}}$





Two different computations suggest:

$$k_{4n} = C \cdot 256^n / n^{\alpha}, \text{ for } \alpha = 3.3257570041744\ldots,$$

so excursions are very probably non-D-finite

Beyond small steps: Walks in $\mathbb{N}^2$ with large steps

quadrant models with steps in $\{-2,-1,0,1\}^2$: 13 110

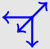
- $|\mathcal{G}_{\mathscr{S}}| < \infty$: 240
  - OS $\neq 0$: 431 → **D-finite**
  - OS $= 0$: 9 → **D-finite?**
- $|\mathcal{G}_{\mathscr{S}}| = \infty$: 12 870
  - α rational: 16 → **non-D-finite?**
  - α irrational: 12 854 → **non-D-finite**

[B., Bousquet-Mélou, Melczer, 2018]

Question: differential finiteness $\Longleftrightarrow$ finiteness of the group?

Answer: ?

Conjecture 1 [B., Bousquet-Mélou, Melczer, 2018]

For the model  the excursions generating function $Q(0,0;t^{1/2})$ equals

$$\frac{1}{3t} - \frac{1}{6t} \cdot \left(\frac{1-12t}{(1+36t)^{1/3}} \cdot {}_2F_1\left(\begin{matrix} \frac{1}{6} & \frac{2}{3} \\ & 1 \end{matrix} \,\middle|\, \frac{108t(1+4t)^2}{(1+36t)^2} \right) + \sqrt{1-12t} \cdot {}_2F_1\left(\begin{matrix} -\frac{1}{6} & \frac{2}{3} \\ 1 & \end{matrix} \,\middle|\, \frac{108t(1+4t)^2}{(1-12t)^2} \right) \right).$$

Conjecture 2 [B., Bousquet-Mélou, Melczer, 2018]

For the model  the excursions generating function $Q(0,0;t)$ equals

$$\frac{(1-24\,U+120\,U^2-144\,U^3)\,(1-4\,U)}{(1-3\,U)\,(1-2\,U)^{3/2}\,(1-6\,U)^{9/2}},$$

where $U = t^4 + 53\,t^8 + 4363\,t^{12} + \cdots$ is the unique series in $\mathbb{Q}[[t]]$ satisfying

$$U\,(1-2\,U)^3\,(1-3\,U)^3\,(1-6\,U)^9 = t^4\,(1-4\,U)^4.$$

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Solution of the “exercise”

Excursions in $\mathbb{Z} \times \mathbb{N}$

- The kernel equation reads (with $K(x,y) = 1 - t(y + \bar{x} + x\bar{y})$):

$$K(x,y)yH(x,y) = y - txH(x,0)$$

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- Let

$$y_0 = \frac{x - t - \sqrt{(t-x)^2 - 4t^2x^3}}{2tx} \qquad = xt + t^2 + (x^2 + \bar{x})t^3 + (3x + \bar{x}^2)t^4 + \cdots$$

be the (unique) root in $\mathbb{Q}[x, \bar{x}][[t]]$ of $K(x, y_0) = 0$.

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Excursions in $\mathbb{Z} \times \mathbb{N}$

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$$(27t^4 - t)A''(t) + (108t^3 - 4)A'(t) + 54t^2A(t) = 0.$$

```
> Zeilberger(1/x * sqrt((t-x)^2 - 4*t^2*x^3)/(2*t^2*x^2), t, x, Dt);
```

The group of the model $\{\uparrow, \leftarrow, \searrow\}$

Step set $\mathscr{S} = \{(-1,0),(0,1),(1,-1)\}$, with characteristic polynomial

$$\chi(x,y) = \frac{1}{x} + y + x \cdot \frac{1}{y} = \bar{x} + y + x\bar{y}$$

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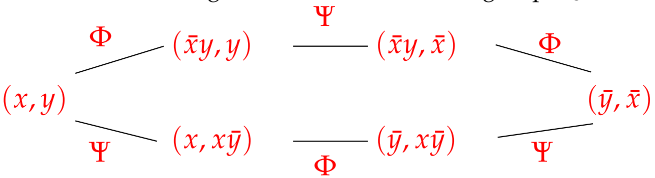
Φ and Ψ are involutions, and generate a finite dihedral group D_3 of order 6:



Diagonal walks in $\mathbb{N}^2$

- Orbit equation:

$$xyQ(x,y) - \bar{x}y^2Q(\bar{x}y,y) + \bar{x}^2yQ(\bar{x}y,\bar{x}) - \bar{x}\bar{y}Q(\bar{y},\bar{x}) + x\bar{y}^2Q(\bar{y},x\bar{y}) - x^2\bar{y}Q(x,x\bar{y}) = \frac{xy - \bar{x}y^2 + \bar{x}^2y - \bar{x}\bar{y} + x\bar{y}^2 - x^2\bar{y}}{1 - t(y + \bar{x} + x\bar{y})}$$

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- Corollary [Bousquet-Mélou & Mishna, 2010]:

$$xyQ(x,y) = [x^{>0}y^{>0}]\ \frac{xy - \bar{x}y^2 + \bar{x}^2y - \bar{x}\bar{y} + x\bar{y}^2 - x^2\bar{y}}{1 - t(y + \bar{x} + x\bar{y})}$$

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$$B(t) = [z^0]Q(z,\bar{z}) = [u^{-1}v^{-1}z^{-1}]\ \frac{\bar{u}\bar{v} - u\bar{v}^2 + u^2\bar{v} - uv + \bar{u}v^2 - \bar{u}^2v}{z(1-zu)(1-v\bar{z})(1-t(\bar{v}+u+\bar{u}v))}$$

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- Creative Telescoping gives a differential equation for $B(t)$:

$$(27t^4 - t)B''(t) + (108t^3 - 4)B'(t) + 54t^2B(t) = 0.$$

Conclusion

We have proved that $A(t)$ and $B(t)$ are both solutions of

$$(27t^4 - t)y''(t) + (108t^3 - 4)y'(t) + 54t^2 y(t) = 0.$$

Solving this equation proves:

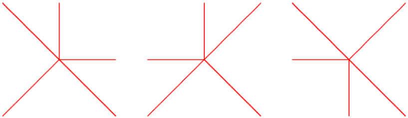
$$A(t) = B(t) = {}_2F_1\left(\begin{matrix}1/3 & 2/3\\ & 2\end{matrix}\,\middle|\, 27\,t^3\right) = \sum_{n=0}^{\infty} \frac{(3n)!}{n!^3}\,\frac{t^{3n}}{n+1}.$$

Thus the two sequences are equal to

$$a_{3n} = b_{3n} = \frac{(3n)!}{n!^2 \cdot (n+1)!}, \qquad \text{and} \quad a_m = b_m = 0 \quad \text{if 3 does not divide } m.$$

Example with infinite group: the scarecrows

[B., Raschel, Salvy, 2014]: $Q_{\mathscr{S}}(0,0;t)$ is not D-finite for the models



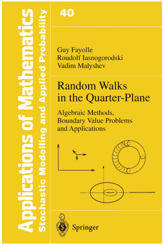
▷ For the 1st and the 3rd, the excursions sequence $[t^n]\, Q_{\mathscr{S}}(0,0;t)$

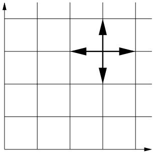
$$1, 0, 0, 2, 4, 8, 28, 108, 372, \ldots$$

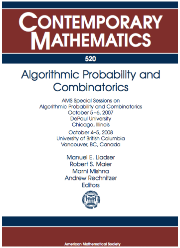
is $\sim K \cdot 5^n \cdot n^{-\alpha}$, with $\alpha = 1 + \pi / \arccos(1/4) = 3.383396\ldots$
[Denisov, Wachtel, 2015]

▷ The irrationality of α prevents $Q_{\mathscr{S}}(0,0;t)$ from being D-finite.
[Katz, 1970; Chudnovsky, 1985; André, 1989]

The group of a model: the simple walk case







The characteristic polynomial $\chi_{\mathscr{S}} := x + \dfrac{1}{x} + y + \dfrac{1}{y}$

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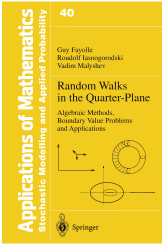
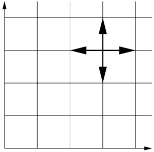
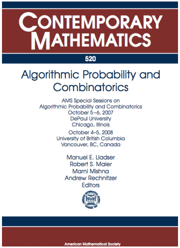
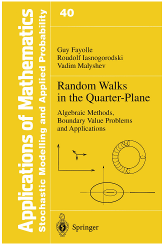


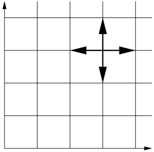


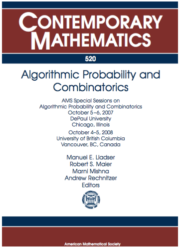


The characteristic polynomial $\chi_{\mathscr{S}} := x + \frac{1}{x} + y + \frac{1}{y}$ is left invariant under

$$\psi(x,y) = \left(x, \frac{1}{y}\right), \quad \phi(x,y) = \left(\frac{1}{x}, y\right),$$







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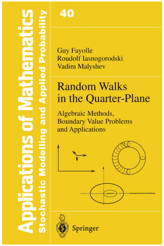
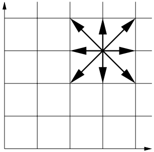
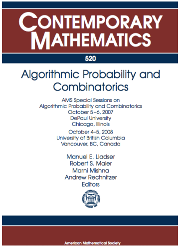
and thus under any element of the group

$$\langle \psi, \phi \rangle = \left\{ (x,y), \left(x, \frac{1}{y}\right), \left(\frac{1}{x}, \frac{1}{y}\right), \left(\frac{1}{x}, y\right) \right\}.$$

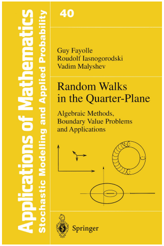


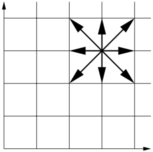


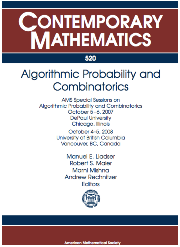


The generating polynomial $\chi_{\mathscr{S}} := \sum_{(i,j)\in\mathscr{S}} x^i y^j = \sum_{i=-1}^{1} B_i(y) x^i = \sum_{j=-1}^{1} A_j(x) y^j$

The group of a model







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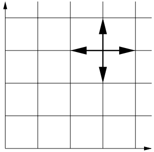
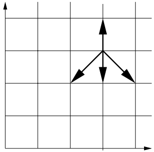
$$\psi(x,y) = \left(x, \frac{A_{-1}(x)}{A_{+1}(x)}\frac{1}{y}\right), \qquad \phi(x,y) = \left(\frac{B_{-1}(y)}{B_{+1}(y)}\frac{1}{x}, y\right),$$

and thus under any element of the (dihedral) group

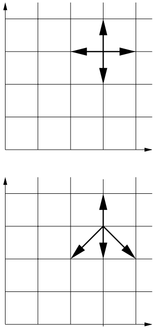
$$\mathcal{G}_{\mathscr{S}} := \langle \psi, \phi \rangle.$$





Order 4,

Examples of groups



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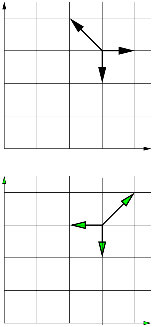
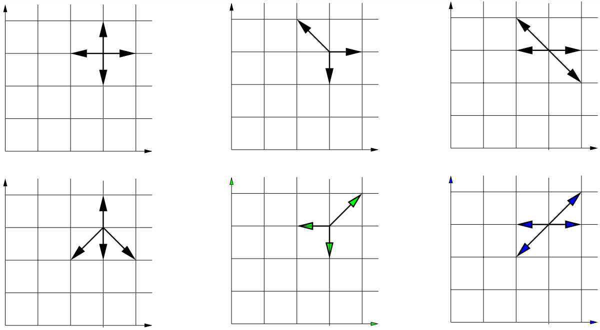


order 6,



Order 4, order 6, order 8,

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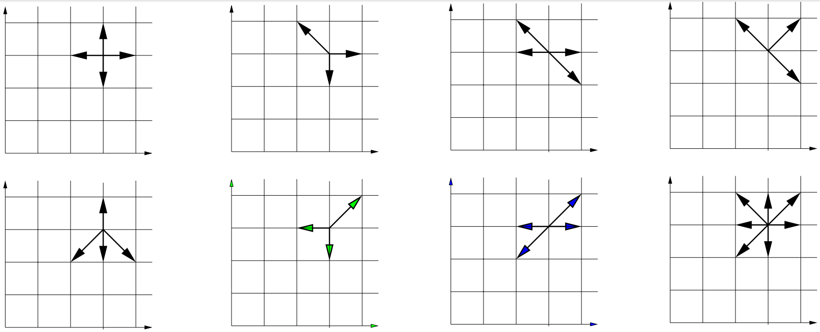

Order 4, order 6, order 8, order ∞.

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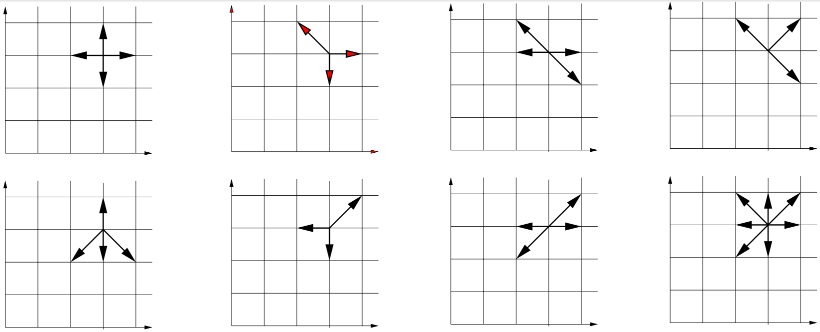

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$$(x,y) \overset{\Phi}{—} \left(\frac{y}{x}, y\right) \overset{\Psi}{—} \left(\frac{y}{x}, \frac{1}{x}\right) \overset{\Phi}{—} \left(\frac{1}{y}, \frac{1}{x}\right)$$

$$(x,y) \overset{\Psi}{—} \left(x, \frac{x}{y}\right) \overset{\Phi}{—} \left(\frac{1}{y}, \frac{x}{y}\right) \overset{\Psi}{—} \left(\frac{1}{y}, \frac{1}{x}\right)$$